wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2026 – 04:22 pm BST

PDB ID	:	5FCJ / pdb_00005fcj
Title	:	Structure of the anisomycin-containing uL3 W255C mutant 80S yeast ribosome
Authors	:	Mailliot, J.; Garreau de Loubresse, N.; Yusupova, G.; Dinman, J.D.; Yusupov, M.
Deposited on	:	2015-12-15
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

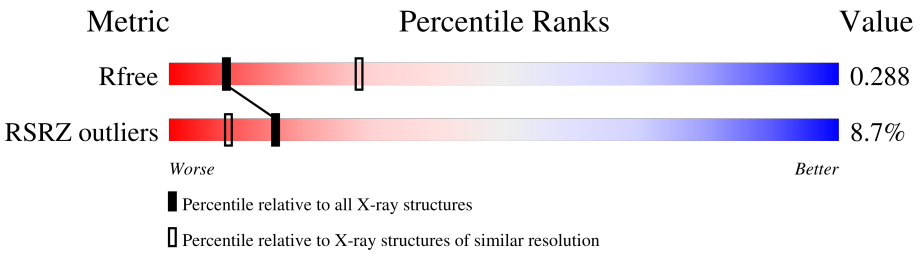
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	1	3406	-	-	-	X
84	MG	1	3414	-	-	-	X
84	MG	1	3449	-	-	-	X
84	MG	1	3500	-	-	-	X
84	MG	1	3518	-	-	-	X
84	MG	1	3563	-	-	-	X
84	MG	1	3567	-	-	-	X
84	MG	1	3569	-	-	-	X
84	MG	1	3570	-	-	-	X
84	MG	1	3586	-	-	-	X
84	MG	1	3650	-	-	-	X
84	MG	1	3705	-	-	-	X
84	MG	1	3709	-	-	-	X
84	MG	2	1904	-	-	-	X
84	MG	2	1910	-	-	-	X
84	MG	2	1917	-	-	-	X
84	MG	2	1920	-	-	-	X
84	MG	2	1921	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	2	1922	-	-	-	X
84	MG	2	1923	-	-	-	X
84	MG	2	1924	-	-	-	X
84	MG	2	1925	-	-	-	X
84	MG	2	1927	-	-	-	X
84	MG	2	1932	-	-	-	X
84	MG	2	1940	-	-	-	X
84	MG	2	1946	-	-	-	X
84	MG	2	1947	-	-	-	X
84	MG	2	1952	-	-	-	X
84	MG	2	1953	-	-	-	X
84	MG	2	1954	-	-	-	X
84	MG	2	1956	-	-	-	X
84	MG	2	1957	-	-	-	X
84	MG	2	1962	-	-	-	X
84	MG	2	1965	-	-	-	X
84	MG	2	1969	-	-	-	X
84	MG	2	1978	-	-	-	X
84	MG	4	203	-	-	-	X
84	MG	5	3457	-	-	-	X
84	MG	5	3532	-	-	-	X
84	MG	5	3533	-	-	-	X
84	MG	5	3608	-	-	-	X
84	MG	5	3641	-	-	-	X
84	MG	5	3693	-	-	-	X
84	MG	6	1909	-	-	-	X
84	MG	6	1921	-	-	-	X
84	MG	6	1926	-	-	-	X
84	MG	6	1927	-	-	-	X
84	MG	6	1930	-	-	-	X
84	MG	6	1937	-	-	-	X
84	MG	6	1938	-	-	-	X
84	MG	6	1951	-	-	-	X
84	MG	6	1952	-	-	-	X
84	MG	6	1955	-	-	-	X
84	MG	6	1956	-	-	-	X
84	MG	6	1959	-	-	-	X
84	MG	6	1971	-	-	-	X
84	MG	6	1975	-	-	-	X
84	MG	6	1993	-	-	-	X
84	MG	6	2002	-	-	-	X

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 410912 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	2	1781	37970	16975	6720	12493	1782	0	1	0
1	6	1795	38260	17105	6763	12596	1796	0	1	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S0	206	1577	1014	278	283	2	0	0	0
2	s0	206	1612	1034	285	291	2	0	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S1	214	1709	1084	310	311	4	0	0	0
3	s1	216	1722	1091	312	315	4	0	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	S2	217	1635	1047	289	297	2	0	0	0
4	s2	217	1635	1047	289	297	2	0	0	0

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	S3	223	1734	1101	313	314	6	0	0	0
5	s3	223	1734	1101	313	314	6	0	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	S4	260	2068	1316	389	360	3	0	0	0
6	s4	260	2068	1316	389	360	3	0	0	0

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	S5	206	1609	1007	300	299	3	0	0	0
7	s5	206	1609	1007	300	299	3	0	0	0

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	S6	226	1799	1129	346	321	3	0	0	0
8	s6	218	1755	1102	337	313	3	0	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	S7	184	1481	951	265	265	0	0	0
9	s7	186	1492	957	267	268	0	0	0

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	S8	188	1489	925	298	264	2	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	s8	188	1489	925	298	264	2	0	0	0

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	S9	185	1494	943	289	261	1	0	0	0
			Total	C	N	O	S			
11	s9	185	1494	943	289	261	1	0	0	0

- Molecule 12 is a protein called 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	C0	96	773	500	126	145	2	0	0	0
			Total	C	N	O	S			
12	c0	96	762	491	125	144	2	0	0	0

- Molecule 13 is a protein called 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
			Total	C	N	O	S			
13	c1	146	1169	748	221	197	3	0	0	0

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	C2	124	890	560	156	172	2	0	0	0
			Total	C	N	O	S			
14	c2	124	890	560	156	172	2	0	0	0

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	C3	150	1192	759	224	207	2	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	c3	150	1192	759	224	207	2	0	0	0

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	C4	127	891	545	182	163	1	0	0	0
			Total	C	N	O	S			
16	c4	128	949	582	188	176	3	0	0	0

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	C5	124	977	622	182	166	7	0	0	0
			Total	C	N	O	S			
17	c5	135	1039	658	196	178	7	0	0	0

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	C6	141	1105	708	203	194	0	0	0
			Total	C	N	O			
18	c6	142	1111	711	204	196	0	0	0

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	C7	120	926	577	177	170	2	0	0	0
			Total	C	N	O	S			
19	c7	117	944	591	179	172	2	0	0	0

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	C8	145	1192	743	237	210	2	0	0	0
			Total	C	N	O	S			
20	c8	145	1192	743	237	210	2	0	0	0

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	C9	143	1112	694	208	208	2	0	0	0
21	c9	143	1112	694	208	208	2	0	0	0

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	D0	107	855	539	156	159	1	0	0	0
22	d0	110	882	554	161	166	1	0	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	D1	87	684	420	125	137	2	0	0	0
23	d1	87	684	420	125	137	2	0	0	0

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	D2	129	1021	650	188	180	3	0	0	0
24	d2	129	1021	650	188	180	3	0	0	0

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	D3	144	1121	708	220	191	2	0	0	0
25	d3	144	1121	708	220	191	2	0	0	0

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
26	D4	134	1073	676	208	189	0	0	0
26	d4	134	1073	676	208	189	0	0	0

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
27	D5	70	563	360	104	99	0	0	0
27	d5	69	558	357	103	98	0	0	0

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	D6	97	769	475	160	129	5	0	0	0
28	d6	97	769	475	160	129	5	0	0	0

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	D7	81	610	382	110	113	5	0	0	0
29	d7	81	610	382	110	113	5	0	0	0

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	D8	63	497	306	99	91	1	0	0	0
30	d8	63	497	306	99	91	1	0	0	0

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	D9	53	442	274	92	72	4	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	d9	53	443	275	92	72	4	0	0	0

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	E0	60	475	299	98	77	1	0	0	0
32	e0	62	491	309	101	80	1	0	0	0

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	E1	71	566	362	106	94	4	0	0	0
33	e1	76	608	388	117	99	4	0	0	0

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	SR	318	2437	1541	418	470	8	0	0	0
34	sR	318	2445	1546	419	472	8	0	0	0

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1104	652	221	231	0	0	0
35	sM	104	680	403	140	137	0	0	0

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	1	3149	67355	30086	12142	21978	3149	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	5	3150	67377	30095	12145	21987	3150	0	0	0

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
37	3	121	2579	1152	461	845	121	0	0	0
37	7	121	2579	1152	461	845	121	0	0	0

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
38	4	158	3353	1500	586	1109	158	0	0	0
38	8	158	3353	1500	586	1109	158	0	0	0

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	L2	252	1914	1191	388	334	1	0	0	0
39	l2	252	1918	1193	389	335	1	0	0	0

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	3067	1942	583	533	9	0	0	0
40	l3	386	3073	1948	583	533	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L3	255	CYS	TRP	engineered mutation	UNP P14126
l3	255	CYS	TRP	engineered mutation	UNP P14126

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	L4	361	2748	1729	522	494	3	0	0	0
41	l4	361	2749	1730	522	494	3	0	0	0

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	L5	296	2375	1501	414	458	2	0	0	0
42	l5	294	2359	1489	412	456	2	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	L6	156	1239	800	222	216	1	0	0	0
43	l6	157	1248	806	224	217	1	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	L7	222	1784	1151	324	308	1	0	0	0
44	l7	223	1791	1155	325	310	1	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	1804	1151	323	327	3	0	0	0
45	l8	231	1763	1130	316	314	3	0	0	0

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	L9	191	1518	963	274	277	4	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	l9	191	1518	963	274	277	4	0	0	0

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	M0	211	1705	1083	322	294	6	0	0	0
			Total	C	N	O	S			
47	m0	213	1733	1101	327	299	6	0	0	0

- Molecule 48 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	M1	169	1353	847	253	249	4	0	0	0
			Total	C	N	O	S			
48	m1	169	1353	847	253	249	4	0	0	0

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	M3	193	1543	962	315	266	0	0	0
			Total	C	N	O			
49	m3	194	1548	965	316	267	0	0	0

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	M4	136	1053	675	199	177	2	0	0	0
			Total	C	N	O	S			
50	m4	137	1059	678	200	179	2	0	0	0

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	M5	203	1720	1077	361	281	1	0	0	0
			Total	C	N	O	S			
51	m5	203	1720	1077	361	281	1	0	0	0

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	M6	197	1555	1003	289	262	1	0	0	0
52	m6	197	1555	1003	289	262	1	0	0	0

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	M7	183	1420	882	281	257	0	0	0
53	m7	155	1227	764	238	225	0	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	M8	185	1441	908	290	241	2	0	0	0
54	m8	185	1441	908	290	241	2	0	0	0

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
55	M9	188	1521	935	326	260	0	0	0
55	m9	188	1521	935	326	260	0	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	N0	172	1445	930	267	244	4	0	0	0
56	n0	172	1445	930	267	244	4	0	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	N1	159	1276	805	246	221	4	0	0	0
57	n1	159	1276	805	246	221	4	0	0	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	N2	100	796	516	131	149	0	0	0
58	n2	98	778	505	127	146	0	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	N3	136	1003	628	189	179	7	0	0	0
59	n3	136	1003	628	189	179	7	0	0	0

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	N4	98	699	443	137	118	1	0	0	0
60	n4	135	1089	682	219	187	1	0	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
61	N5	121	964	620	169	173	2	0	0	0
61	n5	120	959	617	168	172	2	0	0	0

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
62	N6	126	993	625	192	176	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
62	n6	126	993	625	192	176	0	0	0

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
63	N7	135	1092	710	202	180	0	0	0
63	n7	135	1092	710	202	180	0	0	0

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
64	N8	148	1173	749	231	190	3	0	0	0
64	n8	148	1173	749	231	190	3	0	0	0

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
65	N9	58	462	289	100	73	0	0	0
65	n9	58	462	289	100	73	0	0	0

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
66	O0	97	743	479	124	139	1	0	0	0
66	o0	100	767	492	128	146	1	0	0	0

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	O1	109	876	556	167	152	1	0	0	0
67	o1	109	890	565	168	156	1	0	0	0

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	O2	127	1020	647	205	167	1	0	0	0
68	o2	127	1020	647	205	167	1	0	0	0

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
69	O3	106	850	540	165	144	1	0	0	0
69	o3	106	850	540	165	144	1	0	0	0

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
70	O4	112	880	545	179	152	4	0	0	0
70	o4	112	881	546	179	152	4	0	0	0

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
71	O5	119	969	615	186	167	1	0	0	0
71	o5	119	969	615	186	167	1	0	0	0

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
72	O6	99	771	481	156	132	2	0	0	0
72	o6	99	771	481	156	132	2	0	0	0

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
73	O7	87	681	414	148	114	5	0	0	0
73	o7	87	681	414	148	114	5	0	0	0

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
74	O8	77	612	391	115	106	0	0	0
74	o8	77	612	391	115	106	0	0	0

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
75	O9	50	436	272	97	65	2	0	0	0
75	o9	50	436	272	97	65	2	0	0	0

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
76	Q0	52	417	259	86	67	5	0	0	0
76	q0	52	417	259	86	67	5	0	0	0

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
77	Q1	25	233	142	63	27	1	0	0	0
77	q1	25	233	142	63	27	1	0	0	0

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	Q2	105	847	534	170	138	5	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	q2	105	847	534	170	138	5	0	0	0

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
79	Q3	91	694	429	138	121	6	0	0	0
79	q3	91	694	429	138	121	6	0	0	0

- Molecule 80 is a protein called 60S ribosomal protein L12-A (uL11).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
80	m2	150	750	450	150	150	0	0	0

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	p0	143	1077	687	192	195	3	0	0	0

- Molecule 82 is a protein called 60S ribosomal protein P1 alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
82	p1	47	235	141	47	47	0	0	0

- Molecule 83 is a protein called 60S ribosomal protein P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
83	p2	46	230	138	46	46	0	0	0

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
84	2	82	82	82	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
84	S4	1	1	1	0	0
84	D9	1	1	1	0	0
84	SM	1	1	1	0	0
84	1	330	330	330	0	0
84	3	10	10	10	0	0
84	4	14	14	14	0	0
84	L2	2	2	2	0	0
84	L3	1	1	1	0	0
84	L6	1	1	1	0	0
84	L7	1	1	1	0	0
84	M0	1	1	1	0	0
84	M3	1	1	1	0	0
84	M5	1	1	1	0	0
84	M6	1	1	1	0	0
84	M7	4	4	4	0	0
84	N3	1	1	1	0	0
84	N8	2	2	2	0	0
84	O2	1	1	1	0	0
84	O3	1	1	1	0	0
84	O4	2	2	2	0	0
84	O7	2	2	2	0	0

Continued on next page...

Continued from previous page...

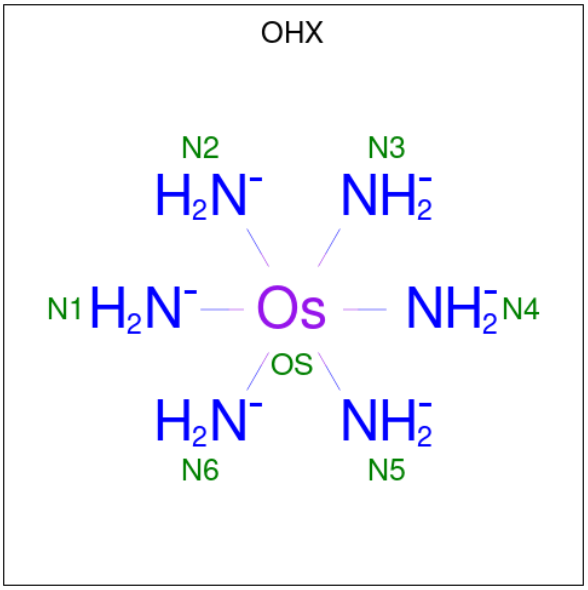
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
84	Q2	1	1	1	0	0
84	6	110	110	110	0	0
84	s8	1	1	1	0	0
84	c1	1	1	1	0	0
84	d6	1	1	1	0	0
84	sM	2	2	2	0	0
84	5	349	349	349	0	0
84	7	10	10	10	0	0
84	8	10	10	10	0	0
84	l2	3	3	3	0	0
84	l3	5	5	5	0	0
84	l6	1	1	1	0	0
84	l7	1	1	1	0	0
84	l8	1	1	1	0	0
84	l9	1	1	1	0	0
84	m1	1	1	1	0	0
84	m5	3	3	3	0	0
84	m6	1	1	1	0	0
84	m7	3	3	3	0	0
84	n0	2	2	2	0	0
84	n3	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	n6	2	Total Mg 2 2	0	0
84	n8	2	Total Mg 2 2	0	0
84	n9	1	Total Mg 1 1	0	0
84	o1	1	Total Mg 1 1	0	0
84	o3	1	Total Mg 1 1	0	0
84	o4	1	Total Mg 1 1	0	0
84	q0	1	Total Mg 1 1	0	0
84	q1	1	Total Mg 1 1	0	0

- Molecule 85 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	2	1	Total N Os 7 6 1	0	0
85	2	1	Total N Os 7 6 1	0	0
85	2	1	Total N Os 7 6 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	2	1	7	6	1	0	0
85	S6	1	7	6	1	0	0
85	S8	1	7	6	1	0	0
85	C3	1	7	6	1	0	0
85	C5	1	7	6	1	0	0
85	C8	1	7	6	1	0	0
85	D9	1	7	6	1	0	0
85	SR	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0
			Total	N	Os		
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	1	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0
85	3	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	3	1	7	6	1	0	0
			Total	N	Os		
85	3	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	4	1	7	6	1	0	0
			Total	N	Os		
85	L3	1	7	6	1	0	0
			Total	N	Os		
85	L3	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	L4	1	7	6	1	0	0
85	M0	1	7	6	1	0	0
85	M5	1	7	6	1	0	0
85	M6	1	7	6	1	0	0
85	M7	1	7	6	1	0	0
85	M9	1	7	6	1	0	0
85	N1	1	7	6	1	0	0
85	N8	1	7	6	1	0	0
85	N9	1	7	6	1	0	0
85	O3	1	7	6	1	0	0
85	O7	1	7	6	1	0	0
85	O7	1	7	6	1	0	0
85	O9	1	7	6	1	0	0
85	Q2	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0
			Total	N	Os		
85	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	6	1	7	6	1	0	0
85	s4	1	7	6	1	0	0
85	s8	1	7	6	1	0	0
85	s9	1	7	6	1	0	0
85	c3	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	c5	1	7	6	1	0	0
85	c8	1	7	6	1	0	0
85	d4	1	7	6	1	0	0
85	sR	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0
			Total	N	Os		
85	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	5	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	7	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0
85	8	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	8	1	7	6	1	0	0
			Total	N	Os		
85	8	1	7	6	1	0	0
			Total	N	Os		
85	l3	1	7	6	1	0	0
			Total	N	Os		
85	l3	1	7	6	1	0	0
			Total	N	Os		
85	l3	1	7	6	1	0	0
			Total	N	Os		
85	l4	1	7	6	1	0	0
			Total	N	Os		
85	l4	1	7	6	1	0	0
			Total	N	Os		
85	l5	1	7	6	1	0	0
			Total	N	Os		
85	l5	1	7	6	1	0	0
			Total	N	Os		
85	l9	1	7	6	1	0	0
			Total	N	Os		
85	m0	1	7	6	1	0	0
			Total	N	Os		
85	m0	1	7	6	1	0	0
			Total	N	Os		
85	m1	1	7	6	1	0	0
			Total	N	Os		
85	m5	1	7	6	1	0	0
			Total	N	Os		
85	m5	1	7	6	1	0	0
			Total	N	Os		
85	m7	1	7	6	1	0	0
			Total	N	Os		
85	n3	1	7	6	1	0	0
			Total	N	Os		
85	n3	1	7	6	1	0	0
			Total	N	Os		
85	n9	1	7	6	1	0	0
			Total	N	Os		
85	o3	1	7	6	1	0	0
			Total	N	Os		
85	o7	1	7	6	1	0	0

Continued on next page...

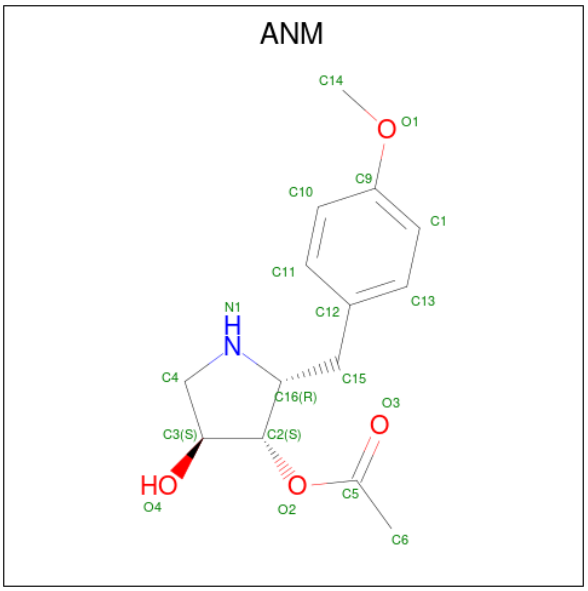
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
85	o9	1	7	6	1	0	0
85	q2	1	7	6	1	0	0

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
86	D6	1	1	1	0	0
86	D7	1	1	1	0	0
86	D9	1	1	1	0	0
86	E1	1	1	1	0	0
86	O7	1	1	1	0	0
86	Q0	1	1	1	0	0
86	Q2	1	1	1	0	0
86	Q3	1	1	1	0	0
86	d6	1	1	1	0	0
86	d7	1	1	1	0	0
86	d9	1	1	1	0	0
86	e1	1	1	1	0	0
86	o7	1	1	1	0	0
86	q0	1	1	1	0	0
86	q2	1	1	1	0	0
86	q3	1	1	1	0	0

- Molecule 87 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
87	1	1	19	14	1	4	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.11Å 287.31Å 303.99Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	49.96 – 3.10 49.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.96-3.10) 89.6 (49.96-3.10)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.291 0.244 , 0.288	Depositor DCC
R_{free} test set	26664 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	410912	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 Ligand geometry (i)

Of 2030 ligands modelled in this entry, 995 are monoatomic - leaving 1035 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3779	-	0,6,6	-	-	-		
85	OHX	5	3831	-	0,6,6	-	-	-		
85	OHX	5	3833	-	0,6,6	-	-	-		
85	OHX	M6	202	-	0,6,6	-	-	-		
85	OHX	5	3827	-	0,6,6	-	-	-		
85	OHX	6	2138	-	0,6,6	-	-	-		
85	OHX	6	2014	-	0,6,6	-	-	-		
85	OHX	1	3822	-	0,6,6	-	-	-		
85	OHX	1	3883	-	0,6,6	-	-	-		
85	OHX	1	4004	-	0,6,6	-	-	-		
85	OHX	1	3762	-	0,6,6	-	-	-		
85	OHX	1	3824	-	0,6,6	-	-	-		
85	OHX	5	4028	-	0,6,6	-	-	-		
85	OHX	1	3733	-	0,6,6	-	-	-		
85	OHX	2	2093	-	0,6,6	-	-	-		
85	OHX	6	2155	-	0,6,6	-	-	-		
85	OHX	5	3843	-	0,6,6	-	-	-		
85	OHX	1	4035	-	0,6,6	-	-	-		
85	OHX	1	4038	-	0,6,6	-	-	-		
85	OHX	6	2068	-	0,6,6	-	-	-		
85	OHX	6	2038	-	0,6,6	-	-	-		
85	OHX	5	3879	-	0,6,6	-	-	-		
85	OHX	1	3850	-	0,6,6	-	-	-		
85	OHX	5	3908	-	0,6,6	-	-	-		
85	OHX	5	3830	-	0,6,6	-	-	-		
85	OHX	1	3815	-	0,6,6	-	-	-		
85	OHX	1	3999	84	0,6,6	-	-	-		
85	OHX	q2	502	-	0,6,6	-	-	-		
85	OHX	2	2067	-	0,6,6	-	-	-		
85	OHX	4	215	-	0,6,6	-	-	-		
85	OHX	5	3755	-	0,6,6	-	-	-		
85	OHX	5	3771	-	0,6,6	-	-	-		
85	OHX	6	2055	-	0,6,6	-	-	-		
85	OHX	5	3992	-	0,6,6	-	-	-		
85	OHX	5	4025	-	0,6,6	-	-	-		
85	OHX	6	2061	-	0,6,6	-	-	-		
85	OHX	2	1999	-	0,6,6	-	-	-		
85	OHX	8	220	-	0,6,6	-	-	-		
85	OHX	2	2108	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3842	-	0,6,6	-	-	-		
85	OHX	5	3855	-	0,6,6	-	-	-		
85	OHX	1	3835	-	0,6,6	-	-	-		
85	OHX	6	2127	-	0,6,6	-	-	-		
85	OHX	5	4003	-	0,6,6	-	-	-		
85	OHX	5	4061	-	0,6,6	-	-	-		
85	OHX	1	3910	-	0,6,6	-	-	-		
85	OHX	7	213	-	0,6,6	-	-	-		
85	OHX	2	1984	-	0,6,6	-	-	-		
85	OHX	1	3790	-	0,6,6	-	-	-		
85	OHX	1	3882	-	0,6,6	-	-	-		
85	OHX	1	3912	-	0,6,6	-	-	-		
85	OHX	m5	304	-	0,6,6	-	-	-		
85	OHX	1	3915	-	0,6,6	-	-	-		
85	OHX	5	4021	-	0,6,6	-	-	-		
85	OHX	5	3914	-	0,6,6	-	-	-		
85	OHX	1	3792	-	0,6,6	-	-	-		
85	OHX	5	3957	-	0,6,6	-	-	-		
85	OHX	2	2117	-	0,6,6	-	-	-		
85	OHX	1	3955	-	0,6,6	-	-	-		
85	OHX	5	3824	-	0,6,6	-	-	-		
85	OHX	6	2072	-	0,6,6	-	-	-		
85	OHX	1	3960	-	0,6,6	-	-	-		
85	OHX	5	3863	-	0,6,6	-	-	-		
85	OHX	5	3743	-	0,6,6	-	-	-		
85	OHX	1	3813	-	0,6,6	-	-	-		
85	OHX	5	3941	-	0,6,6	-	-	-		
85	OHX	5	3761	-	0,6,6	-	-	-		
85	OHX	1	3734	-	0,6,6	-	-	-		
85	OHX	c8	201	-	0,6,6	-	-	-		
85	OHX	5	4038	-	0,6,6	-	-	-		
85	OHX	6	2129	-	0,6,6	-	-	-		
85	OHX	1	3786	-	0,6,6	-	-	-		
85	OHX	6	2060	-	0,6,6	-	-	-		
85	OHX	5	3800	-	0,6,6	-	-	-		
85	OHX	5	3876	-	0,6,6	-	-	-		
85	OHX	1	3830	-	0,6,6	-	-	-		
85	OHX	1	4002	-	0,6,6	-	-	-		
85	OHX	5	3749	-	0,6,6	-	-	-		
85	OHX	8	221	-	0,6,6	-	-	-		
85	OHX	l5	301	-	0,6,6	-	-	-		
85	OHX	2	2016	-	0,6,6	-	-	-		
85	OHX	1	3942	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3777	-	0,6,6	-	-	-		
85	OHX	4	229	-	0,6,6	-	-	-		
85	OHX	5	3849	-	0,6,6	-	-	-		
85	OHX	1	3938	-	0,6,6	-	-	-		
85	OHX	5	4052	-	0,6,6	-	-	-		
85	OHX	1	3836	-	0,6,6	-	-	-		
85	OHX	L3	402	-	0,6,6	-	-	-		
85	OHX	4	222	-	0,6,6	-	-	-		
85	OHX	6	2118	-	0,6,6	-	-	-		
85	OHX	5	3974	-	0,6,6	-	-	-		
85	OHX	5	3883	-	0,6,6	-	-	-		
85	OHX	2	2082	-	0,6,6	-	-	-		
85	OHX	6	2149	-	0,6,6	-	-	-		
85	OHX	5	3790	-	0,6,6	-	-	-		
85	OHX	5	4006	-	0,6,6	-	-	-		
85	OHX	1	3935	-	0,6,6	-	-	-		
85	OHX	6	2100	-	0,6,6	-	-	-		
85	OHX	1	3946	-	0,6,6	-	-	-		
85	OHX	1	3962	-	0,6,6	-	-	-		
85	OHX	6	2048	-	0,6,6	-	-	-		
85	OHX	6	2088	-	0,6,6	-	-	-		
85	OHX	1	3728	-	0,6,6	-	-	-		
85	OHX	5	3958	-	0,6,6	-	-	-		
85	OHX	2	1988	-	0,6,6	-	-	-		
85	OHX	O7	104	84	0,6,6	-	-	-		
85	OHX	6	2092	-	0,6,6	-	-	-		
85	OHX	5	4041	-	0,6,6	-	-	-		
85	OHX	1	3753	-	0,6,6	-	-	-		
85	OHX	1	3797	-	0,6,6	-	-	-		
85	OHX	6	2013	-	0,6,6	-	-	-		
85	OHX	1	3903	-	0,6,6	-	-	-		
85	OHX	6	2084	-	0,6,6	-	-	-		
85	OHX	2	2030	-	0,6,6	-	-	-		
85	OHX	5	3890	-	0,6,6	-	-	-		
85	OHX	5	3889	-	0,6,6	-	-	-		
85	OHX	5	3814	-	0,6,6	-	-	-		
85	OHX	2	2074	-	0,6,6	-	-	-		
85	OHX	1	4005	-	0,6,6	-	-	-		
85	OHX	1	3770	-	0,6,6	-	-	-		
85	OHX	5	4002	-	0,6,6	-	-	-		
85	OHX	2	2103	-	0,6,6	-	-	-		
85	OHX	1	4020	-	0,6,6	-	-	-		
85	OHX	6	2108	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	s4	301	-	0,6,6	-	-	-		
85	OHX	5	3763	-	0,6,6	-	-	-		
85	OHX	5	3874	-	0,6,6	-	-	-		
85	OHX	5	3942	84	0,6,6	-	-	-		
85	OHX	5	3954	-	0,6,6	-	-	-		
85	OHX	1	4023	-	0,6,6	-	-	-		
85	OHX	2	2047	-	0,6,6	-	-	-		
85	OHX	1	3997	-	0,6,6	-	-	-		
85	OHX	1	3937	-	0,6,6	-	-	-		
85	OHX	1	3756	-	0,6,6	-	-	-		
85	OHX	2	2012	-	0,6,6	-	-	-		
85	OHX	1	3730	-	0,6,6	-	-	-		
85	OHX	6	2095	-	0,6,6	-	-	-		
85	OHX	5	3955	-	0,6,6	-	-	-		
85	OHX	5	4013	-	0,6,6	-	-	-		
85	OHX	7	219	-	0,6,6	-	-	-		
85	OHX	m0	301	-	0,6,6	-	-	-		
85	OHX	1	3810	-	0,6,6	-	-	-		
85	OHX	1	3968	-	0,6,6	-	-	-		
85	OHX	5	3960	-	0,6,6	-	-	-		
85	OHX	5	3962	-	0,6,6	-	-	-		
85	OHX	2	2037	-	0,6,6	-	-	-		
85	OHX	1	3796	-	0,6,6	-	-	-		
85	OHX	1	3811	-	0,6,6	-	-	-		
85	OHX	1	3866	-	0,6,6	-	-	-		
85	OHX	1	3987	-	0,6,6	-	-	-		
85	OHX	l5	302	-	0,6,6	-	-	-		
85	OHX	6	2143	-	0,6,6	-	-	-		
85	OHX	m1	202	-	0,6,6	-	-	-		
85	OHX	l3	407	-	0,6,6	-	-	-		
85	OHX	1	3877	-	0,6,6	-	-	-		
85	OHX	6	2037	-	0,6,6	-	-	-		
85	OHX	6	2045	-	0,6,6	-	-	-		
85	OHX	5	3936	-	0,6,6	-	-	-		
85	OHX	1	3738	-	0,6,6	-	-	-		
85	OHX	1	4036	-	0,6,6	-	-	-		
85	OHX	5	3944	-	0,6,6	-	-	-		
85	OHX	1	3995	-	0,6,6	-	-	-		
85	OHX	6	2133	-	0,6,6	-	-	-		
85	OHX	5	3932	-	0,6,6	-	-	-		
85	OHX	1	4008	-	0,6,6	-	-	-		
85	OHX	5	3995	-	0,6,6	-	-	-		
85	OHX	1	4003	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	2	2026	-	0,6,6	-	-	-		
85	OHX	1	3820	-	0,6,6	-	-	-		
85	OHX	3	218	-	0,6,6	-	-	-		
85	OHX	2	2022	-	0,6,6	-	-	-		
85	OHX	6	2009	-	0,6,6	-	-	-		
85	OHX	6	2073	-	0,6,6	-	-	-		
85	OHX	7	221	-	0,6,6	-	-	-		
85	OHX	5	3994	-	0,6,6	-	-	-		
85	OHX	8	217	-	0,6,6	-	-	-		
85	OHX	3	214	-	0,6,6	-	-	-		
85	OHX	2	2031	-	0,6,6	-	-	-		
85	OHX	5	3986	-	0,6,6	-	-	-		
85	OHX	2	2073	-	0,6,6	-	-	-		
85	OHX	1	3747	-	0,6,6	-	-	-		
85	OHX	O3	202	-	0,6,6	-	-	-		
85	OHX	5	3875	-	0,6,6	-	-	-		
85	OHX	7	216	-	0,6,6	-	-	-		
85	OHX	8	213	-	0,6,6	-	-	-		
85	OHX	2	2085	-	0,6,6	-	-	-		
85	OHX	5	4064	-	0,6,6	-	-	-		
85	OHX	2	2069	-	0,6,6	-	-	-		
85	OHX	5	3934	-	0,6,6	-	-	-		
85	OHX	5	4049	-	0,6,6	-	-	-		
85	OHX	O7	105	-	0,6,6	-	-	-		
85	OHX	1	3768	-	0,6,6	-	-	-		
85	OHX	2	2072	-	0,6,6	-	-	-		
85	OHX	5	3802	-	0,6,6	-	-	-		
85	OHX	6	2049	-	0,6,6	-	-	-		
85	OHX	1	3745	-	0,6,6	-	-	-		
85	OHX	c5	201	-	0,6,6	-	-	-		
85	OHX	5	4037	-	0,6,6	-	-	-		
85	OHX	C5	201	-	0,6,6	-	-	-		
85	OHX	2	2110	-	0,6,6	-	-	-		
85	OHX	6	2113	-	0,6,6	-	-	-		
85	OHX	2	1993	-	0,6,6	-	-	-		
85	OHX	6	2044	-	0,6,6	-	-	-		
85	OHX	5	3796	-	0,6,6	-	-	-		
85	OHX	5	3972	-	0,6,6	-	-	-		
85	OHX	1	3793	-	0,6,6	-	-	-		
85	OHX	6	2011	-	0,6,6	-	-	-		
85	OHX	5	3770	-	0,6,6	-	-	-		
85	OHX	5	3866	-	0,6,6	-	-	-		
85	OHX	5	4016	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3869	-	0,6,6	-	-	-		
85	OHX	2	2032	-	0,6,6	-	-	-		
85	OHX	5	4023	-	0,6,6	-	-	-		
85	OHX	5	3976	-	0,6,6	-	-	-		
85	OHX	5	3894	-	0,6,6	-	-	-		
85	OHX	1	3731	-	0,6,6	-	-	-		
85	OHX	1	3948	-	0,6,6	-	-	-		
85	OHX	M5	302	-	0,6,6	-	-	-		
85	OHX	6	2075	-	0,6,6	-	-	-		
85	OHX	1	3892	-	0,6,6	-	-	-		
85	OHX	6	2122	-	0,6,6	-	-	-		
85	OHX	1	3965	-	0,6,6	-	-	-		
85	OHX	5	3782	-	0,6,6	-	-	-		
85	OHX	5	4042	-	0,6,6	-	-	-		
85	OHX	5	3742	-	0,6,6	-	-	-		
85	OHX	6	2097	-	0,6,6	-	-	-		
85	OHX	5	3931	-	0,6,6	-	-	-		
85	OHX	5	4034	-	0,6,6	-	-	-		
85	OHX	n3	202	-	0,6,6	-	-	-		
85	OHX	1	3825	-	0,6,6	-	-	-		
85	OHX	1	4019	-	0,6,6	-	-	-		
85	OHX	1	3808	-	0,6,6	-	-	-		
85	OHX	2	2028	-	0,6,6	-	-	-		
85	OHX	1	3854	-	0,6,6	-	-	-		
85	OHX	1	3981	-	0,6,6	-	-	-		
85	OHX	5	3895	-	0,6,6	-	-	-		
85	OHX	5	4015	-	0,6,6	-	-	-		
85	OHX	1	3809	-	0,6,6	-	-	-		
85	OHX	6	2042	-	0,6,6	-	-	-		
85	OHX	1	3787	-	0,6,6	-	-	-		
85	OHX	5	3745	-	0,6,6	-	-	-		
85	OHX	5	3864	-	0,6,6	-	-	-		
85	OHX	5	3940	84	0,6,6	-	-	-		
85	OHX	1	3992	-	0,6,6	-	-	-		
85	OHX	8	225	-	0,6,6	-	-	-		
85	OHX	3	219	-	0,6,6	-	-	-		
85	OHX	5	3919	-	0,6,6	-	-	-		
85	OHX	1	3959	-	0,6,6	-	-	-		
85	OHX	1	3769	-	0,6,6	-	-	-		
85	OHX	2	2029	-	0,6,6	-	-	-		
85	OHX	6	2101	-	0,6,6	-	-	-		
85	OHX	5	3915	-	0,6,6	-	-	-		
85	OHX	6	2029	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	n9	102	-	0,6,6	-	-	-		
85	OHX	1	4024	-	0,6,6	-	-	-		
85	OHX	1	3776	-	0,6,6	-	-	-		
85	OHX	6	2051	-	0,6,6	-	-	-		
85	OHX	5	3837	-	0,6,6	-	-	-		
85	OHX	1	3772	-	0,6,6	-	-	-		
85	OHX	1	3739	-	0,6,6	-	-	-		
85	OHX	5	3847	-	0,6,6	-	-	-		
85	OHX	4	225	-	0,6,6	-	-	-		
85	OHX	4	217	-	0,6,6	-	-	-		
85	OHX	5	3832	-	0,6,6	-	-	-		
85	OHX	1	3782	-	0,6,6	-	-	-		
85	OHX	1	3904	-	0,6,6	-	-	-		
85	OHX	2	2076	-	0,6,6	-	-	-		
85	OHX	5	3791	-	0,6,6	-	-	-		
85	OHX	5	3943	-	0,6,6	-	-	-		
85	OHX	6	2080	-	0,6,6	-	-	-		
85	OHX	6	2089	-	0,6,6	-	-	-		
85	OHX	6	2130	-	0,6,6	-	-	-		
85	OHX	1	3761	-	0,6,6	-	-	-		
85	OHX	5	3893	-	0,6,6	-	-	-		
85	OHX	s9	201	-	0,6,6	-	-	-		
85	OHX	1	3876	-	0,6,6	-	-	-		
85	OHX	5	3865	-	0,6,6	-	-	-		
85	OHX	3	215	-	0,6,6	-	-	-		
85	OHX	5	3829	-	0,6,6	-	-	-		
85	OHX	5	3787	-	0,6,6	-	-	-		
85	OHX	5	3851	-	0,6,6	-	-	-		
85	OHX	2	2015	-	0,6,6	-	-	-		
85	OHX	1	3774	-	0,6,6	-	-	-		
85	OHX	5	3897	-	0,6,6	-	-	-		
85	OHX	2	2078	-	0,6,6	-	-	-		
85	OHX	1	3949	-	0,6,6	-	-	-		
85	OHX	5	3926	-	0,6,6	-	-	-		
85	OHX	2	1987	-	0,6,6	-	-	-		
85	OHX	1	4026	-	0,6,6	-	-	-		
85	OHX	1	3858	-	0,6,6	-	-	-		
85	OHX	2	1985	-	0,6,6	-	-	-		
85	OHX	6	2017	-	0,6,6	-	-	-		
85	OHX	2	2098	-	0,6,6	-	-	-		
85	OHX	1	3805	-	0,6,6	-	-	-		
85	OHX	6	2115	-	0,6,6	-	-	-		
85	OHX	5	3805	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3807	-	0,6,6	-	-	-		
85	OHX	5	3806	-	0,6,6	-	-	-		
85	OHX	1	3994	-	0,6,6	-	-	-		
85	OHX	4	219	-	0,6,6	-	-	-		
85	OHX	1	3908	-	0,6,6	-	-	-		
85	OHX	1	3954	-	0,6,6	-	-	-		
85	OHX	5	3820	-	0,6,6	-	-	-		
85	OHX	1	3735	-	0,6,6	-	-	-		
85	OHX	6	2082	-	0,6,6	-	-	-		
85	OHX	5	3825	-	0,6,6	-	-	-		
85	OHX	2	2109	-	0,6,6	-	-	-		
85	OHX	5	3896	-	0,6,6	-	-	-		
85	OHX	l9	202	-	0,6,6	-	-	-		
85	OHX	6	2153	-	0,6,6	-	-	-		
85	OHX	1	3763	-	0,6,6	-	-	-		
85	OHX	2	2052	-	0,6,6	-	-	-		
85	OHX	1	3870	-	0,6,6	-	-	-		
85	OHX	2	1998	-	0,6,6	-	-	-		
85	OHX	6	2079	-	0,6,6	-	-	-		
85	OHX	8	222	-	0,6,6	-	-	-		
85	OHX	6	2132	-	0,6,6	-	-	-		
85	OHX	1	4017	-	0,6,6	-	-	-		
85	OHX	1	4027	-	0,6,6	-	-	-		
85	OHX	2	2064	-	0,6,6	-	-	-		
85	OHX	1	3752	-	0,6,6	-	-	-		
85	OHX	8	212	-	0,6,6	-	-	-		
85	OHX	5	4069	-	0,6,6	-	-	-		
85	OHX	1	3914	-	0,6,6	-	-	-		
85	OHX	6	2035	-	0,6,6	-	-	-		
85	OHX	1	3956	-	0,6,6	-	-	-		
85	OHX	2	2024	-	0,6,6	-	-	-		
85	OHX	6	2025	-	0,6,6	-	-	-		
85	OHX	6	2109	-	0,6,6	-	-	-		
85	OHX	5	3812	-	0,6,6	-	-	-		
85	OHX	5	3856	-	0,6,6	-	-	-		
85	OHX	M9	201	-	0,6,6	-	-	-		
85	OHX	6	2107	-	0,6,6	-	-	-		
85	OHX	6	2052	-	0,6,6	-	-	-		
85	OHX	1	3990	-	0,6,6	-	-	-		
85	OHX	5	3756	-	0,6,6	-	-	-		
85	OHX	5	3952	-	0,6,6	-	-	-		
85	OHX	5	4054	-	0,6,6	-	-	-		
85	OHX	6	2020	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	2	1991	-	0,6,6	-	-	-		
85	OHX	3	217	-	0,6,6	-	-	-		
85	OHX	2	2088	-	0,6,6	-	-	-		
85	OHX	6	2012	-	0,6,6	-	-	-		
85	OHX	6	2047	-	0,6,6	-	-	-		
85	OHX	6	2126	-	0,6,6	-	-	-		
85	OHX	5	4050	-	0,6,6	-	-	-		
85	OHX	5	3813	-	0,6,6	-	-	-		
85	OHX	1	3838	-	0,6,6	-	-	-		
85	OHX	6	2070	-	0,6,6	-	-	-		
85	OHX	5	3907	-	0,6,6	-	-	-		
85	OHX	2	2084	-	0,6,6	-	-	-		
85	OHX	5	3798	-	0,6,6	-	-	-		
85	OHX	2	1996	-	0,6,6	-	-	-		
85	OHX	5	3783	-	0,6,6	-	-	-		
85	OHX	6	2135	-	0,6,6	-	-	-		
85	OHX	5	3980	-	0,6,6	-	-	-		
85	OHX	1	3926	-	0,6,6	-	-	-		
85	OHX	2	2018	-	0,6,6	-	-	-		
85	OHX	2	2045	-	0,6,6	-	-	-		
85	OHX	1	4015	-	0,6,6	-	-	-		
85	OHX	6	2071	-	0,6,6	-	-	-		
85	OHX	5	3949	-	0,6,6	-	-	-		
85	OHX	1	4032	-	0,6,6	-	-	-		
85	OHX	6	2154	-	0,6,6	-	-	-		
85	OHX	5	4017	-	0,6,6	-	-	-		
85	OHX	5	3799	-	0,6,6	-	-	-		
85	OHX	1	3817	-	0,6,6	-	-	-		
85	OHX	1	3936	-	0,6,6	-	-	-		
85	OHX	1	3996	-	0,6,6	-	-	-		
85	OHX	2	2119	-	0,6,6	-	-	-		
85	OHX	2	2034	-	0,6,6	-	-	-		
85	OHX	2	2039	-	0,6,6	-	-	-		
85	OHX	5	3775	-	0,6,6	-	-	-		
85	OHX	5	3826	-	0,6,6	-	-	-		
85	OHX	5	3966	-	0,6,6	-	-	-		
85	OHX	5	3848	-	0,6,6	-	-	-		
85	OHX	1	3750	-	0,6,6	-	-	-		
85	OHX	6	2010	-	0,6,6	-	-	-		
85	OHX	1	3951	-	0,6,6	-	-	-		
85	OHX	1	3884	-	0,6,6	-	-	-		
85	OHX	2	2086	-	0,6,6	-	-	-		
85	OHX	2	2036	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3950	-	0,6,6	-	-	-		
85	OHX	5	3990	-	0,6,6	-	-	-		
85	OHX	1	3732	-	0,6,6	-	-	-		
85	OHX	2	2081	-	0,6,6	-	-	-		
85	OHX	2	2041	-	0,6,6	-	-	-		
85	OHX	1	3924	-	0,6,6	-	-	-		
85	OHX	5	4024	-	0,6,6	-	-	-		
85	OHX	2	2005	-	0,6,6	-	-	-		
85	OHX	2	1990	-	0,6,6	-	-	-		
85	OHX	2	2033	-	0,6,6	-	-	-		
85	OHX	2	2063	-	0,6,6	-	-	-		
85	OHX	6	2096	-	0,6,6	-	-	-		
85	OHX	6	2083	-	0,6,6	-	-	-		
85	OHX	5	3838	-	0,6,6	-	-	-		
85	OHX	6	2112	-	0,6,6	-	-	-		
85	OHX	6	2119	-	0,6,6	-	-	-		
85	OHX	1	3973	-	0,6,6	-	-	-		
85	OHX	6	2039	-	0,6,6	-	-	-		
85	OHX	7	215	-	0,6,6	-	-	-		
85	OHX	1	4029	-	0,6,6	-	-	-		
85	OHX	6	2028	-	0,6,6	-	-	-		
85	OHX	1	3963	-	0,6,6	-	-	-		
85	OHX	5	4043	-	0,6,6	-	-	-		
85	OHX	5	3822	-	0,6,6	-	-	-		
85	OHX	5	3910	-	0,6,6	-	-	-		
85	OHX	1	3873	-	0,6,6	-	-	-		
85	OHX	1	3933	-	0,6,6	-	-	-		
85	OHX	6	2144	-	0,6,6	-	-	-		
85	OHX	6	2090	-	0,6,6	-	-	-		
85	OHX	2	2115	-	0,6,6	-	-	-		
85	OHX	2	2068	-	0,6,6	-	-	-		
85	OHX	1	3891	-	0,6,6	-	-	-		
85	OHX	1	4030	-	0,6,6	-	-	-		
85	OHX	5	3868	-	0,6,6	-	-	-		
85	OHX	5	3917	-	0,6,6	-	-	-		
85	OHX	1	3982	-	0,6,6	-	-	-		
85	OHX	c3	201	-	0,6,6	-	-	-		
85	OHX	2	2056	-	0,6,6	-	-	-		
85	OHX	5	3780	-	0,6,6	-	-	-		
85	OHX	1	3991	-	0,6,6	-	-	-		
85	OHX	1	4034	-	0,6,6	-	-	-		
85	OHX	6	2145	-	0,6,6	-	-	-		
85	OHX	5	3899	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3961	-	0,6,6	-	-	-		
85	OHX	4	228	-	0,6,6	-	-	-		
85	OHX	2	2062	-	0,6,6	-	-	-		
85	OHX	6	2111	-	0,6,6	-	-	-		
85	OHX	5	4004	-	0,6,6	-	-	-		
85	OHX	5	3803	-	0,6,6	-	-	-		
85	OHX	5	3923	-	0,6,6	-	-	-		
85	OHX	1	3922	-	0,6,6	-	-	-		
85	OHX	1	3978	-	0,6,6	-	-	-		
85	OHX	5	3981	-	0,6,6	-	-	-		
85	OHX	8	216	-	0,6,6	-	-	-		
85	OHX	2	2053	-	0,6,6	-	-	-		
85	OHX	1	4000	-	0,6,6	-	-	-		
85	OHX	1	3944	-	0,6,6	-	-	-		
85	OHX	1	4014	-	0,6,6	-	-	-		
85	OHX	1	3857	-	0,6,6	-	-	-		
85	OHX	5	3882	-	0,6,6	-	-	-		
85	OHX	5	3920	-	0,6,6	-	-	-		
85	OHX	2	2023	-	0,6,6	-	-	-		
85	OHX	2	2059	-	0,6,6	-	-	-		
85	OHX	2	2101	-	0,6,6	-	-	-		
85	OHX	5	3913	-	0,6,6	-	-	-		
85	OHX	1	3975	-	0,6,6	-	-	-		
85	OHX	5	3758	-	0,6,6	-	-	-		
85	OHX	S6	301	-	0,6,6	-	-	-		
85	OHX	6	2105	-	0,6,6	-	-	-		
85	OHX	2	2057	-	0,6,6	-	-	-		
85	OHX	5	3815	-	0,6,6	-	-	-		
85	OHX	2	2014	-	0,6,6	-	-	-		
85	OHX	5	3921	-	0,6,6	-	-	-		
85	OHX	1	3802	-	0,6,6	-	-	-		
85	OHX	5	3888	-	0,6,6	-	-	-		
85	OHX	5	3939	-	0,6,6	-	-	-		
85	OHX	5	3993	-	0,6,6	-	-	-		
85	OHX	1	3979	-	0,6,6	-	-	-		
85	OHX	1	4037	-	0,6,6	-	-	-		
85	OHX	6	2156	-	0,6,6	-	-	-		
85	OHX	4	226	-	0,6,6	-	-	-		
85	OHX	5	3912	-	0,6,6	-	-	-		
85	OHX	5	3924	-	0,6,6	-	-	-		
85	OHX	1	3972	-	0,6,6	-	-	-		
85	OHX	5	3786	-	0,6,6	-	-	-		
85	OHX	5	3930	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	o3	202	-	0,6,6	-	-	-		
85	OHX	5	3880	-	0,6,6	-	-	-		
85	OHX	5	4062	-	0,6,6	-	-	-		
85	OHX	1	3917	-	0,6,6	-	-	-		
85	OHX	1	3964	-	0,6,6	-	-	-		
85	OHX	1	3888	-	0,6,6	-	-	-		
85	OHX	1	3907	-	0,6,6	-	-	-		
85	OHX	5	3902	-	0,6,6	-	-	-		
85	OHX	2	2038	-	0,6,6	-	-	-		
85	OHX	2	2042	-	0,6,6	-	-	-		
85	OHX	1	3791	-	0,6,6	-	-	-		
85	OHX	5	3903	-	0,6,6	-	-	-		
85	OHX	5	3792	-	0,6,6	-	-	-		
85	OHX	2	2046	-	0,6,6	-	-	-		
85	OHX	5	3938	-	0,6,6	-	-	-		
85	OHX	2	2091	-	0,6,6	-	-	-		
85	OHX	1	3977	-	0,6,6	-	-	-		
85	OHX	6	2128	-	0,6,6	-	-	-		
85	OHX	8	215	-	0,6,6	-	-	-		
85	OHX	1	3989	-	0,6,6	-	-	-		
85	OHX	6	2024	-	0,6,6	-	-	-		
85	OHX	2	1986	-	0,6,6	-	-	-		
85	OHX	1	3984	84	0,6,6	-	-	-		
85	OHX	4	224	-	0,6,6	-	-	-		
85	OHX	5	3948	-	0,6,6	-	-	-		
85	OHX	2	2007	-	0,6,6	-	-	-		
85	OHX	2	2009	-	0,6,6	-	-	-		
85	OHX	1	3851	-	0,6,6	-	-	-		
85	OHX	1	4011	-	0,6,6	-	-	-		
85	OHX	1	3736	-	0,6,6	-	-	-		
85	OHX	6	2066	-	0,6,6	-	-	-		
85	OHX	2	2104	-	0,6,6	-	-	-		
85	OHX	1	3742	-	0,6,6	-	-	-		
85	OHX	1	3988	-	0,6,6	-	-	-		
85	OHX	6	2121	-	0,6,6	-	-	-		
85	OHX	sR	401	-	0,6,6	-	-	-		
85	OHX	1	3945	-	0,6,6	-	-	-		
85	OHX	1	3971	-	0,6,6	-	-	-		
85	OHX	3	212	-	0,6,6	-	-	-		
85	OHX	5	3785	-	0,6,6	-	-	-		
85	OHX	5	3853	-	0,6,6	-	-	-		
85	OHX	1	3920	-	0,6,6	-	-	-		
85	OHX	5	3946	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3860	-	0,6,6	-	-	-		
85	OHX	2	2092	-	0,6,6	-	-	-		
85	OHX	2	2008	-	0,6,6	-	-	-		
85	OHX	5	4063	-	0,6,6	-	-	-		
85	OHX	6	2147	-	0,6,6	-	-	-		
85	OHX	2	2013	-	0,6,6	-	-	-		
85	OHX	5	3751	-	0,6,6	-	-	-		
85	OHX	1	3895	-	0,6,6	-	-	-		
85	OHX	1	3985	-	0,6,6	-	-	-		
85	OHX	5	4057	-	0,6,6	-	-	-		
85	OHX	6	2093	-	0,6,6	-	-	-		
85	OHX	2	2106	-	0,6,6	-	-	-		
85	OHX	7	214	-	0,6,6	-	-	-		
85	OHX	5	3867	-	0,6,6	-	-	-		
85	OHX	1	3940	-	0,6,6	-	-	-		
85	OHX	2	2006	-	0,6,6	-	-	-		
85	OHX	1	3846	-	0,6,6	-	-	-		
85	OHX	1	4009	-	0,6,6	-	-	-		
85	OHX	6	2069	-	0,6,6	-	-	-		
85	OHX	5	4027	-	0,6,6	-	-	-		
85	OHX	2	2043	-	0,6,6	-	-	-		
85	OHX	1	3859	-	0,6,6	-	-	-		
85	OHX	1	3905	-	0,6,6	-	-	-		
85	OHX	5	3878	-	0,6,6	-	-	-		
85	OHX	1	3844	-	0,6,6	-	-	-		
85	OHX	1	3886	-	0,6,6	-	-	-		
85	OHX	1	3918	-	0,6,6	-	-	-		
85	OHX	6	2019	-	0,6,6	-	-	-		
85	OHX	5	3852	-	0,6,6	-	-	-		
85	OHX	2	2065	-	0,6,6	-	-	-		
85	OHX	1	3757	-	0,6,6	-	-	-		
85	OHX	1	3828	-	0,6,6	-	-	-		
85	OHX	5	3977	-	0,6,6	-	-	-		
85	OHX	5	3984	-	0,6,6	-	-	-		
85	OHX	2	2095	-	0,6,6	-	-	-		
85	OHX	5	3816	-	0,6,6	-	-	-		
85	OHX	1	3939	-	0,6,6	-	-	-		
85	OHX	5	3963	-	0,6,6	-	-	-		
85	OHX	5	4005	-	0,6,6	-	-	-		
85	OHX	5	3968	-	0,6,6	-	-	-		
85	OHX	5	3754	-	0,6,6	-	-	-		
85	OHX	5	4020	-	0,6,6	-	-	-		
85	OHX	6	2050	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	N8	203	-	0,6,6	-	-	-		
85	OHX	2	1994	-	0,6,6	-	-	-		
85	OHX	1	3896	-	0,6,6	-	-	-		
85	OHX	1	3925	-	0,6,6	-	-	-		
85	OHX	2	2050	-	0,6,6	-	-	-		
85	OHX	6	2123	-	0,6,6	-	-	-		
85	OHX	2	2058	-	0,6,6	-	-	-		
85	OHX	2	2118	-	0,6,6	-	-	-		
85	OHX	1	3865	-	0,6,6	-	-	-		
85	OHX	6	2117	-	0,6,6	-	-	-		
85	OHX	l3	406	-	0,6,6	-	-	-		
85	OHX	5	4011	-	0,6,6	-	-	-		
85	OHX	5	3810	-	0,6,6	-	-	-		
85	OHX	1	4033	-	0,6,6	-	-	-		
85	OHX	5	3989	-	0,6,6	-	-	-		
85	OHX	5	4007	36	0,6,6	-	-	-		
85	OHX	2	1995	-	0,6,6	-	-	-		
85	OHX	1	3834	-	0,6,6	-	-	-		
85	OHX	1	3867	-	0,6,6	-	-	-		
85	OHX	5	3846	-	0,6,6	-	-	-		
85	OHX	5	4009	-	0,6,6	-	-	-		
85	OHX	2	2094	-	0,6,6	-	-	-		
85	OHX	5	3937	-	0,6,6	-	-	-		
85	OHX	5	3978	-	0,6,6	-	-	-		
85	OHX	5	4032	-	0,6,6	-	-	-		
85	OHX	o9	101	-	0,6,6	-	-	-		
85	OHX	5	4044	-	0,6,6	-	-	-		
85	OHX	1	3967	-	0,6,6	-	-	-		
85	OHX	5	3844	-	0,6,6	-	-	-		
85	OHX	2	2112	-	0,6,6	-	-	-		
85	OHX	1	3806	-	0,6,6	-	-	-		
85	OHX	5	3757	-	0,6,6	-	-	-		
85	OHX	M7	205	-	0,6,6	-	-	-		
85	OHX	5	3916	-	0,6,6	-	-	-		
85	OHX	1	3781	-	0,6,6	-	-	-		
85	OHX	6	2067	-	0,6,6	-	-	-		
85	OHX	5	3841	-	0,6,6	-	-	-		
85	OHX	5	4019	-	0,6,6	-	-	-		
85	OHX	1	4010	-	0,6,6	-	-	-		
85	OHX	5	3768	-	0,6,6	-	-	-		
85	OHX	5	3861	-	0,6,6	-	-	-		
85	OHX	2	2044	-	0,6,6	-	-	-		
85	OHX	1	3863	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3855	-	0,6,6	-	-	-		
87	ANM	1	3401	-	20,20,20	2.93	9 (45%)	22,27,27	2.80	10 (45%)
85	OHX	6	2116	-	0,6,6	-	-	-		
85	OHX	2	2004	-	0,6,6	-	-	-		
85	OHX	5	3925	-	0,6,6	-	-	-		
85	OHX	5	4018	-	0,6,6	-	-	-		
85	OHX	1	3840	-	0,6,6	-	-	-		
85	OHX	5	3953	-	0,6,6	-	-	-		
85	OHX	7	220	-	0,6,6	-	-	-		
85	OHX	8	219	-	0,6,6	-	-	-		
85	OHX	6	2152	-	0,6,6	-	-	-		
85	OHX	1	3832	-	0,6,6	-	-	-		
85	OHX	4	230	-	0,6,6	-	-	-		
85	OHX	3	213	-	0,6,6	-	-	-		
85	OHX	5	3886	-	0,6,6	-	-	-		
85	OHX	5	4033	-	0,6,6	-	-	-		
85	OHX	1	3833	-	0,6,6	-	-	-		
85	OHX	6	2148	-	0,6,6	-	-	-		
85	OHX	5	3951	-	0,6,6	-	-	-		
85	OHX	2	2107	-	0,6,6	-	-	-		
85	OHX	2	2111	-	0,6,6	-	-	-		
85	OHX	6	2086	-	0,6,6	-	-	-		
85	OHX	5	3748	-	0,6,6	-	-	-		
85	OHX	1	3812	-	0,6,6	-	-	-		
85	OHX	5	3881	-	0,6,6	-	-	-		
85	OHX	5	3965	-	0,6,6	-	-	-		
85	OHX	5	3788	-	0,6,6	-	-	-		
85	OHX	1	3767	-	0,6,6	-	-	-		
85	OHX	2	2003	-	0,6,6	-	-	-		
85	OHX	5	4036	-	0,6,6	-	-	-		
85	OHX	6	2063	-	0,6,6	-	-	-		
85	OHX	C8	201	-	0,6,6	-	-	-		
85	OHX	1	3800	-	0,6,6	-	-	-		
85	OHX	5	3795	-	0,6,6	-	-	-		
85	OHX	2	2100	-	0,6,6	-	-	-		
85	OHX	5	4012	-	0,6,6	-	-	-		
85	OHX	5	3781	-	0,6,6	-	-	-		
85	OHX	5	3945	-	0,6,6	-	-	-		
85	OHX	1	3744	-	0,6,6	-	-	-		
85	OHX	1	3765	-	0,6,6	-	-	-		
85	OHX	5	3828	-	0,6,6	-	-	-		
85	OHX	5	3746	-	0,6,6	-	-	-		
85	OHX	6	2078	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3871	-	0,6,6	-	-	-		
85	OHX	1	3821	-	0,6,6	-	-	-		
85	OHX	1	3845	-	0,6,6	-	-	-		
85	OHX	L4	401	-	0,6,6	-	-	-		
85	OHX	6	2098	-	0,6,6	-	-	-		
85	OHX	1	3843	-	0,6,6	-	-	-		
85	OHX	6	2062	-	0,6,6	-	-	-		
85	OHX	5	4022	-	0,6,6	-	-	-		
85	OHX	5	3762	-	0,6,6	-	-	-		
85	OHX	1	3799	-	0,6,6	-	-	-		
85	OHX	6	2016	-	0,6,6	-	-	-		
85	OHX	1	3729	-	0,6,6	-	-	-		
85	OHX	s8	302	-	0,6,6	-	-	-		
85	OHX	1	3759	-	0,6,6	-	-	-		
85	OHX	5	3901	-	0,6,6	-	-	-		
85	OHX	5	3808	-	0,6,6	-	-	-		
85	OHX	6	2136	-	0,6,6	-	-	-		
85	OHX	n3	203	-	0,6,6	-	-	-		
85	OHX	1	3766	-	0,6,6	-	-	-		
85	OHX	1	3966	-	0,6,6	-	-	-		
85	OHX	5	3892	84	0,6,6	-	-	-		
85	OHX	1	3928	-	0,6,6	-	-	-		
85	OHX	2	1983	-	0,6,6	-	-	-		
85	OHX	2	2021	-	0,6,6	-	-	-		
85	OHX	m7	204	-	0,6,6	-	-	-		
85	OHX	2	2075	-	0,6,6	-	-	-		
85	OHX	2	2049	-	0,6,6	-	-	-		
85	OHX	6	2099	-	0,6,6	-	-	-		
85	OHX	6	2018	-	0,6,6	-	-	-		
85	OHX	1	3827	-	0,6,6	-	-	-		
85	OHX	6	2125	84	0,6,6	-	-	-		
85	OHX	1	3842	-	0,6,6	-	-	-		
85	OHX	m0	302	-	0,6,6	-	-	-		
85	OHX	l4	401	-	0,6,6	-	-	-		
85	OHX	2	2027	-	0,6,6	-	-	-		
85	OHX	6	2022	-	0,6,6	-	-	-		
85	OHX	6	2031	-	0,6,6	-	-	-		
85	OHX	2	2089	-	0,6,6	-	-	-		
85	OHX	2	2097	-	0,6,6	-	-	-		
85	OHX	1	3740	-	0,6,6	-	-	-		
85	OHX	1	3778	-	0,6,6	-	-	-		
85	OHX	1	3849	-	0,6,6	-	-	-		
85	OHX	5	3744	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3784	-	0,6,6	-	-	-		
85	OHX	1	3780	-	0,6,6	-	-	-		
85	OHX	1	3930	-	0,6,6	-	-	-		
85	OHX	6	2134	-	0,6,6	-	-	-		
85	OHX	1	3902	-	0,6,6	-	-	-		
85	OHX	6	2124	-	0,6,6	-	-	-		
85	OHX	2	2002	-	0,6,6	-	-	-		
85	OHX	5	3774	-	0,6,6	-	-	-		
85	OHX	3	211	-	0,6,6	-	-	-		
85	OHX	2	2061	-	0,6,6	-	-	-		
85	OHX	1	3885	-	0,6,6	-	-	-		
85	OHX	6	2074	-	0,6,6	-	-	-		
85	OHX	5	3904	-	0,6,6	-	-	-		
85	OHX	6	2103	-	0,6,6	-	-	-		
85	OHX	5	3764	-	0,6,6	-	-	-		
85	OHX	5	3850	-	0,6,6	-	-	-		
85	OHX	1	3898	-	0,6,6	-	-	-		
85	OHX	5	3807	-	0,6,6	-	-	-		
85	OHX	2	2105	-	0,6,6	-	-	-		
85	OHX	1	3901	-	0,6,6	-	-	-		
85	OHX	5	3871	-	0,6,6	-	-	-		
85	OHX	1	3777	-	0,6,6	-	-	-		
85	OHX	5	3959	-	0,6,6	-	-	-		
85	OHX	1	3980	-	0,6,6	-	-	-		
85	OHX	1	3853	-	0,6,6	-	-	-		
85	OHX	2	2099	-	0,6,6	-	-	-		
85	OHX	5	3900	-	0,6,6	-	-	-		
85	OHX	5	4055	-	0,6,6	-	-	-		
85	OHX	1	3961	-	0,6,6	-	-	-		
85	OHX	3	210	-	0,6,6	-	-	-		
85	OHX	Q2	503	84	0,6,6	-	-	-		
85	OHX	1	3958	-	0,6,6	-	-	-		
85	OHX	5	4001	-	0,6,6	-	-	-		
85	OHX	5	3809	-	0,6,6	-	-	-		
85	OHX	1	3875	-	0,6,6	-	-	-		
85	OHX	6	2091	-	0,6,6	-	-	-		
85	OHX	5	4056	-	0,6,6	-	-	-		
85	OHX	5	3870	-	0,6,6	-	-	-		
85	OHX	2	2079	-	0,6,6	-	-	-		
85	OHX	2	2087	-	0,6,6	-	-	-		
85	OHX	5	3836	-	0,6,6	-	-	-		
85	OHX	2	2040	-	0,6,6	-	-	-		
85	OHX	2	2113	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	2	2096	-	0,6,6	-	-	-		
85	OHX	1	3890	-	0,6,6	-	-	-		
85	OHX	6	2034	-	0,6,6	-	-	-		
85	OHX	5	3752	-	0,6,6	-	-	-		
85	OHX	6	2137	-	0,6,6	-	-	-		
85	OHX	2	2011	-	0,6,6	-	-	-		
85	OHX	5	3773	-	0,6,6	-	-	-		
85	OHX	5	3784	-	0,6,6	-	-	-		
85	OHX	SR	401	-	0,6,6	-	-	-		
85	OHX	2	2080	-	0,6,6	-	-	-		
85	OHX	4	221	-	0,6,6	-	-	-		
85	OHX	5	3818	-	0,6,6	-	-	-		
85	OHX	6	2151	-	0,6,6	-	-	-		
85	OHX	5	3766	-	0,6,6	-	-	-		
85	OHX	5	3956	-	0,6,6	-	-	-		
85	OHX	7	217	-	0,6,6	-	-	-		
85	OHX	1	3906	-	0,6,6	-	-	-		
85	OHX	5	4048	-	0,6,6	-	-	-		
85	OHX	1	3773	-	0,6,6	-	-	-		
85	OHX	5	3885	-	0,6,6	-	-	-		
85	OHX	5	3996	-	0,6,6	-	-	-		
85	OHX	1	3794	-	0,6,6	-	-	-		
85	OHX	1	3894	-	0,6,6	-	-	-		
85	OHX	1	3911	-	0,6,6	-	-	-		
85	OHX	1	3976	-	0,6,6	-	-	-		
85	OHX	5	4060	-	0,6,6	-	-	-		
85	OHX	6	2030	-	0,6,6	-	-	-		
85	OHX	4	227	-	0,6,6	-	-	-		
85	OHX	6	2026	-	0,6,6	-	-	-		
85	OHX	1	3889	-	0,6,6	-	-	-		
85	OHX	1	4013	-	0,6,6	-	-	-		
85	OHX	1	3764	84	0,6,6	-	-	-		
85	OHX	1	3847	-	0,6,6	-	-	-		
85	OHX	1	3927	-	0,6,6	-	-	-		
85	OHX	1	3970	-	0,6,6	-	-	-		
85	OHX	5	3769	-	0,6,6	-	-	-		
85	OHX	2	2102	-	0,6,6	-	-	-		
85	OHX	5	3898	-	0,6,6	-	-	-		
85	OHX	1	3874	-	0,6,6	-	-	-		
85	OHX	2	2017	-	0,6,6	-	-	-		
85	OHX	1	3823	-	0,6,6	-	-	-		
85	OHX	1	3880	-	0,6,6	-	-	-		
85	OHX	1	3760	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3814	-	0,6,6	-	-	-		
85	OHX	O9	101	-	0,6,6	-	-	-		
85	OHX	5	3778	-	0,6,6	-	-	-		
85	OHX	1	3909	-	0,6,6	-	-	-		
85	OHX	1	3869	-	0,6,6	-	-	-		
85	OHX	6	2131	-	0,6,6	-	-	-		
85	OHX	5	3983	-	0,6,6	-	-	-		
85	OHX	5	4053	-	0,6,6	-	-	-		
85	OHX	1	3856	-	0,6,6	-	-	-		
85	OHX	1	3974	-	0,6,6	-	-	-		
85	OHX	6	2065	-	0,6,6	-	-	-		
85	OHX	5	3793	-	0,6,6	-	-	-		
85	OHX	5	3872	-	0,6,6	-	-	-		
85	OHX	1	3983	84	0,6,6	-	-	-		
85	OHX	5	3858	-	0,6,6	-	-	-		
85	OHX	1	3749	-	0,6,6	-	-	-		
85	OHX	5	4035	-	0,6,6	-	-	-		
85	OHX	4	220	-	0,6,6	-	-	-		
85	OHX	1	3775	-	0,6,6	-	-	-		
85	OHX	1	3872	-	0,6,6	-	-	-		
85	OHX	1	3931	-	0,6,6	-	-	-		
85	OHX	1	4022	-	0,6,6	-	-	-		
85	OHX	5	3834	-	0,6,6	-	-	-		
85	OHX	5	3999	-	0,6,6	-	-	-		
85	OHX	2	2000	-	0,6,6	-	-	-		
85	OHX	6	2032	-	0,6,6	-	-	-		
85	OHX	5	3811	-	0,6,6	-	-	-		
85	OHX	1	3919	-	0,6,6	-	-	-		
85	OHX	2	2114	-	0,6,6	-	-	-		
85	OHX	5	3891	-	0,6,6	-	-	-		
85	OHX	5	3982	-	0,6,6	-	-	-		
85	OHX	1	3804	-	0,6,6	-	-	-		
85	OHX	1	3899	-	0,6,6	-	-	-		
85	OHX	6	2015	-	0,6,6	-	-	-		
85	OHX	5	4026	-	0,6,6	-	-	-		
85	OHX	6	2021	-	0,6,6	-	-	-		
85	OHX	5	3794	-	0,6,6	-	-	-		
85	OHX	5	3911	-	0,6,6	-	-	-		
85	OHX	5	3884	-	0,6,6	-	-	-		
85	OHX	1	3862	-	0,6,6	-	-	-		
85	OHX	5	4040	-	0,6,6	-	-	-		
85	OHX	2	2051	-	0,6,6	-	-	-		
85	OHX	2	2025	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3751	-	0,6,6	-	-	-		
85	OHX	1	3864	-	0,6,6	-	-	-		
85	OHX	5	3927	-	0,6,6	-	-	-		
85	OHX	1	3932	84	0,6,6	-	-	-		
85	OHX	5	4008	-	0,6,6	-	-	-		
85	OHX	2	2054	-	0,6,6	-	-	-		
85	OHX	5	4059	84	0,6,6	-	-	-		
85	OHX	2	2116	-	0,6,6	-	-	-		
85	OHX	5	4039	-	0,6,6	-	-	-		
85	OHX	6	2057	-	0,6,6	-	-	-		
85	OHX	5	3760	-	0,6,6	-	-	-		
85	OHX	1	3921	-	0,6,6	-	-	-		
85	OHX	5	3909	-	0,6,6	-	-	-		
85	OHX	m5	305	-	0,6,6	-	-	-		
85	OHX	5	4029	-	0,6,6	-	-	-		
85	OHX	1	3878	-	0,6,6	-	-	-		
85	OHX	2	2070	-	0,6,6	-	-	-		
85	OHX	7	211	-	0,6,6	-	-	-		
85	OHX	N1	201	-	0,6,6	-	-	-		
85	OHX	5	3928	-	0,6,6	-	-	-		
85	OHX	5	3859	-	0,6,6	-	-	-		
85	OHX	1	3934	-	0,6,6	-	-	-		
85	OHX	6	2085	-	0,6,6	-	-	-		
85	OHX	o7	502	-	0,6,6	-	-	-		
85	OHX	1	3837	-	0,6,6	-	-	-		
85	OHX	D9	103	-	0,6,6	-	-	-		
85	OHX	1	3998	-	0,6,6	-	-	-		
85	OHX	4	216	-	0,6,6	-	-	-		
85	OHX	1	3816	-	0,6,6	-	-	-		
85	OHX	5	4058	-	0,6,6	-	-	-		
85	OHX	5	3823	-	0,6,6	-	-	-		
85	OHX	5	3873	-	0,6,6	-	-	-		
85	OHX	5	3933	-	0,6,6	-	-	-		
85	OHX	5	3970	-	0,6,6	-	-	-		
85	OHX	6	2139	-	0,6,6	-	-	-		
85	OHX	1	3831	-	0,6,6	-	-	-		
85	OHX	1	3941	-	0,6,6	-	-	-		
85	OHX	N9	101	-	0,6,6	-	-	-		
85	OHX	5	3804	-	0,6,6	-	-	-		
85	OHX	2	2055	-	0,6,6	-	-	-		
85	OHX	1	3795	-	0,6,6	-	-	-		
85	OHX	8	214	-	0,6,6	-	-	-		
85	OHX	1	3829	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3862	-	0,6,6	-	-	-		
85	OHX	1	3900	-	0,6,6	-	-	-		
85	OHX	1	4012	-	0,6,6	-	-	-		
85	OHX	2	2071	-	0,6,6	-	-	-		
85	OHX	1	3897	-	0,6,6	-	-	-		
85	OHX	6	2077	-	0,6,6	-	-	-		
85	OHX	S8	301	-	0,6,6	-	-	-		
85	OHX	5	3821	-	0,6,6	-	-	-		
85	OHX	L3	403	-	0,6,6	-	-	-		
85	OHX	5	3835	-	0,6,6	-	-	-		
85	OHX	5	4000	-	0,6,6	-	-	-		
85	OHX	1	3839	-	0,6,6	-	-	-		
85	OHX	1	4007	-	0,6,6	-	-	-		
85	OHX	1	3755	-	0,6,6	-	-	-		
85	OHX	4	218	-	0,6,6	-	-	-		
85	OHX	2	2010	-	0,6,6	-	-	-		
85	OHX	1	3789	-	0,6,6	-	-	-		
85	OHX	5	3797	84	0,6,6	-	-	-		
85	OHX	6	2058	-	0,6,6	-	-	-		
85	OHX	5	3750	-	0,6,6	-	-	-		
85	OHX	2	2035	-	0,6,6	-	-	-		
85	OHX	1	3887	-	0,6,6	-	-	-		
85	OHX	1	4021	-	0,6,6	-	-	-		
85	OHX	4	231	-	0,6,6	-	-	-		
85	OHX	5	3854	-	0,6,6	-	-	-		
85	OHX	5	3998	-	0,6,6	-	-	-		
85	OHX	8	224	-	0,6,6	-	-	-		
85	OHX	8	211	-	0,6,6	-	-	-		
85	OHX	1	3758	-	0,6,6	-	-	-		
85	OHX	1	3841	-	0,6,6	-	-	-		
85	OHX	1	3819	-	0,6,6	-	-	-		
85	OHX	1	3861	-	0,6,6	-	-	-		
85	OHX	5	3817	-	0,6,6	-	-	-		
85	OHX	6	2106	-	0,6,6	-	-	-		
85	OHX	5	3845	-	0,6,6	-	-	-		
85	OHX	8	223	-	0,6,6	-	-	-		
85	OHX	5	4014	-	0,6,6	-	-	-		
85	OHX	2	2083	-	0,6,6	-	-	-		
85	OHX	5	3979	84	0,6,6	-	-	-		
85	OHX	2	2020	-	0,6,6	-	-	-		
85	OHX	5	4065	-	0,6,6	-	-	-		
85	OHX	6	2064	-	0,6,6	-	-	-		
85	OHX	5	3969	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3748	-	0,6,6	-	-	-		
85	OHX	2	1992	-	0,6,6	-	-	-		
85	OHX	1	3953	-	0,6,6	-	-	-		
85	OHX	5	3997	-	0,6,6	-	-	-		
85	OHX	5	4067	-	0,6,6	-	-	-		
85	OHX	1	3969	-	0,6,6	-	-	-		
85	OHX	6	2027	-	0,6,6	-	-	-		
85	OHX	1	3743	-	0,6,6	-	-	-		
85	OHX	1	3783	-	0,6,6	-	-	-		
85	OHX	1	3741	-	0,6,6	-	-	-		
85	OHX	2	2090	-	0,6,6	-	-	-		
85	OHX	5	3973	-	0,6,6	-	-	-		
85	OHX	1	3788	-	0,6,6	-	-	-		
85	OHX	5	3975	-	0,6,6	-	-	-		
85	OHX	6	2076	-	0,6,6	-	-	-		
85	OHX	1	3943	-	0,6,6	-	-	-		
85	OHX	5	4047	-	0,6,6	-	-	-		
85	OHX	5	3789	-	0,6,6	-	-	-		
85	OHX	1	3893	-	0,6,6	-	-	-		
85	OHX	5	3987	-	0,6,6	-	-	-		
85	OHX	5	3887	-	0,6,6	-	-	-		
85	OHX	5	4066	-	0,6,6	-	-	-		
85	OHX	6	2158	-	0,6,6	-	-	-		
85	OHX	5	3877	-	0,6,6	-	-	-		
85	OHX	1	4028	-	0,6,6	-	-	-		
85	OHX	5	3819	-	0,6,6	-	-	-		
85	OHX	1	3746	-	0,6,6	-	-	-		
85	OHX	5	3839	-	0,6,6	-	-	-		
85	OHX	5	3929	-	0,6,6	-	-	-		
85	OHX	5	3935	-	0,6,6	-	-	-		
85	OHX	6	2146	-	0,6,6	-	-	-		
85	OHX	1	4006	-	0,6,6	-	-	-		
85	OHX	5	3985	-	0,6,6	-	-	-		
85	OHX	1	4031	-	0,6,6	-	-	-		
85	OHX	2	2048	-	0,6,6	-	-	-		
85	OHX	5	3988	-	0,6,6	-	-	-		
85	OHX	d4	201	-	0,6,6	-	-	-		
85	OHX	1	3785	-	0,6,6	-	-	-		
85	OHX	5	3991	-	0,6,6	-	-	-		
85	OHX	6	2056	-	0,6,6	-	-	-		
85	OHX	6	2087	-	0,6,6	-	-	-		
85	OHX	2	2077	-	0,6,6	-	-	-		
85	OHX	5	3905	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	6	2040	-	0,6,6	-	-	-		
85	OHX	6	2140	-	0,6,6	-	-	-		
85	OHX	5	3922	-	0,6,6	-	-	-		
85	OHX	5	3967	-	0,6,6	-	-	-		
85	OHX	1	3986	-	0,6,6	-	-	-		
85	OHX	1	3852	-	0,6,6	-	-	-		
85	OHX	1	4018	-	0,6,6	-	-	-		
85	OHX	3	216	-	0,6,6	-	-	-		
85	OHX	5	4030	-	0,6,6	-	-	-		
85	OHX	5	3857	-	0,6,6	-	-	-		
85	OHX	l3	408	-	0,6,6	-	-	-		
85	OHX	7	212	-	0,6,6	-	-	-		
85	OHX	6	2081	-	0,6,6	-	-	-		
85	OHX	1	3848	-	0,6,6	-	-	-		
85	OHX	6	2141	-	0,6,6	-	-	-		
85	OHX	1	3947	-	0,6,6	-	-	-		
85	OHX	6	2114	-	0,6,6	-	-	-		
85	OHX	5	3964	-	0,6,6	-	-	-		
85	OHX	1	3881	-	0,6,6	-	-	-		
85	OHX	5	4070	-	0,6,6	-	-	-		
85	OHX	8	218	-	0,6,6	-	-	-		
85	OHX	5	4046	-	0,6,6	-	-	-		
85	OHX	6	2036	-	0,6,6	-	-	-		
85	OHX	2	2001	-	0,6,6	-	-	-		
85	OHX	6	2120	-	0,6,6	-	-	-		
85	OHX	5	3906	-	0,6,6	-	-	-		
85	OHX	6	2041	-	0,6,6	-	-	-		
85	OHX	1	3929	-	0,6,6	-	-	-		
85	OHX	4	223	-	0,6,6	-	-	-		
85	OHX	6	2033	-	0,6,6	-	-	-		
85	OHX	5	4031	-	0,6,6	-	-	-		
85	OHX	1	3727	-	0,6,6	-	-	-		
85	OHX	1	3879	-	0,6,6	-	-	-		
85	OHX	6	2157	-	0,6,6	-	-	-		
85	OHX	1	3868	-	0,6,6	-	-	-		
85	OHX	7	218	-	0,6,6	-	-	-		
85	OHX	1	3801	-	0,6,6	-	-	-		
85	OHX	6	2102	-	0,6,6	-	-	-		
85	OHX	6	2046	-	0,6,6	-	-	-		
85	OHX	2	1989	-	0,6,6	-	-	-		
85	OHX	1	3779	-	0,6,6	-	-	-		
85	OHX	1	3798	-	0,6,6	-	-	-		
85	OHX	1	3826	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	1	3916	-	0,6,6	-	-	-		
85	OHX	5	3747	-	0,6,6	-	-	-		
85	OHX	5	3971	-	0,6,6	-	-	-		
85	OHX	1	4001	-	0,6,6	-	-	-		
85	OHX	2	2019	-	0,6,6	-	-	-		
85	OHX	1	3803	-	0,6,6	-	-	-		
85	OHX	1	3913	84	0,6,6	-	-	-		
85	OHX	1	3923	-	0,6,6	-	-	-		
85	OHX	6	2142	-	0,6,6	-	-	-		
85	OHX	5	3765	-	0,6,6	-	-	-		
85	OHX	6	2104	-	0,6,6	-	-	-		
85	OHX	5	4068	84	0,6,6	-	-	-		
85	OHX	5	3918	-	0,6,6	-	-	-		
85	OHX	6	2053	-	0,6,6	-	-	-		
85	OHX	5	3947	-	0,6,6	-	-	-		
85	OHX	1	3737	-	0,6,6	-	-	-		
85	OHX	1	3860	-	0,6,6	-	-	-		
85	OHX	1	3726	-	0,6,6	-	-	-		
85	OHX	1	3993	-	0,6,6	-	-	-		
85	OHX	1	4016	-	0,6,6	-	-	-		
85	OHX	5	4045	-	0,6,6	-	-	-		
85	OHX	1	3957	84	0,6,6	-	-	-		
85	OHX	6	2094	-	0,6,6	-	-	-		
85	OHX	2	1997	-	0,6,6	-	-	-		
85	OHX	6	2054	-	0,6,6	-	-	-		
85	OHX	C3	201	-	0,6,6	-	-	-		
85	OHX	1	3818	-	0,6,6	-	-	-		
85	OHX	5	3753	-	0,6,6	-	-	-		
85	OHX	5	3776	-	0,6,6	-	-	-		
85	OHX	1	3754	-	0,6,6	-	-	-		
85	OHX	1	3771	-	0,6,6	-	-	-		
85	OHX	1	3950	-	0,6,6	-	-	-		
85	OHX	1	3952	-	0,6,6	-	-	-		
85	OHX	6	2150	-	0,6,6	-	-	-		
85	OHX	5	3772	-	0,6,6	-	-	-		
85	OHX	5	4010	-	0,6,6	-	-	-		
85	OHX	5	4051	-	0,6,6	-	-	-		
85	OHX	l4	402	-	0,6,6	-	-	-		
85	OHX	1	4025	-	0,6,6	-	-	-		
85	OHX	5	3759	-	0,6,6	-	-	-		
85	OHX	6	2110	-	0,6,6	-	-	-		
85	OHX	2	2060	-	0,6,6	-	-	-		
85	OHX	5	3767	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	OHX	5	3840	-	0,6,6	-	-	-		
85	OHX	2	2066	-	0,6,6	-	-	-		
85	OHX	5	3801	-	0,6,6	-	-	-		
85	OHX	6	2023	-	0,6,6	-	-	-		
85	OHX	6	2043	-	0,6,6	-	-	-		
85	OHX	6	2059	-	0,6,6	-	-	-		
85	OHX	M0	302	-	0,6,6	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	ANM	1	3401	-	3/3/4/5	3/10/23/23	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	1	3401	ANM	C4-C3	-6.47	1.43	1.53
87	1	3401	ANM	C3-C2	-6.41	1.40	1.53
87	1	3401	ANM	O2-C2	-4.67	1.37	1.44
87	1	3401	ANM	C16-N1	-4.41	1.38	1.48
87	1	3401	ANM	C15-C16	-3.10	1.47	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	1	3401	ANM	C15-C16-N1	-5.90	104.18	111.47
87	1	3401	ANM	C2-O2-C5	-5.34	109.46	117.72
87	1	3401	ANM	O2-C5-O3	-5.31	112.42	122.96
87	1	3401	ANM	C4-C3-C2	-4.14	97.94	103.29
87	1	3401	ANM	O4-C3-C4	-4.08	101.29	110.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
87	1	3401	ANM	C2
87	1	3401	ANM	C3
87	1	3401	ANM	C16

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	1	3401	ANM	C6-C5-O2-C2
87	1	3401	ANM	C10-C9-O1-C14
87	1	3401	ANM	C1-C9-O1-C14

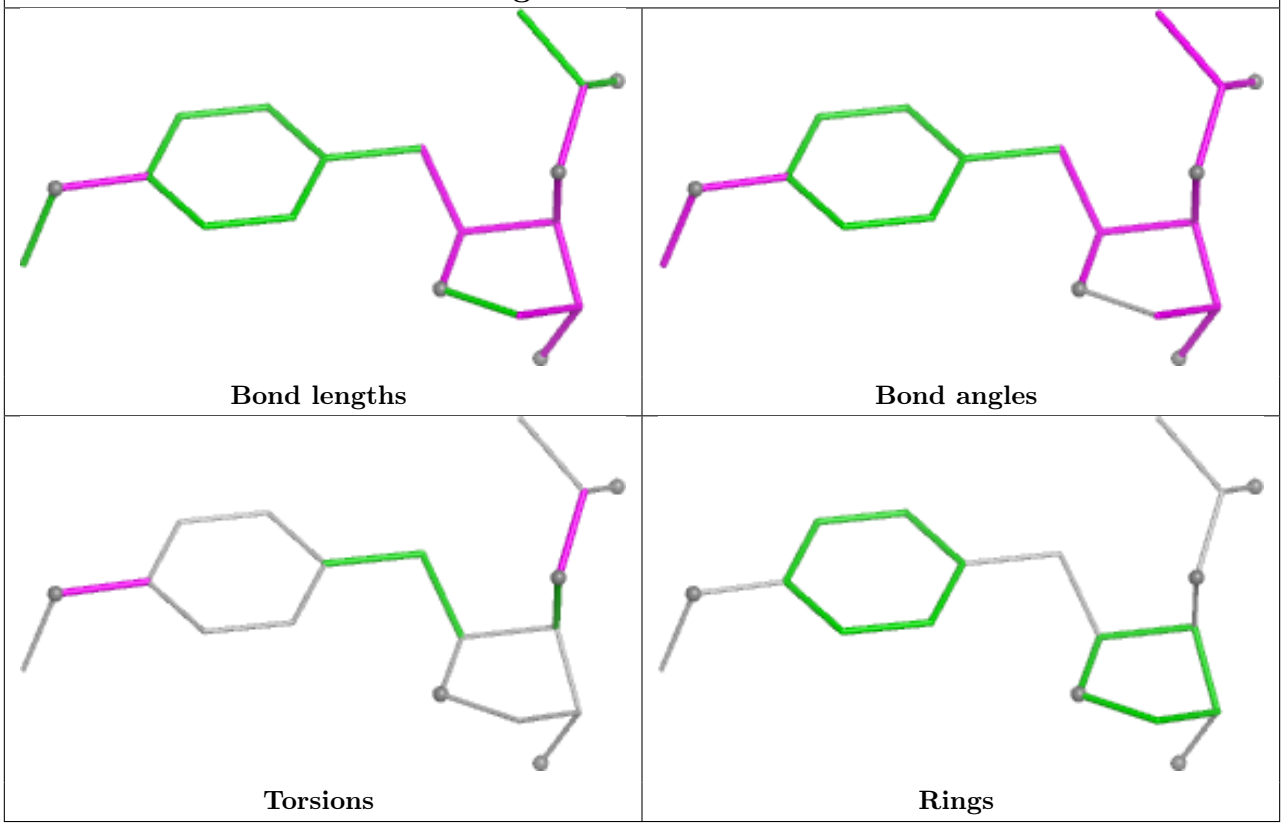
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	C8	201	OHX	0	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ANM 1 3401



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	m2	2
35	sM	1
35	SM	1
12	c0	1
1	2	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	37.86
1	SM	141:ALA	C	151:UNK	N	26.40
1	c0	84:GLU	C	87:UNK	N	8.00

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	3.94
1	m2	23:UNK	C	28:UNK	N	3.86

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	2	1781/1800 (98%)	1.07	199 (11%)	10	5	37, 86, 144, 179	1 (0%)
1	6	1795/1800 (99%)	0.86	155 (8%)	16	9	31, 76, 145, 181	1 (0%)
2	S0	206/251 (82%)	1.23	28 (13%)	7	4	87, 96, 101, 106	0
2	s0	206/251 (82%)	2.04	101 (49%)	0	0	78, 120, 181, 264	0
3	S1	214/254 (84%)	1.66	66 (30%)	1	1	96, 117, 134, 137	0
3	s1	216/254 (85%)	0.86	11 (5%)	33	18	71, 82, 95, 105	0
4	S2	217/253 (85%)	0.94	20 (9%)	14	8	73, 81, 90, 98	0
4	s2	217/253 (85%)	0.84	20 (9%)	14	8	58, 68, 84, 89	0
5	S3	223/239 (93%)	0.91	13 (5%)	29	16	76, 86, 104, 107	0
5	s3	223/239 (93%)	0.91	23 (10%)	12	6	77, 98, 120, 126	0
6	S4	260/260 (100%)	0.93	18 (6%)	23	12	64, 84, 91, 104	0
6	s4	260/260 (100%)	0.87	19 (7%)	21	11	49, 74, 82, 99	0
7	S5	206/224 (91%)	1.22	29 (14%)	6	3	94, 104, 110, 113	0
7	s5	206/224 (91%)	1.04	18 (8%)	16	9	74, 93, 100, 104	0
8	S6	226/236 (95%)	1.29	39 (17%)	4	2	67, 89, 106, 109	0
8	s6	218/236 (92%)	0.94	17 (7%)	19	10	51, 82, 94, 102	0
9	S7	184/189 (97%)	1.16	27 (14%)	6	3	83, 103, 119, 122	0
9	s7	186/189 (98%)	1.07	23 (12%)	8	5	71, 96, 123, 189	0
10	S8	188/200 (94%)	1.21	24 (12%)	7	4	61, 75, 106, 113	0
10	s8	188/200 (94%)	1.02	16 (8%)	16	9	46, 69, 110, 123	0
11	S9	185/196 (94%)	1.22	26 (14%)	6	3	77, 89, 111, 126	0
11	s9	185/196 (94%)	1.19	26 (14%)	6	3	62, 79, 104, 119	0
12	C0	84/96 (87%)	1.22	16 (19%)	3	1	83, 96, 104, 107	0
12	c0	84/96 (87%)	1.47	27 (32%)	1	0	97, 122, 131, 135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	C1	146/155 (94%)	0.92	10 (6%)	23	12	64, 72, 90, 101	0
13	c1	146/155 (94%)	1.03	22 (15%)	5	3	51, 66, 97, 152	0
14	C2	124/142 (87%)	1.33	22 (17%)	4	2	118, 124, 129, 132	0
14	c2	124/142 (87%)	2.20	68 (54%)	0	0	170, 185, 193, 202	0
15	C3	150/150 (100%)	1.03	18 (12%)	9	5	71, 85, 93, 97	0
15	c3	150/150 (100%)	0.71	9 (6%)	27	15	56, 72, 87, 92	0
16	C4	127/136 (93%)	1.79	43 (33%)	1	0	74, 116, 124, 126	0
16	c4	128/136 (94%)	0.95	11 (8%)	16	9	54, 81, 85, 88	0
17	C5	124/141 (87%)	1.11	18 (14%)	6	3	77, 88, 107, 114	0
17	c5	135/141 (95%)	1.25	21 (15%)	5	2	61, 91, 108, 115	0
18	C6	141/142 (99%)	1.44	39 (27%)	1	1	81, 99, 102, 103	0
18	c6	142/142 (100%)	1.54	34 (23%)	2	1	69, 89, 101, 104	0
19	C7	120/136 (88%)	1.42	27 (22%)	2	1	89, 99, 106, 107	0
19	c7	117/136 (86%)	2.38	68 (58%)	0	0	79, 95, 321, 380	0
20	C8	145/145 (100%)	1.19	24 (16%)	4	2	76, 94, 109, 114	0
20	c8	145/145 (100%)	1.04	15 (10%)	12	6	69, 87, 98, 103	0
21	C9	143/143 (100%)	1.55	33 (23%)	2	1	86, 97, 105, 110	0
21	c9	143/143 (100%)	1.03	10 (6%)	22	12	71, 83, 93, 98	0
22	D0	107/120 (89%)	1.48	28 (26%)	1	1	76, 98, 107, 109	0
22	d0	110/120 (91%)	1.32	21 (19%)	3	1	73, 103, 118, 121	0
23	D1	87/87 (100%)	0.91	8 (9%)	14	8	84, 87, 97, 100	0
23	d1	87/87 (100%)	0.99	9 (10%)	12	6	70, 86, 139, 157	0
24	D2	129/129 (100%)	1.01	11 (8%)	16	9	73, 81, 87, 95	0
24	d2	129/129 (100%)	0.84	9 (6%)	22	12	56, 67, 74, 81	0
25	D3	144/144 (100%)	0.92	16 (11%)	10	5	63, 66, 72, 75	0
25	d3	144/144 (100%)	0.43	4 (2%)	55	34	47, 52, 60, 65	0
26	D4	134/134 (100%)	1.09	21 (15%)	5	2	74, 90, 97, 100	0
26	d4	134/134 (100%)	1.01	16 (11%)	9	5	58, 78, 88, 101	0
27	D5	70/107 (65%)	1.35	14 (20%)	3	1	103, 109, 114, 114	0
27	d5	69/107 (64%)	1.23	12 (17%)	4	2	86, 97, 101, 102	0
28	D6	97/97 (100%)	1.30	20 (20%)	2	1	76, 85, 121, 121	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	0.80	7 (7%)	21	11	56, 66, 87, 91	0
29	D7	81/81 (100%)	1.23	11 (13%)	7	4	84, 95, 107, 108	0
29	d7	81/81 (100%)	1.10	7 (8%)	16	9	72, 86, 101, 103	0
30	D8	63/66 (95%)	1.48	14 (22%)	2	1	101, 108, 112, 115	0
30	d8	63/66 (95%)	1.03	5 (7%)	18	10	88, 96, 101, 106	0
31	D9	53/55 (96%)	1.54	13 (24%)	2	1	78, 82, 94, 95	0
31	d9	53/55 (96%)	1.79	19 (35%)	1	0	73, 85, 114, 122	0
32	E0	60/62 (96%)	1.07	8 (13%)	7	4	65, 90, 102, 104	0
32	e0	62/62 (100%)	0.90	5 (8%)	18	10	53, 78, 95, 99	0
33	E1	71/76 (93%)	1.53	14 (19%)	3	1	89, 115, 125, 126	0
33	e1	76/76 (100%)	2.37	44 (57%)	0	0	96, 155, 181, 183	0
34	SR	318/318 (100%)	1.25	54 (16%)	4	2	95, 103, 114, 120	0
34	sR	318/318 (100%)	1.35	57 (17%)	3	1	102, 116, 127, 175	0
35	SM	133/182 (73%)	1.04	18 (13%)	7	4	56, 80, 122, 131	0
35	sM	63/182 (34%)	1.04	9 (14%)	6	3	44, 87, 93, 95	0
36	1	3149/3396 (92%)	0.41	157 (4%)	34	18	31, 53, 104, 189	0
36	5	3150/3396 (92%)	0.36	155 (4%)	35	18	29, 51, 105, 149	0
37	3	121/121 (100%)	0.43	1 (0%)	82	65	43, 66, 77, 80	0
37	7	121/121 (100%)	0.24	1 (0%)	82	65	34, 52, 64, 69	0
38	4	158/158 (100%)	0.35	4 (2%)	58	37	35, 54, 84, 107	0
38	8	158/158 (100%)	0.53	5 (3%)	50	30	40, 61, 93, 104	0
39	L2	252/253 (99%)	0.51	7 (2%)	55	34	39, 52, 65, 70	0
39	l2	252/253 (99%)	0.68	18 (7%)	22	12	37, 55, 73, 146	0
40	L3	386/386 (100%)	0.46	6 (1%)	70	49	38, 53, 64, 73	0
40	l3	386/386 (100%)	0.21	3 (0%)	82	65	30, 43, 58, 82	0
41	L4	361/361 (100%)	0.11	2 (0%)	85	70	33, 44, 56, 62	0
41	l4	361/361 (100%)	0.49	13 (3%)	46	26	36, 51, 66, 72	0
42	L5	296/296 (100%)	0.67	15 (5%)	33	18	52, 69, 81, 90	0
42	l5	294/296 (99%)	0.52	13 (4%)	39	21	37, 55, 77, 101	0
43	L6	156/175 (89%)	0.27	1 (0%)	85	70	42, 49, 58, 71	0
43	l6	157/175 (89%)	0.49	6 (3%)	44	25	42, 54, 65, 71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	L7	222/243 (91%)	0.10	2 (0%) 81 63	36, 42, 58, 72	0
44	l7	223/243 (91%)	0.20	3 (1%) 75 56	33, 41, 69, 86	0
45	L8	233/255 (91%)	0.74	6 (2%) 57 36	58, 71, 89, 96	0
45	l8	231/255 (90%)	1.12	34 (14%) 6 3	65, 80, 101, 106	0
46	L9	191/191 (100%)	0.62	8 (4%) 40 22	51, 59, 67, 72	0
46	l9	191/191 (100%)	0.24	0 100 100	39, 47, 59, 67	0
47	M0	211/220 (95%)	0.45	5 (2%) 59 38	39, 50, 74, 80	0
47	m0	213/220 (96%)	0.46	10 (4%) 36 19	33, 46, 75, 167	0
48	M1	169/173 (97%)	1.01	18 (10%) 11 6	61, 74, 82, 86	0
48	m1	169/173 (97%)	0.51	9 (5%) 32 17	44, 57, 67, 76	0
49	M3	193/198 (97%)	0.49	9 (4%) 36 19	35, 52, 76, 98	0
49	m3	194/198 (97%)	0.59	9 (4%) 37 20	35, 63, 86, 93	0
50	M4	136/137 (99%)	0.39	3 (2%) 62 41	46, 52, 62, 64	0
50	m4	137/137 (100%)	0.24	3 (2%) 62 41	41, 46, 61, 67	0
51	M5	203/203 (100%)	0.68	12 (5%) 28 15	36, 49, 59, 60	0
51	m5	203/203 (100%)	0.85	16 (7%) 18 10	40, 56, 66, 69	0
52	M6	197/198 (99%)	0.38	9 (4%) 37 20	37, 43, 57, 58	0
52	m6	197/198 (99%)	0.18	3 (1%) 72 52	30, 35, 55, 58	0
53	M7	183/183 (100%)	0.65	19 (10%) 11 6	39, 47, 73, 82	0
53	m7	155/183 (84%)	0.30	2 (1%) 75 56	36, 43, 53, 61	0
54	M8	185/185 (100%)	0.37	3 (1%) 70 49	37, 47, 59, 68	0
54	m8	185/185 (100%)	0.39	4 (2%) 62 41	36, 52, 60, 66	0
55	M9	188/188 (100%)	0.82	11 (5%) 28 15	58, 67, 117, 123	0
55	m9	188/188 (100%)	0.79	10 (5%) 32 17	53, 60, 108, 121	0
56	N0	172/172 (100%)	0.35	6 (3%) 47 27	43, 49, 57, 63	0
56	n0	172/172 (100%)	0.34	6 (3%) 47 27	35, 41, 49, 52	0
57	N1	159/159 (100%)	0.31	2 (1%) 75 56	39, 49, 71, 75	0
57	n1	159/159 (100%)	0.24	1 (0%) 85 70	34, 41, 66, 71	0
58	N2	100/120 (83%)	1.18	11 (11%) 10 5	81, 89, 92, 92	0
58	n2	98/120 (81%)	0.92	14 (14%) 6 3	70, 79, 83, 86	0
59	N3	136/136 (100%)	0.28	2 (1%) 72 52	43, 50, 55, 59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
59	n3	136/136 (100%)	0.13	2 (1%)	72	52	30, 39, 48, 51	0
60	N4	98/155 (63%)	1.23	22 (22%)	2	1	49, 63, 112, 120	0
60	n4	135/155 (87%)	1.34	40 (29%)	1	1	38, 87, 303, 442	0
61	N5	121/141 (85%)	0.52	4 (3%)	49	29	51, 60, 72, 88	0
61	n5	120/141 (85%)	0.85	8 (6%)	24	13	50, 65, 80, 86	0
62	N6	126/126 (100%)	0.41	1 (0%)	82	65	40, 53, 61, 64	0
62	n6	126/126 (100%)	0.79	5 (3%)	42	23	46, 60, 71, 75	0
63	N7	135/135 (100%)	0.79	6 (4%)	39	21	71, 79, 92, 98	0
63	n7	135/135 (100%)	1.28	27 (20%)	3	1	75, 86, 100, 107	0
64	N8	148/148 (100%)	0.35	4 (2%)	56	35	30, 48, 62, 72	0
64	n8	148/148 (100%)	0.40	2 (1%)	73	53	31, 54, 63, 65	0
65	N9	58/58 (100%)	0.59	5 (8%)	16	9	35, 53, 81, 89	0
65	n9	58/58 (100%)	0.72	5 (8%)	16	9	32, 49, 69, 73	0
66	O0	97/104 (93%)	0.54	4 (4%)	41	23	67, 73, 84, 87	0
66	o0	100/104 (96%)	0.78	6 (6%)	27	15	66, 76, 86, 92	0
67	O1	109/112 (97%)	0.65	7 (6%)	25	14	52, 62, 76, 82	0
67	o1	109/112 (97%)	0.75	9 (8%)	17	9	44, 56, 81, 163	0
68	O2	127/129 (98%)	0.27	2 (1%)	70	49	32, 44, 49, 53	0
68	o2	127/129 (98%)	0.55	11 (8%)	16	9	31, 50, 57, 61	0
69	O3	106/106 (100%)	0.44	4 (3%)	44	25	37, 42, 56, 60	0
69	o3	106/106 (100%)	0.42	2 (1%)	66	45	34, 43, 59, 65	0
70	O4	112/120 (93%)	1.19	16 (14%)	6	3	52, 67, 82, 87	0
70	o4	112/120 (93%)	1.10	15 (13%)	7	4	51, 66, 88, 91	0
71	O5	119/119 (100%)	0.65	3 (2%)	58	37	49, 60, 66, 70	0
71	o5	119/119 (100%)	0.80	5 (4%)	40	22	57, 68, 76, 81	0
72	O6	99/99 (100%)	0.73	8 (8%)	18	10	51, 60, 77, 83	0
72	o6	99/99 (100%)	0.90	10 (10%)	12	6	59, 67, 77, 85	0
73	O7	87/87 (100%)	0.59	2 (2%)	61	39	37, 43, 60, 73	0
73	o7	87/87 (100%)	0.68	4 (4%)	37	20	37, 46, 74, 90	0
74	O8	77/77 (100%)	0.80	4 (5%)	33	17	75, 80, 87, 87	0
74	o8	77/77 (100%)	1.16	7 (9%)	15	8	81, 89, 108, 120	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	O9	50/50 (100%)	0.73	5 (10%) 12 6	45, 49, 51, 52	0
75	o9	50/50 (100%)	0.42	0 100 100	45, 50, 57, 66	0
76	Q0	52/52 (100%)	0.72	2 (3%) 44 25	48, 52, 61, 65	0
76	q0	52/52 (100%)	0.21	1 (1%) 66 45	36, 39, 47, 51	0
77	Q1	25/25 (100%)	0.98	2 (8%) 18 10	62, 63, 67, 68	0
77	q1	25/25 (100%)	0.91	2 (8%) 18 10	49, 51, 53, 55	0
78	Q2	105/105 (100%)	0.38	1 (0%) 79 61	39, 51, 63, 74	0
78	q2	105/105 (100%)	0.33	2 (1%) 66 45	38, 49, 59, 71	0
79	Q3	91/91 (100%)	0.34	0 100 100	46, 53, 63, 69	0
79	q3	91/91 (100%)	0.37	3 (3%) 49 29	43, 51, 65, 71	0
80	m2	0/150	-	-	-	-
81	p0	143/311 (45%)	1.31	22 (15%) 5 2	83, 101, 174, 180	0
82	p1	0/47	-	-	-	-
83	p2	0/46	-	-	-	-
All	All	32994/35138 (93%)	0.75	2874 (8%) 16 9	29, 66, 117, 442	2 (0%)

The worst 5 of 2874 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	C4	15	GLY	9.6
1	2	194	U	8.9
39	l2	253	GLN	8.6
36	1	1236	G	7.2
1	6	718	U	6.7

5.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3406	1/1	-0.23	0.63	130,130,130,130	0
84	MG	2	1978	1/1	0.22	0.45	104,104,104,104	0
84	MG	2	1962	1/1	0.24	0.56	110,110,110,110	0
84	MG	5	3678	1/1	0.30	0.18	58,58,58,58	0
84	MG	2	1932	1/1	0.39	0.46	68,68,68,68	0
84	MG	5	3457	1/1	0.40	0.47	100,100,100,100	0
84	MG	M3	201	1/1	0.42	0.36	86,86,86,86	0
84	MG	6	1984	1/1	0.44	0.32	70,70,70,70	0
84	MG	5	3739	1/1	0.45	0.39	88,88,88,88	0
84	MG	2	1941	1/1	0.46	0.32	93,93,93,93	0
84	MG	1	3570	1/1	0.47	0.47	67,67,67,67	0
84	MG	2	1940	1/1	0.48	0.49	72,72,72,72	0
84	MG	5	3693	1/1	0.49	0.44	80,80,80,80	0
84	MG	6	1959	1/1	0.53	0.54	86,86,86,86	0
84	MG	1	3701	1/1	0.53	0.15	40,40,40,40	0
84	MG	1	3705	1/1	0.54	0.46	52,52,52,52	0
84	MG	1	3650	1/1	0.55	0.41	81,81,81,81	0
84	MG	2	1954	1/1	0.55	0.42	90,90,90,90	0
84	MG	2	1949	1/1	0.56	0.33	96,96,96,96	0
84	MG	2	1968	1/1	0.56	0.38	85,85,85,85	0
84	MG	2	1937	1/1	0.56	0.40	79,79,79,79	0
84	MG	2	1956	1/1	0.57	0.41	64,64,64,64	0
84	MG	2	1924	1/1	0.58	0.47	86,86,86,86	0
84	MG	6	1971	1/1	0.59	0.41	90,90,90,90	0
84	MG	2	1925	1/1	0.59	0.57	74,74,74,74	0
84	MG	2	1953	1/1	0.60	0.56	84,84,84,84	0
84	MG	5	3697	1/1	0.60	0.23	50,50,50,50	0
84	MG	6	1970	1/1	0.60	0.37	98,98,98,98	0
84	MG	1	3678	1/1	0.61	0.28	65,65,65,65	0
84	MG	6	2002	1/1	0.61	0.47	99,99,99,99	0
84	MG	4	203	1/1	0.61	0.40	68,68,68,68	0
84	MG	5	3608	1/1	0.61	0.56	89,89,89,89	0
84	MG	6	1961	1/1	0.62	0.34	61,61,61,61	0
84	MG	6	1958	1/1	0.63	0.39	47,47,47,47	0
84	MG	1	3414	1/1	0.63	0.45	63,63,63,63	0
84	MG	2	1946	1/1	0.63	0.60	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	6	1902	1/1	0.63	0.32	57,57,57,57	0
84	MG	6	1912	1/1	0.63	0.32	79,79,79,79	0
84	MG	6	1975	1/1	0.63	0.48	79,79,79,79	0
84	MG	6	1926	1/1	0.63	0.45	46,46,46,46	0
84	MG	5	3641	1/1	0.64	0.42	79,79,79,79	0
84	MG	2	1969	1/1	0.64	0.47	66,66,66,66	0
84	MG	2	1926	1/1	0.64	0.36	74,74,74,74	0
84	MG	2	1915	1/1	0.64	0.40	76,76,76,76	0
84	MG	2	1947	1/1	0.64	0.44	93,93,93,93	0
84	MG	5	3655	1/1	0.66	0.33	64,64,64,64	0
84	MG	5	3458	1/1	0.66	0.30	107,107,107,107	0
84	MG	5	3460	1/1	0.66	0.13	44,44,44,44	0
84	MG	6	1938	1/1	0.66	0.50	99,99,99,99	0
84	MG	1	3416	1/1	0.66	0.26	48,48,48,48	0
84	MG	2	1961	1/1	0.67	0.36	75,75,75,75	0
84	MG	1	3652	1/1	0.67	0.18	57,57,57,57	0
84	MG	1	3459	1/1	0.67	0.30	46,46,46,46	0
84	MG	1	3692	1/1	0.67	0.17	45,45,45,45	0
84	MG	2	1979	1/1	0.67	0.39	72,72,72,72	0
84	MG	2	1928	1/1	0.68	0.35	71,71,71,71	0
84	MG	6	1976	1/1	0.68	0.26	91,91,91,91	0
84	MG	D9	102	1/1	0.68	0.33	86,86,86,86	0
84	MG	6	1933	1/1	0.68	0.28	84,84,84,84	0
84	MG	5	3438	1/1	0.68	0.21	45,45,45,45	0
84	MG	6	1930	1/1	0.69	0.45	59,59,59,59	0
84	MG	6	1962	1/1	0.70	0.27	84,84,84,84	0
84	MG	6	1993	1/1	0.70	0.50	95,95,95,95	0
84	MG	6	1969	1/1	0.70	0.39	65,65,65,65	0
84	MG	6	1927	1/1	0.70	0.41	50,50,50,50	0
84	MG	6	1925	1/1	0.70	0.37	72,72,72,72	0
84	MG	1	3659	1/1	0.70	0.40	47,47,47,47	0
84	MG	6	1937	1/1	0.70	0.42	72,72,72,72	0
84	MG	6	2005	1/1	0.71	0.20	61,61,61,61	0
84	MG	2	1974	1/1	0.71	0.21	93,93,93,93	0
84	MG	6	1909	1/1	0.71	0.41	98,98,98,98	0
84	MG	n6	201	1/1	0.71	0.31	65,65,65,65	0
84	MG	S4	301	1/1	0.72	0.18	79,79,79,79	0
84	MG	Q2	502	1/1	0.72	0.15	55,55,55,55	0
84	MG	1	3449	1/1	0.72	0.53	64,64,64,64	0
84	MG	5	3610	1/1	0.72	0.18	37,37,37,37	0
84	MG	6	1904	1/1	0.72	0.32	76,76,76,76	0
84	MG	6	1951	1/1	0.72	0.56	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	2	1975	1/1	0.72	0.40	76,76,76,76	0
84	MG	1	3518	1/1	0.72	0.41	52,52,52,52	0
84	MG	1	3567	1/1	0.72	0.55	50,50,50,50	0
84	MG	2	1973	1/1	0.72	0.35	64,64,64,64	0
84	MG	2	1920	1/1	0.72	0.43	74,74,74,74	0
84	MG	1	3563	1/1	0.73	0.51	54,54,54,54	0
84	MG	2	1958	1/1	0.73	0.29	96,96,96,96	0
84	MG	1	3569	1/1	0.73	0.42	53,53,53,53	0
84	MG	5	3466	1/1	0.73	0.32	68,68,68,68	0
84	MG	2	1912	1/1	0.73	0.39	74,74,74,74	0
84	MG	1	3541	1/1	0.73	0.38	55,55,55,55	0
84	MG	5	3616	1/1	0.73	0.28	40,40,40,40	0
84	MG	2	1955	1/1	0.74	0.38	68,68,68,68	0
84	MG	2	1939	1/1	0.74	0.23	74,74,74,74	0
84	MG	5	3643	1/1	0.74	0.37	55,55,55,55	0
84	MG	2	1904	1/1	0.74	0.51	77,77,77,77	0
84	MG	5	3674	1/1	0.74	0.27	49,49,49,49	0
84	MG	6	1980	1/1	0.74	0.21	68,68,68,68	0
84	MG	6	1963	1/1	0.74	0.40	76,76,76,76	0
84	MG	6	1956	1/1	0.74	0.50	60,60,60,60	0
84	MG	6	2001	1/1	0.74	0.39	73,73,73,73	0
84	MG	l2	302	1/1	0.74	0.21	42,42,42,42	0
84	MG	l6	201	1/1	0.74	0.29	56,56,56,56	0
84	MG	2	1981	1/1	0.74	0.28	76,76,76,76	0
84	MG	5	3480	1/1	0.75	0.15	36,36,36,36	0
84	MG	5	3533	1/1	0.75	0.47	55,55,55,55	0
84	MG	3	201	1/1	0.75	0.29	71,71,71,71	0
84	MG	2	1964	1/1	0.75	0.33	83,83,83,83	0
84	MG	2	1921	1/1	0.75	0.54	81,81,81,81	0
84	MG	1	3624	1/1	0.75	0.13	44,44,44,44	0
84	MG	1	3450	1/1	0.75	0.27	33,33,33,33	0
84	MG	2	1944	1/1	0.75	0.35	91,91,91,91	0
84	MG	5	3657	1/1	0.75	0.20	57,57,57,57	0
84	MG	6	1907	1/1	0.75	0.36	75,75,75,75	0
84	MG	1	3500	1/1	0.75	0.44	44,44,44,44	0
84	MG	d6	102	1/1	0.75	0.23	56,56,56,56	0
84	MG	5	3694	1/1	0.75	0.16	35,35,35,35	0
84	MG	2	1971	1/1	0.75	0.26	77,77,77,77	0
84	MG	2	1909	1/1	0.75	0.35	81,81,81,81	0
84	MG	2	1935	1/1	0.75	0.29	68,68,68,68	0
84	MG	2	1963	1/1	0.75	0.35	78,78,78,78	0
84	MG	1	3709	1/1	0.75	0.43	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3696	1/1	0.76	0.15	55,55,55,55	0
84	MG	5	3404	1/1	0.76	0.20	33,33,33,33	0
84	MG	2	1916	1/1	0.76	0.37	59,59,59,59	0
84	MG	2	1923	1/1	0.76	0.46	56,56,56,56	0
84	MG	6	1952	1/1	0.76	0.41	54,54,54,54	0
84	MG	6	1994	1/1	0.76	0.19	49,49,49,49	0
84	MG	6	1998	1/1	0.76	0.18	58,58,58,58	0
84	MG	5	3687	1/1	0.76	0.26	31,31,31,31	0
84	MG	2	1910	1/1	0.76	0.50	64,64,64,64	0
84	MG	5	3500	1/1	0.76	0.37	47,47,47,47	0
84	MG	1	3601	1/1	0.76	0.28	65,65,65,65	0
84	MG	5	3595	1/1	0.76	0.20	60,60,60,60	0
84	MG	1	3496	1/1	0.76	0.24	39,39,39,39	0
84	MG	l3	403	1/1	0.76	0.26	38,38,38,38	0
84	MG	6	2160	1/1	0.76	0.25	84,84,84,84	0
84	MG	5	3613	1/1	0.76	0.30	58,58,58,58	0
85	OHX	2	2111	7/7	0.76	0.24	112,112,112,112	0
85	OHX	2	2115	7/7	0.76	0.25	115,115,115,115	0
84	MG	5	3415	1/1	0.77	0.31	29,29,29,29	0
84	MG	5	3417	1/1	0.77	0.32	84,84,84,84	0
84	MG	5	3644	1/1	0.77	0.28	72,72,72,72	0
84	MG	2	1943	1/1	0.77	0.31	71,71,71,71	0
84	MG	1	3684	1/1	0.77	0.17	51,51,51,51	0
84	MG	1	3608	1/1	0.77	0.38	87,87,87,87	0
84	MG	6	1955	1/1	0.77	0.48	67,67,67,67	0
84	MG	1	3472	1/1	0.77	0.35	52,52,52,52	0
84	MG	5	3472	1/1	0.77	0.36	50,50,50,50	0
84	MG	1	3699	1/1	0.77	0.32	55,55,55,55	0
84	MG	1	3629	1/1	0.77	0.24	74,74,74,74	0
84	MG	1	3704	1/1	0.77	0.23	34,34,34,34	0
84	MG	1	3643	1/1	0.77	0.37	63,63,63,63	0
84	MG	1	3527	1/1	0.77	0.34	64,64,64,64	0
84	MG	1	3427	1/1	0.77	0.31	48,48,48,48	0
84	MG	1	3589	1/1	0.77	0.17	64,64,64,64	0
84	MG	5	3614	1/1	0.77	0.19	55,55,55,55	0
84	MG	1	3667	1/1	0.77	0.29	62,62,62,62	0
85	OHX	2	2117	7/7	0.77	0.21	128,128,128,128	0
85	OHX	6	2158	7/7	0.77	0.19	140,140,140,140	0
85	OHX	5	4024	7/7	0.77	0.21	116,116,116,116	0
84	MG	6	2159	1/1	0.78	0.38	58,58,58,58	0
84	MG	5	3665	1/1	0.78	0.26	39,39,39,39	0
84	MG	5	3499	1/1	0.78	0.21	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3487	1/1	0.78	0.30	49,49,49,49	0
84	MG	1	3620	1/1	0.78	0.39	54,54,54,54	0
84	MG	5	3553	1/1	0.78	0.38	38,38,38,38	0
84	MG	2	1965	1/1	0.78	0.47	60,60,60,60	0
84	MG	5	3596	1/1	0.78	0.13	40,40,40,40	0
84	MG	5	3723	1/1	0.78	0.15	38,38,38,38	0
84	MG	5	3735	1/1	0.78	0.09	65,65,65,65	0
84	MG	6	1921	1/1	0.78	0.44	56,56,56,56	0
84	MG	7	210	1/1	0.78	0.13	53,53,53,53	0
84	MG	1	3720	1/1	0.78	0.18	56,56,56,56	0
84	MG	2	1950	1/1	0.78	0.31	72,72,72,72	0
84	MG	1	3688	1/1	0.78	0.22	47,47,47,47	0
84	MG	1	3630	1/1	0.78	0.38	56,56,56,56	0
84	MG	5	3623	1/1	0.78	0.33	57,57,57,57	0
84	MG	2	1957	1/1	0.78	0.47	76,76,76,76	0
84	MG	2	1917	1/1	0.78	0.46	62,62,62,62	0
84	MG	2	1959	1/1	0.78	0.40	67,67,67,67	0
84	MG	5	3477	1/1	0.78	0.11	42,42,42,42	0
87	ANM	1	3401	19/19	0.78	0.37	62,62,62,62	19
84	MG	1	3443	1/1	0.79	0.28	43,43,43,43	0
84	MG	2	1952	1/1	0.79	0.49	77,77,77,77	0
84	MG	1	3586	1/1	0.79	0.46	68,68,68,68	0
84	MG	6	1910	1/1	0.79	0.16	74,74,74,74	0
84	MG	6	2006	1/1	0.79	0.34	61,61,61,61	0
84	MG	5	3537	1/1	0.79	0.31	36,36,36,36	0
84	MG	2	1948	1/1	0.79	0.25	94,94,94,94	0
84	MG	5	3698	1/1	0.79	0.25	73,73,73,73	0
84	MG	5	3712	1/1	0.79	0.11	44,44,44,44	0
84	MG	5	3714	1/1	0.79	0.22	34,34,34,34	0
84	MG	1	3658	1/1	0.79	0.24	52,52,52,52	0
84	MG	6	1924	1/1	0.79	0.28	56,56,56,56	0
84	MG	5	3738	1/1	0.79	0.17	45,45,45,45	0
84	MG	1	3597	1/1	0.79	0.28	46,46,46,46	0
84	MG	2	1922	1/1	0.79	0.55	74,74,74,74	0
84	MG	1	3722	1/1	0.79	0.12	60,60,60,60	0
84	MG	1	3673	1/1	0.79	0.29	65,65,65,65	0
84	MG	l3	404	1/1	0.79	0.14	39,39,39,39	0
84	MG	5	3451	1/1	0.79	0.27	33,33,33,33	0
84	MG	1	3538	1/1	0.79	0.39	42,42,42,42	0
85	OHX	2	2102	7/7	0.79	0.22	114,114,114,114	0
84	MG	5	3628	1/1	0.79	0.28	49,49,49,49	0
84	MG	4	213	1/1	0.79	0.18	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	2	1945	1/1	0.79	0.23	63,63,63,63	0
85	OHX	2	2118	7/7	0.79	0.20	132,132,132,132	0
85	OHX	2	2119	7/7	0.79	0.18	144,144,144,144	0
85	OHX	6	2157	7/7	0.79	0.21	115,115,115,115	0
84	MG	1	3484	1/1	0.79	0.28	52,52,52,52	0
84	MG	5	3467	1/1	0.79	0.39	65,65,65,65	0
84	MG	1	3439	1/1	0.79	0.31	60,60,60,60	0
84	MG	2	1927	1/1	0.80	0.48	65,65,65,65	0
84	MG	5	3574	1/1	0.80	0.32	53,53,53,53	0
84	MG	1	3408	1/1	0.80	0.29	50,50,50,50	0
84	MG	1	3460	1/1	0.80	0.27	52,52,52,52	0
84	MG	5	3402	1/1	0.80	0.39	61,61,61,61	0
84	MG	2	1913	1/1	0.80	0.22	63,63,63,63	0
84	MG	O7	102	1/1	0.80	0.17	51,51,51,51	0
84	MG	1	3641	1/1	0.80	0.31	51,51,51,51	0
84	MG	2	1931	1/1	0.80	0.51	65,65,65,65	0
84	MG	2	1914	1/1	0.80	0.44	73,73,73,73	0
84	MG	6	1940	1/1	0.80	0.26	43,43,43,43	0
84	MG	6	1944	1/1	0.80	0.53	69,69,69,69	0
84	MG	6	1985	1/1	0.80	0.36	65,65,65,65	0
84	MG	6	1990	1/1	0.80	0.18	61,61,61,61	0
85	OHX	2	2106	7/7	0.80	0.24	123,123,123,123	0
85	OHX	2	2109	7/7	0.80	0.22	112,112,112,112	0
84	MG	6	1950	1/1	0.80	0.34	72,72,72,72	0
84	MG	1	3437	1/1	0.80	0.19	45,45,45,45	0
84	MG	6	1996	1/1	0.80	0.15	54,54,54,54	0
84	MG	2	1934	1/1	0.80	0.28	72,72,72,72	0
84	MG	1	3508	1/1	0.80	0.23	43,43,43,43	0
85	OHX	1	3931	7/7	0.80	0.21	111,111,111,111	0
85	OHX	6	2131	7/7	0.80	0.21	121,121,121,121	0
85	OHX	6	2155	7/7	0.80	0.25	116,116,116,116	0
84	MG	2	1906	1/1	0.80	0.33	63,63,63,63	0
84	MG	5	3532	1/1	0.80	0.42	50,50,50,50	0
84	MG	6	1915	1/1	0.80	0.36	72,72,72,72	0
85	OHX	5	4061	7/7	0.80	0.26	121,121,121,121	0
85	OHX	5	4070	7/7	0.80	0.20	135,135,135,135	0
84	MG	2	1901	1/1	0.80	0.61	85,85,85,85	0
84	MG	5	3732	1/1	0.81	0.17	52,52,52,52	0
84	MG	1	3534	1/1	0.81	0.45	36,36,36,36	0
84	MG	1	3638	1/1	0.81	0.20	46,46,46,46	0
84	MG	1	3639	1/1	0.81	0.26	59,59,59,59	0
84	MG	5	4074	1/1	0.81	0.28	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	4039	1/1	0.81	0.20	46,46,46,46	0
84	MG	8	202	1/1	0.81	0.28	64,64,64,64	0
84	MG	8	204	1/1	0.81	0.14	56,56,56,56	0
84	MG	8	209	1/1	0.81	0.40	68,68,68,68	0
84	MG	1	3434	1/1	0.81	0.33	52,52,52,52	0
84	MG	5	3462	1/1	0.81	0.25	58,58,58,58	0
84	MG	3	206	1/1	0.81	0.37	59,59,59,59	0
84	MG	1	3501	1/1	0.81	0.38	43,43,43,43	0
84	MG	4	210	1/1	0.81	0.30	58,58,58,58	0
84	MG	n9	101	1/1	0.81	0.13	33,33,33,33	0
84	MG	1	3693	1/1	0.81	0.29	58,58,58,58	0
84	MG	2	1982	1/1	0.81	0.22	65,65,65,65	0
84	MG	5	3483	1/1	0.81	0.37	41,41,41,41	0
84	MG	5	3488	1/1	0.81	0.35	53,53,53,53	0
84	MG	O4	202	1/1	0.81	0.27	67,67,67,67	0
84	MG	1	3417	1/1	0.81	0.36	58,58,58,58	0
84	MG	5	3517	1/1	0.81	0.29	53,53,53,53	0
84	MG	5	3684	1/1	0.81	0.21	77,77,77,77	0
84	MG	1	3526	1/1	0.81	0.24	52,52,52,52	0
85	OHX	1	4012	7/7	0.81	0.21	116,116,116,116	0
84	MG	6	1901	1/1	0.81	0.31	50,50,50,50	0
85	OHX	6	2148	7/7	0.81	0.23	114,114,114,114	0
84	MG	2	1972	1/1	0.81	0.24	71,71,71,71	0
84	MG	5	3541	1/1	0.81	0.34	50,50,50,50	0
84	MG	1	3583	1/1	0.81	0.12	61,61,61,61	0
85	OHX	5	4001	7/7	0.81	0.21	130,130,130,130	0
84	MG	5	3709	1/1	0.81	0.24	61,61,61,61	0
84	MG	5	3571	1/1	0.81	0.43	53,53,53,53	0
84	MG	6	1948	1/1	0.81	0.37	47,47,47,47	0
86	ZN	D7	101	1/1	0.81	0.16	115,115,115,115	0
84	MG	5	3421	1/1	0.81	0.27	50,50,50,50	0
84	MG	1	3402	1/1	0.82	0.37	46,46,46,46	0
84	MG	2	1930	1/1	0.82	0.44	58,58,58,58	0
84	MG	5	3618	1/1	0.82	0.32	40,40,40,40	0
84	MG	5	3621	1/1	0.82	0.39	40,40,40,40	0
85	OHX	2	2110	7/7	0.82	0.20	130,130,130,130	0
84	MG	1	3494	1/1	0.82	0.25	52,52,52,52	0
84	MG	1	3531	1/1	0.82	0.38	45,45,45,45	0
84	MG	5	3520	1/1	0.82	0.35	40,40,40,40	0
84	MG	5	3441	1/1	0.82	0.34	65,65,65,65	0
84	MG	2	1977	1/1	0.82	0.29	75,75,75,75	0
84	MG	1	3436	1/1	0.82	0.31	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	4076	1/1	0.82	0.17	52,52,52,52	0
85	OHX	M9	201	7/7	0.82	0.18	124,124,124,124	0
84	MG	5	4078	1/1	0.82	0.18	40,40,40,40	0
84	MG	3	204	1/1	0.82	0.50	40,40,40,40	0
84	MG	2	1919	1/1	0.82	0.48	73,73,73,73	0
84	MG	2	1907	1/1	0.82	0.41	64,64,64,64	0
84	MG	4	207	1/1	0.82	0.30	49,49,49,49	0
84	MG	1	3616	1/1	0.82	0.50	81,81,81,81	0
84	MG	l2	303	1/1	0.82	0.60	46,46,46,46	0
85	OHX	5	4058	7/7	0.82	0.21	115,115,115,115	0
84	MG	6	1918	1/1	0.82	0.34	58,58,58,58	0
84	MG	1	3512	1/1	0.82	0.35	55,55,55,55	0
85	OHX	7	221	7/7	0.82	0.20	110,110,110,110	0
84	MG	5	3403	1/1	0.82	0.14	45,45,45,45	0
84	MG	1	3621	1/1	0.82	0.21	36,36,36,36	0
84	MG	1	3559	1/1	0.83	0.24	48,48,48,48	0
84	MG	6	1903	1/1	0.83	0.38	45,45,45,45	0
84	MG	6	1936	1/1	0.83	0.27	42,42,42,42	0
84	MG	2	1933	1/1	0.83	0.41	74,74,74,74	0
85	OHX	2	2108	7/7	0.83	0.16	145,145,145,145	0
84	MG	5	3598	1/1	0.83	0.13	42,42,42,42	0
84	MG	5	3470	1/1	0.83	0.20	32,32,32,32	0
84	MG	1	3599	1/1	0.83	0.19	59,59,59,59	0
84	MG	2	1938	1/1	0.83	0.36	75,75,75,75	0
84	MG	6	1942	1/1	0.83	0.43	79,79,79,79	0
84	MG	5	3721	1/1	0.83	0.28	35,35,35,35	0
84	MG	1	3411	1/1	0.83	0.26	51,51,51,51	0
84	MG	5	3484	1/1	0.83	0.30	35,35,35,35	0
85	OHX	1	3960	7/7	0.83	0.19	122,122,122,122	0
84	MG	6	1977	1/1	0.83	0.38	79,79,79,79	0
85	OHX	1	4024	7/7	0.83	0.14	155,155,155,155	0
85	OHX	4	229	7/7	0.83	0.21	113,113,113,113	0
84	MG	1	3707	1/1	0.83	0.31	53,53,53,53	0
85	OHX	N8	203	7/7	0.83	0.18	129,129,129,129	0
84	MG	5	3625	1/1	0.83	0.11	44,44,44,44	0
85	OHX	6	2132	7/7	0.83	0.20	112,112,112,112	0
84	MG	2	1966	1/1	0.83	0.39	67,67,67,67	0
84	MG	5	3637	1/1	0.83	0.23	49,49,49,49	0
85	OHX	6	2156	7/7	0.83	0.21	115,115,115,115	0
84	MG	1	3714	1/1	0.83	0.20	45,45,45,45	0
84	MG	6	1988	1/1	0.83	0.27	73,73,73,73	0
84	MG	1	3715	1/1	0.83	0.24	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3619	1/1	0.83	0.14	35,35,35,35	0
85	OHX	5	4055	7/7	0.83	0.22	114,114,114,114	0
84	MG	O7	103	1/1	0.83	0.14	64,64,64,64	0
84	MG	5	3660	1/1	0.83	0.33	41,41,41,41	0
85	OHX	5	4066	7/7	0.83	0.20	114,114,114,114	0
84	MG	1	3552	1/1	0.83	0.42	44,44,44,44	0
84	MG	1	3556	1/1	0.83	0.34	30,30,30,30	0
84	MG	5	3677	1/1	0.83	0.34	41,41,41,41	0
84	MG	5	3555	1/1	0.83	0.34	44,44,44,44	0
84	MG	5	3503	1/1	0.84	0.36	40,40,40,40	0
84	MG	1	3564	1/1	0.84	0.42	40,40,40,40	0
85	OHX	2	2098	7/7	0.84	0.23	125,125,125,125	0
84	MG	6	1931	1/1	0.84	0.27	48,48,48,48	0
84	MG	5	3522	1/1	0.84	0.32	43,43,43,43	0
85	OHX	2	2107	7/7	0.84	0.18	126,126,126,126	0
84	MG	1	3444	1/1	0.84	0.32	51,51,51,51	0
84	MG	5	3411	1/1	0.84	0.20	34,34,34,34	0
84	MG	5	3680	1/1	0.84	0.25	53,53,53,53	0
84	MG	1	3485	1/1	0.84	0.33	37,37,37,37	0
84	MG	1	3668	1/1	0.84	0.31	66,66,66,66	0
85	OHX	2	2116	7/7	0.84	0.22	109,109,109,109	0
84	MG	2	1967	1/1	0.84	0.16	83,83,83,83	0
84	MG	SM	201	1/1	0.84	0.33	56,56,56,56	0
84	MG	5	3559	1/1	0.84	0.18	40,40,40,40	0
84	MG	1	3681	1/1	0.84	0.12	45,45,45,45	0
84	MG	5	3704	1/1	0.84	0.27	54,54,54,54	0
84	MG	2	1976	1/1	0.84	0.46	68,68,68,68	0
84	MG	5	3588	1/1	0.84	0.29	57,57,57,57	0
84	MG	5	3456	1/1	0.84	0.32	54,54,54,54	0
84	MG	2	1970	1/1	0.84	0.28	76,76,76,76	0
84	MG	1	3689	1/1	0.84	0.22	57,57,57,57	0
84	MG	5	3602	1/1	0.84	0.33	49,49,49,49	0
84	MG	1	3462	1/1	0.84	0.30	38,38,38,38	0
84	MG	5	3461	1/1	0.84	0.12	40,40,40,40	0
84	MG	4	202	1/1	0.84	0.37	57,57,57,57	0
84	MG	5	3463	1/1	0.84	0.29	41,41,41,41	0
84	MG	1	3466	1/1	0.84	0.37	57,57,57,57	0
84	MG	1	3510	1/1	0.84	0.26	31,31,31,31	0
85	OHX	5	3938	7/7	0.84	0.18	115,115,115,115	0
84	MG	4	208	1/1	0.84	0.11	54,54,54,54	0
85	OHX	5	4008	7/7	0.84	0.16	144,144,144,144	0
84	MG	6	1923	1/1	0.84	0.38	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	4043	7/7	0.84	0.36	96,96,96,96	0
84	MG	2	1929	1/1	0.84	0.49	67,67,67,67	0
84	MG	6	2007	1/1	0.84	0.12	61,61,61,61	0
84	MG	6	2008	1/1	0.84	0.28	47,47,47,47	0
84	MG	1	3514	1/1	0.84	0.31	33,33,33,33	0
84	MG	1	3656	1/1	0.84	0.36	46,46,46,46	0
84	MG	c1	201	1/1	0.84	0.32	53,53,53,53	0
84	MG	M7	204	1/1	0.84	0.17	40,40,40,40	0
84	MG	m7	203	1/1	0.84	0.36	40,40,40,40	0
84	MG	l3	405	1/1	0.85	0.37	34,34,34,34	0
84	MG	1	3479	1/1	0.85	0.13	64,64,64,64	0
84	MG	1	3502	1/1	0.85	0.33	39,39,39,39	0
84	MG	1	3593	1/1	0.85	0.12	39,39,39,39	0
84	MG	1	3517	1/1	0.85	0.34	51,51,51,51	0
84	MG	5	3645	1/1	0.85	0.14	33,33,33,33	0
84	MG	5	3508	1/1	0.85	0.32	34,34,34,34	0
84	MG	1	3536	1/1	0.85	0.26	56,56,56,56	0
84	MG	5	3410	1/1	0.85	0.37	42,42,42,42	0
84	MG	1	3600	1/1	0.85	0.32	52,52,52,52	0
84	MG	5	3672	1/1	0.85	0.25	40,40,40,40	0
84	MG	5	3529	1/1	0.85	0.47	58,58,58,58	0
84	MG	6	1973	1/1	0.85	0.21	78,78,78,78	0
85	OHX	2	2112	7/7	0.85	0.19	116,116,116,116	0
85	OHX	2	2113	7/7	0.85	0.20	110,110,110,110	0
84	MG	L2	301	1/1	0.85	0.27	39,39,39,39	0
84	MG	5	3420	1/1	0.85	0.28	60,60,60,60	0
84	MG	6	1929	1/1	0.85	0.28	67,67,67,67	0
84	MG	5	3429	1/1	0.85	0.18	78,78,78,78	0
84	MG	5	3688	1/1	0.85	0.22	33,33,33,33	0
85	OHX	S6	301	7/7	0.85	0.18	117,117,117,117	0
84	MG	1	3486	1/1	0.85	0.37	36,36,36,36	0
84	MG	1	3604	1/1	0.85	0.12	47,47,47,47	0
85	OHX	1	3992	7/7	0.85	0.21	116,116,116,116	0
84	MG	6	1932	1/1	0.85	0.57	62,62,62,62	0
85	OHX	1	4014	7/7	0.85	0.18	110,110,110,110	0
84	MG	1	3520	1/1	0.85	0.26	42,42,42,42	0
84	MG	5	3701	1/1	0.85	0.14	47,47,47,47	0
84	MG	1	3610	1/1	0.85	0.33	42,42,42,42	0
84	MG	5	3589	1/1	0.85	0.28	37,37,37,37	0
84	MG	1	3611	1/1	0.85	0.09	39,39,39,39	0
84	MG	1	3614	1/1	0.85	0.10	55,55,55,55	0
85	OHX	6	2142	7/7	0.85	0.20	117,117,117,117	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3597	1/1	0.85	0.13	29,29,29,29	0
85	OHX	6	2151	7/7	0.85	0.19	127,127,127,127	0
84	MG	1	3665	1/1	0.85	0.29	67,67,67,67	0
84	MG	1	3666	1/1	0.85	0.19	45,45,45,45	0
84	MG	5	3734	1/1	0.85	0.21	60,60,60,60	0
84	MG	1	3718	1/1	0.85	0.09	78,78,78,78	0
84	MG	1	3549	1/1	0.85	0.39	53,53,53,53	0
85	OHX	5	3969	7/7	0.85	0.15	138,138,138,138	0
84	MG	1	3618	1/1	0.85	0.36	62,62,62,62	0
84	MG	5	3469	1/1	0.85	0.27	58,58,58,58	0
84	MG	6	1908	1/1	0.85	0.26	51,51,51,51	0
84	MG	5	3617	1/1	0.85	0.22	46,46,46,46	0
85	OHX	5	4050	7/7	0.85	0.13	158,158,158,158	0
84	MG	1	3571	1/1	0.85	0.28	35,35,35,35	0
84	MG	5	3619	1/1	0.85	0.19	37,37,37,37	0
84	MG	1	3581	1/1	0.85	0.27	45,45,45,45	0
84	MG	1	3679	1/1	0.85	0.14	34,34,34,34	0
84	MG	5	3624	1/1	0.85	0.09	41,41,41,41	0
84	MG	1	3412	1/1	0.85	0.28	42,42,42,42	0
85	OHX	l3	408	7/7	0.85	0.19	111,111,111,111	0
84	MG	6	1917	1/1	0.85	0.44	75,75,75,75	0
84	MG	5	3633	1/1	0.85	0.40	36,36,36,36	0
85	OHX	2	2085	7/7	0.86	0.20	114,114,114,114	0
85	OHX	2	2096	7/7	0.86	0.17	122,122,122,122	0
84	MG	5	3413	1/1	0.86	0.33	41,41,41,41	0
85	OHX	2	2101	7/7	0.86	0.16	129,129,129,129	0
84	MG	5	3527	1/1	0.86	0.40	69,69,69,69	0
84	MG	1	3587	1/1	0.86	0.23	42,42,42,42	0
84	MG	1	3712	1/1	0.86	0.16	41,41,41,41	0
84	MG	5	3667	1/1	0.86	0.24	38,38,38,38	0
84	MG	1	3488	1/1	0.86	0.22	33,33,33,33	0
84	MG	1	3429	1/1	0.86	0.34	51,51,51,51	0
84	MG	1	3471	1/1	0.86	0.25	58,58,58,58	0
84	MG	5	3550	1/1	0.86	0.34	31,31,31,31	0
84	MG	6	1986	1/1	0.86	0.18	57,57,57,57	0
84	MG	1	3628	1/1	0.86	0.31	50,50,50,50	0
84	MG	5	3442	1/1	0.86	0.29	36,36,36,36	0
84	MG	5	3450	1/1	0.86	0.13	58,58,58,58	0
84	MG	6	1941	1/1	0.86	0.38	43,43,43,43	0
84	MG	5	3577	1/1	0.86	0.23	45,45,45,45	0
84	MG	6	1992	1/1	0.86	0.42	60,60,60,60	0
85	OHX	1	3921	7/7	0.86	0.24	110,110,110,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3598	1/1	0.86	0.17	39,39,39,39	0
84	MG	1	3445	1/1	0.86	0.28	40,40,40,40	0
84	MG	5	3459	1/1	0.86	0.26	40,40,40,40	0
84	MG	1	3477	1/1	0.86	0.20	54,54,54,54	0
84	MG	1	3685	1/1	0.86	0.19	39,39,39,39	0
85	OHX	1	4021	7/7	0.86	0.16	128,128,128,128	0
84	MG	5	3601	1/1	0.86	0.29	38,38,38,38	0
85	OHX	1	4028	7/7	0.86	0.19	115,115,115,115	0
84	MG	1	3529	1/1	0.86	0.35	50,50,50,50	0
84	MG	5	3605	1/1	0.86	0.10	37,37,37,37	0
84	MG	1	3405	1/1	0.86	0.43	63,63,63,63	0
84	MG	5	3609	1/1	0.86	0.28	55,55,55,55	0
84	MG	6	2004	1/1	0.86	0.19	70,70,70,70	0
85	OHX	6	2137	7/7	0.86	0.17	127,127,127,127	0
84	MG	2	1936	1/1	0.86	0.24	73,73,73,73	0
84	MG	5	3468	1/1	0.86	0.29	51,51,51,51	0
85	OHX	6	2149	7/7	0.86	0.16	132,132,132,132	0
84	MG	5	3615	1/1	0.86	0.32	56,56,56,56	0
84	MG	1	3647	1/1	0.86	0.32	49,49,49,49	0
84	MG	1	3609	1/1	0.86	0.26	41,41,41,41	0
84	MG	7	209	1/1	0.86	0.32	51,51,51,51	0
84	MG	4	209	1/1	0.86	0.16	54,54,54,54	0
85	OHX	c3	201	7/7	0.86	0.17	113,113,113,113	0
84	MG	5	3474	1/1	0.86	0.22	54,54,54,54	0
84	MG	1	3698	1/1	0.86	0.26	49,49,49,49	0
84	MG	8	206	1/1	0.86	0.34	52,52,52,52	0
84	MG	1	3418	1/1	0.86	0.37	66,66,66,66	0
85	OHX	5	4020	7/7	0.86	0.34	101,101,101,101	0
84	MG	1	3424	1/1	0.86	0.30	45,45,45,45	0
84	MG	6	1964	1/1	0.86	0.28	73,73,73,73	0
84	MG	sM	201	1/1	0.86	0.30	44,44,44,44	0
84	MG	L7	301	1/1	0.86	0.21	42,42,42,42	0
84	MG	1	3415	1/1	0.86	0.33	41,41,41,41	0
85	OHX	5	4060	7/7	0.86	0.16	125,125,125,125	0
84	MG	M7	201	1/1	0.86	0.36	60,60,60,60	0
84	MG	m5	301	1/1	0.86	0.25	48,48,48,48	0
84	MG	5	3406	1/1	0.86	0.18	47,47,47,47	0
85	OHX	7	220	7/7	0.86	0.32	110,110,110,110	0
84	MG	1	3542	1/1	0.86	0.29	46,46,46,46	0
84	MG	1	3545	1/1	0.86	0.40	36,36,36,36	0
85	OHX	2	2059	7/7	0.86	0.19	119,119,119,119	0
85	OHX	2	2075	7/7	0.86	0.22	115,115,115,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3568	1/1	0.87	0.34	40,40,40,40	0
84	MG	1	3706	1/1	0.87	0.57	32,32,32,32	0
84	MG	5	3455	1/1	0.87	0.29	50,50,50,50	0
84	MG	5	3737	1/1	0.87	0.13	52,52,52,52	0
84	MG	6	1965	1/1	0.87	0.23	56,56,56,56	0
85	OHX	S8	301	7/7	0.87	0.16	124,124,124,124	0
85	OHX	1	3905	7/7	0.87	0.26	79,79,79,79	0
84	MG	6	1968	1/1	0.87	0.29	55,55,55,55	0
84	MG	5	4071	1/1	0.87	0.21	43,43,43,43	0
85	OHX	1	3943	7/7	0.87	0.17	112,112,112,112	0
84	MG	5	4072	1/1	0.87	0.23	33,33,33,33	0
85	OHX	1	3974	7/7	0.87	0.15	127,127,127,127	0
84	MG	1	3456	1/1	0.87	0.12	32,32,32,32	0
84	MG	5	3627	1/1	0.87	0.30	34,34,34,34	0
84	MG	1	3442	1/1	0.87	0.10	41,41,41,41	0
85	OHX	1	4016	7/7	0.87	0.38	109,109,109,109	0
85	OHX	1	4020	7/7	0.87	0.21	118,118,118,118	0
84	MG	2	1951	1/1	0.87	0.28	58,58,58,58	0
84	MG	1	3661	1/1	0.87	0.22	55,55,55,55	0
84	MG	5	3638	1/1	0.87	0.12	37,37,37,37	0
85	OHX	1	4029	7/7	0.87	0.41	89,89,89,89	0
84	MG	5	3542	1/1	0.87	0.43	36,36,36,36	0
84	MG	1	3663	1/1	0.87	0.09	36,36,36,36	0
84	MG	6	1911	1/1	0.87	0.31	52,52,52,52	0
85	OHX	6	2095	7/7	0.87	0.18	119,119,119,119	0
85	OHX	6	2127	7/7	0.87	0.15	138,138,138,138	0
84	MG	1	3435	1/1	0.87	0.22	41,41,41,41	0
84	MG	1	3409	1/1	0.87	0.35	40,40,40,40	0
85	OHX	6	2134	7/7	0.87	0.18	112,112,112,112	0
84	MG	6	1916	1/1	0.87	0.30	46,46,46,46	0
84	MG	1	3721	1/1	0.87	0.35	42,42,42,42	0
84	MG	6	1949	1/1	0.87	0.43	76,76,76,76	0
84	MG	5	3578	1/1	0.87	0.48	40,40,40,40	0
84	MG	l7	301	1/1	0.87	0.10	37,37,37,37	0
84	MG	l9	201	1/1	0.87	0.10	45,45,45,45	0
84	MG	5	3471	1/1	0.87	0.32	68,68,68,68	0
84	MG	6	1987	1/1	0.87	0.20	55,55,55,55	0
84	MG	1	3642	1/1	0.87	0.28	48,48,48,48	0
84	MG	1	3723	1/1	0.87	0.22	37,37,37,37	0
85	OHX	2	2034	7/7	0.87	0.20	113,113,113,113	0
85	OHX	5	3959	7/7	0.87	0.17	118,118,118,118	0
84	MG	O4	201	1/1	0.87	0.37	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3988	7/7	0.87	0.18	116,116,116,116	0
84	MG	5	3418	1/1	0.87	0.28	41,41,41,41	0
85	OHX	2	2076	7/7	0.87	0.17	135,135,135,135	0
85	OHX	5	4009	7/7	0.87	0.18	115,115,115,115	0
84	MG	5	3599	1/1	0.87	0.20	43,43,43,43	0
85	OHX	2	2089	7/7	0.87	0.20	113,113,113,113	0
85	OHX	5	4029	7/7	0.87	0.16	128,128,128,128	0
84	MG	2	1918	1/1	0.87	0.46	64,64,64,64	0
84	MG	5	3485	1/1	0.87	0.17	37,37,37,37	0
84	MG	5	3486	1/1	0.87	0.29	48,48,48,48	0
84	MG	2	1911	1/1	0.87	0.56	69,69,69,69	0
84	MG	5	3498	1/1	0.87	0.26	41,41,41,41	0
84	MG	3	203	1/1	0.87	0.20	44,44,44,44	0
84	MG	5	3611	1/1	0.87	0.25	40,40,40,40	0
85	OHX	5	4068	7/7	0.87	0.24	96,96,96,96	0
84	MG	1	3674	1/1	0.87	0.25	37,37,37,37	0
84	MG	5	3501	1/1	0.87	0.39	27,27,27,27	0
84	MG	6	1928	1/1	0.87	0.34	51,51,51,51	0
84	MG	1	3543	1/1	0.87	0.24	34,34,34,34	0
84	MG	5	3722	1/1	0.87	0.19	55,55,55,55	0
84	MG	5	3515	1/1	0.87	0.26	52,52,52,52	0
84	MG	l3	402	1/1	0.88	0.13	32,32,32,32	0
84	MG	4	214	1/1	0.88	0.26	53,53,53,53	0
84	MG	1	3626	1/1	0.88	0.15	44,44,44,44	0
84	MG	1	3697	1/1	0.88	0.15	41,41,41,41	0
84	MG	5	3604	1/1	0.88	0.25	36,36,36,36	0
84	MG	5	3509	1/1	0.88	0.25	47,47,47,47	0
84	MG	1	3672	1/1	0.88	0.18	42,42,42,42	0
84	MG	1	3649	1/1	0.88	0.24	43,43,43,43	0
85	OHX	3	218	7/7	0.88	0.19	125,125,125,125	0
84	MG	m7	201	1/1	0.88	0.10	37,37,37,37	0
84	MG	1	4040	1/1	0.88	0.21	39,39,39,39	0
84	MG	n3	201	1/1	0.88	0.28	28,28,28,28	0
84	MG	6	1979	1/1	0.88	0.27	52,52,52,52	0
85	OHX	6	2112	7/7	0.88	0.17	115,115,115,115	0
84	MG	5	3524	1/1	0.88	0.38	34,34,34,34	0
84	MG	6	1947	1/1	0.88	0.38	53,53,53,53	0
85	OHX	2	2052	7/7	0.88	0.16	117,117,117,117	0
84	MG	N8	201	1/1	0.88	0.14	37,37,37,37	0
84	MG	1	3469	1/1	0.88	0.44	51,51,51,51	0
84	MG	6	1922	1/1	0.88	0.40	48,48,48,48	0
85	OHX	2	2080	7/7	0.88	0.18	112,112,112,112	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3409	1/1	0.88	0.29	58,58,58,58	0
84	MG	1	3503	1/1	0.88	0.41	33,33,33,33	0
84	MG	1	3507	1/1	0.88	0.29	34,34,34,34	0
84	MG	1	3680	1/1	0.88	0.10	40,40,40,40	0
84	MG	5	3725	1/1	0.88	0.24	38,38,38,38	0
84	MG	5	3728	1/1	0.88	0.30	50,50,50,50	0
85	OHX	s8	302	7/7	0.88	0.15	132,132,132,132	0
85	OHX	2	2105	7/7	0.88	0.21	114,114,114,114	0
84	MG	1	3516	1/1	0.88	0.40	40,40,40,40	0
84	MG	5	3473	1/1	0.88	0.30	44,44,44,44	0
84	MG	5	3557	1/1	0.88	0.45	42,42,42,42	0
84	MG	1	3539	1/1	0.88	0.42	44,44,44,44	0
84	MG	5	3561	1/1	0.88	0.49	48,48,48,48	0
85	OHX	5	4004	7/7	0.88	0.15	119,119,119,119	0
84	MG	1	3640	1/1	0.88	0.25	74,74,74,74	0
84	MG	5	3572	1/1	0.88	0.33	28,28,28,28	0
84	MG	6	1995	1/1	0.88	0.43	52,52,52,52	0
85	OHX	2	2114	7/7	0.88	0.12	170,170,170,170	0
84	MG	1	3493	1/1	0.88	0.34	30,30,30,30	0
84	MG	1	3623	1/1	0.88	0.17	51,51,51,51	0
84	MG	5	3584	1/1	0.88	0.11	45,45,45,45	0
84	MG	7	201	1/1	0.88	0.39	49,49,49,49	0
84	MG	7	206	1/1	0.88	0.34	42,42,42,42	0
84	MG	5	3647	1/1	0.88	0.13	41,41,41,41	0
84	MG	5	3585	1/1	0.88	0.16	39,39,39,39	0
84	MG	6	1905	1/1	0.88	0.41	61,61,61,61	0
84	MG	1	3612	1/1	0.88	0.16	40,40,40,40	0
84	MG	4	211	1/1	0.88	0.21	42,42,42,42	0
84	MG	5	3447	1/1	0.88	0.30	34,34,34,34	0
84	MG	6	1934	1/1	0.88	0.32	67,67,67,67	0
85	OHX	1	3973	7/7	0.88	0.38	105,105,105,105	0
84	MG	1	3645	1/1	0.88	0.30	69,69,69,69	0
84	MG	l3	401	1/1	0.88	0.38	29,29,29,29	0
85	OHX	C3	201	7/7	0.89	0.16	115,115,115,115	0
85	OHX	C5	201	7/7	0.89	0.14	127,127,127,127	0
84	MG	5	3528	1/1	0.89	0.24	36,36,36,36	0
84	MG	O2	201	1/1	0.89	0.16	35,35,35,35	0
84	MG	1	3660	1/1	0.89	0.12	47,47,47,47	0
84	MG	1	3633	1/1	0.89	0.27	56,56,56,56	0
84	MG	5	3534	1/1	0.89	0.30	36,36,36,36	0
84	MG	5	3635	1/1	0.89	0.15	66,66,66,66	0
84	MG	1	3695	1/1	0.89	0.21	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3991	7/7	0.89	0.17	119,119,119,119	0
84	MG	1	3585	1/1	0.89	0.33	59,59,59,59	0
85	OHX	1	4002	7/7	0.89	0.17	112,112,112,112	0
84	MG	6	1966	1/1	0.89	0.29	53,53,53,53	0
84	MG	5	3642	1/1	0.89	0.10	37,37,37,37	0
84	MG	2	1942	1/1	0.89	0.25	69,69,69,69	0
84	MG	5	3552	1/1	0.89	0.35	36,36,36,36	0
84	MG	1	3448	1/1	0.89	0.47	64,64,64,64	0
84	MG	5	3646	1/1	0.89	0.09	35,35,35,35	0
84	MG	5	3464	1/1	0.89	0.25	29,29,29,29	0
84	MG	3	205	1/1	0.89	0.27	66,66,66,66	0
84	MG	1	3524	1/1	0.89	0.28	43,43,43,43	0
84	MG	5	3659	1/1	0.89	0.11	41,41,41,41	0
85	OHX	4	230	7/7	0.89	0.38	108,108,108,108	0
84	MG	1	3565	1/1	0.89	0.27	32,32,32,32	0
84	MG	6	1935	1/1	0.89	0.40	44,44,44,44	0
85	OHX	6	2093	7/7	0.89	0.16	117,117,117,117	0
84	MG	m5	303	1/1	0.89	0.32	46,46,46,46	0
84	MG	1	3419	1/1	0.89	0.31	44,44,44,44	0
85	OHX	6	2114	7/7	0.89	0.19	114,114,114,114	0
84	MG	1	3495	1/1	0.89	0.35	41,41,41,41	0
85	OHX	6	2128	7/7	0.89	0.19	112,112,112,112	0
84	MG	n0	202	1/1	0.89	0.11	40,40,40,40	0
84	MG	5	3576	1/1	0.89	0.32	34,34,34,34	0
84	MG	5	3408	1/1	0.89	0.26	42,42,42,42	0
84	MG	1	3422	1/1	0.89	0.23	55,55,55,55	0
85	OHX	6	2141	7/7	0.89	0.33	109,109,109,109	0
84	MG	o1	201	1/1	0.89	0.13	49,49,49,49	0
85	OHX	6	2145	7/7	0.89	0.33	106,106,106,106	0
84	MG	5	3581	1/1	0.89	0.39	35,35,35,35	0
84	MG	5	3583	1/1	0.89	0.19	42,42,42,42	0
84	MG	6	1939	1/1	0.89	0.31	56,56,56,56	0
85	OHX	2	2071	7/7	0.89	0.16	127,127,127,127	0
84	MG	1	3468	1/1	0.89	0.25	59,59,59,59	0
84	MG	1	3433	1/1	0.89	0.23	36,36,36,36	0
85	OHX	2	2077	7/7	0.89	0.17	110,110,110,110	0
84	MG	5	3481	1/1	0.89	0.33	35,35,35,35	0
85	OHX	2	2083	7/7	0.89	0.18	115,115,115,115	0
85	OHX	d4	201	7/7	0.89	0.17	115,115,115,115	0
85	OHX	5	3937	7/7	0.89	0.19	112,112,112,112	0
84	MG	5	3414	1/1	0.89	0.19	31,31,31,31	0
85	OHX	5	3945	7/7	0.89	0.15	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3651	1/1	0.89	0.14	36,36,36,36	0
85	OHX	2	2091	7/7	0.89	0.16	122,122,122,122	0
84	MG	4	212	1/1	0.89	0.15	54,54,54,54	0
84	MG	1	3713	1/1	0.89	0.07	45,45,45,45	0
85	OHX	2	2100	7/7	0.89	0.17	116,116,116,116	0
84	MG	1	3575	1/1	0.89	0.34	40,40,40,40	0
84	MG	5	3491	1/1	0.89	0.36	42,42,42,42	0
84	MG	5	3492	1/1	0.89	0.33	41,41,41,41	0
84	MG	5	3493	1/1	0.89	0.42	34,34,34,34	0
84	MG	1	3653	1/1	0.89	0.10	40,40,40,40	0
85	OHX	5	4033	7/7	0.89	0.31	105,105,105,105	0
84	MG	5	3426	1/1	0.89	0.19	36,36,36,36	0
84	MG	1	3717	1/1	0.89	0.19	60,60,60,60	0
84	MG	5	3435	1/1	0.89	0.15	34,34,34,34	0
84	MG	6	1919	1/1	0.89	0.43	67,67,67,67	0
84	MG	5	3733	1/1	0.89	0.24	32,32,32,32	0
84	MG	6	1920	1/1	0.89	0.36	42,42,42,42	0
85	OHX	5	4063	7/7	0.89	0.18	121,121,121,121	0
84	MG	1	3579	1/1	0.89	0.30	40,40,40,40	0
84	MG	5	3445	1/1	0.89	0.42	49,49,49,49	0
84	MG	1	3458	1/1	0.89	0.30	59,59,59,59	0
84	MG	6	2000	1/1	0.89	0.20	86,86,86,86	0
84	MG	5	3521	1/1	0.89	0.27	39,39,39,39	0
84	MG	1	3557	1/1	0.89	0.41	37,37,37,37	0
84	MG	5	3452	1/1	0.89	0.24	43,43,43,43	0
86	ZN	d7	101	1/1	0.89	0.13	106,106,106,106	0
86	ZN	e1	501	1/1	0.89	0.07	160,160,160,160	0
84	MG	1	3691	1/1	0.89	0.14	54,54,54,54	0
85	OHX	1	3985	7/7	0.90	0.41	97,97,97,97	0
85	OHX	1	3986	7/7	0.90	0.16	112,112,112,112	0
84	MG	1	3578	1/1	0.90	0.19	35,35,35,35	0
84	MG	1	3719	1/1	0.90	0.24	45,45,45,45	0
84	MG	l8	301	1/1	0.90	0.47	83,83,83,83	0
84	MG	5	3690	1/1	0.90	0.18	30,30,30,30	0
84	MG	5	3692	1/1	0.90	0.22	68,68,68,68	0
84	MG	1	3447	1/1	0.90	0.30	37,37,37,37	0
84	MG	m6	201	1/1	0.90	0.18	37,37,37,37	0
84	MG	5	3554	1/1	0.90	0.32	29,29,29,29	0
84	MG	m7	202	1/1	0.90	0.28	36,36,36,36	0
84	MG	1	3670	1/1	0.90	0.33	52,52,52,52	0
84	MG	6	1953	1/1	0.90	0.46	43,43,43,43	0
85	OHX	1	4035	7/7	0.90	0.21	105,105,105,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	4038	7/7	0.90	0.34	100,100,100,100	0
84	MG	1	3457	1/1	0.90	0.27	42,42,42,42	0
84	MG	5	3702	1/1	0.90	0.11	35,35,35,35	0
84	MG	1	3582	1/1	0.90	0.15	45,45,45,45	0
84	MG	5	3620	1/1	0.90	0.28	35,35,35,35	0
84	MG	5	3563	1/1	0.90	0.36	38,38,38,38	0
84	MG	5	3622	1/1	0.90	0.17	55,55,55,55	0
85	OHX	2	2055	7/7	0.90	0.29	111,111,111,111	0
84	MG	5	3718	1/1	0.90	0.08	40,40,40,40	0
85	OHX	2	2060	7/7	0.90	0.17	122,122,122,122	0
85	OHX	2	2067	7/7	0.90	0.28	106,106,106,106	0
84	MG	L3	401	1/1	0.90	0.38	53,53,53,53	0
85	OHX	2	2073	7/7	0.90	0.16	120,120,120,120	0
84	MG	2	1908	1/1	0.90	0.24	78,78,78,78	0
84	MG	5	3573	1/1	0.90	0.33	37,37,37,37	0
84	MG	1	3566	1/1	0.90	0.28	37,37,37,37	0
84	MG	1	4044	1/1	0.90	0.14	51,51,51,51	0
84	MG	5	3629	1/1	0.90	0.28	35,35,35,35	0
84	MG	5	3507	1/1	0.90	0.38	44,44,44,44	0
85	OHX	2	2087	7/7	0.90	0.17	119,119,119,119	0
84	MG	1	3423	1/1	0.90	0.19	36,36,36,36	0
85	OHX	2	2090	7/7	0.90	0.16	121,121,121,121	0
84	MG	1	3498	1/1	0.90	0.31	32,32,32,32	0
84	MG	5	3582	1/1	0.90	0.23	49,49,49,49	0
84	MG	1	3407	1/1	0.90	0.16	45,45,45,45	0
84	MG	1	3682	1/1	0.90	0.24	33,33,33,33	0
84	MG	5	3740	1/1	0.90	0.11	41,41,41,41	0
85	OHX	s9	201	7/7	0.90	0.37	96,96,96,96	0
84	MG	1	3451	1/1	0.90	0.24	47,47,47,47	0
85	OHX	c5	201	7/7	0.90	0.13	128,128,128,128	0
85	OHX	2	2103	7/7	0.90	0.14	132,132,132,132	0
85	OHX	5	3870	7/7	0.90	0.28	76,76,76,76	0
85	OHX	5	3932	7/7	0.90	0.26	75,75,75,75	0
84	MG	5	3587	1/1	0.90	0.19	39,39,39,39	0
84	MG	1	3596	1/1	0.90	0.15	46,46,46,46	0
85	OHX	5	3943	7/7	0.90	0.16	116,116,116,116	0
84	MG	5	4075	1/1	0.90	0.32	33,33,33,33	0
84	MG	1	3662	1/1	0.90	0.14	45,45,45,45	0
84	MG	5	3592	1/1	0.90	0.15	42,42,42,42	0
85	OHX	5	3982	7/7	0.90	0.30	80,80,80,80	0
84	MG	5	3650	1/1	0.90	0.20	46,46,46,46	0
84	MG	7	202	1/1	0.90	0.13	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	7	205	1/1	0.90	0.37	35,35,35,35	0
85	OHX	5	4005	7/7	0.90	0.23	104,104,104,104	0
84	MG	6	1943	1/1	0.90	0.50	58,58,58,58	0
84	MG	5	3525	1/1	0.90	0.29	36,36,36,36	0
84	MG	1	3491	1/1	0.90	0.44	41,41,41,41	0
84	MG	5	3440	1/1	0.90	0.09	40,40,40,40	0
84	MG	8	203	1/1	0.90	0.34	43,43,43,43	0
84	MG	5	3663	1/1	0.90	0.27	62,62,62,62	0
84	MG	5	3476	1/1	0.90	0.32	51,51,51,51	0
85	OHX	5	4044	7/7	0.90	0.16	116,116,116,116	0
84	MG	8	207	1/1	0.90	0.27	51,51,51,51	0
84	MG	8	208	1/1	0.90	0.13	63,63,63,63	0
84	MG	6	1945	1/1	0.90	0.42	66,66,66,66	0
84	MG	8	210	1/1	0.90	0.17	57,57,57,57	0
85	OHX	D9	103	7/7	0.90	0.19	108,108,108,108	0
85	OHX	5	4062	7/7	0.90	0.41	84,84,84,84	0
85	OHX	1	3889	7/7	0.90	0.21	99,99,99,99	0
84	MG	5	3479	1/1	0.90	0.21	35,35,35,35	0
85	OHX	1	3914	7/7	0.90	0.14	111,111,111,111	0
85	OHX	1	3918	7/7	0.90	0.15	121,121,121,121	0
84	MG	6	1946	1/1	0.90	0.33	49,49,49,49	0
84	MG	1	3574	1/1	0.90	0.32	33,33,33,33	0
85	OHX	8	223	7/7	0.90	0.33	95,95,95,95	0
84	MG	6	1978	1/1	0.90	0.18	76,76,76,76	0
85	OHX	l4	402	7/7	0.90	0.41	99,99,99,99	0
85	OHX	1	3950	7/7	0.90	0.15	121,121,121,121	0
84	MG	1	3492	1/1	0.90	0.32	39,39,39,39	0
84	MG	5	3543	1/1	0.90	0.39	37,37,37,37	0
84	MG	5	3685	1/1	0.90	0.10	36,36,36,36	0
84	MG	8	201	1/1	0.91	0.11	42,42,42,42	0
84	MG	5	3566	1/1	0.91	0.40	46,46,46,46	0
85	OHX	6	2077	7/7	0.91	0.18	100,100,100,100	0
85	OHX	6	2088	7/7	0.91	0.37	81,81,81,81	0
85	OHX	6	2090	7/7	0.91	0.17	115,115,115,115	0
84	MG	1	3528	1/1	0.91	0.23	34,34,34,34	0
84	MG	1	3432	1/1	0.91	0.21	49,49,49,49	0
85	OHX	6	2098	7/7	0.91	0.31	99,99,99,99	0
85	OHX	6	2105	7/7	0.91	0.18	115,115,115,115	0
85	OHX	6	2110	7/7	0.91	0.28	103,103,103,103	0
84	MG	1	3694	1/1	0.91	0.31	41,41,41,41	0
84	MG	1	3605	1/1	0.91	0.23	46,46,46,46	0
85	OHX	6	2116	7/7	0.91	0.14	111,111,111,111	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	2	2104	7/7	0.91	0.29	96,96,96,96	0
84	MG	1	3478	1/1	0.91	0.19	40,40,40,40	0
84	MG	5	3518	1/1	0.91	0.32	41,41,41,41	0
84	MG	5	3427	1/1	0.91	0.26	47,47,47,47	0
84	MG	l2	301	1/1	0.91	0.41	48,48,48,48	0
85	OHX	6	2135	7/7	0.91	0.33	92,92,92,92	0
84	MG	5	3695	1/1	0.91	0.19	48,48,48,48	0
84	MG	1	3532	1/1	0.91	0.20	57,57,57,57	0
84	MG	1	3554	1/1	0.91	0.29	32,32,32,32	0
85	OHX	6	2143	7/7	0.91	0.33	97,97,97,97	0
84	MG	1	3631	1/1	0.91	0.33	49,49,49,49	0
85	OHX	6	2146	7/7	0.91	0.26	108,108,108,108	0
84	MG	1	3724	1/1	0.91	0.18	49,49,49,49	0
84	MG	5	3631	1/1	0.91	0.16	41,41,41,41	0
84	MG	1	3470	1/1	0.91	0.27	37,37,37,37	0
85	OHX	6	2154	7/7	0.91	0.31	100,100,100,100	0
84	MG	1	3590	1/1	0.91	0.27	60,60,60,60	0
84	MG	5	3713	1/1	0.91	0.25	33,33,33,33	0
84	MG	1	3482	1/1	0.91	0.17	53,53,53,53	0
84	MG	5	3715	1/1	0.91	0.12	39,39,39,39	0
84	MG	5	3446	1/1	0.91	0.13	45,45,45,45	0
84	MG	5	3720	1/1	0.91	0.15	32,32,32,32	0
84	MG	5	3640	1/1	0.91	0.18	51,51,51,51	0
84	MG	2	1980	1/1	0.91	0.18	58,58,58,58	0
84	MG	5	3449	1/1	0.91	0.13	34,34,34,34	0
85	OHX	sR	401	7/7	0.91	0.13	132,132,132,132	0
85	OHX	5	3860	7/7	0.91	0.14	122,122,122,122	0
85	OHX	1	3855	7/7	0.91	0.34	86,86,86,86	0
84	MG	3	202	1/1	0.91	0.46	67,67,67,67	0
84	MG	6	1960	1/1	0.91	0.21	45,45,45,45	0
84	MG	5	3405	1/1	0.91	0.17	43,43,43,43	0
84	MG	1	3577	1/1	0.91	0.28	46,46,46,46	0
84	MG	n8	202	1/1	0.91	0.15	37,37,37,37	0
85	OHX	1	3922	7/7	0.91	0.40	92,92,92,92	0
85	OHX	1	3930	7/7	0.91	0.24	100,100,100,100	0
85	OHX	5	3976	7/7	0.91	0.20	107,107,107,107	0
84	MG	5	3544	1/1	0.91	0.31	32,32,32,32	0
85	OHX	5	3986	7/7	0.91	0.33	105,105,105,105	0
84	MG	5	3547	1/1	0.91	0.36	33,33,33,33	0
85	OHX	5	3992	7/7	0.91	0.37	97,97,97,97	0
85	OHX	5	3996	7/7	0.91	0.32	92,92,92,92	0
84	MG	q0	202	1/1	0.91	0.08	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3955	7/7	0.91	0.28	108,108,108,108	0
84	MG	5	3549	1/1	0.91	0.41	48,48,48,48	0
84	MG	5	3490	1/1	0.91	0.44	39,39,39,39	0
84	MG	5	3658	1/1	0.91	0.20	46,46,46,46	0
85	OHX	5	4010	7/7	0.91	0.39	75,75,75,75	0
85	OHX	5	4013	7/7	0.91	0.38	96,96,96,96	0
85	OHX	2	2058	7/7	0.91	0.13	89,89,89,89	0
84	MG	5	3607	1/1	0.91	0.11	38,38,38,38	0
84	MG	N3	201	1/1	0.91	0.28	40,40,40,40	0
85	OHX	2	2063	7/7	0.91	0.11	160,160,160,160	0
85	OHX	5	4039	7/7	0.91	0.32	105,105,105,105	0
85	OHX	5	4040	7/7	0.91	0.39	102,102,102,102	0
85	OHX	1	4000	7/7	0.91	0.28	109,109,109,109	0
84	MG	5	3662	1/1	0.91	0.18	34,34,34,34	0
85	OHX	5	4045	7/7	0.91	0.36	99,99,99,99	0
85	OHX	1	4007	7/7	0.91	0.35	101,101,101,101	0
85	OHX	5	4053	7/7	0.91	0.21	105,105,105,105	0
84	MG	5	4073	1/1	0.91	0.42	31,31,31,31	0
84	MG	1	3438	1/1	0.91	0.28	32,32,32,32	0
84	MG	1	3664	1/1	0.91	0.13	36,36,36,36	0
85	OHX	1	4017	7/7	0.91	0.39	68,68,68,68	0
85	OHX	1	4018	7/7	0.91	0.25	88,88,88,88	0
84	MG	1	3474	1/1	0.91	0.30	53,53,53,53	0
84	MG	5	4077	1/1	0.91	0.45	38,38,38,38	0
84	MG	5	3669	1/1	0.91	0.28	39,39,39,39	0
85	OHX	2	2082	7/7	0.91	0.17	114,114,114,114	0
84	MG	5	3612	1/1	0.91	0.28	40,40,40,40	0
85	OHX	1	4030	7/7	0.91	0.35	98,98,98,98	0
85	OHX	8	222	7/7	0.91	0.15	114,114,114,114	0
85	OHX	1	4034	7/7	0.91	0.30	104,104,104,104	0
84	MG	4	201	1/1	0.91	0.41	53,53,53,53	0
85	OHX	1	4037	7/7	0.91	0.34	98,98,98,98	0
84	MG	6	1967	1/1	0.91	0.20	51,51,51,51	0
84	MG	1	3475	1/1	0.91	0.33	40,40,40,40	0
84	MG	5	3416	1/1	0.91	0.21	38,38,38,38	0
84	MG	5	3682	1/1	0.91	0.13	35,35,35,35	0
84	MG	5	3531	1/1	0.92	0.30	56,56,56,56	0
84	MG	5	3673	1/1	0.92	0.20	34,34,34,34	0
85	OHX	6	2103	7/7	0.92	0.13	131,131,131,131	0
84	MG	1	3464	1/1	0.92	0.20	36,36,36,36	0
84	MG	5	3676	1/1	0.92	0.12	63,63,63,63	0
84	MG	1	3489	1/1	0.92	0.48	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3530	1/1	0.92	0.41	41,41,41,41	0
84	MG	6	1991	1/1	0.92	0.08	50,50,50,50	0
84	MG	6	1954	1/1	0.92	0.42	51,51,51,51	0
84	MG	1	4043	1/1	0.92	0.33	33,33,33,33	0
85	OHX	6	2129	7/7	0.92	0.10	152,152,152,152	0
84	MG	1	3515	1/1	0.92	0.33	41,41,41,41	0
84	MG	5	3424	1/1	0.92	0.25	32,32,32,32	0
84	MG	1	3481	1/1	0.92	0.20	45,45,45,45	0
84	MG	1	3558	1/1	0.92	0.30	45,45,45,45	0
85	OHX	6	2136	7/7	0.92	0.30	108,108,108,108	0
84	MG	1	3533	1/1	0.92	0.28	39,39,39,39	0
84	MG	5	3433	1/1	0.92	0.27	42,42,42,42	0
84	MG	5	3434	1/1	0.92	0.29	32,32,32,32	0
84	MG	1	3561	1/1	0.92	0.35	43,43,43,43	0
85	OHX	6	2144	7/7	0.92	0.30	102,102,102,102	0
84	MG	5	3436	1/1	0.92	0.15	30,30,30,30	0
84	MG	5	3556	1/1	0.92	0.25	36,36,36,36	0
84	MG	5	3437	1/1	0.92	0.12	35,35,35,35	0
84	MG	5	3487	1/1	0.92	0.28	32,32,32,32	0
85	OHX	6	2150	7/7	0.92	0.31	100,100,100,100	0
84	MG	1	3404	1/1	0.92	0.22	42,42,42,42	0
85	OHX	6	2153	7/7	0.92	0.25	109,109,109,109	0
84	MG	5	3439	1/1	0.92	0.12	33,33,33,33	0
84	MG	5	3710	1/1	0.92	0.12	44,44,44,44	0
84	MG	m5	302	1/1	0.92	0.12	53,53,53,53	0
85	OHX	1	3864	7/7	0.92	0.19	79,79,79,79	0
85	OHX	1	3877	7/7	0.92	0.12	126,126,126,126	0
85	OHX	1	3884	7/7	0.92	0.15	109,109,109,109	0
84	MG	5	3565	1/1	0.92	0.38	49,49,49,49	0
84	MG	1	3467	1/1	0.92	0.22	47,47,47,47	0
84	MG	3	208	1/1	0.92	0.25	65,65,65,65	0
84	MG	1	3671	1/1	0.92	0.11	45,45,45,45	0
84	MG	5	3717	1/1	0.92	0.11	39,39,39,39	0
84	MG	n0	201	1/1	0.92	0.09	43,43,43,43	0
84	MG	5	3632	1/1	0.92	0.30	42,42,42,42	0
85	OHX	5	3909	7/7	0.92	0.17	88,88,88,88	0
84	MG	1	3613	1/1	0.92	0.15	45,45,45,45	0
85	OHX	1	3935	7/7	0.92	0.31	88,88,88,88	0
84	MG	1	3506	1/1	0.92	0.42	42,42,42,42	0
85	OHX	1	3949	7/7	0.92	0.23	101,101,101,101	0
85	OHX	5	3944	7/7	0.92	0.35	74,74,74,74	0
84	MG	n6	202	1/1	0.92	0.28	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3952	7/7	0.92	0.16	111,111,111,111	0
84	MG	5	3575	1/1	0.92	0.31	31,31,31,31	0
84	MG	4	206	1/1	0.92	0.21	35,35,35,35	0
85	OHX	5	3978	7/7	0.92	0.28	92,92,92,92	0
85	OHX	5	3980	7/7	0.92	0.20	102,102,102,102	0
84	MG	1	3646	1/1	0.92	0.12	53,53,53,53	0
84	MG	5	3727	1/1	0.92	0.15	62,62,62,62	0
85	OHX	2	2026	7/7	0.92	0.14	118,118,118,118	0
85	OHX	5	3989	7/7	0.92	0.36	81,81,81,81	0
85	OHX	2	2027	7/7	0.92	0.12	128,128,128,128	0
84	MG	1	3588	1/1	0.92	0.24	42,42,42,42	0
85	OHX	2	2040	7/7	0.92	0.21	110,110,110,110	0
84	MG	5	3505	1/1	0.92	0.38	36,36,36,36	0
84	MG	1	3521	1/1	0.92	0.33	31,31,31,31	0
85	OHX	1	4006	7/7	0.92	0.38	102,102,102,102	0
85	OHX	2	2057	7/7	0.92	0.15	126,126,126,126	0
85	OHX	1	4010	7/7	0.92	0.35	104,104,104,104	0
84	MG	6	1972	1/1	0.92	0.29	51,51,51,51	0
85	OHX	5	4014	7/7	0.92	0.29	96,96,96,96	0
85	OHX	5	4016	7/7	0.92	0.29	90,90,90,90	0
85	OHX	5	4018	7/7	0.92	0.29	105,105,105,105	0
85	OHX	5	4019	7/7	0.92	0.25	109,109,109,109	0
84	MG	1	3540	1/1	0.92	0.30	35,35,35,35	0
84	MG	5	3736	1/1	0.92	0.18	48,48,48,48	0
84	MG	5	3511	1/1	0.92	0.49	62,62,62,62	0
85	OHX	5	4031	7/7	0.92	0.24	106,106,106,106	0
84	MG	5	3401	1/1	0.92	0.21	32,32,32,32	0
85	OHX	5	4034	7/7	0.92	0.29	84,84,84,84	0
84	MG	2	1905	1/1	0.92	0.59	63,63,63,63	0
84	MG	5	3651	1/1	0.92	0.28	46,46,46,46	0
84	MG	6	1913	1/1	0.92	0.32	51,51,51,51	0
84	MG	1	3595	1/1	0.92	0.22	50,50,50,50	0
84	MG	1	3622	1/1	0.92	0.14	35,35,35,35	0
85	OHX	5	4046	7/7	0.92	0.36	75,75,75,75	0
85	OHX	5	4047	7/7	0.92	0.24	101,101,101,101	0
85	OHX	5	4048	7/7	0.92	0.25	104,104,104,104	0
84	MG	1	3655	1/1	0.92	0.10	41,41,41,41	0
85	OHX	5	4052	7/7	0.92	0.35	94,94,94,94	0
85	OHX	1	4032	7/7	0.92	0.36	88,88,88,88	0
84	MG	1	3687	1/1	0.92	0.11	48,48,48,48	0
85	OHX	5	4056	7/7	0.92	0.25	104,104,104,104	0
84	MG	6	1981	1/1	0.92	0.33	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	4036	7/7	0.92	0.24	104,104,104,104	0
85	OHX	2	2084	7/7	0.92	0.27	98,98,98,98	0
84	MG	1	3525	1/1	0.92	0.30	46,46,46,46	0
84	MG	5	3600	1/1	0.92	0.07	34,34,34,34	0
85	OHX	3	219	7/7	0.92	0.33	95,95,95,95	0
85	OHX	4	225	7/7	0.92	0.14	113,113,113,113	0
84	MG	5	3666	1/1	0.92	0.11	37,37,37,37	0
84	MG	1	3461	1/1	0.92	0.21	36,36,36,36	0
84	MG	7	204	1/1	0.92	0.29	40,40,40,40	0
85	OHX	2	2093	7/7	0.92	0.26	103,103,103,103	0
85	OHX	6	2068	7/7	0.92	0.18	90,90,90,90	0
85	OHX	8	224	7/7	0.92	0.41	94,94,94,94	0
84	MG	5	3668	1/1	0.92	0.43	71,71,71,71	0
85	OHX	6	2080	7/7	0.92	0.28	109,109,109,109	0
85	OHX	6	2084	7/7	0.92	0.14	117,117,117,117	0
84	MG	1	3455	1/1	0.92	0.26	32,32,32,32	0
85	OHX	2	2099	7/7	0.92	0.14	128,128,128,128	0
84	MG	7	208	1/1	0.92	0.27	43,43,43,43	0
84	MG	5	3422	1/1	0.93	0.20	37,37,37,37	0
84	MG	1	3562	1/1	0.93	0.29	48,48,48,48	0
84	MG	3	207	1/1	0.93	0.06	44,44,44,44	0
85	OHX	6	2130	7/7	0.93	0.37	88,88,88,88	0
84	MG	5	3724	1/1	0.93	0.13	42,42,42,42	0
84	MG	1	3708	1/1	0.93	0.25	60,60,60,60	0
85	OHX	6	2133	7/7	0.93	0.24	85,85,85,85	0
84	MG	1	3627	1/1	0.93	0.12	45,45,45,45	0
84	MG	5	3649	1/1	0.93	0.18	35,35,35,35	0
84	MG	6	2003	1/1	0.93	0.46	63,63,63,63	0
85	OHX	1	3920	7/7	0.93	0.12	121,121,121,121	0
85	OHX	6	2139	7/7	0.93	0.38	84,84,84,84	0
85	OHX	2	2025	7/7	0.93	0.16	108,108,108,108	0
84	MG	5	3593	1/1	0.93	0.31	54,54,54,54	0
85	OHX	1	3923	7/7	0.93	0.32	91,91,91,91	0
85	OHX	1	3929	7/7	0.93	0.33	83,83,83,83	0
84	MG	5	3652	1/1	0.93	0.08	44,44,44,44	0
84	MG	1	3453	1/1	0.93	0.24	33,33,33,33	0
84	MG	1	3476	1/1	0.93	0.18	42,42,42,42	0
85	OHX	1	3940	7/7	0.93	0.37	88,88,88,88	0
84	MG	5	3478	1/1	0.93	0.12	45,45,45,45	0
85	OHX	1	3946	7/7	0.93	0.29	99,99,99,99	0
84	MG	4	204	1/1	0.93	0.33	51,51,51,51	0
84	MG	4	205	1/1	0.93	0.35	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3538	1/1	0.93	0.33	41,41,41,41	0
84	MG	5	3540	1/1	0.93	0.34	28,28,28,28	0
84	MG	1	3505	1/1	0.93	0.16	38,38,38,38	0
85	OHX	1	3967	7/7	0.93	0.33	94,94,94,94	0
85	OHX	1	3969	7/7	0.93	0.25	103,103,103,103	0
84	MG	5	3482	1/1	0.93	0.10	33,33,33,33	0
84	MG	1	3440	1/1	0.93	0.12	48,48,48,48	0
85	OHX	1	3980	7/7	0.93	0.36	83,83,83,83	0
85	OHX	1	3981	7/7	0.93	0.22	95,95,95,95	0
85	OHX	1	3982	7/7	0.93	0.25	107,107,107,107	0
85	OHX	5	3849	7/7	0.93	0.17	90,90,90,90	0
85	OHX	1	3984	7/7	0.93	0.25	102,102,102,102	0
84	MG	5	3606	1/1	0.93	0.20	41,41,41,41	0
85	OHX	5	3871	7/7	0.93	0.24	77,77,77,77	0
85	OHX	5	3894	7/7	0.93	0.40	80,80,80,80	0
85	OHX	5	3897	7/7	0.93	0.28	81,81,81,81	0
85	OHX	5	3906	7/7	0.93	0.18	101,101,101,101	0
84	MG	1	3544	1/1	0.93	0.41	35,35,35,35	0
85	OHX	5	3919	7/7	0.93	0.26	97,97,97,97	0
85	OHX	1	3990	7/7	0.93	0.29	99,99,99,99	0
84	MG	5	3546	1/1	0.93	0.46	39,39,39,39	0
84	MG	1	3634	1/1	0.93	0.18	39,39,39,39	0
85	OHX	1	3993	7/7	0.93	0.34	87,87,87,87	0
85	OHX	1	3998	7/7	0.93	0.30	102,102,102,102	0
84	MG	5	3548	1/1	0.93	0.27	29,29,29,29	0
85	OHX	5	3958	7/7	0.93	0.28	98,98,98,98	0
85	OHX	2	2078	7/7	0.93	0.28	105,105,105,105	0
85	OHX	5	3961	7/7	0.93	0.20	102,102,102,102	0
85	OHX	5	3962	7/7	0.93	0.17	111,111,111,111	0
85	OHX	1	4003	7/7	0.93	0.27	108,108,108,108	0
85	OHX	5	3973	7/7	0.93	0.24	96,96,96,96	0
85	OHX	2	2079	7/7	0.93	0.15	115,115,115,115	0
84	MG	1	3637	1/1	0.93	0.19	42,42,42,42	0
84	MG	7	203	1/1	0.93	0.34	58,58,58,58	0
84	MG	1	3519	1/1	0.93	0.46	38,38,38,38	0
85	OHX	5	3983	7/7	0.93	0.27	83,83,83,83	0
85	OHX	5	3984	7/7	0.93	0.28	86,86,86,86	0
85	OHX	5	3985	7/7	0.93	0.34	97,97,97,97	0
85	OHX	1	4013	7/7	0.93	0.23	104,104,104,104	0
84	MG	5	3551	1/1	0.93	0.28	35,35,35,35	0
84	MG	5	3679	1/1	0.93	0.29	42,42,42,42	0
85	OHX	5	3990	7/7	0.93	0.38	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3425	1/1	0.93	0.14	49,49,49,49	0
84	MG	1	3592	1/1	0.93	0.18	61,61,61,61	0
85	OHX	5	3997	7/7	0.93	0.32	87,87,87,87	0
84	MG	1	3615	1/1	0.93	0.16	31,31,31,31	0
84	MG	1	3551	1/1	0.93	0.36	37,37,37,37	0
85	OHX	1	4023	7/7	0.93	0.27	109,109,109,109	0
85	OHX	2	2092	7/7	0.93	0.26	106,106,106,106	0
85	OHX	1	4025	7/7	0.93	0.37	101,101,101,101	0
84	MG	5	3686	1/1	0.93	0.11	44,44,44,44	0
84	MG	1	3446	1/1	0.93	0.18	47,47,47,47	0
85	OHX	2	2097	7/7	0.93	0.23	110,110,110,110	0
85	OHX	1	4031	7/7	0.93	0.19	102,102,102,102	0
85	OHX	5	4017	7/7	0.93	0.12	128,128,128,128	0
84	MG	6	1983	1/1	0.93	0.21	73,73,73,73	0
85	OHX	1	4033	7/7	0.93	0.23	100,100,100,100	0
84	MG	8	205	1/1	0.93	0.25	48,48,48,48	0
85	OHX	5	4023	7/7	0.93	0.31	89,89,89,89	0
84	MG	5	3689	1/1	0.93	0.08	30,30,30,30	0
85	OHX	5	4026	7/7	0.93	0.30	105,105,105,105	0
84	MG	1	3523	1/1	0.93	0.34	41,41,41,41	0
84	MG	5	3560	1/1	0.93	0.31	35,35,35,35	0
84	MG	M0	301	1/1	0.93	0.18	43,43,43,43	0
84	MG	1	3535	1/1	0.93	0.31	43,43,43,43	0
84	MG	M6	201	1/1	0.93	0.13	45,45,45,45	0
84	MG	5	3504	1/1	0.93	0.34	37,37,37,37	0
85	OHX	5	4042	7/7	0.93	0.29	100,100,100,100	0
85	OHX	4	227	7/7	0.93	0.37	85,85,85,85	0
85	OHX	4	228	7/7	0.93	0.32	85,85,85,85	0
84	MG	5	3569	1/1	0.93	0.46	29,29,29,29	0
84	MG	5	3700	1/1	0.93	0.09	38,38,38,38	0
85	OHX	4	231	7/7	0.93	0.25	103,103,103,103	0
84	MG	1	3430	1/1	0.93	0.20	36,36,36,36	0
84	MG	M7	203	1/1	0.93	0.29	38,38,38,38	0
85	OHX	5	4051	7/7	0.93	0.28	100,100,100,100	0
85	OHX	O9	101	7/7	0.93	0.40	77,77,77,77	0
84	MG	1	3537	1/1	0.93	0.25	33,33,33,33	0
85	OHX	6	2070	7/7	0.93	0.28	98,98,98,98	0
84	MG	5	3705	1/1	0.93	0.16	36,36,36,36	0
85	OHX	6	2079	7/7	0.93	0.16	110,110,110,110	0
84	MG	5	3706	1/1	0.93	0.26	37,37,37,37	0
85	OHX	6	2083	7/7	0.93	0.14	116,116,116,116	0
84	MG	1	3702	1/1	0.93	0.21	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2086	7/7	0.93	0.32	103,103,103,103	0
85	OHX	5	4064	7/7	0.93	0.34	90,90,90,90	0
84	MG	1	3490	1/1	0.93	0.20	42,42,42,42	0
84	MG	5	3711	1/1	0.93	0.11	32,32,32,32	0
85	OHX	6	2091	7/7	0.93	0.15	110,110,110,110	0
85	OHX	7	213	7/7	0.93	0.16	79,79,79,79	0
84	MG	5	3512	1/1	0.93	0.14	31,31,31,31	0
84	MG	5	3636	1/1	0.93	0.28	44,44,44,44	0
85	OHX	8	221	7/7	0.93	0.29	92,92,92,92	0
84	MG	1	3677	1/1	0.93	0.19	43,43,43,43	0
85	OHX	6	2101	7/7	0.93	0.22	105,105,105,105	0
84	MG	5	3465	1/1	0.93	0.12	41,41,41,41	0
84	MG	5	3716	1/1	0.93	0.22	29,29,29,29	0
84	MG	5	3419	1/1	0.93	0.11	41,41,41,41	0
85	OHX	l5	301	7/7	0.93	0.17	106,106,106,106	0
85	OHX	m0	302	7/7	0.93	0.22	88,88,88,88	0
85	OHX	m1	202	7/7	0.93	0.21	107,107,107,107	0
85	OHX	o9	101	7/7	0.93	0.26	87,87,87,87	0
84	MG	O3	201	1/1	0.93	0.12	42,42,42,42	0
84	MG	1	3452	1/1	0.93	0.36	38,38,38,38	0
85	OHX	SR	401	7/7	0.93	0.11	134,134,134,134	0
86	ZN	q2	501	1/1	0.93	0.20	64,64,64,64	0
85	OHX	6	2123	7/7	0.93	0.28	102,102,102,102	0
84	MG	5	3671	1/1	0.94	0.22	35,35,35,35	0
84	MG	L2	302	1/1	0.94	0.12	41,41,41,41	0
84	MG	1	3584	1/1	0.94	0.46	54,54,54,54	0
85	OHX	5	3839	7/7	0.94	0.17	84,84,84,84	0
84	MG	5	3454	1/1	0.94	0.26	37,37,37,37	0
84	MG	1	3573	1/1	0.94	0.47	33,33,33,33	0
85	OHX	5	3864	7/7	0.94	0.18	78,78,78,78	0
84	MG	6	1906	1/1	0.94	0.31	51,51,51,51	0
84	MG	1	3431	1/1	0.94	0.08	51,51,51,51	0
85	OHX	5	3886	7/7	0.94	0.20	82,82,82,82	0
85	OHX	1	4015	7/7	0.94	0.31	91,91,91,91	0
84	MG	3	209	1/1	0.94	0.07	74,74,74,74	0
84	MG	5	3626	1/1	0.94	0.24	33,33,33,33	0
85	OHX	5	3907	7/7	0.94	0.12	116,116,116,116	0
84	MG	M5	301	1/1	0.94	0.11	39,39,39,39	0
85	OHX	5	3914	7/7	0.94	0.21	93,93,93,93	0
84	MG	n8	201	1/1	0.94	0.30	50,50,50,50	0
84	MG	5	3741	1/1	0.94	0.22	54,54,54,54	0
84	MG	5	3683	1/1	0.94	0.11	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	1	3703	1/1	0.94	0.12	33,33,33,33	0
85	OHX	5	3940	7/7	0.94	0.21	99,99,99,99	0
84	MG	o3	201	1/1	0.94	0.18	49,49,49,49	0
85	OHX	1	4027	7/7	0.94	0.31	103,103,103,103	0
84	MG	5	3497	1/1	0.94	0.34	30,30,30,30	0
85	OHX	5	3947	7/7	0.94	0.33	79,79,79,79	0
85	OHX	5	3955	7/7	0.94	0.21	104,104,104,104	0
85	OHX	2	2008	7/7	0.94	0.14	105,105,105,105	0
85	OHX	2	2012	7/7	0.94	0.12	107,107,107,107	0
84	MG	6	1982	1/1	0.94	0.09	46,46,46,46	0
84	MG	1	3522	1/1	0.94	0.26	32,32,32,32	0
85	OHX	5	3964	7/7	0.94	0.29	106,106,106,106	0
85	OHX	5	3966	7/7	0.94	0.28	108,108,108,108	0
85	OHX	5	3967	7/7	0.94	0.13	116,116,116,116	0
84	MG	5	3545	1/1	0.94	0.34	30,30,30,30	0
85	OHX	5	3972	7/7	0.94	0.30	87,87,87,87	0
84	MG	5	3591	1/1	0.94	0.21	33,33,33,33	0
85	OHX	5	3975	7/7	0.94	0.36	85,85,85,85	0
85	OHX	1	3770	7/7	0.94	0.16	74,74,74,74	0
85	OHX	5	3977	7/7	0.94	0.38	70,70,70,70	0
85	OHX	1	3788	7/7	0.94	0.15	86,86,86,86	0
85	OHX	1	3806	7/7	0.94	0.14	92,92,92,92	0
85	OHX	1	3813	7/7	0.94	0.22	77,77,77,77	0
85	OHX	3	216	7/7	0.94	0.23	108,108,108,108	0
85	OHX	1	3820	7/7	0.94	0.14	87,87,87,87	0
85	OHX	2	2039	7/7	0.94	0.10	133,133,133,133	0
85	OHX	4	221	7/7	0.94	0.30	88,88,88,88	0
85	OHX	5	3987	7/7	0.94	0.38	81,81,81,81	0
85	OHX	1	3858	7/7	0.94	0.12	128,128,128,128	0
84	MG	s8	301	1/1	0.94	0.13	47,47,47,47	0
85	OHX	1	3865	7/7	0.94	0.20	93,93,93,93	0
85	OHX	1	3873	7/7	0.94	0.14	112,112,112,112	0
85	OHX	5	3993	7/7	0.94	0.24	101,101,101,101	0
85	OHX	5	3994	7/7	0.94	0.30	97,97,97,97	0
84	MG	5	3428	1/1	0.94	0.37	39,39,39,39	0
85	OHX	1	3881	7/7	0.94	0.28	87,87,87,87	0
85	OHX	5	3998	7/7	0.94	0.42	83,83,83,83	0
85	OHX	5	4000	7/7	0.94	0.19	106,106,106,106	0
84	MG	5	3594	1/1	0.94	0.07	40,40,40,40	0
85	OHX	5	4002	7/7	0.94	0.31	102,102,102,102	0
85	OHX	1	3888	7/7	0.94	0.28	85,85,85,85	0
84	MG	1	3441	1/1	0.94	0.20	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3903	7/7	0.94	0.23	77,77,77,77	0
84	MG	1	3690	1/1	0.94	0.17	48,48,48,48	0
85	OHX	1	3909	7/7	0.94	0.24	83,83,83,83	0
84	MG	5	3696	1/1	0.94	0.08	31,31,31,31	0
84	MG	6	1914	1/1	0.94	0.34	41,41,41,41	0
85	OHX	6	2081	7/7	0.94	0.17	110,110,110,110	0
85	OHX	1	3919	7/7	0.94	0.22	99,99,99,99	0
85	OHX	2	2061	7/7	0.94	0.15	115,115,115,115	0
85	OHX	2	2062	7/7	0.94	0.26	106,106,106,106	0
85	OHX	6	2087	7/7	0.94	0.30	109,109,109,109	0
84	MG	1	3725	1/1	0.94	0.31	52,52,52,52	0
85	OHX	6	2089	7/7	0.94	0.28	85,85,85,85	0
84	MG	5	3699	1/1	0.94	0.18	42,42,42,42	0
85	OHX	5	4027	7/7	0.94	0.29	92,92,92,92	0
85	OHX	1	3925	7/7	0.94	0.12	116,116,116,116	0
85	OHX	5	4030	7/7	0.94	0.37	89,89,89,89	0
85	OHX	2	2068	7/7	0.94	0.13	122,122,122,122	0
84	MG	1	3463	1/1	0.94	0.26	32,32,32,32	0
84	MG	1	3548	1/1	0.94	0.19	31,31,31,31	0
85	OHX	1	3932	7/7	0.94	0.39	71,71,71,71	0
85	OHX	1	3934	7/7	0.94	0.29	94,94,94,94	0
85	OHX	5	4041	7/7	0.94	0.33	96,96,96,96	0
84	MG	1	4041	1/1	0.94	0.22	41,41,41,41	0
85	OHX	6	2108	7/7	0.94	0.22	102,102,102,102	0
85	OHX	1	3936	7/7	0.94	0.20	98,98,98,98	0
85	OHX	1	3937	7/7	0.94	0.38	88,88,88,88	0
84	MG	2	1960	1/1	0.94	0.53	72,72,72,72	0
85	OHX	1	3941	7/7	0.94	0.26	107,107,107,107	0
85	OHX	6	2119	7/7	0.94	0.23	106,106,106,106	0
84	MG	5	3648	1/1	0.94	0.07	61,61,61,61	0
84	MG	5	3603	1/1	0.94	0.35	47,47,47,47	0
84	MG	5	3707	1/1	0.94	0.07	43,43,43,43	0
84	MG	5	3708	1/1	0.94	0.13	44,44,44,44	0
85	OHX	5	4054	7/7	0.94	0.31	87,87,87,87	0
84	MG	1	3711	1/1	0.94	0.14	46,46,46,46	0
84	MG	5	3516	1/1	0.94	0.28	31,31,31,31	0
85	OHX	5	4057	7/7	0.94	0.30	96,96,96,96	0
84	MG	5	3407	1/1	0.94	0.22	33,33,33,33	0
85	OHX	1	3965	7/7	0.94	0.14	109,109,109,109	0
84	MG	5	3653	1/1	0.94	0.12	67,67,67,67	0
85	OHX	2	2086	7/7	0.94	0.28	104,104,104,104	0
85	OHX	1	3972	7/7	0.94	0.33	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3654	1/1	0.94	0.12	42,42,42,42	0
84	MG	1	3607	1/1	0.94	0.24	42,42,42,42	0
85	OHX	5	4067	7/7	0.94	0.21	93,93,93,93	0
85	OHX	1	3976	7/7	0.94	0.27	91,91,91,91	0
85	OHX	1	3978	7/7	0.94	0.24	92,92,92,92	0
84	MG	5	3444	1/1	0.94	0.15	32,32,32,32	0
84	MG	5	3562	1/1	0.94	0.19	32,32,32,32	0
84	MG	1	3483	1/1	0.94	0.21	45,45,45,45	0
84	MG	5	3564	1/1	0.94	0.30	38,38,38,38	0
85	OHX	2	2094	7/7	0.94	0.20	108,108,108,108	0
84	MG	1	3594	1/1	0.94	0.24	48,48,48,48	0
85	OHX	1	3988	7/7	0.94	0.30	104,104,104,104	0
85	OHX	8	225	7/7	0.94	0.34	101,101,101,101	0
85	OHX	1	3989	7/7	0.94	0.31	104,104,104,104	0
84	MG	5	3523	1/1	0.94	0.22	27,27,27,27	0
84	MG	6	1997	1/1	0.94	0.24	63,63,63,63	0
84	MG	5	3570	1/1	0.94	0.22	31,31,31,31	0
84	MG	5	3448	1/1	0.94	0.24	28,28,28,28	0
85	OHX	1	3996	7/7	0.94	0.26	97,97,97,97	0
85	OHX	1	3997	7/7	0.94	0.35	82,82,82,82	0
85	OHX	s4	301	7/7	0.94	0.23	110,110,110,110	0
84	MG	m1	201	1/1	0.94	0.15	48,48,48,48	0
84	MG	2	1902	1/1	0.94	0.38	55,55,55,55	0
84	MG	1	3683	1/1	0.94	0.20	34,34,34,34	0
85	OHX	5	3852	7/7	0.95	0.20	71,71,71,71	0
85	OHX	1	4019	7/7	0.95	0.32	85,85,85,85	0
85	OHX	1	3872	7/7	0.95	0.20	98,98,98,98	0
85	OHX	5	3867	7/7	0.95	0.22	85,85,85,85	0
84	MG	5	3489	1/1	0.95	0.20	34,34,34,34	0
84	MG	5	3423	1/1	0.95	0.34	45,45,45,45	0
85	OHX	5	3878	7/7	0.95	0.16	80,80,80,80	0
85	OHX	5	3884	7/7	0.95	0.10	129,129,129,129	0
85	OHX	5	3885	7/7	0.95	0.26	92,92,92,92	0
85	OHX	1	3879	7/7	0.95	0.20	101,101,101,101	0
84	MG	5	3535	1/1	0.95	0.24	49,49,49,49	0
85	OHX	5	3895	7/7	0.95	0.28	76,76,76,76	0
85	OHX	1	4026	7/7	0.95	0.34	90,90,90,90	0
85	OHX	5	3905	7/7	0.95	0.27	93,93,93,93	0
84	MG	5	3670	1/1	0.95	0.28	35,35,35,35	0
84	MG	1	3511	1/1	0.95	0.43	39,39,39,39	0
84	MG	5	3719	1/1	0.95	0.07	32,32,32,32	0
85	OHX	5	3911	7/7	0.95	0.30	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3913	7/7	0.95	0.20	88,88,88,88	0
85	OHX	1	3897	7/7	0.95	0.14	109,109,109,109	0
85	OHX	1	3899	7/7	0.95	0.28	91,91,91,91	0
85	OHX	5	3930	7/7	0.95	0.35	75,75,75,75	0
84	MG	5	3425	1/1	0.95	0.07	31,31,31,31	0
85	OHX	5	3934	7/7	0.95	0.27	91,91,91,91	0
84	MG	1	3454	1/1	0.95	0.27	34,34,34,34	0
85	OHX	1	3906	7/7	0.95	0.30	85,85,85,85	0
84	MG	5	3496	1/1	0.95	0.28	56,56,56,56	0
85	OHX	5	3941	7/7	0.95	0.29	90,90,90,90	0
85	OHX	1	3912	7/7	0.95	0.13	110,110,110,110	0
84	MG	5	3675	1/1	0.95	0.30	59,59,59,59	0
85	OHX	1	3917	7/7	0.95	0.10	133,133,133,133	0
85	OHX	5	3946	7/7	0.95	0.21	100,100,100,100	0
84	MG	1	3603	1/1	0.95	0.28	38,38,38,38	0
85	OHX	5	3948	7/7	0.95	0.26	92,92,92,92	0
85	OHX	5	3950	7/7	0.95	0.30	101,101,101,101	0
85	OHX	5	3951	7/7	0.95	0.24	92,92,92,92	0
85	OHX	5	3952	7/7	0.95	0.32	77,77,77,77	0
85	OHX	5	3954	7/7	0.95	0.26	82,82,82,82	0
84	MG	6	1957	1/1	0.95	0.40	63,63,63,63	0
85	OHX	5	3957	7/7	0.95	0.27	84,84,84,84	0
84	MG	5	3630	1/1	0.95	0.10	31,31,31,31	0
84	MG	1	3572	1/1	0.95	0.29	33,33,33,33	0
85	OHX	5	3960	7/7	0.95	0.23	105,105,105,105	0
85	OHX	4	223	7/7	0.95	0.20	97,97,97,97	0
84	MG	5	3730	1/1	0.95	0.07	43,43,43,43	0
85	OHX	5	3963	7/7	0.95	0.17	108,108,108,108	0
84	MG	5	3430	1/1	0.95	0.20	33,33,33,33	0
84	MG	5	3681	1/1	0.95	0.25	40,40,40,40	0
84	MG	L6	201	1/1	0.95	0.09	48,48,48,48	0
85	OHX	5	3968	7/7	0.95	0.19	86,86,86,86	0
84	MG	1	3413	1/1	0.95	0.28	43,43,43,43	0
85	OHX	5	3970	7/7	0.95	0.33	90,90,90,90	0
84	MG	1	3710	1/1	0.95	0.18	40,40,40,40	0
85	OHX	L4	401	7/7	0.95	0.25	92,92,92,92	0
85	OHX	M0	302	7/7	0.95	0.16	86,86,86,86	0
84	MG	1	3403	1/1	0.95	0.38	51,51,51,51	0
84	MG	1	3644	1/1	0.95	0.22	41,41,41,41	0
84	MG	5	3639	1/1	0.95	0.15	40,40,40,40	0
85	OHX	6	2027	7/7	0.95	0.14	78,78,78,78	0
85	OHX	5	3981	7/7	0.95	0.27	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2040	7/7	0.95	0.14	89,89,89,89	0
85	OHX	6	2048	7/7	0.95	0.11	117,117,117,117	0
85	OHX	6	2054	7/7	0.95	0.21	84,84,84,84	0
85	OHX	6	2058	7/7	0.95	0.17	99,99,99,99	0
85	OHX	6	2063	7/7	0.95	0.10	134,134,134,134	0
84	MG	1	3426	1/1	0.95	0.47	50,50,50,50	0
85	OHX	6	2069	7/7	0.95	0.24	86,86,86,86	0
84	MG	1	3410	1/1	0.95	0.30	35,35,35,35	0
85	OHX	6	2074	7/7	0.95	0.16	106,106,106,106	0
85	OHX	1	3939	7/7	0.95	0.30	94,94,94,94	0
84	MG	1	3550	1/1	0.95	0.21	40,40,40,40	0
84	MG	5	3691	1/1	0.95	0.19	43,43,43,43	0
84	MG	1	3669	1/1	0.95	0.23	48,48,48,48	0
85	OHX	1	3945	7/7	0.95	0.09	162,162,162,162	0
84	MG	5	3513	1/1	0.95	0.27	32,32,32,32	0
84	MG	5	3514	1/1	0.95	0.31	30,30,30,30	0
84	MG	1	3648	1/1	0.95	0.25	37,37,37,37	0
84	MG	5	3558	1/1	0.95	0.34	37,37,37,37	0
85	OHX	1	3953	7/7	0.95	0.18	108,108,108,108	0
85	OHX	1	3954	7/7	0.95	0.31	96,96,96,96	0
84	MG	5	3475	1/1	0.95	0.38	32,32,32,32	0
85	OHX	1	3957	7/7	0.95	0.28	111,111,111,111	0
84	MG	o4	201	1/1	0.95	0.26	52,52,52,52	0
85	OHX	1	3962	7/7	0.95	0.19	101,101,101,101	0
85	OHX	6	2100	7/7	0.95	0.20	96,96,96,96	0
85	OHX	5	4015	7/7	0.95	0.26	98,98,98,98	0
85	OHX	1	3964	7/7	0.95	0.26	89,89,89,89	0
85	OHX	6	2102	7/7	0.95	0.25	104,104,104,104	0
84	MG	1	3480	1/1	0.95	0.23	36,36,36,36	0
85	OHX	1	3966	7/7	0.95	0.09	175,175,175,175	0
84	MG	q1	101	1/1	0.95	0.36	47,47,47,47	0
85	OHX	5	4022	7/7	0.95	0.30	94,94,94,94	0
85	OHX	2	1991	7/7	0.95	0.14	97,97,97,97	0
85	OHX	1	3970	7/7	0.95	0.25	94,94,94,94	0
85	OHX	6	2113	7/7	0.95	0.31	86,86,86,86	0
85	OHX	2	2000	7/7	0.95	0.12	89,89,89,89	0
85	OHX	5	4028	7/7	0.95	0.30	86,86,86,86	0
85	OHX	6	2115	7/7	0.95	0.17	106,106,106,106	0
85	OHX	2	2003	7/7	0.95	0.14	101,101,101,101	0
85	OHX	6	2118	7/7	0.95	0.21	109,109,109,109	0
85	OHX	5	4032	7/7	0.95	0.28	86,86,86,86	0
84	MG	1	3580	1/1	0.95	0.18	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2121	7/7	0.95	0.26	108,108,108,108	0
85	OHX	5	4037	7/7	0.95	0.29	89,89,89,89	0
85	OHX	6	2122	7/7	0.95	0.30	92,92,92,92	0
85	OHX	1	3975	7/7	0.95	0.32	85,85,85,85	0
85	OHX	6	2126	7/7	0.95	0.24	96,96,96,96	0
84	MG	6	1999	1/1	0.95	0.27	49,49,49,49	0
85	OHX	1	3977	7/7	0.95	0.26	98,98,98,98	0
84	MG	1	3465	1/1	0.95	0.16	42,42,42,42	0
85	OHX	1	3979	7/7	0.95	0.26	94,94,94,94	0
84	MG	1	3553	1/1	0.95	0.27	30,30,30,30	0
84	MG	5	3703	1/1	0.95	0.10	36,36,36,36	0
85	OHX	2	2032	7/7	0.95	0.10	121,121,121,121	0
85	OHX	5	4049	7/7	0.95	0.32	85,85,85,85	0
85	OHX	1	3983	7/7	0.95	0.29	78,78,78,78	0
84	MG	7	207	1/1	0.95	0.06	36,36,36,36	0
85	OHX	2	2037	7/7	0.95	0.21	106,106,106,106	0
84	MG	1	3509	1/1	0.95	0.23	33,33,33,33	0
85	OHX	1	3987	7/7	0.95	0.29	79,79,79,79	0
85	OHX	6	2140	7/7	0.95	0.25	101,101,101,101	0
84	MG	1	3700	1/1	0.95	0.25	36,36,36,36	0
85	OHX	2	2044	7/7	0.95	0.13	113,113,113,113	0
85	OHX	2	2045	7/7	0.95	0.21	90,90,90,90	0
85	OHX	5	4059	7/7	0.95	0.34	74,74,74,74	0
85	OHX	2	2047	7/7	0.95	0.20	101,101,101,101	0
85	OHX	2	2049	7/7	0.95	0.21	100,100,100,100	0
85	OHX	2	2050	7/7	0.95	0.32	102,102,102,102	0
85	OHX	6	2147	7/7	0.95	0.29	100,100,100,100	0
85	OHX	1	3994	7/7	0.95	0.32	92,92,92,92	0
85	OHX	1	3995	7/7	0.95	0.14	86,86,86,86	0
84	MG	1	3654	1/1	0.95	0.13	45,45,45,45	0
85	OHX	1	3799	7/7	0.95	0.12	88,88,88,88	0
85	OHX	5	4069	7/7	0.95	0.11	129,129,129,129	0
85	OHX	6	2152	7/7	0.95	0.21	107,107,107,107	0
85	OHX	1	3800	7/7	0.95	0.13	88,88,88,88	0
85	OHX	7	218	7/7	0.95	0.28	92,92,92,92	0
84	MG	5	3526	1/1	0.95	0.30	38,38,38,38	0
85	OHX	1	3810	7/7	0.95	0.12	99,99,99,99	0
85	OHX	8	218	7/7	0.95	0.30	79,79,79,79	0
84	MG	1	3428	1/1	0.95	0.26	48,48,48,48	0
84	MG	5	3453	1/1	0.95	0.10	42,42,42,42	0
85	OHX	1	3826	7/7	0.95	0.13	93,93,93,93	0
85	OHX	1	3828	7/7	0.95	0.12	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	4011	7/7	0.95	0.25	100,100,100,100	0
85	OHX	1	3837	7/7	0.95	0.20	71,71,71,71	0
84	MG	1	3636	1/1	0.95	0.27	46,46,46,46	0
85	OHX	1	3856	7/7	0.95	0.16	107,107,107,107	0
85	OHX	l5	302	7/7	0.95	0.20	107,107,107,107	0
85	OHX	l9	202	7/7	0.95	0.19	92,92,92,92	0
85	OHX	m0	301	7/7	0.95	0.14	109,109,109,109	0
85	OHX	c8	201	7/7	0.95	0.12	117,117,117,117	0
84	MG	5	3530	1/1	0.95	0.26	41,41,41,41	0
85	OHX	m7	204	7/7	0.95	0.34	84,84,84,84	0
84	MG	1	3617	1/1	0.95	0.13	43,43,43,43	0
85	OHX	5	3819	7/7	0.95	0.14	78,78,78,78	0
86	ZN	Q2	501	1/1	0.95	0.17	64,64,64,64	0
85	OHX	5	3838	7/7	0.95	0.15	101,101,101,101	0
84	MG	1	4042	1/1	0.95	0.08	45,45,45,45	0
85	OHX	5	3843	7/7	0.95	0.14	91,91,91,91	0
85	OHX	1	3869	7/7	0.95	0.20	91,91,91,91	0
85	OHX	1	3822	7/7	0.96	0.11	95,95,95,95	0
85	OHX	5	3933	7/7	0.96	0.30	77,77,77,77	0
85	OHX	1	3823	7/7	0.96	0.18	73,73,73,73	0
85	OHX	5	3935	7/7	0.96	0.18	92,92,92,92	0
85	OHX	5	3936	7/7	0.96	0.25	98,98,98,98	0
85	OHX	6	2072	7/7	0.96	0.22	92,92,92,92	0
85	OHX	1	3968	7/7	0.96	0.28	86,86,86,86	0
85	OHX	6	2075	7/7	0.96	0.23	96,96,96,96	0
85	OHX	2	2016	7/7	0.96	0.20	108,108,108,108	0
85	OHX	5	3942	7/7	0.96	0.22	98,98,98,98	0
85	OHX	2	2081	7/7	0.96	0.22	109,109,109,109	0
85	OHX	1	3971	7/7	0.96	0.32	98,98,98,98	0
85	OHX	1	3835	7/7	0.96	0.16	85,85,85,85	0
85	OHX	2	2017	7/7	0.96	0.14	89,89,89,89	0
85	OHX	1	3840	7/7	0.96	0.17	82,82,82,82	0
85	OHX	6	2085	7/7	0.96	0.22	78,78,78,78	0
85	OHX	1	3843	7/7	0.96	0.24	79,79,79,79	0
85	OHX	1	3847	7/7	0.96	0.20	91,91,91,91	0
85	OHX	2	2021	7/7	0.96	0.19	99,99,99,99	0
85	OHX	2	2022	7/7	0.96	0.12	107,107,107,107	0
85	OHX	2	2023	7/7	0.96	0.27	90,90,90,90	0
85	OHX	5	3956	7/7	0.96	0.31	76,76,76,76	0
85	OHX	1	3862	7/7	0.96	0.23	74,74,74,74	0
84	MG	1	3555	1/1	0.96	0.22	35,35,35,35	0
84	MG	5	3661	1/1	0.96	0.14	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2096	7/7	0.96	0.21	100,100,100,100	0
85	OHX	6	2097	7/7	0.96	0.16	103,103,103,103	0
85	OHX	1	3868	7/7	0.96	0.22	83,83,83,83	0
84	MG	5	3580	1/1	0.96	0.42	37,37,37,37	0
85	OHX	1	3870	7/7	0.96	0.22	97,97,97,97	0
85	OHX	5	3965	7/7	0.96	0.30	88,88,88,88	0
85	OHX	1	3871	7/7	0.96	0.21	100,100,100,100	0
85	OHX	2	2028	7/7	0.96	0.19	94,94,94,94	0
85	OHX	6	2104	7/7	0.96	0.26	103,103,103,103	0
85	OHX	2	2029	7/7	0.96	0.12	108,108,108,108	0
85	OHX	6	2106	7/7	0.96	0.25	96,96,96,96	0
85	OHX	6	2107	7/7	0.96	0.23	99,99,99,99	0
85	OHX	1	3875	7/7	0.96	0.20	100,100,100,100	0
85	OHX	5	3974	7/7	0.96	0.26	89,89,89,89	0
85	OHX	6	2109	7/7	0.96	0.24	84,84,84,84	0
85	OHX	2	2030	7/7	0.96	0.22	103,103,103,103	0
84	MG	M7	202	1/1	0.96	0.31	41,41,41,41	0
84	MG	5	3412	1/1	0.96	0.27	39,39,39,39	0
85	OHX	2	2095	7/7	0.96	0.29	96,96,96,96	0
85	OHX	1	3886	7/7	0.96	0.20	101,101,101,101	0
85	OHX	2	2035	7/7	0.96	0.17	95,95,95,95	0
85	OHX	6	2117	7/7	0.96	0.21	86,86,86,86	0
85	OHX	2	2036	7/7	0.96	0.14	103,103,103,103	0
85	OHX	1	3890	7/7	0.96	0.18	102,102,102,102	0
85	OHX	1	3894	7/7	0.96	0.11	114,114,114,114	0
85	OHX	1	3896	7/7	0.96	0.23	88,88,88,88	0
85	OHX	1	4001	7/7	0.96	0.19	108,108,108,108	0
85	OHX	6	2124	7/7	0.96	0.22	89,89,89,89	0
84	MG	1	3473	1/1	0.96	0.32	45,45,45,45	0
85	OHX	5	3991	7/7	0.96	0.28	87,87,87,87	0
85	OHX	1	3898	7/7	0.96	0.28	85,85,85,85	0
85	OHX	1	4004	7/7	0.96	0.31	85,85,85,85	0
85	OHX	2	2038	7/7	0.96	0.27	93,93,93,93	0
85	OHX	5	3995	7/7	0.96	0.27	80,80,80,80	0
84	MG	1	3504	1/1	0.96	0.26	40,40,40,40	0
84	MG	5	3431	1/1	0.96	0.20	37,37,37,37	0
85	OHX	2	2041	7/7	0.96	0.10	119,119,119,119	0
85	OHX	2	2042	7/7	0.96	0.11	110,110,110,110	0
85	OHX	1	3910	7/7	0.96	0.23	84,84,84,84	0
85	OHX	1	3911	7/7	0.96	0.19	103,103,103,103	0
85	OHX	5	4003	7/7	0.96	0.22	86,86,86,86	0
84	MG	5	3586	1/1	0.96	0.19	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
84	MG	5	3726	1/1	0.96	0.09	33,33,33,33	0
85	OHX	5	4006	7/7	0.96	0.32	89,89,89,89	0
85	OHX	5	4007	7/7	0.96	0.30	63,63,63,63	0
85	OHX	6	2138	7/7	0.96	0.25	77,77,77,77	0
85	OHX	1	3915	7/7	0.96	0.28	69,69,69,69	0
85	OHX	1	3916	7/7	0.96	0.29	87,87,87,87	0
85	OHX	5	4012	7/7	0.96	0.26	89,89,89,89	0
85	OHX	2	2046	7/7	0.96	0.18	105,105,105,105	0
84	MG	5	3432	1/1	0.96	0.20	31,31,31,31	0
84	MG	5	3536	1/1	0.96	0.43	46,46,46,46	0
85	OHX	1	4022	7/7	0.96	0.37	77,77,77,77	0
84	MG	5	3729	1/1	0.96	0.26	52,52,52,52	0
84	MG	1	3499	1/1	0.96	0.34	39,39,39,39	0
85	OHX	2	2054	7/7	0.96	0.10	122,122,122,122	0
84	MG	1	3675	1/1	0.96	0.12	41,41,41,41	0
85	OHX	5	4021	7/7	0.96	0.32	82,82,82,82	0
85	OHX	2	2056	7/7	0.96	0.10	127,127,127,127	0
85	OHX	1	3926	7/7	0.96	0.32	81,81,81,81	0
85	OHX	1	3927	7/7	0.96	0.28	92,92,92,92	0
85	OHX	5	4025	7/7	0.96	0.32	93,93,93,93	0
85	OHX	1	3928	7/7	0.96	0.23	95,95,95,95	0
84	MG	N8	202	1/1	0.96	0.08	35,35,35,35	0
84	MG	1	3676	1/1	0.96	0.19	48,48,48,48	0
84	MG	5	3495	1/1	0.96	0.23	35,35,35,35	0
84	MG	5	3519	1/1	0.96	0.41	34,34,34,34	0
85	OHX	1	3933	7/7	0.96	0.14	92,92,92,92	0
84	MG	5	3568	1/1	0.96	0.36	35,35,35,35	0
84	MG	1	3421	1/1	0.96	0.29	41,41,41,41	0
84	MG	1	3560	1/1	0.96	0.28	40,40,40,40	0
85	OHX	3	212	7/7	0.96	0.15	81,81,81,81	0
85	OHX	5	4038	7/7	0.96	0.27	91,91,91,91	0
85	OHX	3	215	7/7	0.96	0.16	98,98,98,98	0
85	OHX	2	2066	7/7	0.96	0.19	93,93,93,93	0
84	MG	2	1903	1/1	0.96	0.40	55,55,55,55	0
84	MG	1	3632	1/1	0.96	0.12	50,50,50,50	0
85	OHX	C8	201	7/7	0.96	0.10	97,97,97,97	0
85	OHX	5	3799	7/7	0.96	0.13	82,82,82,82	0
85	OHX	5	3802	7/7	0.96	0.14	70,70,70,70	0
85	OHX	5	3818	7/7	0.96	0.10	90,90,90,90	0
85	OHX	4	222	7/7	0.96	0.26	83,83,83,83	0
85	OHX	5	3837	7/7	0.96	0.27	72,72,72,72	0
85	OHX	1	3942	7/7	0.96	0.25	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	2	2069	7/7	0.96	0.11	112,112,112,112	0
85	OHX	2	2070	7/7	0.96	0.24	95,95,95,95	0
84	MG	1	3497	1/1	0.96	0.39	33,33,33,33	0
85	OHX	1	3947	7/7	0.96	0.23	85,85,85,85	0
85	OHX	1	3780	7/7	0.96	0.11	100,100,100,100	0
84	MG	1	3546	1/1	0.96	0.19	36,36,36,36	0
85	OHX	L3	402	7/7	0.96	0.29	86,86,86,86	0
85	OHX	5	3869	7/7	0.96	0.17	79,79,79,79	0
85	OHX	1	3795	7/7	0.96	0.13	83,83,83,83	0
85	OHX	2	2074	7/7	0.96	0.23	101,101,101,101	0
85	OHX	5	3873	7/7	0.96	0.22	68,68,68,68	0
85	OHX	5	3874	7/7	0.96	0.17	87,87,87,87	0
85	OHX	5	3876	7/7	0.96	0.31	76,76,76,76	0
85	OHX	M7	205	7/7	0.96	0.23	101,101,101,101	0
85	OHX	5	3879	7/7	0.96	0.15	103,103,103,103	0
85	OHX	5	4065	7/7	0.96	0.13	92,92,92,92	0
85	OHX	5	3880	7/7	0.96	0.18	91,91,91,91	0
85	OHX	5	3881	7/7	0.96	0.10	106,106,106,106	0
84	MG	5	3656	1/1	0.96	0.06	36,36,36,36	0
84	MG	5	3502	1/1	0.96	0.35	32,32,32,32	0
85	OHX	O3	202	7/7	0.96	0.32	85,85,85,85	0
85	OHX	5	3891	7/7	0.96	0.21	84,84,84,84	0
85	OHX	7	217	7/7	0.96	0.16	95,95,95,95	0
85	OHX	5	3893	7/7	0.96	0.10	111,111,111,111	0
85	OHX	7	219	7/7	0.96	0.26	80,80,80,80	0
85	OHX	1	3956	7/7	0.96	0.22	100,100,100,100	0
85	OHX	1	3807	7/7	0.96	0.14	76,76,76,76	0
85	OHX	8	215	7/7	0.96	0.14	94,94,94,94	0
85	OHX	8	217	7/7	0.96	0.17	101,101,101,101	0
85	OHX	5	3896	7/7	0.96	0.21	77,77,77,77	0
85	OHX	8	219	7/7	0.96	0.25	90,90,90,90	0
85	OHX	6	2036	7/7	0.96	0.11	110,110,110,110	0
85	OHX	5	3901	7/7	0.96	0.15	110,110,110,110	0
85	OHX	5	3903	7/7	0.96	0.11	110,110,110,110	0
85	OHX	5	3904	7/7	0.96	0.22	76,76,76,76	0
85	OHX	1	3958	7/7	0.96	0.29	84,84,84,84	0
85	OHX	l3	407	7/7	0.96	0.24	78,78,78,78	0
84	MG	5	3443	1/1	0.96	0.13	38,38,38,38	0
85	OHX	l4	401	7/7	0.96	0.21	96,96,96,96	0
85	OHX	1	3961	7/7	0.96	0.21	104,104,104,104	0
85	OHX	6	2057	7/7	0.96	0.10	108,108,108,108	0
85	OHX	5	3910	7/7	0.96	0.14	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3812	7/7	0.96	0.14	88,88,88,88	0
85	OHX	5	3912	7/7	0.96	0.20	108,108,108,108	0
85	OHX	6	2061	7/7	0.96	0.18	98,98,98,98	0
85	OHX	6	2062	7/7	0.96	0.10	126,126,126,126	0
85	OHX	5	3916	7/7	0.96	0.27	85,85,85,85	0
85	OHX	5	3918	7/7	0.96	0.31	84,84,84,84	0
84	MG	1	3602	1/1	0.96	0.35	41,41,41,41	0
85	OHX	5	3921	7/7	0.96	0.25	95,95,95,95	0
85	OHX	5	3922	7/7	0.96	0.17	97,97,97,97	0
85	OHX	5	3926	7/7	0.96	0.15	104,104,104,104	0
85	OHX	5	3928	7/7	0.96	0.20	91,91,91,91	0
85	OHX	2	2015	7/7	0.96	0.13	106,106,106,106	0
85	OHX	1	3829	7/7	0.97	0.17	82,82,82,82	0
85	OHX	5	3939	7/7	0.97	0.26	83,83,83,83	0
85	OHX	1	3833	7/7	0.97	0.22	78,78,78,78	0
85	OHX	2	2064	7/7	0.97	0.19	92,92,92,92	0
85	OHX	1	3836	7/7	0.97	0.20	83,83,83,83	0
85	OHX	2	2065	7/7	0.97	0.20	104,104,104,104	0
85	OHX	1	3839	7/7	0.97	0.19	80,80,80,80	0
84	MG	6	1989	1/1	0.97	0.11	74,74,74,74	0
85	OHX	1	3842	7/7	0.97	0.13	96,96,96,96	0
84	MG	5	3510	1/1	0.97	0.29	36,36,36,36	0
85	OHX	1	3844	7/7	0.97	0.20	71,71,71,71	0
85	OHX	1	3845	7/7	0.97	0.28	77,77,77,77	0
85	OHX	6	2120	7/7	0.97	0.22	85,85,85,85	0
85	OHX	1	3938	7/7	0.97	0.26	92,92,92,92	0
85	OHX	5	3953	7/7	0.97	0.20	81,81,81,81	0
85	OHX	1	3846	7/7	0.97	0.18	97,97,97,97	0
84	MG	5	3539	1/1	0.97	0.27	29,29,29,29	0
85	OHX	1	3849	7/7	0.97	0.18	80,80,80,80	0
85	OHX	6	2125	7/7	0.97	0.24	87,87,87,87	0
85	OHX	1	3850	7/7	0.97	0.29	83,83,83,83	0
85	OHX	1	3851	7/7	0.97	0.26	82,82,82,82	0
85	OHX	1	3944	7/7	0.97	0.18	100,100,100,100	0
85	OHX	1	3852	7/7	0.97	0.10	110,110,110,110	0
84	MG	1	3420	1/1	0.97	0.08	38,38,38,38	0
84	MG	1	3547	1/1	0.97	0.32	33,33,33,33	0
84	MG	5	3590	1/1	0.97	0.18	34,34,34,34	0
85	OHX	1	3859	7/7	0.97	0.10	119,119,119,119	0
85	OHX	1	3951	7/7	0.97	0.28	81,81,81,81	0
85	OHX	3	213	7/7	0.97	0.15	97,97,97,97	0
85	OHX	3	214	7/7	0.97	0.17	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3860	7/7	0.97	0.25	82,82,82,82	0
85	OHX	2	2072	7/7	0.97	0.23	106,106,106,106	0
85	OHX	5	3971	7/7	0.97	0.23	94,94,94,94	0
85	OHX	3	217	7/7	0.97	0.29	85,85,85,85	0
85	OHX	1	3863	7/7	0.97	0.15	95,95,95,95	0
85	OHX	2	2033	7/7	0.97	0.26	94,94,94,94	0
85	OHX	4	218	7/7	0.97	0.19	77,77,77,77	0
85	OHX	4	219	7/7	0.97	0.11	93,93,93,93	0
85	OHX	4	220	7/7	0.97	0.17	96,96,96,96	0
84	MG	5	3664	1/1	0.97	0.12	53,53,53,53	0
85	OHX	5	3979	7/7	0.97	0.23	85,85,85,85	0
85	OHX	1	3866	7/7	0.97	0.22	91,91,91,91	0
85	OHX	1	3867	7/7	0.97	0.22	75,75,75,75	0
85	OHX	4	224	7/7	0.97	0.26	82,82,82,82	0
85	OHX	1	3959	7/7	0.97	0.25	84,84,84,84	0
84	MG	1	3606	1/1	0.97	0.21	34,34,34,34	0
85	OHX	2	1985	7/7	0.97	0.14	84,84,84,84	0
85	OHX	2	1988	7/7	0.97	0.12	90,90,90,90	0
85	OHX	2	1990	7/7	0.97	0.12	95,95,95,95	0
84	MG	1	3625	1/1	0.97	0.32	63,63,63,63	0
85	OHX	2	1993	7/7	0.97	0.11	99,99,99,99	0
85	OHX	L3	403	7/7	0.97	0.20	86,86,86,86	0
85	OHX	2	1995	7/7	0.97	0.10	91,91,91,91	0
85	OHX	2	1997	7/7	0.97	0.11	115,115,115,115	0
85	OHX	M5	302	7/7	0.97	0.21	88,88,88,88	0
85	OHX	2	1998	7/7	0.97	0.11	89,89,89,89	0
84	MG	1	3591	1/1	0.97	0.08	44,44,44,44	0
85	OHX	1	3882	7/7	0.97	0.19	90,90,90,90	0
85	OHX	1	3883	7/7	0.97	0.17	106,106,106,106	0
84	MG	1	3513	1/1	0.97	0.38	38,38,38,38	0
85	OHX	5	3999	7/7	0.97	0.29	76,76,76,76	0
85	OHX	2	2005	7/7	0.97	0.14	94,94,94,94	0
85	OHX	6	2032	7/7	0.97	0.10	87,87,87,87	0
85	OHX	5	3770	7/7	0.97	0.12	63,63,63,63	0
85	OHX	5	3784	7/7	0.97	0.12	70,70,70,70	0
85	OHX	5	3786	7/7	0.97	0.11	75,75,75,75	0
85	OHX	5	3788	7/7	0.97	0.09	78,78,78,78	0
85	OHX	5	3795	7/7	0.97	0.13	104,104,104,104	0
85	OHX	5	3796	7/7	0.97	0.11	89,89,89,89	0
85	OHX	6	2033	7/7	0.97	0.15	74,74,74,74	0
85	OHX	5	3800	7/7	0.97	0.11	78,78,78,78	0
85	OHX	1	3887	7/7	0.97	0.13	99,99,99,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3810	7/7	0.97	0.11	87,87,87,87	0
85	OHX	5	3816	7/7	0.97	0.18	66,66,66,66	0
85	OHX	5	3817	7/7	0.97	0.14	67,67,67,67	0
85	OHX	6	2037	7/7	0.97	0.09	112,112,112,112	0
85	OHX	1	3756	7/7	0.97	0.10	68,68,68,68	0
85	OHX	5	3821	7/7	0.97	0.11	74,74,74,74	0
85	OHX	5	3824	7/7	0.97	0.14	82,82,82,82	0
85	OHX	5	3827	7/7	0.97	0.20	76,76,76,76	0
85	OHX	5	3832	7/7	0.97	0.09	103,103,103,103	0
85	OHX	5	3836	7/7	0.97	0.15	81,81,81,81	0
85	OHX	6	2042	7/7	0.97	0.15	100,100,100,100	0
85	OHX	6	2047	7/7	0.97	0.11	91,91,91,91	0
85	OHX	1	3765	7/7	0.97	0.11	79,79,79,79	0
85	OHX	5	3840	7/7	0.97	0.22	73,73,73,73	0
85	OHX	6	2049	7/7	0.97	0.16	85,85,85,85	0
85	OHX	5	3845	7/7	0.97	0.11	87,87,87,87	0
85	OHX	5	3846	7/7	0.97	0.24	58,58,58,58	0
85	OHX	6	2051	7/7	0.97	0.12	93,93,93,93	0
85	OHX	5	3850	7/7	0.97	0.10	107,107,107,107	0
85	OHX	6	2052	7/7	0.97	0.10	110,110,110,110	0
85	OHX	5	3854	7/7	0.97	0.24	80,80,80,80	0
85	OHX	5	3855	7/7	0.97	0.24	83,83,83,83	0
85	OHX	5	3856	7/7	0.97	0.08	120,120,120,120	0
85	OHX	5	4036	7/7	0.97	0.24	82,82,82,82	0
85	OHX	5	3857	7/7	0.97	0.21	71,71,71,71	0
85	OHX	5	3858	7/7	0.97	0.23	82,82,82,82	0
85	OHX	2	2048	7/7	0.97	0.20	87,87,87,87	0
85	OHX	5	3862	7/7	0.97	0.27	77,77,77,77	0
85	OHX	1	3891	7/7	0.97	0.26	81,81,81,81	0
85	OHX	5	3866	7/7	0.97	0.19	87,87,87,87	0
85	OHX	1	3892	7/7	0.97	0.22	95,95,95,95	0
85	OHX	6	2059	7/7	0.97	0.11	106,106,106,106	0
85	OHX	6	2060	7/7	0.97	0.07	138,138,138,138	0
85	OHX	1	3893	7/7	0.97	0.28	81,81,81,81	0
85	OHX	1	3776	7/7	0.97	0.15	69,69,69,69	0
85	OHX	1	3778	7/7	0.97	0.11	84,84,84,84	0
85	OHX	5	3875	7/7	0.97	0.11	112,112,112,112	0
85	OHX	6	2064	7/7	0.97	0.08	141,141,141,141	0
85	OHX	6	2065	7/7	0.97	0.12	94,94,94,94	0
85	OHX	6	2067	7/7	0.97	0.16	98,98,98,98	0
84	MG	3	220	1/1	0.97	0.16	46,46,46,46	0
85	OHX	1	3781	7/7	0.97	0.14	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3883	7/7	0.97	0.20	91,91,91,91	0
85	OHX	1	3783	7/7	0.97	0.13	70,70,70,70	0
85	OHX	1	3900	7/7	0.97	0.25	83,83,83,83	0
85	OHX	6	2073	7/7	0.97	0.25	86,86,86,86	0
85	OHX	5	3887	7/7	0.97	0.23	72,72,72,72	0
85	OHX	5	3889	7/7	0.97	0.24	72,72,72,72	0
85	OHX	5	3890	7/7	0.97	0.20	97,97,97,97	0
85	OHX	1	3901	7/7	0.97	0.15	106,106,106,106	0
85	OHX	1	3902	7/7	0.97	0.25	88,88,88,88	0
85	OHX	1	3784	7/7	0.97	0.10	77,77,77,77	0
85	OHX	6	2078	7/7	0.97	0.22	98,98,98,98	0
85	OHX	2	2009	7/7	0.97	0.15	95,95,95,95	0
85	OHX	2	2051	7/7	0.97	0.26	93,93,93,93	0
85	OHX	5	3899	7/7	0.97	0.26	80,80,80,80	0
85	OHX	5	3900	7/7	0.97	0.17	103,103,103,103	0
85	OHX	1	3907	7/7	0.97	0.20	96,96,96,96	0
85	OHX	5	3902	7/7	0.97	0.24	87,87,87,87	0
85	OHX	1	3797	7/7	0.97	0.11	76,76,76,76	0
84	MG	6	1974	1/1	0.97	0.06	50,50,50,50	0
85	OHX	2	2053	7/7	0.97	0.08	130,130,130,130	0
85	OHX	2	2013	7/7	0.97	0.19	105,105,105,105	0
85	OHX	1	3913	7/7	0.97	0.28	70,70,70,70	0
85	OHX	8	212	7/7	0.97	0.11	91,91,91,91	0
85	OHX	8	213	7/7	0.97	0.19	83,83,83,83	0
85	OHX	5	3908	7/7	0.97	0.25	84,84,84,84	0
85	OHX	8	216	7/7	0.97	0.27	86,86,86,86	0
85	OHX	1	3999	7/7	0.97	0.24	82,82,82,82	0
85	OHX	2	2014	7/7	0.97	0.18	89,89,89,89	0
85	OHX	1	3809	7/7	0.97	0.10	107,107,107,107	0
85	OHX	8	220	7/7	0.97	0.09	120,120,120,120	0
84	MG	5	3579	1/1	0.97	0.37	32,32,32,32	0
85	OHX	6	2092	7/7	0.97	0.18	96,96,96,96	0
84	MG	1	3657	1/1	0.97	0.33	50,50,50,50	0
85	OHX	5	3915	7/7	0.97	0.22	91,91,91,91	0
85	OHX	6	2094	7/7	0.97	0.20	96,96,96,96	0
85	OHX	5	3917	7/7	0.97	0.24	86,86,86,86	0
84	MG	5	3506	1/1	0.97	0.46	47,47,47,47	0
85	OHX	1	4005	7/7	0.97	0.24	95,95,95,95	0
85	OHX	1	3816	7/7	0.97	0.14	84,84,84,84	0
85	OHX	1	3817	7/7	0.97	0.18	75,75,75,75	0
85	OHX	5	3923	7/7	0.97	0.23	85,85,85,85	0
85	OHX	5	3924	7/7	0.97	0.27	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3925	7/7	0.97	0.25	81,81,81,81	0
85	OHX	6	2099	7/7	0.97	0.27	95,95,95,95	0
85	OHX	5	3927	7/7	0.97	0.18	87,87,87,87	0
85	OHX	m5	304	7/7	0.97	0.12	74,74,74,74	0
85	OHX	1	4008	7/7	0.97	0.20	82,82,82,82	0
85	OHX	1	4009	7/7	0.97	0.23	83,83,83,83	0
85	OHX	q2	502	7/7	0.97	0.17	61,61,61,61	0
85	OHX	2	2018	7/7	0.97	0.14	106,106,106,106	0
86	ZN	E1	501	1/1	0.97	0.05	115,115,115,115	0
84	MG	5	3731	1/1	0.97	0.21	37,37,37,37	0
84	MG	1	3576	1/1	0.97	0.47	28,28,28,28	0
85	OHX	1	3924	7/7	0.97	0.25	76,76,76,76	0
84	MG	1	3716	1/1	0.97	0.07	33,33,33,33	0
84	MG	5	3567	1/1	0.97	0.38	30,30,30,30	0
85	OHX	2	1999	7/7	0.98	0.10	84,84,84,84	0
85	OHX	5	3841	7/7	0.98	0.08	97,97,97,97	0
85	OHX	5	3842	7/7	0.98	0.11	91,91,91,91	0
85	OHX	1	3777	7/7	0.98	0.09	84,84,84,84	0
85	OHX	5	3844	7/7	0.98	0.15	70,70,70,70	0
85	OHX	2	2031	7/7	0.98	0.17	95,95,95,95	0
84	MG	1	3686	1/1	0.98	0.07	37,37,37,37	0
85	OHX	2	2002	7/7	0.98	0.09	84,84,84,84	0
85	OHX	1	3848	7/7	0.98	0.15	90,90,90,90	0
84	MG	sM	202	1/1	0.98	0.08	43,43,43,43	0
85	OHX	5	3853	7/7	0.98	0.11	83,83,83,83	0
84	MG	5	3494	1/1	0.98	0.34	30,30,30,30	0
85	OHX	1	3786	7/7	0.98	0.09	101,101,101,101	0
85	OHX	2	2020	7/7	0.98	0.10	103,103,103,103	0
85	OHX	4	226	7/7	0.98	0.15	106,106,106,106	0
85	OHX	1	3853	7/7	0.98	0.14	93,93,93,93	0
85	OHX	5	3859	7/7	0.98	0.17	81,81,81,81	0
85	OHX	1	3854	7/7	0.98	0.18	74,74,74,74	0
85	OHX	5	3861	7/7	0.98	0.09	103,103,103,103	0
85	OHX	1	3789	7/7	0.98	0.10	88,88,88,88	0
85	OHX	5	3863	7/7	0.98	0.24	86,86,86,86	0
85	OHX	1	3792	7/7	0.98	0.13	80,80,80,80	0
85	OHX	1	3857	7/7	0.98	0.21	79,79,79,79	0
85	OHX	1	3793	7/7	0.98	0.08	89,89,89,89	0
85	OHX	5	3868	7/7	0.98	0.09	96,96,96,96	0
85	OHX	2	2006	7/7	0.98	0.08	113,113,113,113	0
85	OHX	1	3796	7/7	0.98	0.09	79,79,79,79	0
85	OHX	6	2111	7/7	0.98	0.21	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3872	7/7	0.98	0.19	65,65,65,65	0
85	OHX	2	2007	7/7	0.98	0.12	94,94,94,94	0
85	OHX	1	3798	7/7	0.98	0.11	75,75,75,75	0
85	OHX	M6	202	7/7	0.98	0.19	80,80,80,80	0
85	OHX	2	2088	7/7	0.98	0.19	94,94,94,94	0
85	OHX	5	3877	7/7	0.98	0.19	80,80,80,80	0
85	OHX	2	1994	7/7	0.98	0.11	99,99,99,99	0
85	OHX	1	3801	7/7	0.98	0.12	81,81,81,81	0
85	OHX	1	3804	7/7	0.98	0.10	88,88,88,88	0
85	OHX	O7	104	7/7	0.98	0.12	77,77,77,77	0
85	OHX	5	3882	7/7	0.98	0.26	67,67,67,67	0
85	OHX	O7	105	7/7	0.98	0.18	76,76,76,76	0
85	OHX	1	3805	7/7	0.98	0.13	72,72,72,72	0
85	OHX	6	2010	7/7	0.98	0.15	73,73,73,73	0
85	OHX	6	2016	7/7	0.98	0.13	71,71,71,71	0
85	OHX	6	2017	7/7	0.98	0.09	85,85,85,85	0
85	OHX	5	3888	7/7	0.98	0.22	91,91,91,91	0
85	OHX	6	2022	7/7	0.98	0.09	87,87,87,87	0
85	OHX	2	2024	7/7	0.98	0.19	89,89,89,89	0
85	OHX	6	2028	7/7	0.98	0.10	89,89,89,89	0
85	OHX	5	3892	7/7	0.98	0.20	80,80,80,80	0
85	OHX	6	2029	7/7	0.98	0.11	110,110,110,110	0
85	OHX	6	2030	7/7	0.98	0.18	74,74,74,74	0
85	OHX	6	2031	7/7	0.98	0.15	76,76,76,76	0
85	OHX	2	1986	7/7	0.98	0.10	81,81,81,81	0
85	OHX	1	3808	7/7	0.98	0.12	93,93,93,93	0
85	OHX	5	3898	7/7	0.98	0.19	80,80,80,80	0
85	OHX	6	2034	7/7	0.98	0.08	91,91,91,91	0
85	OHX	5	4035	7/7	0.98	0.18	63,63,63,63	0
85	OHX	6	2035	7/7	0.98	0.20	71,71,71,71	0
85	OHX	2	2010	7/7	0.98	0.19	88,88,88,88	0
85	OHX	1	3742	7/7	0.98	0.10	65,65,65,65	0
85	OHX	6	2039	7/7	0.98	0.12	83,83,83,83	0
85	OHX	1	3874	7/7	0.98	0.18	91,91,91,91	0
85	OHX	6	2041	7/7	0.98	0.13	74,74,74,74	0
85	OHX	1	3811	7/7	0.98	0.11	78,78,78,78	0
85	OHX	6	2043	7/7	0.98	0.18	77,77,77,77	0
85	OHX	6	2044	7/7	0.98	0.14	81,81,81,81	0
85	OHX	6	2046	7/7	0.98	0.10	95,95,95,95	0
85	OHX	1	3876	7/7	0.98	0.23	86,86,86,86	0
85	OHX	1	3747	7/7	0.98	0.10	64,64,64,64	0
85	OHX	1	3878	7/7	0.98	0.18	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	6	2050	7/7	0.98	0.15	92,92,92,92	0
85	OHX	1	3750	7/7	0.98	0.11	76,76,76,76	0
85	OHX	1	3880	7/7	0.98	0.20	89,89,89,89	0
85	OHX	6	2053	7/7	0.98	0.17	84,84,84,84	0
85	OHX	1	3814	7/7	0.98	0.16	71,71,71,71	0
85	OHX	6	2055	7/7	0.98	0.10	95,95,95,95	0
85	OHX	6	2056	7/7	0.98	0.17	82,82,82,82	0
85	OHX	1	3751	7/7	0.98	0.10	67,67,67,67	0
85	OHX	1	3755	7/7	0.98	0.14	67,67,67,67	0
85	OHX	1	3819	7/7	0.98	0.09	90,90,90,90	0
85	OHX	1	3885	7/7	0.98	0.24	78,78,78,78	0
85	OHX	2	2011	7/7	0.98	0.18	98,98,98,98	0
85	OHX	1	3757	7/7	0.98	0.10	70,70,70,70	0
85	OHX	1	3759	7/7	0.98	0.11	79,79,79,79	0
85	OHX	1	3825	7/7	0.98	0.16	83,83,83,83	0
85	OHX	5	3929	7/7	0.98	0.20	76,76,76,76	0
85	OHX	1	3762	7/7	0.98	0.08	66,66,66,66	0
85	OHX	6	2066	7/7	0.98	0.17	83,83,83,83	0
85	OHX	1	3827	7/7	0.98	0.20	72,72,72,72	0
84	MG	1	3635	1/1	0.98	0.23	41,41,41,41	0
85	OHX	1	3767	7/7	0.98	0.09	69,69,69,69	0
85	OHX	1	3830	7/7	0.98	0.12	86,86,86,86	0
85	OHX	7	211	7/7	0.98	0.08	74,74,74,74	0
85	OHX	7	212	7/7	0.98	0.16	70,70,70,70	0
85	OHX	5	3773	7/7	0.98	0.12	64,64,64,64	0
85	OHX	7	214	7/7	0.98	0.17	71,71,71,71	0
85	OHX	7	215	7/7	0.98	0.10	82,82,82,82	0
85	OHX	7	216	7/7	0.98	0.13	87,87,87,87	0
85	OHX	5	3775	7/7	0.98	0.10	60,60,60,60	0
85	OHX	5	3783	7/7	0.98	0.08	77,77,77,77	0
85	OHX	6	2071	7/7	0.98	0.19	79,79,79,79	0
85	OHX	1	3895	7/7	0.98	0.23	70,70,70,70	0
85	OHX	5	3787	7/7	0.98	0.09	63,63,63,63	0
85	OHX	1	3963	7/7	0.98	0.23	88,88,88,88	0
85	OHX	5	3793	7/7	0.98	0.08	87,87,87,87	0
85	OHX	8	214	7/7	0.98	0.11	102,102,102,102	0
85	OHX	5	3794	7/7	0.98	0.10	69,69,69,69	0
85	OHX	1	3831	7/7	0.98	0.17	86,86,86,86	0
85	OHX	1	3832	7/7	0.98	0.21	75,75,75,75	0
85	OHX	6	2076	7/7	0.98	0.22	81,81,81,81	0
85	OHX	1	3768	7/7	0.98	0.08	83,83,83,83	0
85	OHX	1	3834	7/7	0.98	0.10	99,99,99,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3803	7/7	0.98	0.10	63,63,63,63	0
85	OHX	5	3804	7/7	0.98	0.12	63,63,63,63	0
85	OHX	5	3806	7/7	0.98	0.09	74,74,74,74	0
85	OHX	5	3807	7/7	0.98	0.10	74,74,74,74	0
85	OHX	5	3809	7/7	0.98	0.12	88,88,88,88	0
85	OHX	l3	406	7/7	0.98	0.16	79,79,79,79	0
85	OHX	1	3769	7/7	0.98	0.10	63,63,63,63	0
85	OHX	5	3813	7/7	0.98	0.10	81,81,81,81	0
85	OHX	2	1989	7/7	0.98	0.08	92,92,92,92	0
85	OHX	1	3771	7/7	0.98	0.10	76,76,76,76	0
85	OHX	6	2082	7/7	0.98	0.19	91,91,91,91	0
85	OHX	1	3838	7/7	0.98	0.24	68,68,68,68	0
85	OHX	5	3820	7/7	0.98	0.12	81,81,81,81	0
85	OHX	3	210	7/7	0.98	0.10	77,77,77,77	0
85	OHX	5	3822	7/7	0.98	0.18	64,64,64,64	0
85	OHX	5	3823	7/7	0.98	0.15	76,76,76,76	0
85	OHX	3	211	7/7	0.98	0.20	85,85,85,85	0
85	OHX	m5	305	7/7	0.98	0.18	94,94,94,94	0
85	OHX	1	3904	7/7	0.98	0.14	82,82,82,82	0
85	OHX	n3	203	7/7	0.98	0.20	76,76,76,76	0
85	OHX	o3	202	7/7	0.98	0.20	82,82,82,82	0
85	OHX	5	3828	7/7	0.98	0.22	73,73,73,73	0
85	OHX	5	3830	7/7	0.98	0.16	64,64,64,64	0
85	OHX	5	3831	7/7	0.98	0.13	77,77,77,77	0
85	OHX	1	3773	7/7	0.98	0.09	73,73,73,73	0
85	OHX	5	3834	7/7	0.98	0.13	79,79,79,79	0
86	ZN	d6	101	1/1	0.98	0.04	60,60,60,60	0
85	OHX	1	3774	7/7	0.98	0.09	74,74,74,74	0
85	OHX	1	3841	7/7	0.98	0.17	62,62,62,62	0
85	OHX	1	3908	7/7	0.98	0.16	103,103,103,103	0
85	OHX	1	3775	7/7	0.98	0.09	83,83,83,83	0
85	OHX	5	3847	7/7	0.99	0.15	67,67,67,67	0
85	OHX	5	3848	7/7	0.99	0.19	80,80,80,80	0
85	OHX	1	3746	7/7	0.99	0.07	65,65,65,65	0
85	OHX	2	1996	7/7	0.99	0.10	83,83,83,83	0
85	OHX	5	3851	7/7	0.99	0.10	52,52,52,52	0
85	OHX	1	3794	7/7	0.99	0.08	62,62,62,62	0
85	OHX	1	3748	7/7	0.99	0.09	72,72,72,72	0
85	OHX	1	3749	7/7	0.99	0.10	67,67,67,67	0
85	OHX	2	2004	7/7	0.99	0.09	86,86,86,86	0
85	OHX	2	1987	7/7	0.99	0.09	74,74,74,74	0
85	OHX	1	3753	7/7	0.99	0.07	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	1	3754	7/7	0.99	0.08	63,63,63,63	0
85	OHX	2	1992	7/7	0.99	0.07	89,89,89,89	0
85	OHX	1	3802	7/7	0.99	0.15	75,75,75,75	0
85	OHX	1	3803	7/7	0.99	0.18	74,74,74,74	0
85	OHX	N1	201	7/7	0.99	0.06	59,59,59,59	0
85	OHX	2	1984	7/7	0.99	0.10	78,78,78,78	0
85	OHX	N9	101	7/7	0.99	0.08	56,56,56,56	0
85	OHX	5	3865	7/7	0.99	0.12	87,87,87,87	0
85	OHX	2	2043	7/7	0.99	0.18	89,89,89,89	0
85	OHX	1	3758	7/7	0.99	0.06	67,67,67,67	0
84	MG	5	3634	1/1	0.99	0.06	31,31,31,31	0
85	OHX	1	3760	7/7	0.99	0.10	68,68,68,68	0
85	OHX	Q2	503	7/7	0.99	0.20	59,59,59,59	0
85	OHX	1	3861	7/7	0.99	0.16	67,67,67,67	0
85	OHX	6	2011	7/7	0.99	0.08	61,61,61,61	0
85	OHX	6	2012	7/7	0.99	0.08	67,67,67,67	0
85	OHX	5	4011	7/7	0.99	0.20	63,63,63,63	0
85	OHX	6	2013	7/7	0.99	0.09	70,70,70,70	0
85	OHX	6	2014	7/7	0.99	0.08	62,62,62,62	0
85	OHX	6	2015	7/7	0.99	0.11	75,75,75,75	0
85	OHX	1	3761	7/7	0.99	0.06	60,60,60,60	0
85	OHX	5	3742	7/7	0.99	0.13	46,46,46,46	0
85	OHX	5	3743	7/7	0.99	0.10	43,43,43,43	0
85	OHX	5	3745	7/7	0.99	0.07	43,43,43,43	0
85	OHX	5	3746	7/7	0.99	0.12	54,54,54,54	0
85	OHX	5	3747	7/7	0.99	0.11	53,53,53,53	0
85	OHX	5	3748	7/7	0.99	0.07	55,55,55,55	0
85	OHX	5	3749	7/7	0.99	0.10	52,52,52,52	0
85	OHX	5	3750	7/7	0.99	0.09	54,54,54,54	0
85	OHX	5	3751	7/7	0.99	0.09	52,52,52,52	0
85	OHX	5	3753	7/7	0.99	0.12	68,68,68,68	0
85	OHX	5	3754	7/7	0.99	0.06	50,50,50,50	0
85	OHX	5	3755	7/7	0.99	0.07	50,50,50,50	0
85	OHX	5	3756	7/7	0.99	0.06	60,60,60,60	0
85	OHX	5	3757	7/7	0.99	0.07	58,58,58,58	0
85	OHX	5	3758	7/7	0.99	0.09	55,55,55,55	0
85	OHX	5	3759	7/7	0.99	0.07	62,62,62,62	0
85	OHX	5	3760	7/7	0.99	0.07	56,56,56,56	0
85	OHX	5	3761	7/7	0.99	0.05	55,55,55,55	0
85	OHX	5	3762	7/7	0.99	0.08	63,63,63,63	0
85	OHX	5	3763	7/7	0.99	0.08	61,61,61,61	0
85	OHX	5	3764	7/7	0.99	0.06	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3765	7/7	0.99	0.06	59,59,59,59	0
85	OHX	5	3766	7/7	0.99	0.07	63,63,63,63	0
85	OHX	5	3767	7/7	0.99	0.09	63,63,63,63	0
85	OHX	5	3768	7/7	0.99	0.07	58,58,58,58	0
85	OHX	5	3769	7/7	0.99	0.07	52,52,52,52	0
85	OHX	2	2001	7/7	0.99	0.08	83,83,83,83	0
85	OHX	5	3771	7/7	0.99	0.06	66,66,66,66	0
85	OHX	5	3772	7/7	0.99	0.08	61,61,61,61	0
85	OHX	6	2018	7/7	0.99	0.08	60,60,60,60	0
85	OHX	5	3774	7/7	0.99	0.08	53,53,53,53	0
85	OHX	6	2019	7/7	0.99	0.10	77,77,77,77	0
85	OHX	5	3776	7/7	0.99	0.10	86,86,86,86	0
85	OHX	5	3777	7/7	0.99	0.07	59,59,59,59	0
85	OHX	5	3778	7/7	0.99	0.07	64,64,64,64	0
85	OHX	5	3779	7/7	0.99	0.08	65,65,65,65	0
85	OHX	5	3780	7/7	0.99	0.07	59,59,59,59	0
85	OHX	5	3781	7/7	0.99	0.11	65,65,65,65	0
85	OHX	5	3782	7/7	0.99	0.09	76,76,76,76	0
85	OHX	6	2020	7/7	0.99	0.06	69,69,69,69	0
85	OHX	6	2021	7/7	0.99	0.06	74,74,74,74	0
85	OHX	5	3785	7/7	0.99	0.09	68,68,68,68	0
85	OHX	5	3920	7/7	0.99	0.14	73,73,73,73	0
85	OHX	1	3763	7/7	0.99	0.07	68,68,68,68	0
85	OHX	6	2023	7/7	0.99	0.07	71,71,71,71	0
85	OHX	6	2024	7/7	0.99	0.06	71,71,71,71	0
85	OHX	5	3789	7/7	0.99	0.07	59,59,59,59	0
85	OHX	5	3790	7/7	0.99	0.08	58,58,58,58	0
85	OHX	5	3791	7/7	0.99	0.07	73,73,73,73	0
85	OHX	5	3792	7/7	0.99	0.09	81,81,81,81	0
85	OHX	6	2025	7/7	0.99	0.09	73,73,73,73	0
85	OHX	6	2026	7/7	0.99	0.08	71,71,71,71	0
85	OHX	1	3764	7/7	0.99	0.16	64,64,64,64	0
85	OHX	5	3931	7/7	0.99	0.18	68,68,68,68	0
85	OHX	2	1983	7/7	0.99	0.11	75,75,75,75	0
85	OHX	5	3797	7/7	0.99	0.14	57,57,57,57	0
85	OHX	5	3798	7/7	0.99	0.07	80,80,80,80	0
85	OHX	1	3766	7/7	0.99	0.07	76,76,76,76	0
85	OHX	1	3815	7/7	0.99	0.16	71,71,71,71	0
85	OHX	5	3801	7/7	0.99	0.10	69,69,69,69	0
85	OHX	1	3726	7/7	0.99	0.10	43,43,43,43	0
85	OHX	1	3727	7/7	0.99	0.10	52,52,52,52	0
85	OHX	1	3818	7/7	0.99	0.19	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	5	3805	7/7	0.99	0.13	73,73,73,73	0
85	OHX	1	3729	7/7	0.99	0.10	53,53,53,53	0
85	OHX	1	3730	7/7	0.99	0.14	55,55,55,55	0
85	OHX	8	211	7/7	0.99	0.07	55,55,55,55	0
85	OHX	5	3808	7/7	0.99	0.12	67,67,67,67	0
85	OHX	1	3821	7/7	0.99	0.14	77,77,77,77	0
85	OHX	1	3731	7/7	0.99	0.09	50,50,50,50	0
85	OHX	5	3811	7/7	0.99	0.13	73,73,73,73	0
85	OHX	5	3812	7/7	0.99	0.09	74,74,74,74	0
85	OHX	5	3949	7/7	0.99	0.19	63,63,63,63	0
85	OHX	6	2038	7/7	0.99	0.11	71,71,71,71	0
85	OHX	5	3814	7/7	0.99	0.08	84,84,84,84	0
85	OHX	5	3815	7/7	0.99	0.15	68,68,68,68	0
85	OHX	1	3772	7/7	0.99	0.07	74,74,74,74	0
85	OHX	1	3824	7/7	0.99	0.12	56,56,56,56	0
85	OHX	1	3732	7/7	0.99	0.10	57,57,57,57	0
85	OHX	1	3733	7/7	0.99	0.07	47,47,47,47	0
85	OHX	1	3734	7/7	0.99	0.08	56,56,56,56	0
85	OHX	1	3735	7/7	0.99	0.08	54,54,54,54	0
85	OHX	6	2045	7/7	0.99	0.10	87,87,87,87	0
85	OHX	1	3736	7/7	0.99	0.08	63,63,63,63	0
85	OHX	1	3737	7/7	0.99	0.05	56,56,56,56	0
85	OHX	5	3825	7/7	0.99	0.14	68,68,68,68	0
85	OHX	5	3826	7/7	0.99	0.11	62,62,62,62	0
85	OHX	1	3779	7/7	0.99	0.11	71,71,71,71	0
85	OHX	1	3738	7/7	0.99	0.06	56,56,56,56	0
85	OHX	5	3829	7/7	0.99	0.12	68,68,68,68	0
85	OHX	1	3739	7/7	0.99	0.05	62,62,62,62	0
85	OHX	1	3782	7/7	0.99	0.07	77,77,77,77	0
85	OHX	4	215	7/7	0.99	0.07	54,54,54,54	0
85	OHX	5	3833	7/7	0.99	0.08	61,61,61,61	0
85	OHX	4	216	7/7	0.99	0.06	58,58,58,58	0
85	OHX	n3	202	7/7	0.99	0.09	72,72,72,72	0
85	OHX	5	3835	7/7	0.99	0.14	73,73,73,73	0
85	OHX	n9	102	7/7	0.99	0.10	59,59,59,59	0
85	OHX	4	217	7/7	0.99	0.08	68,68,68,68	0
85	OHX	o7	502	7/7	0.99	0.13	79,79,79,79	0
85	OHX	1	3740	7/7	0.99	0.09	60,60,60,60	0
85	OHX	1	3741	7/7	0.99	0.08	55,55,55,55	0
86	ZN	D6	500	1/1	0.99	0.03	81,81,81,81	0
85	OHX	1	3785	7/7	0.99	0.09	66,66,66,66	0
86	ZN	D9	101	1/1	0.99	0.03	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	OHX	2	2019	7/7	0.99	0.16	87,87,87,87	0
86	ZN	Q0	500	1/1	0.99	0.03	48,48,48,48	0
85	OHX	1	3787	7/7	0.99	0.09	73,73,73,73	0
86	ZN	Q3	501	1/1	0.99	0.03	58,58,58,58	0
85	OHX	1	3743	7/7	0.99	0.09	60,60,60,60	0
85	OHX	1	3745	7/7	0.99	0.10	66,66,66,66	0
86	ZN	d9	101	1/1	0.99	0.04	86,86,86,86	0
85	OHX	1	3948	7/7	0.99	0.19	70,70,70,70	0
85	OHX	1	3790	7/7	0.99	0.12	72,72,72,72	0
86	ZN	q3	501	1/1	0.99	0.03	57,57,57,57	0
85	OHX	1	3791	7/7	0.99	0.09	73,73,73,73	0
85	OHX	1	3744	7/7	1.00	0.06	54,54,54,54	0
85	OHX	1	3728	7/7	1.00	0.08	44,44,44,44	0
85	OHX	5	3744	7/7	1.00	0.10	40,40,40,40	0
86	ZN	O7	101	1/1	1.00	0.02	42,42,42,42	0
86	ZN	o7	501	1/1	1.00	0.02	45,45,45,45	0
86	ZN	q0	201	1/1	1.00	0.02	36,36,36,36	0
85	OHX	6	2009	7/7	1.00	0.10	57,57,57,57	0
85	OHX	1	3752	7/7	1.00	0.05	59,59,59,59	0
85	OHX	5	3752	7/7	1.00	0.06	40,40,40,40	0

5.5 Other polymers (i)

There are no such residues in this entry.