Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:28 AM UTC

PDB ID	:	2RDB / pdb_00002rdb
Title	:	X-ray Crystal Structure of Toluene/o-Xylene Monooxygenase Hydroxylase I100W Mutant
Authors	:	Murray, L.J.; Garcia-Serres, R.; McCormick, M.S.; Davydov, R.; Naik, S.; Hoffman, B.M.; Huynh, B.H.; Lippard, S.J.
Deposited on	:	2007-09-21
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

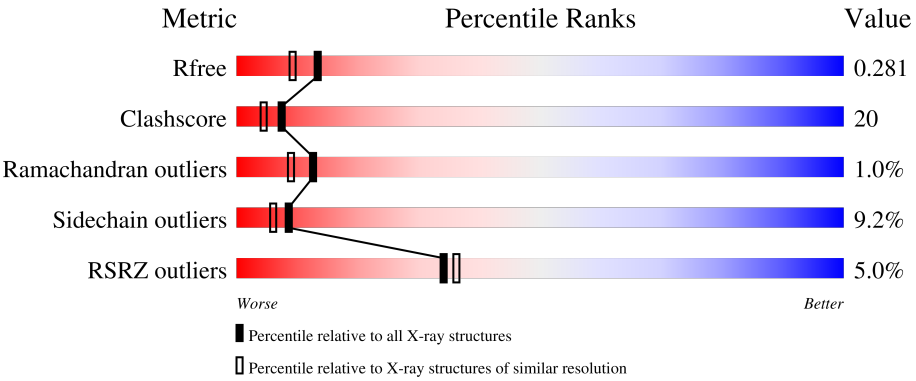
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	498	4% 41% 45% 12%
2	B	330	2% 54% 34% 8%
3	C	86	20% 24% 42% 23% 7%

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
5	P6G	A	4974	-	-	X	-
7	MPO	B	4401	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7556 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 protein called Toluene, o-xylene monooxygenase oxygenase subunit;alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			4035	2580	676	753	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	TRP	ILE	engineered mutation	UNP O87798

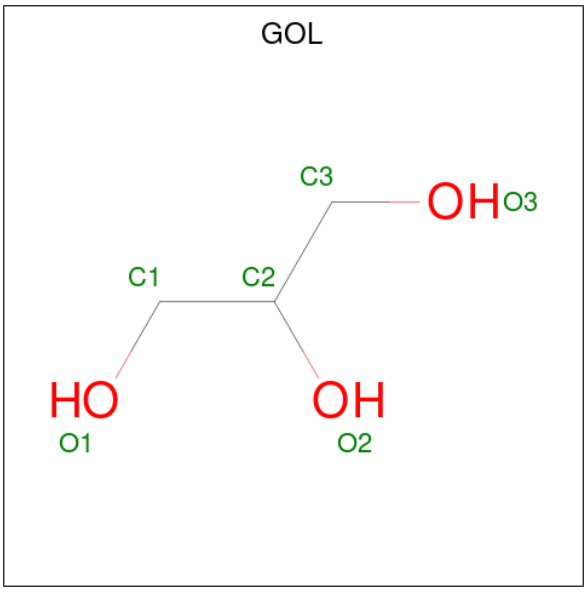
- Molecule 2 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2641	1674	467	490	10			

- Molecule 3 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;gamma.

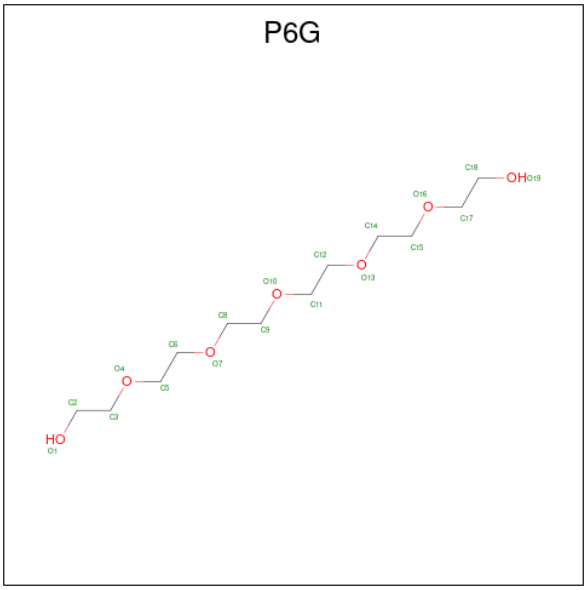
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total	C	N	O	S	0	0	0
			676	425	120	126	5			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).

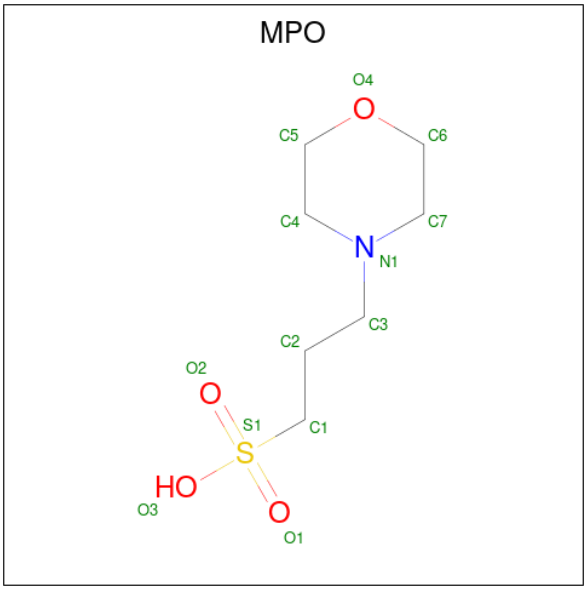


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 19 12 7	0	0

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Fe 2 2	0	0

- Molecule 7 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O S 13 7 1 4 1	0	0

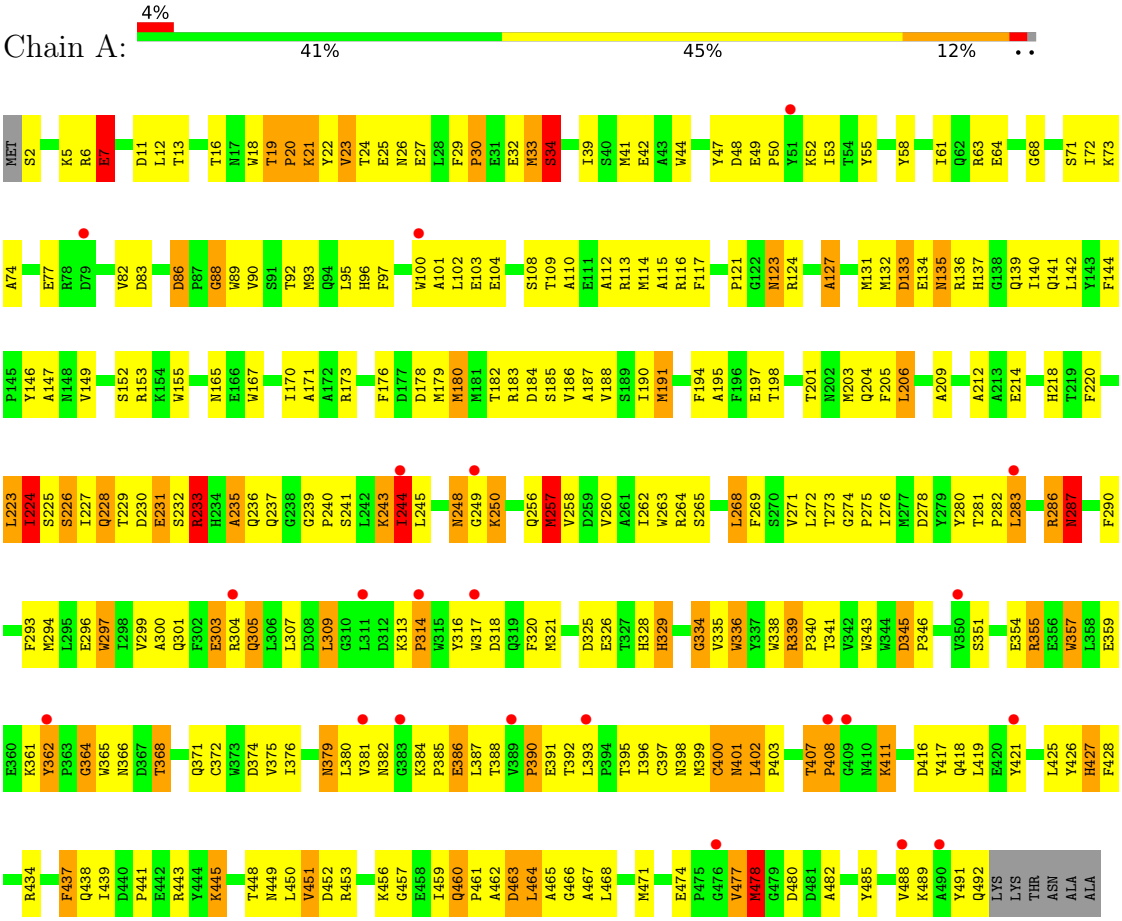
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	82	Total O 82 82	0	0
8	B	72	Total O 72 72	0	0
8	C	4	Total O 4 4	0	0

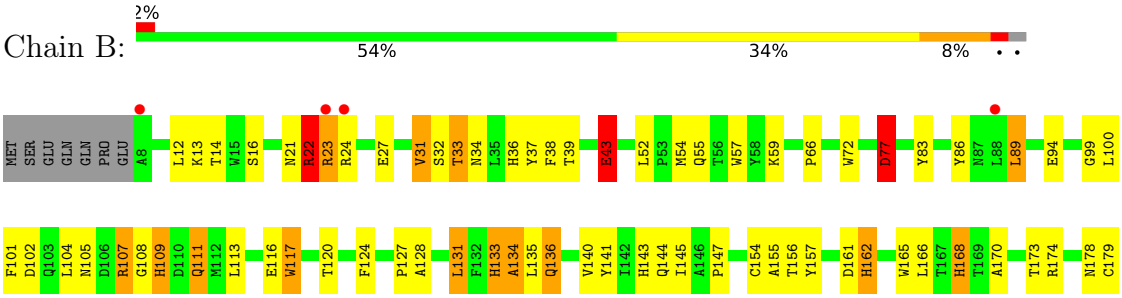
3 Residue-property plots (i)

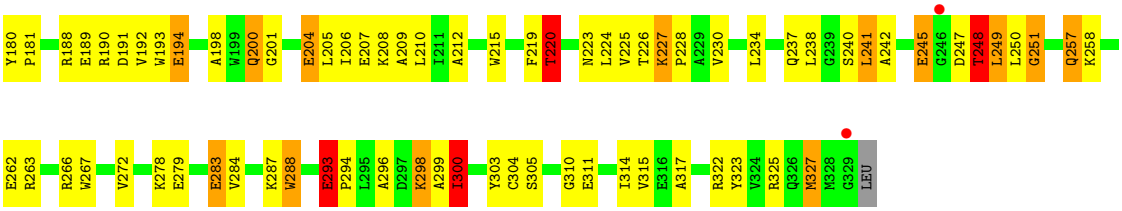
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Toluene, o-xylene monooxygenase oxygenase subunit;alpha

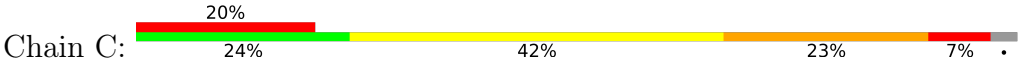


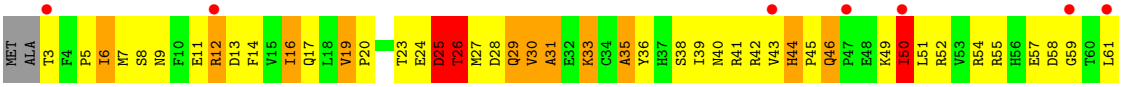
• Molecule 2: Toluene, o-xylene monooxygenase oxygenase subunit;beta

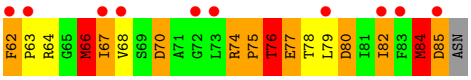




• Molecule 3: Toluene, o-xylene monooxygenase oxygenase subunit;gamma







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.42Å 182.42Å 67.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.84 – 2.10 36.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.7 (36.84-2.10) 84.6 (36.84-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.284 0.218 , 0.281	Depositor DCC
R_{free} test set	3687 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.952	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7556	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FE, MPO, P6G

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.95	96/4166 (2.3%)	1.75	105/5664 (1.9%)
2	B	2.00	53/2713 (2.0%)	1.81	53/3688 (1.4%)
3	C	1.87	13/690 (1.9%)	1.87	22/934 (2.4%)
All	All	1.96	162/7569 (2.1%)	1.79	180/10286 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	131	LEU	C-O	-12.20	1.09	1.24
2	B	135	LEU	N-CA	10.76	1.60	1.46
1	A	374	ASP	N-CA	10.56	1.58	1.46
2	B	300	ILE	CA-CB	10.22	1.67	1.54
1	A	34	SER	CA-C	-9.19	1.43	1.52
2	B	212	ALA	CA-CB	8.81	1.64	1.52
1	A	241	SER	C-O	-8.43	1.14	1.24
2	B	155	ALA	C-O	-8.40	1.13	1.24
1	A	451	VAL	CA-CB	8.28	1.65	1.54
1	A	117	PHE	CA-CB	7.91	1.66	1.54
2	B	298	LYS	N-CA	7.87	1.55	1.46
2	B	59	LYS	C-O	7.86	1.33	1.24
1	A	114	MET	CA-C	7.76	1.63	1.52
1	A	241	SER	CA-C	-7.74	1.42	1.52
3	C	46	GLN	C-N	7.48	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	ALA	C-O	7.37	1.32	1.24
1	A	92	THR	C-O	-7.32	1.15	1.24
2	B	162	HIS	CA-CB	7.21	1.64	1.53
1	A	133	ASP	CA-CB	7.18	1.64	1.53
2	B	156	THR	CA-CB	7.16	1.64	1.53
3	C	77	GLU	C-O	7.10	1.32	1.24
2	B	230	VAL	N-CA	7.10	1.54	1.46
1	A	400	CYS	C-O	7.04	1.33	1.24
1	A	357	TRP	N-CA	7.02	1.54	1.46
1	A	52	LYS	C-O	-6.99	1.15	1.23
1	A	11	ASP	C-O	-6.92	1.16	1.24
1	A	82	VAL	CA-CB	6.90	1.63	1.54
2	B	37	TYR	CD1-CE1	6.89	1.59	1.38
1	A	180	MET	CA-C	6.87	1.62	1.52
1	A	235	ALA	CA-C	-6.82	1.43	1.52
1	A	457	GLY	N-CA	-6.80	1.36	1.45
2	B	325	ARG	CZ-NH2	6.76	1.42	1.33
3	C	39	ILE	CA-CB	6.70	1.61	1.54
1	A	63	ARG	CA-C	6.70	1.61	1.52
2	B	241	LEU	CA-C	6.62	1.61	1.52
1	A	376	ILE	CA-CB	6.62	1.62	1.54
1	A	235	ALA	C-O	-6.59	1.15	1.24
2	B	288	TRP	C-O	-6.58	1.16	1.24
1	A	112	ALA	CA-CB	-6.53	1.43	1.53
2	B	287	LYS	C-O	-6.52	1.16	1.24
1	A	64	GLU	CB-CG	6.47	1.71	1.52
1	A	124	ARG	C-O	-6.43	1.16	1.24
1	A	230	ASP	C-O	-6.41	1.15	1.24
1	A	283	LEU	N-CA	6.35	1.54	1.46
3	C	80	ASP	CA-C	6.33	1.61	1.52
2	B	248	THR	CA-CB	6.29	1.63	1.53
1	A	191	MET	CA-C	-6.29	1.44	1.52
3	C	16	ILE	N-CA	6.28	1.53	1.46
1	A	362	TYR	C-N	6.20	1.40	1.33
3	C	19	VAL	N-CA	6.20	1.54	1.46
1	A	462	ALA	CA-C	6.19	1.60	1.53
1	A	187	ALA	CA-C	-6.16	1.44	1.52
1	A	448	THR	N-CA	-6.14	1.38	1.46
2	B	43	GLU	CG-CD	6.10	1.67	1.52
2	B	283	GLU	CG-CD	6.10	1.67	1.52
1	A	18	TRP	C-O	6.09	1.31	1.23
1	A	182	THR	N-CA	6.09	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	LEU	N-CA	-6.08	1.39	1.46
1	A	135	ASN	N-CA	-6.07	1.39	1.46
2	B	191	ASP	CA-CB	-6.05	1.43	1.53
2	B	225	VAL	CA-CB	6.03	1.62	1.54
3	C	8	SER	C-O	-6.02	1.16	1.24
2	B	192	VAL	N-CA	-6.01	1.39	1.46
1	A	97	PHE	N-CA	-5.99	1.39	1.46
2	B	117	TRP	C-O	-5.99	1.17	1.24
1	A	110	ALA	C-O	-5.99	1.16	1.24
1	A	26	ASN	N-CA	5.98	1.53	1.46
1	A	42	GLU	CA-C	5.95	1.60	1.52
1	A	147	ALA	C-O	-5.94	1.16	1.24
2	B	193	TRP	N-CA	5.93	1.53	1.46
1	A	346	PRO	C-O	5.92	1.30	1.23
1	A	257	MET	N-CA	5.91	1.53	1.46
1	A	171	ALA	CA-C	5.89	1.60	1.52
1	A	19	THR	C-O	-5.86	1.17	1.24
2	B	209	ALA	N-CA	5.83	1.53	1.46
1	A	460	GLN	CA-CB	5.83	1.62	1.53
1	A	29	PHE	N-CA	-5.81	1.39	1.46
2	B	39	THR	CA-C	5.80	1.60	1.52
1	A	63	ARG	C-O	5.79	1.30	1.24
2	B	89	LEU	C-O	-5.77	1.17	1.24
1	A	110	ALA	CA-CB	-5.75	1.43	1.53
3	C	43	VAL	CA-C	5.74	1.59	1.52
2	B	133	HIS	CA-C	5.74	1.60	1.52
2	B	238	LEU	CA-C	5.72	1.60	1.52
2	B	14	THR	CA-C	-5.71	1.46	1.53
1	A	95	LEU	CA-C	5.69	1.60	1.52
1	A	464	LEU	CG-CD1	5.69	1.71	1.52
1	A	334	GLY	C-O	5.65	1.30	1.23
3	C	38	SER	CA-C	5.64	1.59	1.52
2	B	77	ASP	C-O	-5.61	1.17	1.24
1	A	368	THR	N-CA	5.59	1.53	1.46
1	A	434	ARG	C-O	-5.59	1.17	1.24
1	A	381	VAL	N-CA	5.58	1.53	1.46
1	A	33	MET	SD-CE	5.57	1.93	1.79
1	A	392	THR	CA-CB	-5.56	1.45	1.53
1	A	132	MET	C-O	5.55	1.30	1.24
1	A	97	PHE	CG-CD2	5.55	1.50	1.38
1	A	268	LEU	C-O	5.54	1.30	1.24
2	B	107	ARG	CZ-NH2	5.54	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	59	LYS	CG-CD	5.53	1.69	1.52
1	A	438	GLN	C-O	5.53	1.30	1.24
2	B	99	GLY	N-CA	-5.52	1.38	1.45
1	A	108	SER	C-O	5.52	1.30	1.24
2	B	120	THR	N-CA	-5.50	1.39	1.46
2	B	77	ASP	CA-C	-5.47	1.47	1.52
2	B	201	GLY	N-CA	5.46	1.52	1.45
2	B	101	PHE	N-CA	5.46	1.52	1.46
2	B	38	PHE	C-O	-5.46	1.17	1.24
1	A	465	ALA	CA-CB	5.45	1.61	1.53
1	A	402	LEU	CG-CD2	5.45	1.70	1.52
2	B	204	GLU	CA-CB	5.45	1.61	1.53
2	B	86	TYR	N-CA	-5.44	1.39	1.46
2	B	262	GLU	C-O	-5.44	1.17	1.24
1	A	194	PHE	CA-C	5.42	1.59	1.52
2	B	155	ALA	CA-C	-5.42	1.45	1.52
1	A	437	PHE	CD2-CE2	5.42	1.54	1.38
1	A	314	PRO	CA-C	5.41	1.58	1.52
1	A	393	LEU	CG-CD2	5.41	1.70	1.52
1	A	149	VAL	CA-CB	5.41	1.61	1.54
2	B	191	ASP	CA-C	-5.41	1.45	1.52
1	A	376	ILE	N-CA	-5.40	1.39	1.46
1	A	427	HIS	C-O	5.39	1.30	1.24
2	B	299	ALA	C-O	5.38	1.30	1.24
1	A	20	PRO	C-O	5.36	1.30	1.23
2	B	31	VAL	N-CA	5.35	1.53	1.46
3	C	17	GLN	CA-C	-5.35	1.46	1.52
3	C	9	ASN	CA-C	5.33	1.59	1.53
1	A	140	ILE	CA-CB	5.31	1.61	1.54
2	B	157	TYR	N-CA	-5.30	1.39	1.46
1	A	16	THR	CA-CB	-5.29	1.45	1.54
1	A	190	ILE	CA-CB	5.27	1.60	1.54
1	A	226	SER	C-O	-5.24	1.18	1.24
3	C	84	MET	N-CA	5.24	1.52	1.46
1	A	186	VAL	CA-CB	5.22	1.60	1.54
1	A	136	ARG	CZ-NH2	-5.22	1.26	1.33
1	A	72	ILE	CA-CB	5.21	1.60	1.54
2	B	317	ALA	CA-CB	5.21	1.61	1.53
2	B	22	ARG	N-CA	5.17	1.52	1.46
2	B	134	ALA	CA-CB	-5.16	1.45	1.53
1	A	271	VAL	CA-C	-5.14	1.47	1.53
1	A	198	THR	C-O	-5.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	304	CYS	C-O	-5.13	1.17	1.24
1	A	61	ILE	CA-C	5.13	1.59	1.52
1	A	371	GLN	CD-NE2	5.13	1.44	1.33
1	A	73	LYS	CA-C	5.12	1.59	1.52
1	A	488	VAL	CA-CB	5.12	1.61	1.54
1	A	297	TRP	CA-CB	-5.10	1.46	1.54
1	A	123	ASN	CA-C	5.08	1.59	1.52
1	A	137	HIS	C-O	-5.08	1.18	1.24
2	B	165	TRP	CA-C	5.05	1.59	1.52
3	C	35	ALA	CA-CB	5.05	1.62	1.53
1	A	88	GLY	CA-C	5.05	1.58	1.52
1	A	127	ALA	CA-C	5.05	1.59	1.52
1	A	343	TRP	N-CA	5.04	1.52	1.46
1	A	245	LEU	C-O	-5.04	1.18	1.24
1	A	173	ARG	CA-C	-5.04	1.45	1.52
2	B	168	HIS	C-O	5.04	1.30	1.24
1	A	104	GLU	N-CA	5.03	1.52	1.46
1	A	407	THR	CA-C	5.02	1.59	1.52
1	A	477	VAL	C-O	-5.02	1.18	1.23
1	A	407	THR	CA-CB	5.01	1.61	1.53
1	A	287	ASN	N-CA	5.01	1.52	1.46

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	227	LYS	CA-C-N	-14.31	103.53	119.28
2	B	227	LYS	C-N-CA	-14.31	103.53	119.28
1	A	339	ARG	CA-C-N	-12.90	106.45	119.87
1	A	339	ARG	C-N-CA	-12.90	106.45	119.87
1	A	287	ASN	N-CA-C	11.40	135.08	110.80
1	A	101	ALA	N-CA-C	11.03	123.30	111.28
2	B	251	GLY	N-CA-C	-10.02	100.71	112.73
3	C	76	THR	N-CA-CB	-9.83	104.27	114.10
2	B	192	VAL	N-CA-C	-9.75	101.06	110.42
1	A	209	ALA	N-CA-C	9.52	121.66	111.28
2	B	157	TYR	N-CA-C	-9.01	100.88	112.23
2	B	155	ALA	N-CA-C	-8.82	101.59	111.82
1	A	250	LYS	N-CA-C	8.57	121.86	110.88
2	B	191	ASP	N-CA-C	8.23	121.28	111.33
1	A	132	MET	N-CA-C	8.19	120.94	111.11
2	B	300	ILE	CB-CA-C	-8.04	101.28	112.14
3	C	25	ASP	N-CA-C	7.97	120.08	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	TRP	N-CA-C	-7.91	102.74	111.36
1	A	265	SER	N-CA-C	-7.89	102.62	111.14
1	A	364	GLY	N-CA-C	-7.87	105.12	114.48
1	A	86	ASP	CA-C-N	-7.69	111.79	119.56
1	A	86	ASP	C-N-CA	-7.69	111.79	119.56
1	A	232	SER	N-CA-C	7.66	120.30	111.11
1	A	29	PHE	CA-C-N	-7.64	112.14	119.85
1	A	29	PHE	C-N-CA	-7.64	112.14	119.85
1	A	142	LEU	N-CA-C	-7.60	103.86	113.43
2	B	86	TYR	N-CA-C	-7.52	102.44	111.69
2	B	220	THR	N-CA-C	-7.49	102.47	111.69
1	A	451	VAL	N-CA-C	-7.37	103.67	110.82
2	B	293	GLU	CA-C-N	-7.29	111.01	119.47
2	B	293	GLU	C-N-CA	-7.29	111.01	119.47
2	B	147	PRO	N-CA-C	7.28	122.99	114.03
1	A	7	GLU	N-CA-C	-7.28	103.50	112.38
1	A	49	GLU	CA-C-N	-7.26	112.70	120.47
1	A	49	GLU	C-N-CA	-7.26	112.70	120.47
1	A	335	VAL	N-CA-C	7.26	118.05	110.72
1	A	19	THR	CA-C-N	7.21	127.25	119.89
1	A	19	THR	C-N-CA	7.21	127.25	119.89
1	A	438	GLN	N-CA-C	7.21	120.98	111.75
3	C	33	LYS	CA-C-N	7.18	130.13	120.65
3	C	33	LYS	C-N-CA	7.18	130.13	120.65
2	B	162	HIS	N-CA-CB	7.18	120.67	110.12
1	A	188	VAL	CB-CA-C	-7.16	102.34	112.22
1	A	248	ASN	CA-C-N	-7.08	107.54	121.41
1	A	248	ASN	C-N-CA	-7.08	107.54	121.41
2	B	198	ALA	N-CA-C	-7.07	103.61	111.82
1	A	355	ARG	N-CA-C	7.03	119.02	111.36
2	B	299	ALA	CA-C-N	6.94	129.97	120.46
2	B	299	ALA	C-N-CA	6.94	129.97	120.46
1	A	239	GLY	CA-C-N	6.91	127.48	119.47
1	A	239	GLY	C-N-CA	6.91	127.48	119.47
1	A	146	TYR	N-CA-C	-6.87	104.00	112.38
2	B	77	ASP	CA-C-N	6.84	126.47	119.56
2	B	77	ASP	C-N-CA	6.84	126.47	119.56
1	A	380	LEU	N-CA-C	-6.80	103.99	112.90
3	C	82	ILE	N-CA-C	6.79	118.93	109.29
3	C	74	ARG	CA-C-N	-6.68	112.78	119.93
3	C	74	ARG	C-N-CA	-6.68	112.78	119.93
1	A	478	MET	CA-C-N	-6.66	114.39	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	478	MET	C-N-CA	-6.66	114.39	121.45
1	A	198	THR	CA-C-N	6.63	128.64	120.22
1	A	198	THR	C-N-CA	6.63	128.64	120.22
1	A	345	ASP	CB-CA-C	-6.58	103.61	110.33
2	B	131	LEU	CA-C-N	6.46	128.83	120.44
2	B	131	LEU	C-N-CA	6.46	128.83	120.44
1	A	437	PHE	N-CA-C	6.46	118.89	111.02
1	A	329	HIS	N-CA-C	-6.41	104.22	111.07
1	A	58	TYR	N-CA-C	-6.39	104.00	110.97
1	A	191	MET	CB-CG-SD	6.38	131.84	112.70
2	B	161	ASP	N-CA-C	6.37	117.88	111.07
2	B	225	VAL	CB-CA-C	-6.34	100.89	111.29
2	B	55	GLN	N-CA-C	-6.33	104.29	111.07
2	B	245	GLU	N-CA-C	6.33	120.85	113.20
2	B	178	ASN	N-CA-C	-6.32	103.69	111.40
1	A	110	ALA	N-CA-C	-6.29	104.52	111.82
3	C	26	THR	N-CA-C	-6.29	99.66	109.72
1	A	190	ILE	N-CA-C	6.26	116.31	110.42
1	A	231	GLU	N-CA-C	6.20	117.71	111.07
1	A	463	ASP	N-CA-C	-6.20	100.12	108.86
1	A	74	ALA	N-CA-C	-6.19	104.98	112.54
2	B	205	LEU	CD1-CG-CD2	6.16	124.35	110.80
2	B	241	LEU	N-CA-C	6.14	118.48	111.11
2	B	165	TRP	N-CA-C	-6.11	104.54	111.14
2	B	219	PHE	N-CA-C	6.10	121.43	111.37
3	C	50	ILE	CB-CA-C	6.09	119.90	110.83
1	A	393	LEU	N-CA-C	-6.09	102.48	110.39
1	A	375	VAL	N-CA-C	6.03	116.69	110.36
1	A	489	LYS	N-CA-C	6.01	118.60	111.33
2	B	170	ALA	CA-C-N	5.99	128.77	120.63
2	B	170	ALA	C-N-CA	5.99	128.77	120.63
2	B	31	VAL	N-CA-C	5.98	118.75	112.83
2	B	234	LEU	CA-C-N	-5.95	113.19	122.42
2	B	234	LEU	C-N-CA	-5.95	113.19	122.42
1	A	25	GLU	CA-C-N	5.95	128.85	120.28
1	A	25	GLU	C-N-CA	5.95	128.85	120.28
1	A	34	SER	N-CA-C	-5.94	105.03	112.93
1	A	488	VAL	CA-C-N	5.93	128.50	120.38
1	A	488	VAL	C-N-CA	5.93	128.50	120.38
2	B	124	PHE	N-CA-C	5.91	120.56	113.23
1	A	451	VAL	CA-C-N	5.89	128.98	120.79
1	A	451	VAL	C-N-CA	5.89	128.98	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	456	LYS	CA-C-N	-5.86	113.38	122.69
1	A	456	LYS	C-N-CA	-5.86	113.38	122.69
2	B	257	GLN	N-CA-C	-5.82	104.90	112.23
2	B	194	GLU	N-CA-C	5.81	118.56	111.82
1	A	48	ASP	N-CA-C	5.79	119.79	107.70
1	A	83	ASP	N-CA-C	5.76	120.04	113.19
1	A	459	ILE	N-CA-C	-5.72	99.39	107.75
2	B	173	THR	N-CA-C	-5.70	104.68	111.69
2	B	322	ARG	N-CA-CB	-5.69	101.54	110.30
1	A	241	SER	CB-CA-C	-5.68	101.20	110.85
1	A	382	ASN	N-CA-C	5.67	119.28	112.93
1	A	53	ILE	N-CA-CB	5.67	118.84	111.19
3	C	79	LEU	N-CA-C	5.66	118.19	109.07
2	B	136	GLN	CA-C-N	5.64	127.83	120.28
2	B	136	GLN	C-N-CA	5.64	127.83	120.28
1	A	379	ASN	N-CA-C	5.63	117.42	111.28
1	A	233	ARG	N-CA-C	-5.62	105.25	111.71
3	C	41	ARG	N-CA-C	-5.60	106.50	113.55
3	C	59	GLY	CA-C-N	5.59	128.70	120.82
3	C	59	GLY	C-N-CA	5.59	128.70	120.82
1	A	144	PHE	CA-C-N	-5.58	113.92	119.56
1	A	144	PHE	C-N-CA	-5.58	113.92	119.56
3	C	44	HIS	CA-C-N	5.58	125.90	119.93
3	C	44	HIS	C-N-CA	5.58	125.90	119.93
1	A	244	ILE	N-CA-C	5.57	118.01	111.05
1	A	439	ILE	CA-C-N	-5.53	117.41	122.28
1	A	439	ILE	C-N-CA	-5.53	117.41	122.28
1	A	102	LEU	N-CA-C	5.53	118.23	111.82
1	A	227	ILE	N-CA-C	-5.50	104.17	111.05
1	A	30	PRO	CB-CA-C	-5.50	103.78	110.98
1	A	23	VAL	N-CA-C	-5.45	100.84	108.80
3	C	66	MET	N-CA-C	5.44	118.12	110.23
2	B	237	GLN	CA-C-N	-5.41	113.04	120.28
2	B	237	GLN	C-N-CA	-5.41	113.04	120.28
1	A	149	VAL	N-CA-CB	5.38	117.86	110.54
2	B	200	GLN	N-CA-C	-5.38	106.56	113.23
1	A	326	GLU	N-CA-C	5.35	122.20	110.80
1	A	401	ASN	N-CA-C	-5.35	106.05	112.58
2	B	32	SER	CB-CA-C	-5.34	100.05	109.02
1	A	224	ILE	CB-CA-C	-5.30	104.98	112.14
2	B	117	TRP	N-CA-C	5.30	116.75	110.97
1	A	41	MET	N-CA-C	-5.29	104.56	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	GLY	N-CA-C	5.28	118.87	112.49
2	B	272	VAL	N-CA-C	-5.28	105.39	110.72
1	A	248	ASN	O-C-N	-5.25	117.06	122.84
2	B	33	THR	N-CA-C	5.24	118.77	109.96
2	B	303	TYR	CA-C-N	5.24	127.83	120.28
2	B	303	TYR	C-N-CA	5.24	127.83	120.28
1	A	282	PRO	CA-C-N	5.24	127.30	120.28
1	A	282	PRO	C-N-CA	5.24	127.30	120.28
1	A	42	GLU	N-CA-C	5.23	117.65	111.33
1	A	194	PHE	CA-C-N	5.23	127.55	120.44
1	A	194	PHE	C-N-CA	5.23	127.55	120.44
1	A	55	TYR	CA-C-N	-5.22	113.65	119.19
1	A	55	TYR	C-N-CA	-5.22	113.65	119.19
1	A	218	HIS	N-CA-C	5.20	117.02	111.36
1	A	11	ASP	N-CA-C	5.19	117.36	111.02
1	A	286	ARG	CA-C-N	5.17	131.41	121.54
1	A	286	ARG	C-N-CA	5.17	131.41	121.54
1	A	271	VAL	N-CA-C	-5.15	107.81	112.96
1	A	402	LEU	CA-C-N	5.12	125.36	119.83
1	A	402	LEU	C-N-CA	5.12	125.36	119.83
3	C	19	VAL	N-CA-C	5.12	119.95	108.88
1	A	149	VAL	CB-CA-C	-5.11	105.25	112.14
3	C	75	PRO	CA-C-N	-5.10	118.85	126.86
3	C	75	PRO	C-N-CA	-5.10	118.85	126.86
1	A	141	GLN	CA-CB-CG	-5.09	103.92	114.10
1	A	281	THR	N-CA-C	-5.09	100.23	109.44
1	A	297	TRP	N-CA-C	5.08	120.32	113.72
1	A	11	ASP	O-C-N	-5.08	116.64	122.08
1	A	263	TRP	CA-C-O	5.07	126.14	120.82
3	C	62	PHE	CA-C-N	-5.06	115.15	120.66
3	C	62	PHE	C-N-CA	-5.06	115.15	120.66
3	C	24	GLU	N-CA-C	5.06	119.30	113.18
2	B	283	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	391	GLU	CA-CB-CG	-5.05	103.99	114.10
1	A	194	PHE	N-CA-C	5.05	117.56	111.40
1	A	390	PRO	N-CA-C	5.02	119.19	111.57
1	A	453	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4035	0	3782	178	0
2	B	2641	0	2537	95	0
3	C	676	0	667	56	0
4	A	12	0	15	4	0
5	A	19	0	25	19	0
6	A	2	0	0	0	0
7	B	13	0	15	2	0
8	A	82	0	0	8	0
8	B	72	0	0	2	0
8	C	4	0	0	0	0
All	All	7556	0	7041	295	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (295) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:HIS:HE1	2:B:227:LYS:NZ	1.33	1.23
5:A:4974:P6G:C17	2:B:54:MET:HE2	1.78	1.12
1:A:372:CYS:HB3	3:C:42:ARG:HG2	1.25	1.11
2:B:162:HIS:CE1	2:B:227:LYS:NZ	2.20	1.10
2:B:72:TRP:H	7:B:4401:MPO:H71	1.19	1.05
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.19	1.02
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.42	1.01
1:A:427:HIS:CE1	3:C:76:THR:HG23	1.96	1.00
3:C:28:ASP:OD1	3:C:64:ARG:HB3	1.61	1.00
2:B:162:HIS:CE1	2:B:227:LYS:HZ3	1.76	1.00
1:A:427:HIS:HE1	3:C:76:THR:CG2	1.75	0.99
3:C:75:PRO:O	3:C:76:THR:HB	1.64	0.97
2:B:111:GLN:H	2:B:111:GLN:NE2	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.16	0.94
5:A:4974:P6G:H172	2:B:54:MET:HE2	1.50	0.91
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.19	0.88
5:A:4974:P6G:H171	2:B:54:MET:HE2	1.52	0.87
2:B:249:LEU:C	2:B:249:LEU:HD23	1.99	0.86
3:C:50:ILE:HD13	3:C:64:ARG:HH12	1.43	0.83
3:C:54:ARG:HG3	3:C:80:ASP:HB2	1.59	0.83
2:B:162:HIS:CE1	2:B:227:LYS:HZ2	1.93	0.83
2:B:162:HIS:HE1	2:B:227:LYS:HZ3	0.85	0.82
3:C:50:ILE:HD13	3:C:64:ARG:NH1	1.94	0.82
2:B:77:ASP:HB2	2:B:154:CYS:SG	2.20	0.81
1:A:340:PRO:O	1:A:478:MET:HB3	1.80	0.80
3:C:6:ILE:HG13	3:C:19:VAL:O	1.83	0.79
1:A:387:LEU:HD23	3:C:40:ASN:O	1.83	0.78
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.02	0.77
5:A:4974:P6G:H172	2:B:54:MET:CE	2.14	0.77
3:C:13:ASP:OD1	3:C:42:ARG:HD2	1.85	0.76
3:C:46:GLN:O	3:C:49:LYS:HB2	1.87	0.73
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.27	0.70
1:A:139:GLN:HE22	2:B:83:TYR:H	1.39	0.70
5:A:4974:P6G:H151	8:A:4987:HOH:O	1.92	0.69
1:A:127:ALA:CA	1:A:237:GLN:HE22	2.05	0.69
3:C:67:ILE:HG13	3:C:70:ASP:OD2	1.92	0.69
1:A:50:PRO:HD2	1:A:236:GLN:OE1	1.94	0.68
1:A:305:GLN:HE21	1:A:305:GLN:HA	1.59	0.68
1:A:441:PRO:O	1:A:445:LYS:HG3	1.94	0.68
1:A:116:ARG:HD2	1:A:116:ARG:O	1.94	0.68
5:A:4974:P6G:H181	2:B:54:MET:HA	1.76	0.68
1:A:418:GLN:HE22	3:C:78:THR:H	1.41	0.68
1:A:336:TRP:O	1:A:339:ARG:HG2	1.94	0.67
3:C:75:PRO:O	3:C:76:THR:CB	2.41	0.67
2:B:117:TRP:CE3	2:B:245:GLU:HG2	2.30	0.66
3:C:11:GLU:HG2	3:C:12:ARG:HG3	1.75	0.66
1:A:113:ARG:HH11	2:B:144:GLN:NE2	1.90	0.66
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.77	0.66
5:A:4974:P6G:C17	2:B:54:MET:CE	2.64	0.66
2:B:220:THR:HA	2:B:224:LEU:HD12	1.78	0.65
1:A:398:ASN:HD22	1:A:427:HIS:H	1.45	0.64
2:B:145:ILE:HG23	2:B:215:TRP:HB2	1.79	0.64
1:A:491:TYR:O	1:A:492:GLN:HB2	1.97	0.64
2:B:111:GLN:H	2:B:111:GLN:HE21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:GLN:NE2	2:B:111:GLN:N	2.42	0.64
1:A:372:CYS:HB3	3:C:42:ARG:CG	2.15	0.64
5:A:4974:P6G:H181	2:B:54:MET:CA	2.29	0.63
1:A:427:HIS:CE1	3:C:76:THR:CG2	2.65	0.62
2:B:117:TRP:CZ2	2:B:242:ALA:HA	2.34	0.62
2:B:72:TRP:N	7:B:4401:MPO:H71	2.04	0.62
1:A:116:ARG:NH2	2:B:210:LEU:O	2.33	0.62
1:A:317:TRP:O	1:A:321:MET:HG2	1.99	0.62
3:C:26:THR:HG22	3:C:64:ARG:O	2.01	0.61
1:A:127:ALA:N	1:A:237:GLN:NE2	2.49	0.61
3:C:25:ASP:O	3:C:67:ILE:HG22	2.02	0.60
1:A:368:THR:CG2	1:A:411:LYS:HG2	2.32	0.60
1:A:21:LYS:HE3	1:A:22:TYR:CZ	2.37	0.59
3:C:25:ASP:OD2	3:C:33:LYS:NZ	2.30	0.59
2:B:33:THR:HB	2:B:34:ASN:HD22	1.65	0.59
1:A:2:SER:N	2:B:105:ASN:HD22	2.01	0.59
1:A:127:ALA:HA	1:A:237:GLN:HE22	1.67	0.59
3:C:57:GLU:OE1	3:C:74:ARG:NH2	2.35	0.59
3:C:51:LEU:HA	3:C:82:ILE:O	2.02	0.59
3:C:74:ARG:O	3:C:75:PRO:C	2.43	0.59
1:A:2:SER:HB2	2:B:105:ASN:HD21	1.67	0.59
2:B:249:LEU:C	2:B:249:LEU:CD2	2.75	0.58
1:A:100[B]:TRP:CH2	4:A:4975:GOL:H31	2.38	0.58
2:B:206:ILE:HD13	2:B:226:THR:HG21	1.86	0.58
2:B:311:GLU:O	2:B:315:VAL:HG23	2.03	0.58
2:B:143:HIS:C	2:B:143:HIS:CD2	2.81	0.58
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.39	0.58
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.05	0.57
1:A:318:ASP:O	1:A:321:MET:HB2	2.04	0.56
1:A:357:TRP:CZ2	1:A:361:LYS:HG3	2.40	0.56
1:A:135:ASN:O	1:A:139:GLN:HG3	2.04	0.56
1:A:278:ASP:OD2	1:A:362:TYR:OH	2.22	0.56
1:A:351:SER:OG	1:A:354:GLU:HG3	2.05	0.56
1:A:2:SER:HB2	2:B:105:ASN:ND2	2.21	0.55
1:A:379:ASN:HD22	1:A:384:LYS:HB2	1.71	0.55
1:A:387:LEU:CD2	3:C:40:ASN:O	2.55	0.55
1:A:191:MET:O	1:A:195:ALA:HB3	2.06	0.55
3:C:50:ILE:HB	3:C:85:ASP:HA	1.88	0.55
1:A:22:TYR:CD1	2:B:204:GLU:HB2	2.42	0.55
1:A:133:ASP:OD2	1:A:233:ARG:HD2	2.07	0.55
1:A:225:SER:O	1:A:229:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:THR:HA	3:C:66:MET:O	2.07	0.54
1:A:304:ARG:HA	1:A:304:ARG:HE	1.72	0.54
1:A:357:TRP:CH2	1:A:361:LYS:HG3	2.41	0.54
1:A:416:ASP:OD2	1:A:427:HIS:CD2	2.59	0.54
1:A:449:ASN:OD1	1:A:449:ASN:C	2.51	0.54
1:A:204:GLN:HB2	1:A:269:PHE:HZ	1.73	0.54
3:C:27:MET:HE2	3:C:66:MET:HG2	1.90	0.54
1:A:303:GLU:OE1	1:A:313:LYS:HE2	2.08	0.53
2:B:180:TYR:N	2:B:181:PRO:HD3	2.24	0.53
3:C:13:ASP:OD2	3:C:42:ARG:NH1	2.41	0.53
1:A:100[B]:TRP:CZ3	4:A:4975:GOL:H31	2.43	0.53
3:C:35:ALA:O	3:C:36:TYR:C	2.50	0.53
1:A:474:GLU:O	1:A:478:MET:HG3	2.09	0.53
1:A:294:MET:O	1:A:299:VAL:HG23	2.08	0.53
3:C:25:ASP:O	3:C:67:ILE:HA	2.09	0.53
1:A:223:LEU:HD23	1:A:224:ILE:HD13	1.90	0.52
1:A:243:LYS:HG3	1:A:309:LEU:CD1	2.40	0.52
1:A:33:MET:HE2	2:B:57:TRP:CE2	2.45	0.52
2:B:27:GLU:O	2:B:31:VAL:HG22	2.10	0.52
2:B:220:THR:HG21	2:B:288:TRP:HB3	1.92	0.52
2:B:249:LEU:HD23	2:B:249:LEU:O	2.09	0.52
1:A:96:HIS:O	1:A:100[A]:TRP:CD1	2.63	0.51
1:A:109:THR:HG23	2:B:144:GLN:HB2	1.91	0.51
1:A:139:GLN:NE2	2:B:83:TYR:H	2.06	0.51
2:B:94:GLU:OE1	2:B:168:HIS:HE1	1.94	0.51
1:A:416:ASP:HB2	3:C:16:ILE:CD1	2.40	0.51
1:A:127:ALA:CA	1:A:237:GLN:NE2	2.74	0.51
2:B:226:THR:O	2:B:227:LYS:C	2.52	0.51
1:A:86:ASP:OD1	1:A:88:GLY:N	2.43	0.51
1:A:89:TRP:O	1:A:90:VAL:C	2.51	0.51
1:A:385:PRO:O	1:A:388:THR:N	2.38	0.51
1:A:399:MET:HE3	1:A:437:PHE:N	2.26	0.51
2:B:21:ASN:C	2:B:23:ARG:H	2.18	0.51
1:A:32:GLU:OE1	5:A:4974:P6G:O19	2.29	0.51
1:A:345:ASP:HB3	1:A:482:ALA:HA	1.92	0.50
2:B:12:LEU:CD1	2:B:16:SER:HA	2.41	0.50
1:A:184:ASP:H	5:A:4974:P6G:H122	1.76	0.50
2:B:145:ILE:HG13	2:B:145:ILE:O	2.11	0.50
2:B:296:ALA:O	2:B:300:ILE:HD12	2.12	0.50
1:A:355:ARG:NH1	1:A:366:ASN:OD1	2.37	0.50
1:A:384:LYS:HB3	1:A:387:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HG22	2:B:207:GLU:HB3	1.93	0.50
1:A:268:LEU:HG	1:A:272:LEU:HD12	1.94	0.50
1:A:379:ASN:ND2	1:A:384:LYS:HD3	2.27	0.50
1:A:386:GLU:HG2	1:A:387:LEU:HD12	1.93	0.50
2:B:127:PRO:HA	2:B:189:GLU:HB3	1.93	0.49
1:A:103:GLU:CG	1:A:176:PHE:CD2	2.96	0.49
1:A:443:ARG:HG3	2:B:52:LEU:HD11	1.93	0.49
2:B:179:CYS:C	2:B:181:PRO:HD3	2.37	0.49
1:A:296:GLU:HG2	1:A:297:TRP:CD1	2.47	0.49
1:A:206:LEU:HD13	1:A:228:GLN:HG2	1.93	0.49
2:B:43:GLU:CD	2:B:43:GLU:H	2.21	0.49
1:A:167:TRP:HB3	1:A:450:LEU:CD2	2.42	0.49
1:A:359:GLU:OE1	1:A:366:ASN:HB2	2.13	0.49
1:A:273:THR:HA	4:A:3287:GOL:H32	1.95	0.49
1:A:13:THR:O	2:B:166:LEU:HD21	2.13	0.49
1:A:379:ASN:HD22	1:A:384:LYS:HD3	1.77	0.49
5:A:4974:P6G:C18	2:B:54:MET:HE2	2.41	0.49
3:C:14:PHE:CE2	3:C:42:ARG:HD3	2.48	0.48
1:A:197:GLU:CD	1:A:231:GLU:OE2	2.55	0.48
1:A:30:PRO:O	1:A:34:SER:HB2	2.13	0.48
1:A:463:ASP:HB2	8:A:4990:HOH:O	2.13	0.48
1:A:34:SER:O	1:A:185:SER:HB3	2.14	0.48
1:A:274:GLY:HA2	1:A:290:PHE:CG	2.49	0.48
1:A:203:MET:O	1:A:204:GLN:C	2.56	0.48
1:A:467:ALA:O	1:A:468:LEU:C	2.54	0.48
3:C:7:MET:HG2	3:C:76:THR:O	2.13	0.48
3:C:11:GLU:CG	3:C:12:ARG:HG3	2.44	0.48
3:C:63:PRO:HD2	3:C:66:MET:HB3	1.96	0.48
2:B:204:GLU:O	2:B:208:LYS:HB2	2.12	0.48
2:B:154:CYS:HB3	2:B:267:TRP:CD2	2.49	0.48
2:B:66:PRO:HG2	2:B:288:TRP:CZ2	2.49	0.47
2:B:117:TRP:NE1	2:B:247:ASP:HB2	2.29	0.47
1:A:417:TYR:O	1:A:428:PHE:HB2	2.14	0.47
1:A:103:GLU:CD	1:A:176:PHE:CD2	2.93	0.47
1:A:294:MET:HE3	1:A:294:MET:HB3	1.75	0.47
1:A:416:ASP:OD1	1:A:416:ASP:C	2.58	0.47
2:B:133:HIS:O	2:B:136:GLN:HB3	2.15	0.47
3:C:54:ARG:CG	3:C:80:ASP:HB2	2.38	0.47
1:A:127:ALA:HB2	1:A:237:GLN:NE2	2.30	0.46
1:A:131:MET:HE2	1:A:131:MET:HB3	1.68	0.46
1:A:153:ARG:NH2	8:A:4995:HOH:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:HB2	1:A:269:PHE:CZ	2.51	0.46
1:A:461:PRO:O	1:A:466:GLY:HA3	2.15	0.46
1:A:249:GLY:C	1:A:250:LYS:HG2	2.41	0.46
1:A:426:TYR:OH	1:A:445:LYS:O	2.29	0.46
1:A:103:GLU:HG3	1:A:176:PHE:CD2	2.51	0.46
1:A:339:ARG:NH1	1:A:485:TYR:OH	2.48	0.46
1:A:33:MET:SD	5:A:4974:P6G:H182	2.56	0.46
2:B:128:ALA:HB2	8:B:4436:HOH:O	2.15	0.46
1:A:368:THR:HB	1:A:408:PRO:HD2	1.98	0.46
1:A:47:TYR:C	1:A:47:TYR:CD2	2.94	0.46
1:A:317:TRP:O	1:A:320:PHE:HB3	2.15	0.46
1:A:89:TRP:CD1	1:A:93:MET:HE2	2.51	0.45
1:A:300:ALA:HB3	1:A:301:GLN:OE1	2.15	0.45
1:A:443:ARG:HA	2:B:52:LEU:HD21	1.99	0.45
1:A:364:GLY:O	1:A:365:TRP:C	2.57	0.45
3:C:50:ILE:N	3:C:84:MET:O	2.25	0.45
1:A:339:ARG:HD2	1:A:480:ASP:HA	1.98	0.45
2:B:131:LEU:O	2:B:134:ALA:HB3	2.17	0.45
1:A:395:THR:OG1	3:C:16:ILE:HG22	2.17	0.45
1:A:96:HIS:O	1:A:100[B]:TRP:HB2	2.17	0.45
2:B:245:GLU:HG3	8:B:4454:HOH:O	2.16	0.45
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.52	0.45
1:A:183:ARG:HH11	5:A:4974:P6G:C9	2.30	0.45
1:A:449:ASN:OD1	1:A:451:VAL:N	2.43	0.44
1:A:183:ARG:NH1	5:A:4974:P6G:H91	2.33	0.44
1:A:204:GLN:NE2	4:A:3287:GOL:H11	2.32	0.44
1:A:275:PRO:HD3	1:A:328:HIS:HB2	1.99	0.44
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.53	0.44
1:A:153:ARG:NH1	2:B:12:LEU:HD21	2.32	0.44
1:A:341:THR:HB	1:A:471:MET:HE1	2.00	0.44
1:A:395:THR:HG23	3:C:7:MET:HE3	1.99	0.44
2:B:77:ASP:OD2	2:B:77:ASP:C	2.59	0.44
3:C:26:THR:O	3:C:27:MET:C	2.59	0.44
1:A:21:LYS:HG2	1:A:22:TYR:CE2	2.52	0.44
1:A:39:ILE:HD13	1:A:248:ASN:HB2	1.99	0.44
1:A:113:ARG:NH1	2:B:144:GLN:HE21	2.01	0.44
3:C:13:ASP:CG	3:C:42:ARG:HH11	2.25	0.44
1:A:39:ILE:HB	1:A:44:TRP:HE1	1.83	0.44
2:B:323:TYR:CE1	2:B:327:MET:HE3	2.52	0.44
3:C:19:VAL:HG12	3:C:20:PRO:O	2.18	0.44
3:C:27:MET:HG3	3:C:62:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLU:HG3	1:A:235:ALA:HB2	2.00	0.44
1:A:258:VAL:O	1:A:262:ILE:HG13	2.17	0.44
2:B:109:HIS:HD2	2:B:248:THR:HG23	1.83	0.44
1:A:183:ARG:O	8:A:4994:HOH:O	2.21	0.44
2:B:104:LEU:HD23	2:B:104:LEU:HA	1.32	0.43
1:A:39:ILE:HB	1:A:44:TRP:NE1	2.34	0.43
1:A:134:GLU:OE2	1:A:134:GLU:HA	2.17	0.43
1:A:421:TYR:HE2	1:A:445:LYS:HE2	1.83	0.43
1:A:460:GLN:HA	1:A:461:PRO:C	2.44	0.43
2:B:263:ARG:HB2	2:B:266:ARG:NH2	2.34	0.43
2:B:283:GLU:CD	2:B:283:GLU:H	2.26	0.43
3:C:55:ARG:HD2	3:C:58:ASP:OD1	2.18	0.43
1:A:7:GLU:CD	1:A:7:GLU:H	2.26	0.43
1:A:223:LEU:CD2	1:A:224:ILE:HD13	2.47	0.43
2:B:241:LEU:O	2:B:245:GLU:HB2	2.19	0.43
1:A:179:MET:HE2	1:A:179:MET:HA	2.00	0.43
1:A:416:ASP:HB2	3:C:16:ILE:HD12	2.01	0.43
2:B:168:HIS:HD2	2:B:257:GLN:NE2	1.99	0.43
1:A:176:PHE:HB3	1:A:180:MET:HE2	1.99	0.43
1:A:314:PRO:HB3	1:A:316:TYR:CE2	2.53	0.43
1:A:334:GLY:O	1:A:338:TRP:HB2	2.19	0.43
5:A:4974:P6G:H81	5:A:4974:P6G:H111	1.42	0.43
1:A:152:SER:HB3	1:A:155:TRP:CD1	2.53	0.43
3:C:27:MET:HE2	3:C:66:MET:CG	2.49	0.43
1:A:165:ASN:HB3	1:A:170:ILE:HD11	2.01	0.43
1:A:244:ILE:O	1:A:244:ILE:HG13	2.08	0.43
1:A:293:PHE:CD2	1:A:293:PHE:C	2.97	0.43
1:A:22:TYR:CG	2:B:204:GLU:HB2	2.54	0.42
1:A:116:ARG:HG2	2:B:141:TYR:HB2	2.00	0.42
5:A:4974:P6G:H52	5:A:4974:P6G:H82	1.53	0.42
2:B:293:GLU:O	2:B:294:PRO:C	2.58	0.42
8:A:5005:HOH:O	2:B:36:HIS:HD2	2.02	0.42
1:A:121:PRO:HD2	8:A:4986:HOH:O	2.19	0.42
1:A:22:TYR:CD2	1:A:22:TYR:N	2.87	0.42
2:B:131:LEU:O	2:B:131:LEU:HD12	2.20	0.42
3:C:30:VAL:HG12	3:C:31:ALA:N	2.34	0.42
3:C:52:ARG:NH2	3:C:61:LEU:HG	2.35	0.42
1:A:299:VAL:O	1:A:303:GLU:CG	2.68	0.42
1:A:123:ASN:ND2	8:A:5006:HOH:O	2.52	0.42
1:A:418:GLN:NE2	3:C:78:THR:H	2.12	0.42
2:B:250:LEU:HD12	2:B:250:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:HB2	1:A:220:PHE:HD2	1.85	0.42
5:A:4974:P6G:H171	2:B:54:MET:HB2	2.02	0.42
2:B:108:GLY:C	2:B:111:GLN:NE2	2.78	0.42
2:B:305:SER:HB3	2:B:314:ILE:HD11	2.02	0.42
3:C:44:HIS:HA	3:C:45:PRO:HD2	1.76	0.42
1:A:183:ARG:HH11	5:A:4974:P6G:H91	1.85	0.42
1:A:411:LYS:HB3	1:A:411:LYS:NZ	2.35	0.42
5:A:4974:P6G:C18	2:B:54:MET:CE	2.98	0.42
1:A:178:ASP:O	1:A:183:ARG:HG2	2.20	0.41
2:B:190:ARG:O	2:B:194:GLU:N	2.36	0.41
2:B:145:ILE:HG23	2:B:215:TRP:CB	2.47	0.41
1:A:402:LEU:HB3	1:A:403:PRO:HD2	2.02	0.41
1:A:260:VAL:O	1:A:264:ARG:HG3	2.20	0.41
1:A:449:ASN:O	1:A:452:ASP:HB2	2.20	0.41
2:B:223:ASN:O	2:B:228:PRO:HD3	2.20	0.41
1:A:6:ARG:O	1:A:7:GLU:C	2.61	0.41
1:A:191:MET:SD	1:A:257:MET:HB3	2.61	0.41
1:A:313:LYS:NZ	8:A:5053:HOH:O	2.51	0.41
3:C:6:ILE:HD11	3:C:19:VAL:HB	2.01	0.41
1:A:396:ILE:HG22	1:A:397:CYS:O	2.21	0.41
1:A:478:MET:HG3	1:A:478:MET:H	1.72	0.41
3:C:23:THR:HA	3:C:68:VAL:CG1	2.50	0.41
1:A:2:SER:N	2:B:102:ASP:O	2.54	0.41
1:A:12:LEU:HD11	2:B:174:ARG:NH1	2.36	0.41
1:A:19:THR:HA	1:A:20:PRO:HD2	1.83	0.41
1:A:297:TRP:HA	1:A:301:GLN:HE22	1.86	0.41
1:A:68:GLY:O	1:A:71:SER:HB2	2.21	0.41
2:B:250:LEU:O	2:B:251:GLY:C	2.59	0.41
1:A:153:ARG:CZ	2:B:12:LEU:HD21	2.52	0.40
1:A:400:CYS:O	1:A:401:ASN:HB2	2.22	0.40
1:A:402:LEU:HB3	1:A:403:PRO:CD	2.51	0.40
1:A:325:ASP:O	1:A:329:HIS:HD2	2.04	0.40
1:A:201:THR:O	1:A:205:PHE:HB2	2.22	0.40
1:A:398:ASN:ND2	1:A:427:HIS:H	2.16	0.40
1:A:127:ALA:CB	1:A:237:GLN:HE22	2.34	0.40
3:C:26:THR:OG1	3:C:29:GLN:CD	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	490/498 (98%)	442 (90%)	44 (9%)	4 (1%)	16 12
2	B	320/330 (97%)	292 (91%)	25 (8%)	3 (1%)	14 10
3	C	81/86 (94%)	70 (86%)	9 (11%)	2 (2%)	4 1
All	All	891/914 (98%)	804 (90%)	78 (9%)	9 (1%)	12 9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	GLU
1	A	287	ASN
2	B	310	GLY
1	A	408	PRO
1	A	445	LYS
2	B	327	MET
3	C	77	GLU
2	B	22	ARG
3	C	31	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	418/422 (99%)	388 (93%)	30 (7%)	13 11
2	B	274/282 (97%)	248 (90%)	26 (10%)	8 5
3	C	77/79 (98%)	62 (80%)	15 (20%)	1 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	769/783 (98%)	698 (91%)	71 (9%)	8 6

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	7	GLU
1	A	21	LYS
1	A	34	SER
1	A	77	GLU
1	A	206	LEU
1	A	214	GLU
1	A	223	LEU
1	A	224	ILE
1	A	226	SER
1	A	228	GLN
1	A	233	ARG
1	A	243	LYS
1	A	244	ILE
1	A	256	GLN
1	A	257	MET
1	A	276	ILE
1	A	280	TYR
1	A	283	LEU
1	A	287	ASN
1	A	303	GLU
1	A	305	GLN
1	A	307	LEU
1	A	309	LEU
1	A	407	THR
1	A	411	LYS
1	A	419	LEU
1	A	464	LEU
1	A	477	VAL
1	A	478	MET
2	B	13	LYS
2	B	22	ARG
2	B	23	ARG
2	B	24	ARG
2	B	43	GLU
2	B	77	ASP
2	B	89	LEU

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Mol	Chain	Res	Type
2	B	100	LEU
2	B	107	ARG
2	B	109	HIS
2	B	111	GLN
2	B	113	LEU
2	B	116	GLU
2	B	140	VAL
2	B	188	ARG
2	B	200	GLN
2	B	220	THR
2	B	240	SER
2	B	248	THR
2	B	258	LYS
2	B	278	LYS
2	B	279	GLU
2	B	284	VAL
2	B	293	GLU
2	B	298	LYS
2	B	300	ILE
3	C	3	THR
3	C	5	PRO
3	C	6	ILE
3	C	12	ARG
3	C	25	ASP
3	C	26	THR
3	C	29	GLN
3	C	30	VAL
3	C	50	ILE
3	C	66	MET
3	C	67	ILE
3	C	70	ASP
3	C	76	THR
3	C	84	MET
3	C	85	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	139	GLN
1	A	237	GLN
1	A	305	GLN

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Mol	Chain	Res	Type
1	A	379	ASN
1	A	398	ASN
1	A	418	GLN
1	A	427	HIS
2	B	34	ASN
2	B	36	HIS
2	B	87	ASN
2	B	105	ASN
2	B	109	HIS
2	B	111	GLN
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
2	B	223	ASN
2	B	326	GLN
3	C	40	ASN
3	C	56	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	GOL	A	4975	6	5,5,5	1.07	0	5,5,5	1.86	2 (40%)
7	MPO	B	4401	-	13,13,13	3.15	7 (53%)	17,17,17	4.01	10 (58%)
5	P6G	A	4974	-	18,18,18	1.49	3 (16%)	17,17,17	1.28	3 (17%)
4	GOL	A	3287	-	5,5,5	0.40	0	5,5,5	1.00	0

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
4	GOL	A	4975	6	-	2/4/4/4	-
7	MPO	B	4401	-	-	5/7/15/15	0/1/1/1
5	P6G	A	4974	-	-	12/16/16/16	-
4	GOL	A	3287	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4401	MPO	O2-S1	5.48	1.60	1.45
7	B	4401	MPO	C4-N1	-5.46	1.32	1.46
7	B	4401	MPO	C4-C5	-4.19	1.34	1.50
7	B	4401	MPO	O1-S1	4.08	1.56	1.45
5	A	4974	P6G	O19-C18	-3.78	1.22	1.42
7	B	4401	MPO	C3-N1	3.09	1.54	1.47
7	B	4401	MPO	C1-S1	-2.94	1.73	1.77
5	A	4974	P6G	C15-C14	2.35	1.60	1.49
7	B	4401	MPO	C2-C3	2.21	1.60	1.51
5	A	4974	P6G	O13-C14	2.18	1.51	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	4401	MPO	O2-S1-C1	7.69	118.35	106.73
7	B	4401	MPO	C5-C4-N1	7.52	121.54	110.12
7	B	4401	MPO	O3-S1-O2	-6.25	95.76	111.40
7	B	4401	MPO	C7-N1-C4	4.65	118.85	108.84
7	B	4401	MPO	C3-C2-C1	4.42	127.90	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	4401	MPO	C6-O4-C5	4.25	123.63	109.88
7	B	4401	MPO	C3-N1-C4	4.09	122.14	111.24
7	B	4401	MPO	C2-C1-S1	4.03	119.42	113.25
7	B	4401	MPO	C3-N1-C7	2.91	119.00	111.24
4	A	4975	GOL	O2-C2-C3	2.87	121.06	109.18
7	B	4401	MPO	O4-C6-C7	-2.79	105.77	111.77
5	A	4974	P6G	O16-C15-C14	2.55	121.96	110.35
5	A	4974	P6G	O16-C17-C18	2.41	120.71	110.11
4	A	4975	GOL	O2-C2-C1	2.38	119.04	109.18
5	A	4974	P6G	O19-C18-C17	2.25	125.06	111.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

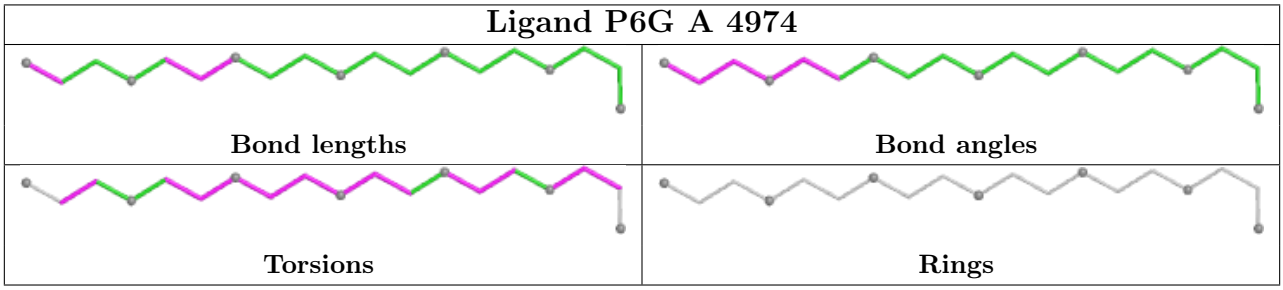
Mol	Chain	Res	Type	Atoms
4	A	4975	GOL	C1-C2-C3-O3
4	A	3287	GOL	O1-C1-C2-C3
5	A	4974	P6G	C8-C9-O10-C11
7	B	4401	MPO	C2-C3-N1-C4
5	A	4974	P6G	C5-C6-O7-C8
5	A	4974	P6G	O13-C14-C15-O16
5	A	4974	P6G	O7-C8-C9-O10
5	A	4974	P6G	O16-C17-C18-O19
5	A	4974	P6G	O1-C2-C3-O4
5	A	4974	P6G	C15-C14-O13-C12
4	A	4975	GOL	O2-C2-C3-O3
4	A	3287	GOL	O1-C1-C2-O2
5	A	4974	P6G	O10-C11-C12-O13
7	B	4401	MPO	C2-C1-S1-O3
7	B	4401	MPO	C2-C1-S1-O1
7	B	4401	MPO	C2-C1-S1-O2
5	A	4974	P6G	C11-C12-O13-C14
5	A	4974	P6G	O4-C5-C6-O7
5	A	4974	P6G	C2-C3-O4-C5
4	A	3287	GOL	O2-C2-C3-O3
7	B	4401	MPO	C1-C2-C3-N1
5	A	4974	P6G	C12-C11-O10-C9

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4975	GOL	2	0
7	B	4401	MPO	2	0
5	A	4974	P6G	19	0
4	A	3287	GOL	2	0

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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	A	491/498 (98%)	0.57	22 (4%) 38 40	23, 50, 65, 81	1 (0%)
2	B	322/330 (97%)	0.40	6 (1%) 66 69	33, 45, 65, 92	0
3	C	83/86 (96%)	1.39	17 (20%) 2 3	48, 63, 78, 85	0
All	All	896/914 (98%)	0.58	45 (5%) 34 36	23, 49, 69, 92	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	85	ASP	3.8
3	C	3	THR	3.7
2	B	329	GLY	3.5
3	C	67	ILE	3.4
3	C	82	ILE	2.9
3	C	62	PHE	2.9
1	A	100[A]	TRP	2.9
3	C	43	VAL	2.9
1	A	51	TYR	2.9
1	A	409	GLY	2.9
1	A	393	LEU	2.8
2	B	8	ALA	2.7
3	C	79	LEU	2.6
3	C	63	PRO	2.6
3	C	50	ILE	2.6
1	A	421	TYR	2.6
1	A	408	PRO	2.6
1	A	381	VAL	2.5
2	B	23	ARG	2.5
1	A	490	ALA	2.4
3	C	59	GLY	2.4
3	C	47	PRO	2.4
1	A	249	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	72	GLY	2.3
3	C	73	LEU	2.3
1	A	362	TYR	2.3
1	A	389	VAL	2.2
1	A	350	VAL	2.2
1	A	488	VAL	2.2
1	A	283	LEU	2.2
2	B	88	LEU	2.2
1	A	383	GLY	2.2
3	C	83	PHE	2.1
3	C	12	ARG	2.1
1	A	317	TRP	2.1
1	A	476	GLY	2.1
2	B	246	GLY	2.1
1	A	244	ILE	2.1
3	C	61	LEU	2.1
1	A	79	ASP	2.1
1	A	304	ARG	2.1
2	B	24	ARG	2.1
3	C	68	VAL	2.1
1	A	311	LEU	2.0
1	A	314	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 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, 95^{th} 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
7	MPO	B	4401	13/13	0.76	0.18	60,66,72,77	0

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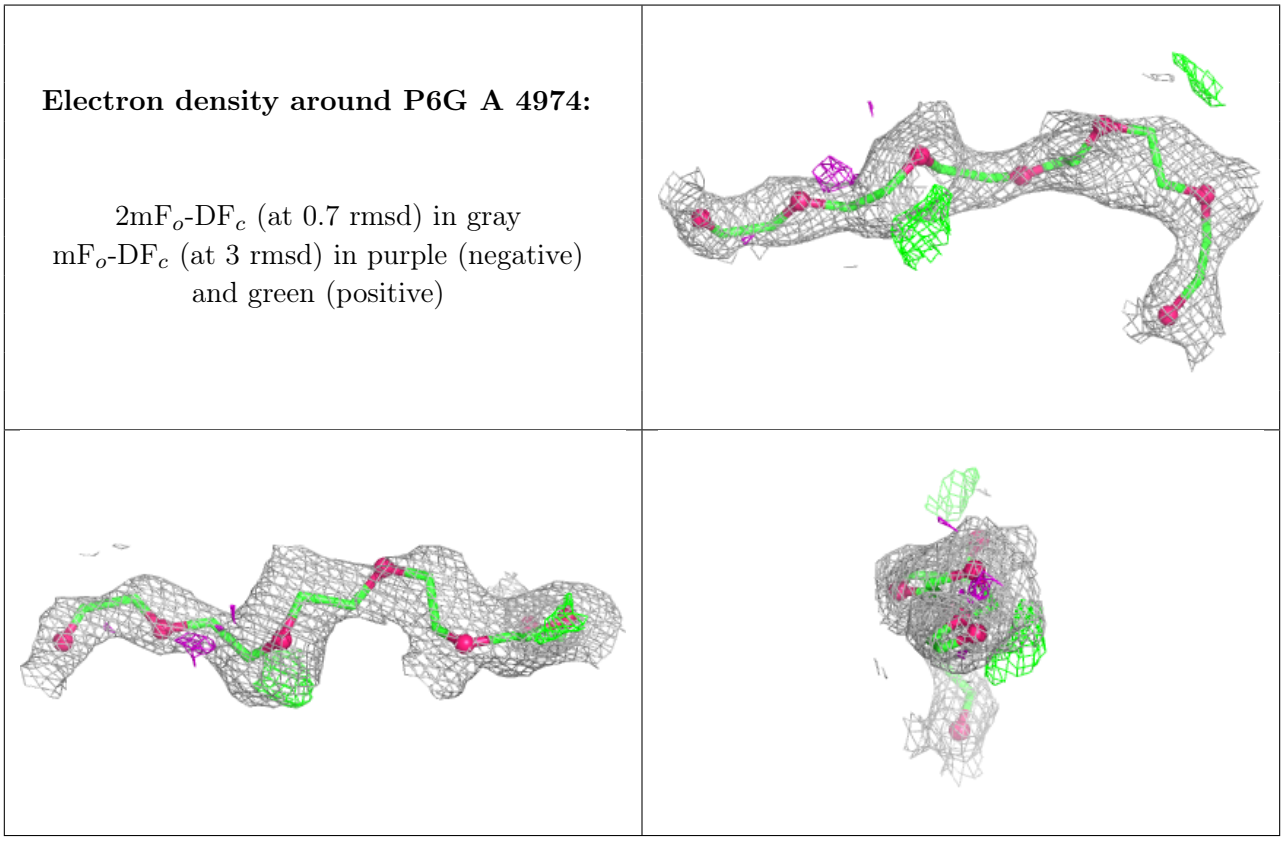
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	P6G	A	4974	19/19	0.86	0.15	47,56,72,76	0
4	GOL	A	3287	6/6	0.88	0.15	83,87,88,89	0
4	GOL	A	4975	6/6	0.95	0.13	43,57,61,65	0
6	FE	A	500	1/1	0.99	0.02	45,45,45,45	0
6	FE	A	499	1/1	1.00	0.01	39,39,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6G A 4974:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.