Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 12:25 PM EDT

PDB ID	:	5REQ / pdb_00005req
Title	:	Methylmalonyl-COA MUTASE, Y89F Mutant, substrate complex
Authors	:	Evans, P.R.; Thomae, N.H.
Deposited on	:	1998-08-03
Resolution	:	2.20 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 (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:

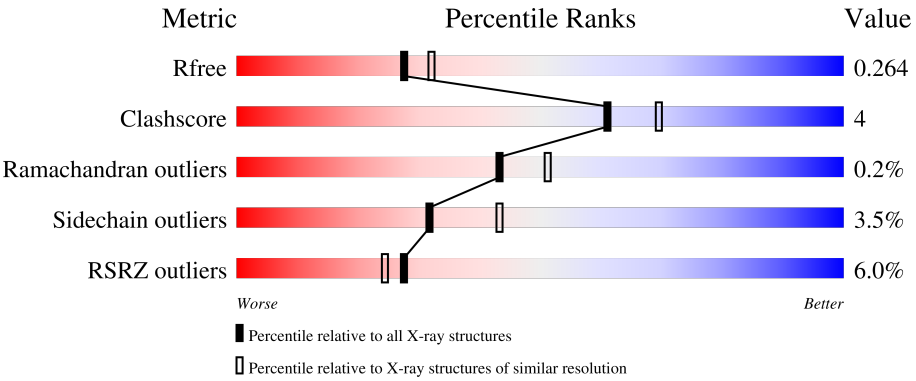
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	727	2% 69% 27%
1	C	727	4% 69% 26% 5%
2	B	637	7% 69% 25%
2	D	637	12% 72% 22%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22112 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 PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	5574	3526	966	1058	24	0	0	0
1	C	725	Total 5574	C 3526	N 966	O 1058	S 24	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PHE	TYR	engineered mutation	UNP P11653
C	89	PHE	TYR	engineered mutation	UNP P11653

- Molecule 2 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT).

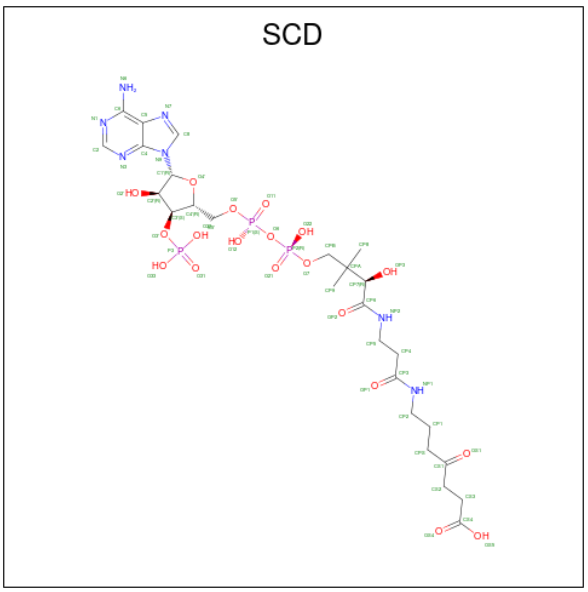
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	4722	2976	821	912	13	0	0	0
2	D	619	Total 4722	C 2976	N 821	O 912	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

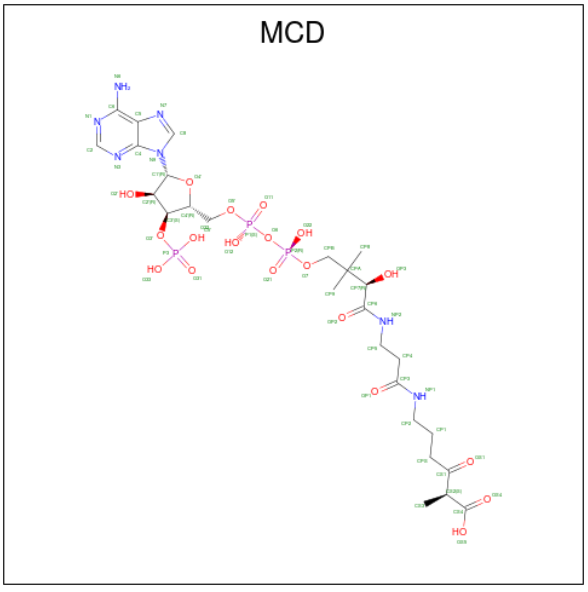
- Molecule 3 is SUCCINYL(CARBADETHIA)-COENZYME A (CCD ID: SCD) (formula:

$C_{26}H_{42}N_7O_{19}P_3$).



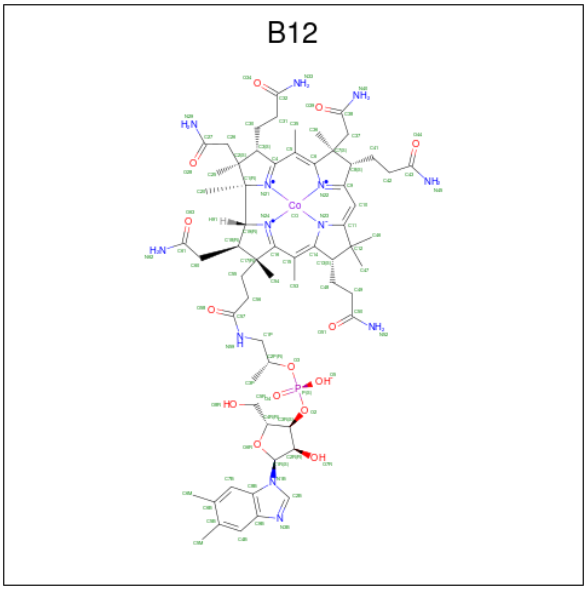
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			55	26	7	19	3		
3	C	1	Total	C	N	O	P	0	1
			55	26	7	19	3		

- Molecule 4 is METHYLMALONYL(CARBADETHIA)-COENZYME A (CCD ID: MCD) (formula: $C_{26}H_{42}N_7O_{19}P_3$).



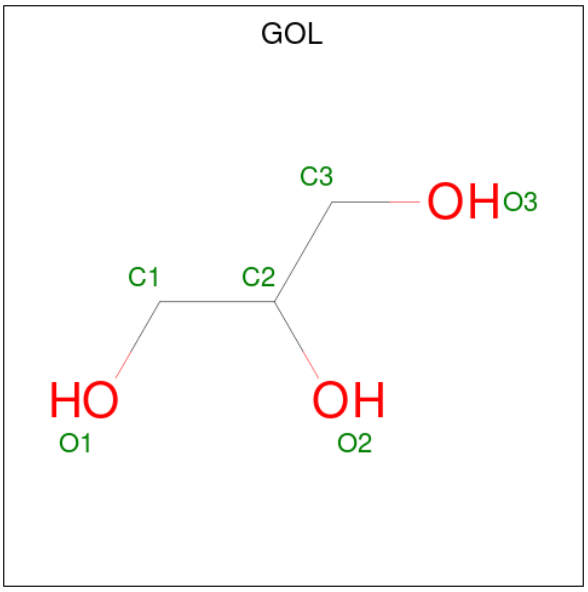
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			55	26	7	19	3		
4	C	1	Total	C	N	O	P	0	1
			55	26	7	19	3		

- Molecule 5 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
5	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	356	Total O 356 356	0	0
7	B	192	Total O 192 192	0	0
7	C	353	Total O 353 353	0	0
7	D	193	Total O 193 193	0	0

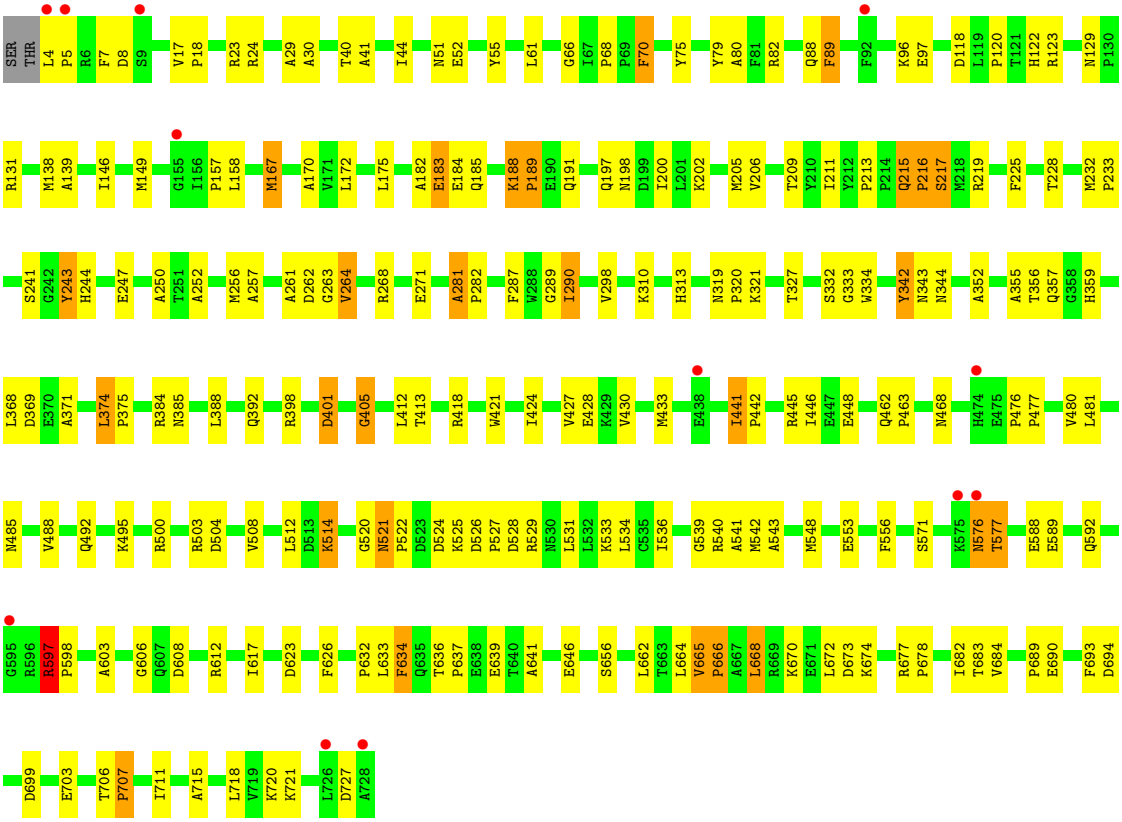
3 Residue-property plots (i)

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: PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT)

Chain A:

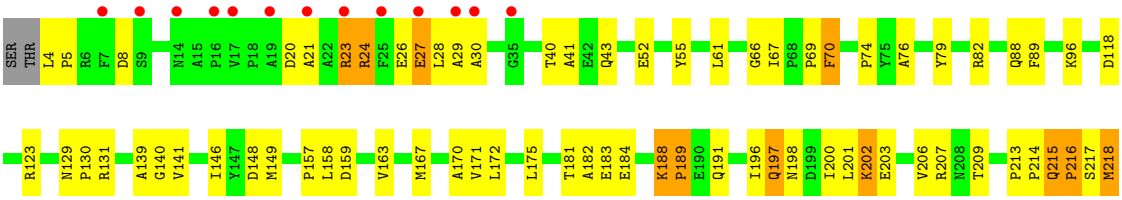


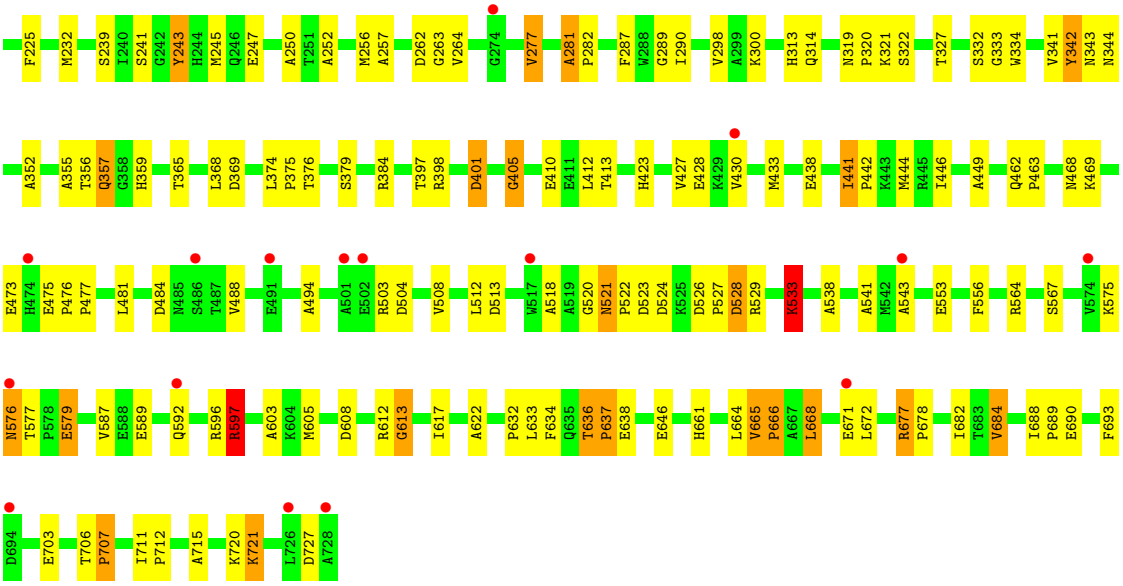


• Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT)

Chain C:

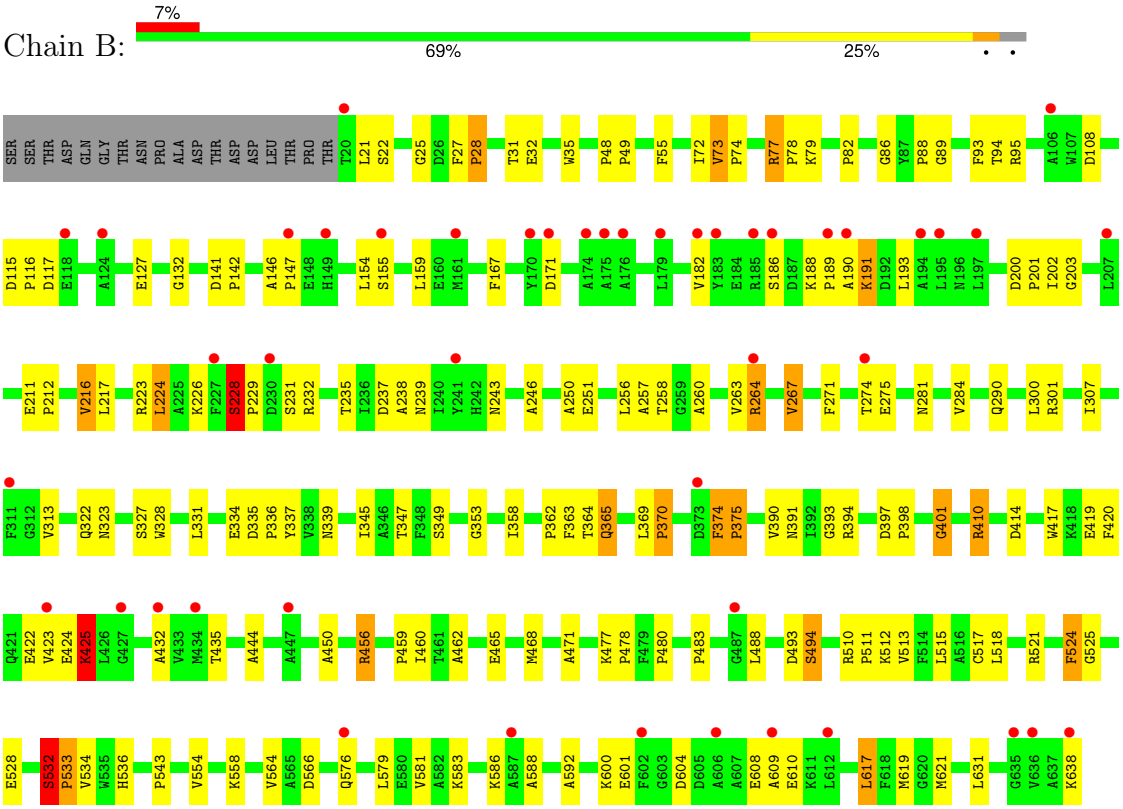






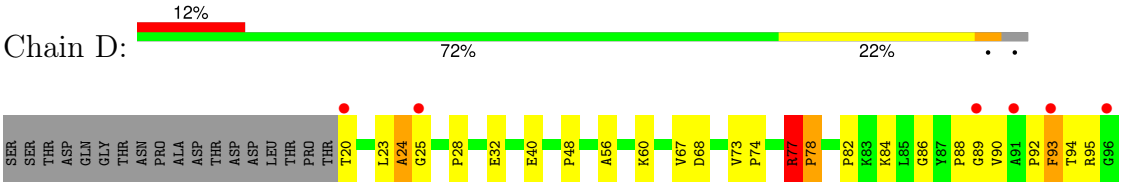
• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT)

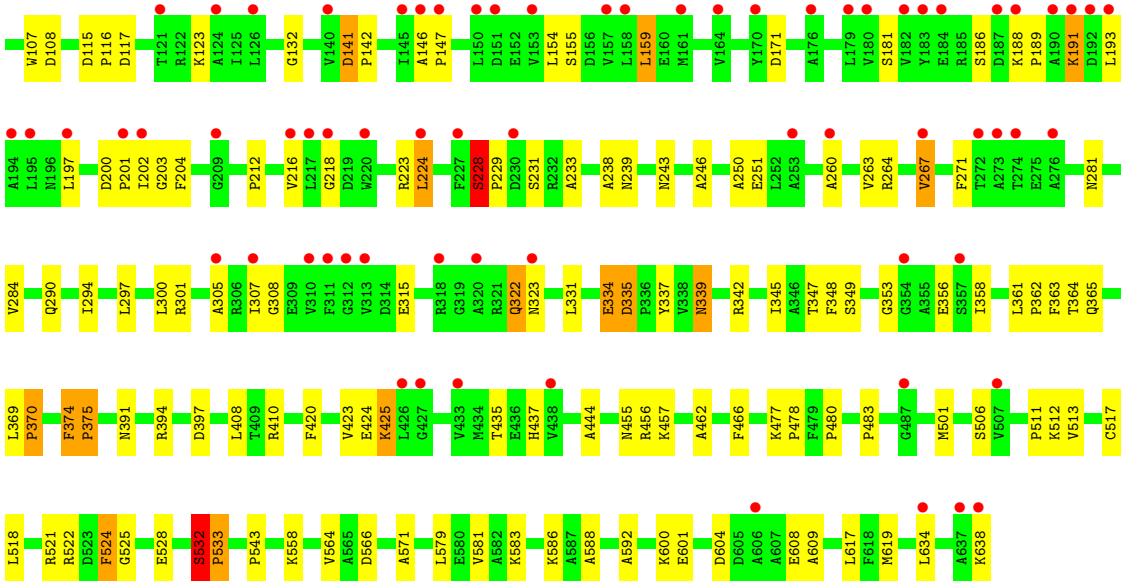
Chain B:



• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT)

Chain D:




W107 D108 D115 P116 D117 T121 R122 K123 A124 I125 L126 G132 V140 D141 P142 I145 A146 P147 L150 D151 E152 V153 L154 S155 D156 V157 L158 L159 E160 M161 V164 Y170 D171 A176 L179 V180 S181 V182 Y183 E184 R185 S186 D187 K188 P189 A190 K191 D192 L193
A194 L195 N196 L197 D200 P201 I202 G203 F204 Q209 P212 V216 L217 G218 D219 W220 R223 L224 F227 S228 P229 D230 S231 R232 A233 A238 N239 N243 A246 A250 E251 L252 A253 A260 V263 R264 V267 F271 T272 A273 T274 E275 A276 N281
V284 Q290 I294 L297 L300 R301 A305 R306 I307 G308 E309 V310 F311 G312 V313 D314 E315 H318 G319 A320 R321 Q322 N323 L331 E334 D335 P336 Y337 V338 N339 R342 I345 A346 T347 F348 S349 G353 G354 A355 E356 S357 I358 L361 P362 F363 T364 Q365
L369 P370 F374 P375 N391 R394 D397 L408 T409 R410 F420 V423 E424 K425 L426 G427 V433 M434 T435 E436 H437 V438 A444 N455 R456 K457 A462 F466 K477 P478 F479 P480 P483 G487 M501 S506 V507 P511 K512 V513 C517
L518 R521 R522 D523 F524 G525 E528 S532 P533 P543 K558 V564 A565 D566 A571 L579 E580 V581 A582 K583 K586 A587 A588 A592 K600 E601 D604 D605 A606 A607 E608 A609 L617 F618 M619 L634 A637 K638

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.20Å 161.89Å 88.70Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.8 (20.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.292 0.230 , 0.264	Depositor DCC
R_{free} test set	8387 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22112	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: MCD, SCD, B12, GOL

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	0.63	0/5691	2.19	293/7728 (3.8%)
1	C	0.64	0/5691	2.19	290/7728 (3.8%)
2	B	0.56	0/4812	2.04	224/6533 (3.4%)
2	D	0.55	0/4812	2.03	196/6533 (3.0%)
All	All	0.60	0/21006	2.12	1003/28522 (3.5%)

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	9
1	C	0	12
2	B	0	2
2	D	0	4
All	All	0	27

There are no bond length outliers.

All (1003) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	ARG	CD-NE-CZ	18.37	150.12	124.40
1	C	384	ARG	CD-NE-CZ	12.37	141.72	124.40
2	B	77	ARG	CD-NE-CZ	12.03	141.24	124.40
1	A	576	ASN	CA-CB-CG	11.68	124.28	112.60
1	C	41	ALA	CA-C-N	11.67	140.21	120.72
1	C	41	ALA	C-N-CA	11.67	140.21	120.72
2	D	77	ARG	CD-NE-CZ	11.32	140.24	124.40
1	C	597	ARG	CD-NE-CZ	11.30	140.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	597	ARG	CD-NE-CZ	11.18	140.05	124.40
1	C	462	GLN	CA-C-O	10.68	126.23	119.29
1	C	333	GLY	O-C-N	-10.51	112.09	122.18
1	A	70	PHE	CA-CB-CG	10.39	124.19	113.80
1	C	690	GLU	CA-C-N	9.96	133.63	120.28
1	C	690	GLU	C-N-CA	9.96	133.63	120.28
1	C	596	ARG	CD-NE-CZ	9.92	138.29	124.40
1	C	476	PRO	N-CA-CB	9.67	108.60	103.19
1	A	690	GLU	CA-C-N	9.59	135.94	120.60
1	A	690	GLU	C-N-CA	9.59	135.94	120.60
2	D	335	ASP	CA-CB-CG	9.55	122.15	112.60
1	A	319	ASN	CA-C-O	9.44	126.31	119.32
1	A	693	PHE	CA-CB-CG	9.41	123.21	113.80
1	C	576	ASN	CA-CB-CG	9.33	121.93	112.60
1	C	225	PHE	CA-CB-CG	9.28	123.08	113.80
1	A	41	ALA	CA-C-N	9.00	139.12	121.58
1	A	41	ALA	C-N-CA	9.00	139.12	121.58
2	B	524	PHE	CA-CB-CG	8.94	122.74	113.80
1	A	333	GLY	O-C-N	-8.93	113.61	122.18
2	D	238	ALA	CA-C-N	8.84	133.74	120.31
2	D	238	ALA	C-N-CA	8.84	133.74	120.31
1	C	693	PHE	CA-CB-CG	8.75	122.55	113.80
1	C	89	PHE	CA-CB-CG	8.73	122.53	113.80
1	A	287	PHE	CA-CB-CG	8.72	122.52	113.80
2	B	601	GLU	CA-C-N	8.67	138.49	121.58
2	B	601	GLU	C-N-CA	8.67	138.49	121.58
1	C	423	HIS	CA-CB-CG	8.66	122.46	113.80
1	C	287	PHE	CA-CB-CG	8.63	122.44	113.80
2	B	238	ALA	CA-C-N	8.63	132.71	120.28
2	B	238	ALA	C-N-CA	8.63	132.71	120.28
2	D	524	PHE	CA-CB-CG	8.53	122.33	113.80
1	C	727	ASP	CA-CB-CG	8.42	121.02	112.60
2	B	93	PHE	CA-C-N	8.30	131.74	120.54
2	B	93	PHE	C-N-CA	8.30	131.74	120.54
1	A	384	ARG	CD-NE-CZ	8.27	135.98	124.40
2	D	93	PHE	CA-C-N	8.21	131.12	120.44
2	D	93	PHE	C-N-CA	8.21	131.12	120.44
2	B	339	ASN	CA-C-N	8.20	130.89	120.56
2	B	339	ASN	C-N-CA	8.20	130.89	120.56
2	D	337	TYR	CA-C-N	8.16	133.36	120.47
2	D	337	TYR	C-N-CA	8.16	133.36	120.47
1	A	313	HIS	CA-C-N	8.11	131.49	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	HIS	C-N-CA	8.11	131.49	120.38
2	D	339	ASN	CA-C-N	8.10	131.05	120.60
2	D	339	ASN	C-N-CA	8.10	131.05	120.60
2	D	528	GLU	CA-C-N	8.05	128.92	119.98
2	D	528	GLU	C-N-CA	8.05	128.92	119.98
2	B	117	ASP	CA-CB-CG	8.04	120.64	112.60
2	B	78	PRO	CA-C-N	8.00	133.40	120.60
2	B	78	PRO	C-N-CA	8.00	133.40	120.60
2	B	600	LYS	CA-C-N	7.98	134.05	120.72
2	B	600	LYS	C-N-CA	7.98	134.05	120.72
2	D	521	ARG	CA-C-N	7.94	131.25	120.38
2	D	521	ARG	C-N-CA	7.94	131.25	120.38
2	B	32	GLU	CA-C-N	7.87	131.16	120.54
2	B	32	GLU	C-N-CA	7.87	131.16	120.54
1	C	313	HIS	CA-C-N	7.84	131.83	120.38
1	C	313	HIS	C-N-CA	7.84	131.83	120.38
2	B	369	LEU	CA-C-O	7.82	126.76	120.19
2	B	86	GLY	O-C-N	-7.82	114.39	122.60
2	B	335	ASP	CA-CB-CG	7.81	120.41	112.60
2	B	154	LEU	CA-C-N	7.80	130.73	120.28
2	B	154	LEU	C-N-CA	7.80	130.73	120.28
1	A	333	GLY	CA-C-N	7.79	131.05	120.38
1	A	333	GLY	C-N-CA	7.79	131.05	120.38
2	D	307	ILE	CA-C-N	7.79	128.75	120.03
2	D	307	ILE	C-N-CA	7.79	128.75	120.03
1	C	52	GLU	N-CA-C	7.78	122.45	113.19
1	C	149	MET	CA-C-N	7.77	130.54	120.44
1	C	149	MET	C-N-CA	7.77	130.54	120.44
1	C	183	GLU	O-C-N	-7.72	114.06	122.09
2	D	601	GLU	CA-C-N	7.71	136.62	121.58
2	D	601	GLU	C-N-CA	7.71	136.62	121.58
1	A	369	ASP	CA-C-N	7.65	130.87	120.38
1	A	369	ASP	C-N-CA	7.65	130.87	120.38
1	A	699	ASP	CA-CB-CG	7.65	120.25	112.60
1	C	213	PRO	CA-C-N	7.65	127.20	119.24
1	C	213	PRO	C-N-CA	7.65	127.20	119.24
1	A	149	MET	CA-C-N	7.63	130.36	120.44
1	A	149	MET	C-N-CA	7.63	130.36	120.44
1	C	41	ALA	O-C-N	-7.62	113.31	122.22
1	A	327	THR	N-CA-C	7.61	121.52	109.50
1	A	334	TRP	CA-C-N	7.60	131.23	120.28
1	A	334	TRP	C-N-CA	7.60	131.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	633	LEU	CA-C-N	7.59	134.96	123.05
1	C	633	LEU	C-N-CA	7.59	134.96	123.05
1	A	526	ASP	CA-CB-CG	7.51	120.11	112.60
2	D	466	PHE	CA-C-O	7.51	126.27	120.26
2	B	239	ASN	CA-C-N	7.49	129.99	120.56
2	B	239	ASN	C-N-CA	7.49	129.99	120.56
1	C	184	GLU	CA-C-N	7.49	134.84	121.66
1	C	184	GLU	C-N-CA	7.49	134.84	121.66
2	B	202	ILE	CA-C-N	7.47	128.27	119.98
2	B	202	ILE	C-N-CA	7.47	128.27	119.98
1	A	79	TYR	CA-C-N	7.46	130.28	120.28
1	A	79	TYR	C-N-CA	7.46	130.28	120.28
1	A	633	LEU	O-C-N	-7.46	113.55	122.65
1	C	55	TYR	N-CA-C	7.44	121.46	112.38
2	D	89	GLY	CA-C-N	7.44	133.42	122.71
2	D	89	GLY	C-N-CA	7.44	133.42	122.71
2	D	600	LYS	CA-C-N	7.43	134.15	121.14
2	D	600	LYS	C-N-CA	7.43	134.15	121.14
1	A	146	ILE	CA-C-N	7.42	130.55	120.54
1	A	146	ILE	C-N-CA	7.42	130.55	120.54
1	C	319	ASN	CA-C-O	7.39	125.72	119.66
1	C	521	ASN	CA-CB-CG	7.38	119.98	112.60
1	A	727	ASP	CA-CB-CG	7.37	119.97	112.60
1	C	333	GLY	CA-C-N	7.36	130.47	120.38
1	C	333	GLY	C-N-CA	7.36	130.47	120.38
1	C	677	ARG	O-C-N	-7.35	114.92	121.17
2	D	78	PRO	CA-C-N	7.34	132.34	120.60
2	D	78	PRO	C-N-CA	7.34	132.34	120.60
1	C	320	PRO	CA-C-N	7.33	130.83	120.28
1	C	320	PRO	C-N-CA	7.33	130.83	120.28
1	C	216	PRO	CA-C-N	7.30	130.07	120.28
1	C	216	PRO	C-N-CA	7.30	130.07	120.28
1	A	424	ILE	CA-C-N	7.28	129.91	120.44
1	A	424	ILE	C-N-CA	7.28	129.91	120.44
1	A	526	ASP	CA-C-O	7.26	126.44	119.62
2	B	424	GLU	CA-C-N	7.24	130.71	120.28
2	B	424	GLU	C-N-CA	7.24	130.71	120.28
1	A	89	PHE	CA-CB-CG	7.23	121.03	113.80
1	A	678	PRO	CA-C-N	7.22	132.96	120.68
1	A	678	PRO	C-N-CA	7.22	132.96	120.68
1	A	398	ARG	N-CA-C	7.21	120.00	111.71
1	C	209	THR	N-CA-CB	7.21	121.99	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	PRO	CA-C-N	7.20	130.65	120.28
1	A	320	PRO	C-N-CA	7.20	130.65	120.28
1	C	369	ASP	CA-C-N	7.20	130.24	120.38
1	C	369	ASP	C-N-CA	7.20	130.24	120.38
2	D	132	GLY	N-CA-C	7.19	124.89	115.40
1	C	319	ASN	CA-C-N	7.19	126.81	119.19
1	C	319	ASN	C-N-CA	7.19	126.81	119.19
1	A	343	ASN	CA-C-N	7.17	129.90	120.28
1	A	343	ASN	C-N-CA	7.17	129.90	120.28
1	C	61	LEU	N-CA-C	7.17	121.47	112.87
1	A	633	LEU	CA-C-N	7.14	132.75	122.40
1	A	633	LEU	C-N-CA	7.14	132.75	122.40
2	D	154	LEU	CA-C-N	7.14	129.84	120.28
2	D	154	LEU	C-N-CA	7.14	129.84	120.28
2	B	95	ARG	N-CA-C	7.13	119.91	111.71
1	A	225	PHE	CA-CB-CG	7.10	120.90	113.80
1	A	342	TYR	CA-C-N	7.08	131.08	120.31
1	A	342	TYR	C-N-CA	7.08	131.08	120.31
1	C	375	PRO	N-CA-CB	7.08	109.51	103.35
1	C	82	ARG	CD-NE-CZ	7.07	134.30	124.40
2	B	228	SER	CA-C-N	7.07	126.70	119.56
2	B	228	SER	C-N-CA	7.07	126.70	119.56
1	C	327	THR	N-CA-C	7.07	121.05	109.24
2	D	363	PHE	CA-CB-CG	7.06	120.86	113.80
2	B	401	GLY	O-C-N	-7.01	115.36	122.65
1	A	662	LEU	N-CA-C	6.98	120.69	111.75
1	C	334	TRP	CA-C-N	6.98	131.77	120.60
1	C	334	TRP	C-N-CA	6.98	131.77	120.60
2	B	89	GLY	CA-C-N	6.98	132.76	122.71
2	B	89	GLY	C-N-CA	6.98	132.76	122.71
1	A	206	VAL	CB-CA-C	-6.96	99.87	111.29
1	A	526	ASP	CA-C-N	6.95	126.93	119.28
1	A	526	ASP	C-N-CA	6.95	126.93	119.28
1	A	577	THR	CA-C-N	6.94	126.46	119.24
1	A	577	THR	C-N-CA	6.94	126.46	119.24
1	C	130	PRO	CA-C-N	6.93	130.26	120.28
1	C	130	PRO	C-N-CA	6.93	130.26	120.28
1	C	298	VAL	O-C-N	-6.93	115.12	121.91
1	C	633	LEU	O-C-N	-6.89	114.25	122.65
2	B	511	PRO	N-CA-CB	6.88	109.44	103.31
1	C	24	ARG	CD-NE-CZ	6.88	134.03	124.40
2	B	28	PRO	N-CA-CB	6.88	109.33	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	241	SER	N-CA-C	6.87	121.03	109.76
2	D	146	ALA	CA-C-N	6.84	126.81	119.28
2	D	146	ALA	C-N-CA	6.84	126.81	119.28
1	C	677	ARG	CA-CB-CG	6.84	127.79	114.10
2	B	301	ARG	CA-C-O	-6.83	113.31	120.55
2	D	322	GLN	CA-C-O	6.83	127.87	120.43
1	A	52	GLU	CA-C-N	6.83	132.12	120.72
1	A	52	GLU	C-N-CA	6.83	132.12	120.72
1	A	209	THR	N-CA-CB	6.82	121.43	111.54
2	D	117	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	673	ASP	CA-C-N	6.82	130.34	120.38
1	A	673	ASP	C-N-CA	6.82	130.34	120.38
1	C	678	PRO	CA-C-N	6.80	132.24	120.68
1	C	678	PRO	C-N-CA	6.80	132.24	120.68
2	D	267	VAL	CA-C-N	6.79	129.94	120.29
2	D	267	VAL	C-N-CA	6.79	129.94	120.29
2	D	543	PRO	N-CA-CB	6.79	109.25	103.35
1	A	334	TRP	O-C-N	-6.77	114.94	122.12
2	D	24	ALA	CA-C-N	6.75	132.35	120.74
2	D	24	ALA	C-N-CA	6.75	132.35	120.74
2	B	528	GLU	CA-C-N	6.74	127.46	119.98
2	B	528	GLU	C-N-CA	6.74	127.46	119.98
1	C	526	ASP	CA-C-N	6.72	126.34	119.56
1	C	526	ASP	C-N-CA	6.72	126.34	119.56
2	D	423	VAL	CA-C-N	6.71	129.28	120.28
2	D	423	VAL	C-N-CA	6.71	129.28	120.28
2	D	239	ASN	CA-C-N	6.71	129.25	120.60
2	D	239	ASN	C-N-CA	6.71	129.25	120.60
1	C	707	PRO	N-CA-CB	6.71	109.15	103.25
2	D	525	GLY	CA-C-N	6.70	127.56	119.99
2	D	525	GLY	C-N-CA	6.70	127.56	119.99
2	B	423	VAL	CA-C-N	6.69	129.25	120.28
2	B	423	VAL	C-N-CA	6.69	129.25	120.28
1	A	183	GLU	O-C-N	-6.69	115.13	122.09
2	D	32	GLU	CA-C-N	6.66	129.54	120.54
2	D	32	GLU	C-N-CA	6.66	129.54	120.54
2	D	48	PRO	CA-C-N	6.66	126.61	119.28
2	D	48	PRO	C-N-CA	6.66	126.61	119.28
1	A	216	PRO	CA-C-N	6.66	129.20	120.28
1	A	216	PRO	C-N-CA	6.66	129.20	120.28
2	D	353	GLY	CA-C-N	6.65	131.69	120.91
2	D	353	GLY	C-N-CA	6.65	131.69	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	243	TYR	CA-C-N	6.64	129.18	120.28
1	C	243	TYR	C-N-CA	6.64	129.18	120.28
1	A	243	TYR	CA-C-N	6.63	129.46	120.38
1	A	243	TYR	C-N-CA	6.63	129.46	120.38
1	C	5	PRO	N-CA-CB	6.62	109.21	103.31
1	A	641	ALA	CA-C-N	6.61	129.04	120.44
1	A	641	ALA	C-N-CA	6.61	129.04	120.44
2	B	146	ALA	CA-C-N	6.60	126.54	119.28
2	B	146	ALA	C-N-CA	6.60	126.54	119.28
1	A	241	SER	N-CA-C	6.60	120.59	109.76
2	D	462	ALA	CA-C-N	6.59	133.83	121.97
2	D	462	ALA	C-N-CA	6.59	133.83	121.97
1	A	612	ARG	CA-C-N	6.58	127.24	119.94
1	A	612	ARG	C-N-CA	6.58	127.24	119.94
1	A	626	PHE	CA-CB-CG	6.58	120.38	113.80
2	B	77	ARG	CA-C-N	6.58	126.82	119.32
2	B	77	ARG	C-N-CA	6.58	126.82	119.32
2	B	48	PRO	CA-C-N	6.55	126.49	119.28
2	B	48	PRO	C-N-CA	6.55	126.49	119.28
1	A	52	GLU	N-CA-C	6.55	120.73	112.87
2	D	420	PHE	CA-CB-CG	6.55	120.35	113.80
1	C	334	TRP	O-C-N	-6.54	115.19	122.12
1	A	388	LEU	CA-C-N	6.54	128.94	120.44
1	A	388	LEU	C-N-CA	6.54	128.94	120.44
2	D	370	PRO	N-CA-CB	6.53	108.99	103.25
1	C	504	ASP	CA-C-N	6.52	126.29	119.05
1	C	504	ASP	C-N-CA	6.52	126.29	119.05
2	D	533	PRO	N-CA-CB	6.52	110.50	103.33
2	D	202	ILE	CA-C-N	6.51	127.20	119.98
2	D	202	ILE	C-N-CA	6.51	127.20	119.98
1	A	646	GLU	N-CA-C	6.50	120.31	112.38
2	D	455	ASN	CA-C-N	6.50	131.82	122.40
2	D	455	ASN	C-N-CA	6.50	131.82	122.40
1	C	131	ARG	N-CA-C	6.49	119.17	111.71
1	A	711	ILE	CA-C-N	6.49	126.41	119.28
1	A	711	ILE	C-N-CA	6.49	126.41	119.28
2	D	82	PRO	N-CA-CB	6.49	108.99	103.35
2	D	95	ARG	N-CA-C	6.48	119.16	111.71
1	A	677	ARG	O-C-N	-6.47	115.43	121.32
1	C	413	THR	CA-C-N	6.47	129.24	120.44
1	C	413	THR	C-N-CA	6.47	129.24	120.44
1	A	244	HIS	CA-C-N	6.46	128.94	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	HIS	C-N-CA	6.46	128.94	120.28
1	A	368	LEU	N-CA-C	6.46	119.13	111.71
2	B	212	PRO	N-CA-CB	6.45	108.91	103.17
1	C	198	ASN	CA-CB-CG	6.45	119.05	112.60
1	C	313	HIS	O-C-N	-6.45	115.28	122.12
2	B	132	GLY	N-CA-C	6.44	123.91	115.40
1	A	344	ASN	CA-C-N	6.43	128.67	120.56
1	A	344	ASN	C-N-CA	6.43	128.67	120.56
2	B	257	ALA	CA-C-N	6.43	128.90	120.28
2	B	257	ALA	C-N-CA	6.43	128.90	120.28
1	A	369	ASP	O-C-N	-6.43	114.14	122.37
1	C	88	GLN	CA-C-N	6.42	129.94	120.95
1	C	88	GLN	C-N-CA	6.42	129.94	120.95
2	D	424	GLU	CA-C-N	6.41	129.51	120.28
2	D	424	GLU	C-N-CA	6.41	129.51	120.28
1	A	17	VAL	CA-C-O	6.41	122.93	119.15
1	A	188	LYS	CA-C-N	6.40	126.32	119.28
1	A	188	LYS	C-N-CA	6.40	126.32	119.28
2	B	95	ARG	CG-CD-NE	6.40	126.08	112.00
1	C	70	PHE	O-C-N	-6.40	114.58	122.57
2	D	67	VAL	CA-C-N	6.39	133.08	122.66
2	D	67	VAL	C-N-CA	6.39	133.08	122.66
1	A	504	ASP	CA-C-N	6.39	126.14	119.05
1	A	504	ASP	C-N-CA	6.39	126.14	119.05
1	C	410	GLU	CA-C-O	-6.38	113.78	120.55
2	B	73	VAL	CA-C-N	6.37	125.95	119.19
2	B	73	VAL	C-N-CA	6.37	125.95	119.19
2	B	397	ASP	CA-C-N	6.37	126.28	119.28
2	B	397	ASP	C-N-CA	6.37	126.28	119.28
2	D	363	PHE	CA-C-N	6.36	134.65	121.94
2	D	363	PHE	C-N-CA	6.36	134.65	121.94
2	B	480	PRO	N-CA-CB	6.35	108.84	103.25
1	A	184	GLU	CA-C-N	6.34	133.85	122.06
1	A	184	GLU	C-N-CA	6.34	133.85	122.06
1	C	427	VAL	CA-C-N	6.34	129.41	120.28
1	C	427	VAL	C-N-CA	6.34	129.41	120.28
1	C	527	PRO	N-CA-CB	6.34	109.59	103.51
1	A	694	ASP	CA-C-N	6.32	128.75	120.28
1	A	694	ASP	C-N-CA	6.32	128.75	120.28
1	C	477	PRO	N-CA-CB	6.32	108.94	103.31
1	C	183	GLU	CA-C-N	6.31	130.70	120.60
1	C	183	GLU	C-N-CA	6.31	130.70	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	343	ASN	CA-C-N	6.31	129.37	120.28
1	C	343	ASN	C-N-CA	6.31	129.37	120.28
1	C	352	ALA	CA-C-O	6.31	127.11	120.42
1	A	170	ALA	CA-C-N	6.31	129.38	120.42
1	A	170	ALA	C-N-CA	6.31	129.38	120.42
1	A	129	ASN	CA-C-N	6.30	126.04	119.05
1	A	129	ASN	C-N-CA	6.30	126.04	119.05
1	A	556	PHE	N-CA-C	6.30	120.17	112.23
1	C	215	GLN	CA-C-N	6.30	126.04	119.05
1	C	215	GLN	C-N-CA	6.30	126.04	119.05
1	A	707	PRO	N-CA-CB	6.29	108.78	103.25
1	C	262	ASP	CA-C-N	6.29	126.96	119.98
1	C	262	ASP	C-N-CA	6.29	126.96	119.98
2	D	511	PRO	N-CA-CB	6.28	108.82	103.35
1	A	129	ASN	CA-C-O	6.28	125.66	119.51
1	C	430	VAL	O-C-N	-6.28	114.72	122.57
2	B	536	HIS	CA-C-N	6.26	128.68	120.60
2	B	536	HIS	C-N-CA	6.26	128.68	120.60
2	D	28	PRO	N-CA-CB	6.25	108.75	103.25
1	C	170	ALA	CA-C-N	6.25	129.02	120.46
1	C	170	ALA	C-N-CA	6.25	129.02	120.46
2	D	263	VAL	N-CA-C	-6.24	104.66	110.53
1	A	588	GLU	CA-C-N	6.23	129.25	120.28
1	A	588	GLU	C-N-CA	6.23	129.25	120.28
1	A	321	LYS	CA-C-N	6.22	128.62	120.28
1	A	321	LYS	C-N-CA	6.22	128.62	120.28
1	A	319	ASN	CA-C-N	6.22	126.12	119.28
1	A	319	ASN	C-N-CA	6.22	126.12	119.28
2	B	25	GLY	O-C-N	-6.22	115.62	122.84
1	A	633	LEU	CA-C-O	6.21	129.07	121.99
1	C	206	VAL	CB-CA-C	-6.21	101.10	111.29
2	B	337	TYR	CA-C-N	6.21	130.95	120.64
2	B	337	TYR	C-N-CA	6.21	130.95	120.64
1	A	182	ALA	CA-C-N	6.21	128.92	120.54
1	A	182	ALA	C-N-CA	6.21	128.92	120.54
1	A	462	GLN	CA-C-O	6.20	123.32	119.29
1	A	715	ALA	CA-C-N	6.20	128.59	120.60
1	A	715	ALA	C-N-CA	6.20	128.59	120.60
2	D	308	GLY	CA-C-N	6.20	128.59	120.28
2	D	308	GLY	C-N-CA	6.20	128.59	120.28
1	C	314	GLN	O-C-N	-6.20	115.14	122.20
1	A	477	PRO	N-CA-CB	6.19	108.82	103.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	PRO	N-CA-CB	6.19	108.82	103.31
2	B	374	PHE	CA-C-N	6.19	126.09	119.28
2	B	374	PHE	C-N-CA	6.19	126.09	119.28
1	C	79	TYR	CA-C-N	6.19	128.89	120.54
1	C	79	TYR	C-N-CA	6.19	128.89	120.54
1	A	157	PRO	N-CA-CB	6.18	108.67	103.17
1	A	413	THR	CA-C-N	6.18	128.48	120.44
1	A	413	THR	C-N-CA	6.18	128.48	120.44
1	C	412	LEU	CA-C-N	6.18	128.48	120.44
1	C	412	LEU	C-N-CA	6.18	128.48	120.44
1	A	548	MET	CA-C-N	6.18	129.06	120.29
1	A	548	MET	C-N-CA	6.18	129.06	120.29
1	A	213	PRO	CA-C-N	6.18	125.67	119.24
1	A	213	PRO	C-N-CA	6.18	125.67	119.24
2	B	94	THR	CA-C-N	6.18	129.17	120.28
2	B	94	THR	C-N-CA	6.18	129.17	120.28
1	A	401	ASP	CA-C-N	6.17	125.90	119.05
1	A	401	ASP	C-N-CA	6.17	125.90	119.05
1	A	82	ARG	CD-NE-CZ	6.16	133.03	124.40
2	B	483	PRO	N-CA-CB	6.16	108.80	103.31
2	D	189	PRO	N-CA-CB	6.16	108.65	103.17
2	B	190	ALA	N-CA-C	6.16	118.78	111.33
2	D	397	ASP	CA-C-N	6.15	126.33	119.32
2	D	397	ASP	C-N-CA	6.15	126.33	119.32
2	D	115	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	633	LEU	CA-C-O	6.15	129.00	121.99
1	A	520	GLY	O-C-N	-6.14	115.74	122.68
2	D	228	SER	CA-C-N	6.14	126.67	120.04
2	D	228	SER	C-N-CA	6.14	126.67	120.04
1	A	232	MET	CA-C-N	6.13	125.75	119.56
1	A	232	MET	C-N-CA	6.13	125.75	119.56
1	C	612	ARG	CA-C-N	6.13	126.74	119.94
1	C	612	ARG	C-N-CA	6.13	126.74	119.94
1	A	521	ASN	CA-CB-CG	6.13	118.73	112.60
1	C	522	PRO	N-CA-CB	6.12	108.20	103.30
1	A	41	ALA	O-C-N	-6.12	114.23	122.43
1	C	410	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	197	GLN	O-C-N	-6.12	115.67	122.03
2	B	363	PHE	CA-C-N	6.11	135.82	121.52
2	B	363	PHE	C-N-CA	6.11	135.82	121.52
2	D	586	LYS	CA-C-N	6.11	128.97	120.29
2	D	586	LYS	C-N-CA	6.11	128.97	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	463	PRO	N-CA-CB	6.11	108.66	103.35
2	D	212	PRO	N-CA-CB	6.10	108.60	103.17
2	B	534	VAL	CA-C-N	6.10	128.45	120.28
2	B	534	VAL	C-N-CA	6.10	128.45	120.28
1	C	398	ARG	N-CA-C	6.10	117.93	111.28
1	C	504	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	371	ALA	CA-C-N	6.08	129.22	123.08
1	A	371	ALA	C-N-CA	6.08	129.22	123.08
2	B	82	PRO	N-CA-CB	6.08	108.64	103.35
1	C	188	LYS	CA-C-N	6.07	125.96	119.28
1	C	188	LYS	C-N-CA	6.07	125.96	119.28
2	D	77	ARG	CA-C-N	6.07	126.51	119.47
2	D	77	ARG	C-N-CA	6.07	126.51	119.47
1	C	637	PRO	CA-C-N	6.07	128.90	120.29
1	C	637	PRO	C-N-CA	6.07	128.90	120.29
2	D	571	ALA	CA-C-N	6.07	128.41	120.28
2	D	571	ALA	C-N-CA	6.07	128.41	120.28
2	B	363	PHE	CA-CB-CG	6.06	119.86	113.80
2	D	243	ASN	N-CA-C	6.06	119.78	112.38
1	C	463	PRO	N-CA-CB	6.06	108.62	103.35
2	B	420	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	262	ASP	CA-C-N	6.03	126.78	120.03
1	A	262	ASP	C-N-CA	6.03	126.78	120.03
1	C	52	GLU	CA-C-N	6.03	133.34	121.58
1	C	52	GLU	C-N-CA	6.03	133.34	121.58
2	B	532	SER	CA-C-N	6.03	126.19	119.32
2	B	532	SER	C-N-CA	6.03	126.19	119.32
2	B	229	PRO	CA-C-N	6.03	129.47	120.31
2	B	229	PRO	C-N-CA	6.03	129.47	120.31
1	C	197	GLN	O-C-N	-6.02	115.77	122.03
1	C	298	VAL	CA-C-N	6.02	128.34	120.28
1	C	298	VAL	C-N-CA	6.02	128.34	120.28
1	C	577	THR	CA-C-N	6.01	126.17	119.32
1	C	577	THR	C-N-CA	6.01	126.17	119.32
2	D	115	ASP	CA-C-N	6.01	125.22	118.97
2	D	115	ASP	C-N-CA	6.01	125.22	118.97
1	C	401	ASP	CA-C-N	6.00	125.72	119.05
1	C	401	ASP	C-N-CA	6.00	125.72	119.05
2	B	159	LEU	N-CA-C	6.00	119.86	112.54
1	C	397	THR	O-C-N	-6.00	114.45	122.49
1	C	181	THR	CA-C-N	6.00	128.63	120.54
1	C	181	THR	C-N-CA	6.00	128.63	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	PRO	N-CA-CB	6.00	108.64	103.31
1	A	608	ASP	CA-CB-CG	5.99	118.59	112.60
2	B	267	VAL	CA-C-N	5.99	128.31	120.28
2	B	267	VAL	C-N-CA	5.99	128.31	120.28
1	A	636	THR	CA-C-N	5.98	125.60	119.56
1	A	636	THR	C-N-CA	5.98	125.60	119.56
2	B	370	PRO	N-CA-CB	5.97	108.51	103.25
1	C	182	ALA	CA-C-N	5.97	128.60	120.54
1	C	182	ALA	C-N-CA	5.97	128.60	120.54
2	D	480	PRO	N-CA-CB	5.97	108.50	103.25
2	D	301	ARG	CA-C-O	-5.97	114.51	120.90
2	B	232	ARG	CD-NE-CZ	5.96	132.75	124.40
1	C	129	ASN	CA-C-N	5.96	125.67	119.05
1	C	129	ASN	C-N-CA	5.96	125.67	119.05
2	D	483	PRO	N-CA-CB	5.96	108.63	103.27
1	C	636	THR	CA-C-N	5.95	125.66	119.05
1	C	636	THR	C-N-CA	5.95	125.66	119.05
2	D	260	ALA	CA-C-N	5.94	128.24	120.28
2	D	260	ALA	C-N-CA	5.94	128.24	120.28
2	B	189	PRO	CA-C-N	5.93	128.51	120.38
2	B	189	PRO	C-N-CA	5.93	128.51	120.38
1	C	342	TYR	CA-C-N	5.93	128.82	120.28
1	C	342	TYR	C-N-CA	5.93	128.82	120.28
1	A	428	GLU	CA-C-N	5.93	129.32	120.31
1	A	428	GLU	C-N-CA	5.93	129.32	120.31
1	C	526	ASP	CA-C-O	5.93	125.05	119.59
2	B	258	THR	CA-C-N	5.93	126.52	119.94
2	B	258	THR	C-N-CA	5.93	126.52	119.94
1	C	521	ASN	O-C-N	-5.92	116.04	121.37
2	B	543	PRO	N-CA-CB	5.92	108.83	103.33
1	A	52	GLU	O-C-N	-5.91	114.57	122.43
1	C	263	GLY	O-C-N	-5.91	116.52	122.19
2	D	294	ILE	CA-C-N	5.91	128.20	120.28
2	D	294	ILE	C-N-CA	5.91	128.20	120.28
2	D	374	PHE	CA-C-N	5.91	125.45	119.19
2	D	374	PHE	C-N-CA	5.91	125.45	119.19
2	D	141	ASP	CA-C-N	5.90	125.60	119.05
2	D	141	ASP	C-N-CA	5.90	125.60	119.05
1	C	711	ILE	CA-C-N	5.89	125.59	119.05
1	C	711	ILE	C-N-CA	5.89	125.59	119.05
2	D	609	ALA	CA-C-N	5.89	128.17	120.28
2	D	609	ALA	C-N-CA	5.89	128.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	69	PRO	CA-C-N	5.89	130.76	122.46
1	C	69	PRO	C-N-CA	5.89	130.76	122.46
2	D	147	PRO	CA-C-N	5.89	133.06	121.58
2	D	147	PRO	C-N-CA	5.89	133.06	121.58
2	D	455	ASN	CA-C-O	5.88	126.23	119.35
1	C	589	GLU	CA-C-N	5.88	128.09	120.44
1	C	589	GLU	C-N-CA	5.88	128.09	120.44
1	A	405	GLY	O-C-N	-5.88	116.54	122.65
2	B	521	ARG	CA-C-N	5.88	128.48	120.54
2	B	521	ARG	C-N-CA	5.88	128.48	120.54
2	B	307	ILE	CA-C-N	5.88	126.50	119.98
2	B	307	ILE	C-N-CA	5.88	126.50	119.98
1	C	613	GLY	CA-C-N	5.87	128.07	120.44
1	C	613	GLY	C-N-CA	5.87	128.07	120.44
2	D	532	SER	CA-C-N	5.87	125.56	119.05
2	D	532	SER	C-N-CA	5.87	125.56	119.05
2	B	141	ASP	CA-C-N	5.87	125.56	119.05
2	B	141	ASP	C-N-CA	5.87	125.56	119.05
1	A	55	TYR	N-CA-C	5.87	118.62	111.82
2	B	115	ASP	CA-C-N	5.87	125.07	118.97
2	B	115	ASP	C-N-CA	5.87	125.07	118.97
1	C	494	ALA	CA-C-N	5.86	128.13	120.28
1	C	494	ALA	C-N-CA	5.86	128.13	120.28
1	A	412	LEU	CA-C-N	5.86	128.06	120.44
1	A	412	LEU	C-N-CA	5.86	128.06	120.44
1	C	428	GLU	CA-C-N	5.86	128.13	120.28
1	C	428	GLU	C-N-CA	5.86	128.13	120.28
2	D	200	ASP	CA-C-N	5.86	125.56	119.05
2	D	200	ASP	C-N-CA	5.86	125.56	119.05
1	C	468	ASN	CA-CB-CG	5.86	118.45	112.60
1	C	438	GLU	CA-C-N	5.85	128.12	120.28
1	C	438	GLU	C-N-CA	5.85	128.12	120.28
1	C	556	PHE	N-CA-C	5.84	119.59	112.23
2	D	444	ALA	CA-C-N	5.83	128.03	120.44
2	D	444	ALA	C-N-CA	5.83	128.03	120.44
1	C	146	ILE	O-C-N	-5.82	116.22	121.87
1	C	216	PRO	N-CA-CB	5.82	109.73	103.33
1	A	80	ALA	CA-C-O	-5.82	114.38	120.55
1	A	205	MET	CA-C-O	-5.82	114.71	120.82
1	A	527	PRO	N-CA-CB	5.81	109.67	103.39
1	C	608	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	527	PRO	CA-C-N	5.80	130.41	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	527	PRO	C-N-CA	5.80	130.41	120.72
1	C	518	ALA	CA-C-O	-5.80	114.41	120.55
1	C	140	GLY	O-C-N	-5.79	118.36	123.92
2	D	84	LYS	CA-C-O	-5.79	113.99	120.54
1	A	146	ILE	O-C-N	-5.79	116.25	121.87
2	B	264	ARG	CD-NE-CZ	5.79	132.50	124.40
1	A	215	GLN	CA-C-N	5.78	125.47	119.05
1	A	215	GLN	C-N-CA	5.78	125.47	119.05
1	A	589	GLU	CA-C-N	5.78	128.50	120.29
1	A	589	GLU	C-N-CA	5.78	128.50	120.29
2	D	478	PRO	N-CA-CB	5.78	108.34	103.25
1	A	703	GLU	CA-CB-CG	5.77	125.64	114.10
2	B	417	TRP	CA-C-N	5.77	128.02	120.28
2	B	417	TRP	C-N-CA	5.77	128.02	120.28
1	A	684	VAL	N-CA-CB	5.77	119.37	111.41
1	A	7	PHE	N-CA-C	5.77	119.94	113.02
2	D	25	GLY	CA-C-N	5.77	131.23	121.14
2	D	25	GLY	C-N-CA	5.77	131.23	121.14
1	A	504	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	66	GLY	O-C-N	-5.76	115.22	122.41
1	C	43	GLN	CA-C-O	5.76	128.12	120.98
1	A	636	THR	N-CA-C	-5.75	101.67	110.07
1	C	703	GLU	CA-CB-CG	5.75	125.61	114.10
2	D	466	PHE	O-C-N	-5.75	118.88	121.53
1	A	639	GLU	CA-C-N	5.75	128.45	120.29
1	A	639	GLU	C-N-CA	5.75	128.45	120.29
2	B	450	ALA	CA-C-N	5.74	127.90	120.44
2	B	450	ALA	C-N-CA	5.74	127.90	120.44
2	B	576	GLN	N-CA-C	5.74	118.02	111.02
1	C	333	GLY	CA-C-O	5.73	127.19	121.00
1	C	672	LEU	CA-C-N	5.73	127.95	120.28
1	C	672	LEU	C-N-CA	5.73	127.95	120.28
1	C	711	ILE	CA-C-O	5.72	123.06	118.71
2	D	203	GLY	CA-C-N	5.72	127.88	120.44
2	D	203	GLY	C-N-CA	5.72	127.88	120.44
2	B	200	ASP	CA-C-N	5.71	125.39	119.05
2	B	200	ASP	C-N-CA	5.71	125.39	119.05
1	A	445	ARG	CA-C-N	5.71	128.28	120.46
1	A	445	ARG	C-N-CA	5.71	128.28	120.46
1	A	677	ARG	CA-CB-CG	5.71	125.52	114.10
1	C	148	ASP	CA-C-N	5.71	127.93	120.28
1	C	148	ASP	C-N-CA	5.71	127.93	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	412	LEU	O-C-N	-5.71	116.07	122.12
1	A	219	ARG	CA-C-N	5.71	127.75	120.56
1	A	219	ARG	C-N-CA	5.71	127.75	120.56
2	B	462	ALA	CA-C-N	5.70	132.24	121.97
2	B	462	ALA	C-N-CA	5.70	132.24	121.97
1	A	313	HIS	O-C-N	-5.70	116.08	122.12
1	C	587	VAL	CA-C-N	5.70	127.92	120.28
1	C	587	VAL	C-N-CA	5.70	127.92	120.28
1	A	522	PRO	N-CA-CB	5.70	108.37	103.36
1	C	332	SER	CA-C-O	5.69	127.39	120.62
1	A	66	GLY	CA-C-N	5.69	132.66	122.13
1	A	66	GLY	C-N-CA	5.69	132.66	122.13
1	C	343	ASN	O-C-N	-5.69	115.56	122.22
2	D	339	ASN	O-C-N	-5.69	114.99	122.39
2	B	72	ILE	CB-CG1-CD1	5.69	125.75	113.80
1	A	198	ASN	CA-CB-CG	5.68	118.28	112.60
1	C	523	ASP	CA-C-N	5.68	128.16	120.38
1	C	523	ASP	C-N-CA	5.68	128.16	120.38
1	A	97	GLU	CA-C-N	5.67	127.82	120.44
1	A	97	GLU	C-N-CA	5.67	127.82	120.44
2	B	127	GLU	CA-C-N	5.67	126.23	119.94
2	B	127	GLU	C-N-CA	5.67	126.23	119.94
2	D	116	PRO	N-CA-CB	5.67	109.30	103.23
1	A	666	PRO	N-CA-CB	5.67	109.29	103.23
2	D	455	ASN	O-C-N	-5.65	115.28	122.34
2	B	390	VAL	O-C-N	-5.64	115.52	122.18
1	A	427	VAL	CA-C-N	5.64	128.89	120.31
1	A	427	VAL	C-N-CA	5.64	128.89	120.31
2	B	78	PRO	O-C-N	-5.64	115.75	122.24
2	B	494	SER	CA-C-N	5.64	127.84	120.28
2	B	494	SER	C-N-CA	5.64	127.84	120.28
1	C	123	ARG	CA-C-N	5.64	131.32	120.66
1	C	123	ARG	C-N-CA	5.64	131.32	120.66
1	C	488	VAL	N-CA-CB	5.64	117.15	110.55
1	C	677	ARG	CA-C-N	5.64	126.13	120.04
1	C	677	ARG	C-N-CA	5.64	126.13	120.04
1	C	157	PRO	N-CA-CB	5.64	108.19	103.17
1	C	30	ALA	CA-C-N	5.63	128.87	120.31
1	C	30	ALA	C-N-CA	5.63	128.87	120.31
2	D	141	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	368	LEU	CA-C-N	5.63	132.00	122.65
1	A	368	LEU	C-N-CA	5.63	132.00	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	88	PRO	N-CA-CB	5.63	108.58	103.34
1	C	520	GLY	O-C-N	-5.63	116.32	122.68
2	B	419	GLU	CA-C-N	5.62	127.75	120.44
2	B	419	GLU	C-N-CA	5.62	127.75	120.44
2	B	586	LYS	CA-C-N	5.62	127.82	120.28
2	B	586	LYS	C-N-CA	5.62	127.82	120.28
2	B	362	PRO	N-CA-CB	5.62	108.24	103.35
2	B	328	TRP	CA-C-N	5.62	128.37	120.28
2	B	328	TRP	C-N-CA	5.62	128.37	120.28
1	A	531	LEU	N-CA-C	5.61	118.33	111.82
1	C	118	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	720	LYS	CA-C-N	5.61	127.80	120.28
1	C	720	LYS	C-N-CA	5.61	127.80	120.28
1	C	665	VAL	CA-C-N	5.61	125.27	119.05
1	C	665	VAL	C-N-CA	5.61	125.27	119.05
1	C	715	ALA	CA-C-N	5.60	128.11	120.77
1	C	715	ALA	C-N-CA	5.60	128.11	120.77
1	A	528	ASP	CA-C-N	5.60	132.48	122.06
1	A	528	ASP	C-N-CA	5.60	132.48	122.06
2	D	361	LEU	CA-C-O	5.60	126.00	120.17
2	B	35	TRP	CA-C-N	5.60	128.10	120.54
2	B	35	TRP	C-N-CA	5.60	128.10	120.54
2	B	211	GLU	CA-C-O	5.60	124.89	120.19
1	C	449	ALA	CA-C-N	5.60	128.82	120.31
1	C	449	ALA	C-N-CA	5.60	128.82	120.31
1	A	637	PRO	CA-C-N	5.58	130.13	120.58
1	A	637	PRO	C-N-CA	5.58	130.13	120.58
1	C	528	ASP	CA-C-N	5.58	132.44	122.06
1	C	528	ASP	C-N-CA	5.58	132.44	122.06
2	B	345	ILE	CA-C-N	5.56	128.19	120.29
2	B	345	ILE	C-N-CA	5.56	128.19	120.29
1	A	539	GLY	CA-C-N	5.56	128.76	120.31
1	A	539	GLY	C-N-CA	5.56	128.76	120.31
1	C	282	PRO	N-CA-CB	5.56	109.04	103.48
2	B	375	PRO	N-CA-CB	5.56	109.39	103.39
2	B	116	PRO	N-CA-CB	5.55	109.17	103.23
2	B	55	PHE	N-CA-CB	5.55	118.26	109.82
1	A	18	PRO	N-CA-CB	5.55	109.08	103.25
2	D	86	GLY	O-C-N	-5.55	116.77	122.60
2	D	457	LYS	CA-C-N	5.55	131.29	123.30
2	D	457	LYS	C-N-CA	5.55	131.29	123.30
2	D	369	LEU	CA-C-O	5.54	125.58	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	251	GLU	CB-CG-CD	5.53	122.01	112.60
1	A	632	PRO	N-CA-CB	5.53	109.19	103.38
1	C	721	LYS	CA-C-N	5.53	127.63	120.44
1	C	721	LYS	C-N-CA	5.53	127.63	120.44
2	D	362	PRO	N-CA-CB	5.53	108.59	103.39
2	B	608	GLU	CA-C-N	5.53	127.95	120.38
2	B	608	GLU	C-N-CA	5.53	127.95	120.38
2	D	24	ALA	O-C-N	-5.52	114.37	122.43
1	A	441	ILE	CA-C-N	5.52	124.98	119.24
1	A	441	ILE	C-N-CA	5.52	124.98	119.24
1	A	158	LEU	N-CA-C	5.52	119.88	113.20
1	C	579	GLU	CA-C-N	5.52	127.51	120.56
1	C	579	GLU	C-N-CA	5.52	127.51	120.56
1	C	202	LYS	CA-C-N	5.51	127.94	120.44
1	C	202	LYS	C-N-CA	5.51	127.94	120.44
2	B	263	VAL	N-CA-C	-5.51	105.48	110.82
2	D	229	PRO	CA-C-N	5.50	130.04	120.68
2	D	229	PRO	C-N-CA	5.50	130.04	120.68
1	A	281	ALA	CA-C-N	5.50	125.17	119.56
1	A	281	ALA	C-N-CA	5.50	125.17	119.56
2	D	223	ARG	CA-C-N	5.50	132.02	122.56
2	D	223	ARG	C-N-CA	5.50	132.02	122.56
2	B	25	GLY	CA-C-N	5.50	130.76	121.14
2	B	25	GLY	C-N-CA	5.50	130.76	121.14
1	C	622	ALA	CA-C-N	5.50	129.90	120.72
1	C	622	ALA	C-N-CA	5.50	129.90	120.72
1	A	216	PRO	N-CA-CB	5.49	109.37	103.33
2	B	478	PRO	N-CA-CB	5.48	108.07	103.25
2	B	339	ASN	O-C-N	-5.48	115.09	122.43
1	A	448	GLU	CA-C-N	5.47	127.62	120.28
1	A	448	GLU	C-N-CA	5.47	127.62	120.28
2	B	190	ALA	O-C-N	-5.47	116.32	122.12
1	C	189	PRO	N-CA-CB	5.47	109.30	103.39
2	D	345	ILE	CA-C-N	5.46	127.54	120.44
2	D	345	ILE	C-N-CA	5.46	127.54	120.44
2	B	465	GLU	O-C-N	-5.46	116.88	123.27
2	D	78	PRO	O-C-N	-5.46	115.57	122.17
1	A	233	PRO	N-CA-CB	5.46	108.75	103.51
2	B	191	LYS	CA-C-N	5.45	131.26	121.66
2	B	191	LYS	C-N-CA	5.45	131.26	121.66
1	C	661	HIS	N-CA-C	5.45	117.98	111.71
1	C	232	MET	CA-C-N	5.45	125.54	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	232	MET	C-N-CA	5.45	125.54	119.87
1	C	488	VAL	CB-CA-C	-5.45	104.99	111.97
1	A	524	ASP	N-CA-C	5.45	117.22	111.28
2	B	533	PRO	N-CA-CB	5.44	109.47	103.26
2	B	108	ASP	CA-CB-CG	5.43	118.03	112.60
2	D	48	PRO	N-CA-CB	5.43	108.35	103.08
1	A	333	GLY	CA-C-O	5.43	126.86	121.00
1	C	281	ALA	O-C-N	-5.43	115.61	120.71
2	D	204	PHE	CA-C-N	5.43	127.87	120.54
2	D	204	PHE	C-N-CA	5.43	127.87	120.54
2	B	229	PRO	N-CA-CB	5.43	108.72	103.51
1	C	344	ASN	CA-C-N	5.43	127.40	120.56
1	C	344	ASN	C-N-CA	5.43	127.40	120.56
1	A	44	ILE	N-CA-C	-5.42	101.80	107.60
2	B	48	PRO	N-CA-CB	5.42	108.34	103.08
1	A	476	PRO	N-CA-CB	5.42	108.33	103.08
2	D	159	LEU	N-CA-C	5.42	119.15	112.54
2	D	364	THR	CA-C-N	5.42	129.26	120.60
2	D	364	THR	C-N-CA	5.42	129.26	120.60
2	D	466	PHE	CB-CA-C	-5.42	107.36	111.20
1	C	524	ASP	N-CA-C	5.41	117.88	111.33
1	A	61	LEU	N-CA-C	5.40	118.97	112.38
1	A	257	ALA	N-CA-C	5.40	117.17	111.28
1	A	189	PRO	N-CA-CB	5.40	109.22	103.39
1	A	332	SER	CA-C-O	5.40	127.04	120.62
1	C	28	LEU	CA-C-N	5.40	127.45	120.44
1	C	28	LEU	C-N-CA	5.40	127.45	120.44
1	A	118	ASP	CA-CB-CG	5.39	118.00	112.60
2	D	191	LYS	N-CA-C	5.39	119.48	113.01
2	D	462	ALA	O-C-N	-5.39	115.26	122.00
2	B	251	GLU	CB-CG-CD	5.39	121.77	112.60
2	B	155	SER	N-CA-C	5.39	117.16	111.28
2	D	68	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	263	GLY	O-C-N	-5.39	116.95	122.17
1	A	282	PRO	N-CA-CB	5.39	108.87	103.48
1	C	678	PRO	N-CA-CB	5.38	108.31	103.20
2	D	315	GLU	N-CA-C	5.38	117.15	111.28
2	B	422	GLU	CA-C-N	5.38	128.06	120.42
2	B	422	GLU	C-N-CA	5.38	128.06	120.42
1	C	262	ASP	O-C-N	-5.38	116.49	122.09
2	B	525	GLY	CA-C-N	5.38	126.06	119.99
2	B	525	GLY	C-N-CA	5.38	126.06	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	214	PRO	N-CA-CB	5.38	109.01	103.15
1	C	541	ALA	CA-C-N	5.38	131.81	121.54
1	C	541	ALA	C-N-CA	5.38	131.81	121.54
2	B	617	LEU	N-CA-CB	5.37	118.99	110.55
2	B	536	HIS	O-C-N	-5.37	115.23	122.43
1	C	441	ILE	CA-C-N	5.37	124.83	119.24
1	C	441	ILE	C-N-CA	5.37	124.83	119.24
1	A	421	TRP	CA-C-N	5.37	125.94	119.98
1	A	421	TRP	C-N-CA	5.37	125.94	119.98
2	B	335	ASP	CA-C-N	5.37	124.98	119.56
2	B	335	ASP	C-N-CA	5.37	124.98	119.56
1	A	290	ILE	N-CA-CB	5.36	118.73	112.35
2	B	349	SER	CA-C-N	5.36	127.46	120.28
2	B	349	SER	C-N-CA	5.36	127.46	120.28
1	C	322	SER	O-C-N	-5.36	116.44	122.12
2	B	609	ALA	N-CA-C	5.35	117.81	111.33
1	A	261	ALA	O-C-N	-5.35	116.05	122.15
2	B	365	GLN	N-CA-C	5.35	119.06	112.54
2	D	123	LYS	CA-C-N	5.35	127.76	120.54
2	D	123	LYS	C-N-CA	5.35	127.76	120.54
2	B	327	SER	N-CA-C	5.35	117.93	109.96
1	A	598	PRO	N-CA-CB	5.35	108.08	103.27
2	D	229	PRO	N-CA-CB	5.34	108.28	103.20
2	B	142	PRO	N-CA-CB	5.34	109.21	103.33
2	B	147	PRO	CA-C-N	5.34	132.00	121.58
2	B	147	PRO	C-N-CA	5.34	132.00	121.58
1	C	556	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	484	ASP	CA-CB-CG	5.34	117.94	112.60
2	B	456	ARG	O-C-N	-5.34	113.29	122.20
2	D	349	SER	CA-C-N	5.34	127.43	120.28
2	D	349	SER	C-N-CA	5.34	127.43	120.28
1	C	159	ASP	CA-CB-CG	5.33	117.93	112.60
2	D	558	LYS	O-C-N	-5.33	116.47	122.12
2	D	604	ASP	CA-C-N	5.33	131.18	122.65
2	D	604	ASP	C-N-CA	5.33	131.18	122.65
1	C	52	GLU	O-C-N	-5.32	113.89	122.41
1	C	66	GLY	N-CA-C	5.32	122.69	115.30
1	C	469	LYS	CA-C-N	5.32	130.50	122.68
1	C	469	LYS	C-N-CA	5.32	130.50	122.68
1	A	281	ALA	O-C-N	-5.32	115.21	121.32
1	A	665	VAL	CA-C-N	5.31	124.50	118.97
1	A	665	VAL	C-N-CA	5.31	124.50	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	182	VAL	CA-C-N	5.31	128.39	120.31
2	B	182	VAL	C-N-CA	5.31	128.39	120.31
1	A	500	ARG	CA-C-N	5.31	127.83	120.29
1	A	500	ARG	C-N-CA	5.31	127.83	120.29
2	D	566	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	398	PRO	N-CA-CB	5.31	109.12	103.39
1	C	368	LEU	N-CA-C	5.31	118.86	112.38
1	C	632	PRO	N-CA-CB	5.30	108.29	103.15
2	D	425	LYS	CA-C-N	5.30	131.92	121.58
2	D	425	LYS	C-N-CA	5.30	131.92	121.58
1	C	597	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	A	82	ARG	CA-C-O	5.30	124.62	119.22
2	B	510	ARG	CA-C-O	5.30	124.16	119.71
1	C	603	ALA	CA-C-O	5.30	126.33	120.71
2	B	444	ALA	CA-C-N	5.29	127.64	120.44
2	B	444	ALA	C-N-CA	5.29	127.64	120.44
1	A	184	GLU	O-C-N	-5.29	115.34	122.43
2	B	235	THR	N-CA-CB	5.29	119.50	110.87
1	C	646	GLU	N-CA-C	5.29	117.80	111.71
1	A	689	PRO	N-CA-CB	5.29	107.95	103.35
1	C	538	ALA	CA-C-N	5.29	125.85	119.98
1	C	538	ALA	C-N-CA	5.29	125.85	119.98
1	A	720	LYS	CA-C-N	5.28	127.36	120.28
1	A	720	LYS	C-N-CA	5.28	127.36	120.28
2	B	631	LEU	CA-C-N	5.28	127.30	120.44
2	B	631	LEU	C-N-CA	5.28	127.30	120.44
1	A	244	HIS	CA-CB-CG	-5.28	108.52	113.80
2	B	167	PHE	CA-CB-CG	5.28	119.08	113.80
2	D	78	PRO	N-CA-CB	5.28	109.21	103.30
2	B	201	PRO	N-CA-CB	5.28	109.13	103.33
2	B	604	ASP	CA-C-N	5.28	131.09	122.65
2	B	604	ASP	C-N-CA	5.28	131.09	122.65
2	D	335	ASP	CA-C-N	5.28	124.89	119.56
2	D	335	ASP	C-N-CA	5.28	124.89	119.56
2	B	217	LEU	CA-C-N	5.27	125.95	119.99
2	B	217	LEU	C-N-CA	5.27	125.95	119.99
1	A	298	VAL	CA-C-N	5.27	127.34	120.28
1	A	298	VAL	C-N-CA	5.27	127.34	120.28
2	B	260	ALA	CA-C-N	5.27	127.34	120.28
2	B	260	ALA	C-N-CA	5.27	127.34	120.28
1	C	158	LEU	CA-C-N	5.27	129.64	120.68
1	C	158	LEU	C-N-CA	5.27	129.64	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	184	GLU	N-CA-C	5.27	118.81	112.38
1	C	433	MET	N-CA-C	5.27	117.10	111.36
2	B	588	ALA	N-CA-C	5.27	119.57	113.20
1	C	8	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	175	LEU	CA-C-N	5.26	127.33	120.28
1	A	175	LEU	C-N-CA	5.26	127.33	120.28
1	C	198	ASN	N-CA-CB	-5.26	103.91	111.70
2	D	437	HIS	CA-CB-CG	-5.26	108.54	113.80
1	A	634	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	211	ILE	N-CA-CB	5.25	119.89	111.23
1	A	433	MET	N-CA-C	5.25	117.91	111.82
2	D	108	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	88	GLN	CA-C-N	5.25	128.80	121.24
1	A	88	GLN	C-N-CA	5.25	128.80	121.24
1	C	26	GLU	CA-C-O	-5.25	114.96	120.63
2	D	88	PRO	N-CA-CB	5.25	108.17	103.19
2	D	218	GLY	CA-C-N	5.25	127.31	120.28
2	D	218	GLY	C-N-CA	5.25	127.31	120.28
1	A	217	SER	CA-C-N	5.24	128.27	120.31
1	A	217	SER	C-N-CA	5.24	128.27	120.31
2	B	189	PRO	N-CA-CB	5.23	108.74	103.25
2	D	142	PRO	N-CA-CB	5.23	109.08	103.33
2	B	610	GLU	N-CA-C	5.22	117.72	111.71
1	A	668	LEU	CA-C-N	5.22	127.59	120.54
1	A	668	LEU	C-N-CA	5.22	127.59	120.54
1	C	20	ASP	CA-C-N	5.22	128.04	120.79
1	C	20	ASP	C-N-CA	5.22	128.04	120.79
1	C	172	LEU	O-C-N	-5.22	116.26	120.38
2	B	31	THR	CA-C-N	5.21	127.21	120.44
2	B	31	THR	C-N-CA	5.21	127.21	120.44
1	A	673	ASP	O-C-N	-5.21	116.68	122.09
1	A	646	GLU	CA-C-N	5.20	130.53	122.26
1	A	646	GLU	C-N-CA	5.20	130.53	122.26
2	D	56	ALA	CA-C-N	5.20	127.25	120.28
2	D	56	ALA	C-N-CA	5.20	127.25	120.28
1	C	553	GLU	CA-C-N	5.19	127.55	120.54
1	C	553	GLU	C-N-CA	5.19	127.55	120.54
2	B	364	THR	CA-C-N	5.19	129.39	120.72
2	B	364	THR	C-N-CA	5.19	129.39	120.72
1	C	158	LEU	N-CA-C	5.19	119.60	113.16
1	A	29	ALA	CA-C-N	5.19	127.23	120.28
1	A	29	ALA	C-N-CA	5.19	127.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	243	ASN	CA-C-N	5.18	131.69	122.06
2	B	243	ASN	C-N-CA	5.18	131.69	122.06
1	C	379	SER	CA-C-N	5.18	127.74	120.28
1	C	379	SER	C-N-CA	5.18	127.74	120.28
1	A	488	VAL	N-CA-CB	5.17	117.19	110.57
1	C	341	VAL	N-CA-C	5.17	119.28	112.04
1	C	368	LEU	CA-C-N	5.17	131.23	122.65
1	C	368	LEU	C-N-CA	5.17	131.23	122.65
1	C	666	PRO	N-CA-CB	5.17	109.02	103.33
2	D	601	GLU	O-C-N	-5.17	115.33	122.46
2	B	510	ARG	CA-C-N	5.17	125.08	119.76
2	B	510	ARG	C-N-CA	5.17	125.08	119.76
2	B	203	GLY	CA-C-N	5.16	127.15	120.44
2	B	203	GLY	C-N-CA	5.16	127.15	120.44
1	A	213	PRO	N-CA-CB	5.16	108.09	103.08
1	A	674	LYS	CA-C-N	5.16	132.26	121.94
1	A	674	LYS	C-N-CA	5.16	132.26	121.94
2	D	455	ASN	CA-CB-CG	5.16	117.76	112.60
1	A	603	ALA	N-CA-C	5.15	117.89	109.59
1	A	468	ASN	CA-CB-CG	5.15	117.75	112.60
1	C	29	ALA	CA-C-N	5.15	127.19	120.28
1	C	29	ALA	C-N-CA	5.15	127.19	120.28
1	C	401	ASP	CA-C-O	5.15	127.22	120.16
2	B	275	GLU	CA-C-N	5.15	127.14	120.44
2	B	275	GLU	C-N-CA	5.15	127.14	120.44
1	C	76	ALA	N-CA-C	5.15	116.89	111.28
2	D	375	PRO	N-CA-CB	5.15	108.98	103.52
2	B	425	LYS	CA-C-N	5.15	132.24	121.94
2	B	425	LYS	C-N-CA	5.15	132.24	121.94
2	B	336	PRO	N-CA-CB	5.14	108.45	103.51
2	B	353	GLY	CA-C-N	5.14	128.56	121.26
2	B	353	GLY	C-N-CA	5.14	128.56	121.26
1	A	30	ALA	CA-C-N	5.14	128.13	120.31
1	A	30	ALA	C-N-CA	5.14	128.13	120.31
2	B	79	LYS	CA-C-N	5.14	131.61	121.58
2	B	79	LYS	C-N-CA	5.14	131.61	121.58
2	D	305	ALA	CA-C-N	5.14	128.13	120.31
2	D	305	ALA	C-N-CA	5.14	128.13	120.31
1	C	636	THR	N-CA-C	-5.14	102.56	110.07
1	C	300	LYS	O-C-N	-5.14	116.75	122.09
1	A	385	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	228	THR	O-C-N	-5.13	116.68	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	617	ILE	CA-C-O	-5.13	115.73	121.17
1	C	264	VAL	O-C-N	-5.13	116.81	121.94
2	D	181	SER	CA-C-N	5.13	127.48	120.46
2	D	181	SER	C-N-CA	5.13	127.48	120.46
1	A	198	ASN	N-CA-CB	-5.12	104.39	112.13
1	A	690	GLU	O-C-N	-5.12	116.22	122.22
2	B	390	VAL	CA-C-O	5.12	125.16	119.42
2	D	588	ALA	N-CA-C	5.12	119.25	113.15
2	D	634	LEU	N-CA-C	5.12	119.29	113.19
1	A	553	GLU	CA-C-N	5.12	127.45	120.54
1	A	553	GLU	C-N-CA	5.12	127.45	120.54
2	D	608	GLU	CA-C-N	5.12	127.40	120.38
2	D	608	GLU	C-N-CA	5.12	127.40	120.38
1	A	252	ALA	CA-C-N	5.12	128.09	120.31
1	A	252	ALA	C-N-CA	5.12	128.09	120.31
1	C	321	LYS	O-C-N	-5.12	116.23	122.22
1	A	261	ALA	N-CA-C	-5.12	105.78	111.36
1	C	141	VAL	N-CA-C	5.12	116.18	109.58
2	B	393	GLY	CA-C-N	5.11	127.64	120.28
2	B	393	GLY	C-N-CA	5.11	127.64	120.28
1	C	264	VAL	CA-C-N	5.11	127.13	120.28
1	C	264	VAL	C-N-CA	5.11	127.13	120.28
2	D	115	ASP	CA-C-O	5.11	124.31	119.76
1	C	475	GLU	CA-C-N	5.11	123.39	119.66
1	C	475	GLU	C-N-CA	5.11	123.39	119.66
1	A	68	PRO	N-CA-CB	5.11	108.03	103.08
1	A	131	ARG	N-CA-C	5.11	118.61	112.38
1	A	352	ALA	CA-C-N	5.11	127.08	120.44
1	A	352	ALA	C-N-CA	5.11	127.08	120.44
1	A	664	LEU	N-CA-C	5.11	116.93	111.36
2	D	94	THR	CA-C-N	5.11	127.63	120.28
2	D	94	THR	C-N-CA	5.11	127.63	120.28
2	D	408	LEU	N-CA-C	5.11	116.84	111.28
2	B	488	LEU	N-CA-C	5.10	117.74	110.24
1	C	175	LEU	CA-C-N	5.10	127.12	120.28
1	C	175	LEU	C-N-CA	5.10	127.12	120.28
1	C	475	GLU	CA-C-O	5.10	124.30	119.76
1	C	314	GLN	CA-C-N	5.10	132.14	121.94
1	C	314	GLN	C-N-CA	5.10	132.14	121.94
1	A	172	LEU	CA-C-N	5.10	124.71	119.05
1	A	172	LEU	C-N-CA	5.10	124.71	119.05
1	C	27	GLU	CA-C-N	5.09	127.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	27	GLU	C-N-CA	5.09	127.06	120.44
1	C	689	PRO	N-CA-CB	5.09	107.78	103.35
1	A	75	TYR	O-C-N	-5.09	116.74	123.21
2	B	223	ARG	CA-C-N	5.09	131.31	122.56
2	B	223	ARG	C-N-CA	5.09	131.31	122.56
2	D	23	LEU	O-C-N	-5.09	116.80	121.79
2	D	506	SER	N-CA-C	5.09	117.72	111.82
1	A	672	LEU	CA-C-N	5.08	127.40	120.54
1	A	672	LEU	C-N-CA	5.08	127.40	120.54
1	A	51	ASN	CA-C-N	5.08	130.44	120.99
1	A	51	ASN	C-N-CA	5.08	130.44	120.99
1	C	163	VAL	CA-C-O	5.08	125.67	120.39
1	C	541	ALA	O-C-N	-5.08	114.87	122.39
1	A	374	LEU	CA-C-O	5.08	126.43	120.69
1	A	343	ASN	O-C-N	-5.07	116.03	122.27
1	C	533	LYS	O-C-N	-5.07	116.82	122.09
2	B	49	PRO	N-CA-CB	5.07	108.86	103.39
2	B	191	LYS	N-CA-C	5.06	119.09	113.01
1	A	448	GLU	O-C-N	-5.06	116.86	122.07
1	A	264	VAL	CA-C-N	5.06	127.06	120.28
1	A	264	VAL	C-N-CA	5.06	127.06	120.28
1	A	504	ASP	CA-C-O	5.05	124.24	119.59
2	B	432	ALA	CA-C-N	5.05	127.38	120.46
2	B	432	ALA	C-N-CA	5.05	127.38	120.46
2	B	77	ARG	CA-C-O	5.05	126.04	120.94
1	A	8	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	120	PRO	N-CA-CB	5.05	108.65	103.15
1	C	684	VAL	N-CA-CB	5.05	118.89	111.52
2	D	40	GLU	N-CA-C	5.05	116.47	111.07
2	B	190	ALA	CA-C-N	5.04	131.16	121.18
2	B	190	ALA	C-N-CA	5.04	131.16	121.18
2	D	408	LEU	CA-C-N	5.04	126.99	120.44
2	D	408	LEU	C-N-CA	5.04	126.99	120.44
2	D	501	MET	CA-C-N	5.04	127.03	120.28
2	D	501	MET	C-N-CA	5.04	127.03	120.28
1	A	385	ASN	CA-C-N	5.04	127.34	120.54
1	A	385	ASN	C-N-CA	5.04	127.34	120.54
2	B	78	PRO	N-CA-CB	5.04	109.00	103.26
2	B	237	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	337	TYR	O-C-N	-5.03	115.85	122.39
2	B	256	LEU	CA-C-N	5.03	126.98	120.44
2	B	256	LEU	C-N-CA	5.03	126.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	410	ARG	CA-CB-CG	5.03	124.16	114.10
1	C	184	GLU	O-C-N	-5.03	115.85	122.39
1	C	634	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	513	ASP	O-C-N	-5.03	116.08	122.27
1	A	536	ILE	CA-C-N	5.03	126.97	120.44
1	A	536	ILE	C-N-CA	5.03	126.97	120.44
1	C	245	MET	CA-C-O	-5.03	115.54	120.82
1	A	185	GLN	CA-C-N	5.03	130.69	121.85
1	A	185	GLN	C-N-CA	5.03	130.69	121.85
1	C	175	LEU	O-C-N	-5.02	116.80	122.12
1	A	70	PHE	O-C-N	-5.02	115.82	122.40
2	B	493	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	257	ALA	N-CA-C	5.02	116.44	111.07
1	C	575	LYS	CA-C-N	5.02	131.12	121.54
1	C	575	LYS	C-N-CA	5.02	131.12	121.54
1	C	405	GLY	O-C-N	-5.02	117.43	122.65
1	A	271	GLU	O-C-N	-5.01	116.80	122.12
1	A	189	PRO	CA-C-N	5.01	129.09	120.72
1	A	189	PRO	C-N-CA	5.01	129.09	120.72
1	C	277	VAL	O-C-N	-5.01	117.01	121.87
2	D	201	PRO	N-CA-CB	5.01	108.84	103.33
2	B	414	ASP	N-CA-C	5.01	116.74	111.28
1	A	418	ARG	CA-C-N	5.00	126.99	120.28
1	A	418	ARG	C-N-CA	5.00	126.99	120.28
2	D	155	SER	N-CA-C	5.00	116.73	111.28
1	A	682	ILE	N-CA-CB	5.00	118.82	111.52
2	D	243	ASN	CA-C-N	5.00	131.44	122.38
2	D	243	ASN	C-N-CA	5.00	131.44	122.38
1	C	617	ILE	CA-C-O	-5.00	115.87	121.17

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	MET	Mainchain
1	A	183	GLU	Mainchain
1	A	281	ALA	Mainchain
1	A	342	TYR	Mainchain
1	A	356	THR	Mainchain
1	A	40	THR	Mainchain
1	A	405	GLY	Mainchain
1	A	540	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	70	PHE	Mainchain
2	B	401	GLY	Mainchain
2	B	456	ARG	Mainchain
1	C	167	MET	Mainchain
1	C	277	VAL	Mainchain
1	C	281	ALA	Mainchain
1	C	342	TYR	Mainchain
1	C	356	THR	Mainchain
1	C	357	GLN	Mainchain
1	C	376	THR	Mainchain
1	C	40	THR	Mainchain
1	C	405	GLY	Mainchain
1	C	677	ARG	Mainchain
1	C	70	PHE	Mainchain
1	C	74	PRO	Mainchain
2	D	228	SER	Mainchain
2	D	24	ALA	Mainchain
2	D	348	PHE	Mainchain
2	D	456	ARG	Mainchain

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	5574	0	5486	37	2
1	C	5574	0	5486	42	0
2	B	4722	0	4642	34	0
2	D	4722	0	4642	33	2
3	A	55	0	37	2	0
3	C	55	0	37	1	0
4	A	55	0	37	3	0
4	C	55	0	37	2	0
5	A	91	0	88	17	0
5	C	91	0	88	16	0
6	B	12	0	16	1	0
6	D	12	0	16	2	0
7	A	356	0	0	0	0
7	B	192	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	353	0	0	4	0
7	D	193	0	0	0	0
All	All	22112	0	20612	173	2

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 4.

All (173) 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)
5:A:1800:B12:H531	5:A:1800:B12:H552	1.46	0.96
5:A:1800:B12:H421	5:A:1800:B12:H363	1.46	0.95
1:C:21:ALA:HB3	7:C:4310:HOH:O	1.72	0.89
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.24	0.85
5:C:2800:B12:H552	5:C:2800:B12:H531	1.64	0.80
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.32	0.77
5:C:2800:B12:H353	5:C:2800:B12:H302	1.67	0.77
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.65	0.76
1:C:27:GLU:HB2	7:C:4284:HOH:O	1.84	0.75
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.69	0.74
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.69	0.74
1:A:247:GLU:HB3	5:A:1800:B12:H532	1.71	0.73
1:C:706:THR:HB	1:C:707:PRO:HD2	1.71	0.72
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.36	0.72
2:B:468:MET:HE2	2:B:471:ALA:HA	1.73	0.71
1:A:706:THR:HB	1:A:707:PRO:HD2	1.73	0.71
5:A:1800:B12:H363	5:A:1800:B12:C42	2.11	0.70
1:C:4:LEU:HB3	2:D:264:ARG:HG2	1.76	0.68
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.77	0.67
2:B:617:LEU:HD22	2:B:621:MET:HE1	1.76	0.67
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.43	0.66
1:C:188:LYS:H	1:C:191:GLN:NE2	1.93	0.66
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.76	0.66
1:C:247:GLU:HB3	5:C:2800:B12:H532	1.77	0.66
5:A:1800:B12:H353	5:A:1800:B12:H302	1.76	0.65
2:D:370:PRO:HB3	2:D:375:PRO:HG2	1.79	0.65
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.79	0.64
2:D:564:VAL:HG22	2:D:592:ALA:HB3	1.78	0.64
3:A:1801[A]:SCD:OP2	3:A:1801[A]:SCD:HPB1	1.97	0.64
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.78	0.64
2:B:224:LEU:HD21	2:B:231:SER:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:HD2	7:C:4304:HOH:O	1.99	0.62
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.81	0.62
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.81	0.62
2:D:197:LEU:HB2	2:D:233:ALA:HA	1.81	0.62
1:A:188:LYS:H	1:A:191:GLN:NE2	1.99	0.61
5:C:2800:B12:H531	5:C:2800:B12:C55	2.30	0.61
3:C:2801[A]:SCD:HPB1	3:C:2801[A]:SCD:OP2	1.99	0.60
5:A:1800:B12:H531	5:A:1800:B12:C55	2.28	0.59
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.85	0.59
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.85	0.58
2:D:197:LEU:HD12	2:D:233:ALA:CB	2.34	0.58
6:B:3002:GOL:O3	6:B:3002:GOL:O1	1.99	0.58
2:D:532:SER:HB3	2:D:533:PRO:HD3	1.85	0.58
2:B:284:VAL:HG11	2:B:322:GLN:HE21	1.68	0.57
2:D:284:VAL:HG11	2:D:322:GLN:HE21	1.69	0.57
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.87	0.57
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.52	0.57
1:A:4:LEU:HB3	2:B:264:ARG:HG2	1.85	0.57
5:A:1800:B12:H312	5:A:1800:B12:H251	1.88	0.56
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.87	0.56
4:C:2802[B]:MCD:HPB1	4:C:2802[B]:MCD:OP2	2.05	0.56
5:A:1800:B12:H2B	5:A:1800:B12:O7R	2.06	0.56
1:C:374:LEU:HB2	1:C:481:LEU:HD23	1.87	0.56
2:D:356:GLU:HA	6:D:3004:GOL:H2	1.89	0.55
5:C:2800:B12:H301	5:C:2800:B12:H203	1.87	0.55
5:A:1800:B12:H203	5:A:1800:B12:H301	1.89	0.55
5:A:1800:B12:H312	5:A:1800:B12:C25	2.37	0.54
1:C:638:GLU:HA	1:C:671:GLU:HG3	1.89	0.54
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.89	0.54
2:B:391:ASN:ND2	2:B:394:ARG:HE	2.05	0.54
2:D:281:ASN:ND2	2:D:323:ASN:HD21	2.05	0.53
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.89	0.53
2:B:216:VAL:HG23	7:B:5409:HOH:O	2.07	0.53
1:C:706:THR:HB	1:C:707:PRO:CD	2.37	0.53
2:D:224:LEU:HD21	2:D:231:SER:HB3	1.89	0.53
2:D:513:VAL:HG13	2:D:564:VAL:HG12	1.92	0.52
4:A:1802[B]:MCD:NP2	4:A:1802[B]:MCD:HP92	2.21	0.52
1:A:512:LEU:HD21	1:A:543:ALA:HB1	1.92	0.52
1:C:512:LEU:HD21	1:C:543:ALA:HB1	1.92	0.52
6:D:3004:GOL:O1	6:D:3004:GOL:O3	2.22	0.52
1:C:357:GLN:HE22	2:D:290:GLN:NE2	2.05	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ASP:HA	1:C:533:LYS:HE3	1.92	0.51
4:A:1802[B]:MCD:HPB1	4:A:1802[B]:MCD:OP2	2.11	0.51
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.93	0.51
2:B:513:VAL:HG13	2:B:564:VAL:HG12	1.93	0.51
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.92	0.50
5:C:2800:B12:H372	5:C:2800:B12:H351	1.94	0.50
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.94	0.50
2:D:77:ARG:HB3	2:D:78:PRO:HD2	1.93	0.50
2:B:554:VAL:HG12	2:B:558:LYS:HD2	1.93	0.49
1:C:250:ALA:HB2	1:C:446:ILE:HG12	1.95	0.49
5:C:2800:B12:C25	5:C:2800:B12:H312	2.43	0.49
1:C:665:VAL:N	1:C:666:PRO:HD2	2.27	0.49
5:C:2800:B12:H312	5:C:2800:B12:H251	1.95	0.49
1:A:706:THR:HB	1:A:707:PRO:CD	2.41	0.48
1:A:359:HIS:CE1	1:A:401:ASP:H	2.32	0.48
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.10	0.48
1:A:122:HIS:HA	1:A:167:MET:HE1	1.96	0.48
1:C:359:HIS:CE1	1:C:401:ASP:H	2.31	0.48
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.62	0.48
1:C:139:ALA:HB1	5:C:2800:B12:H362	1.96	0.48
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.79	0.48
1:A:503:ARG:HD2	1:A:508:VAL:HG21	1.95	0.48
1:C:188:LYS:HB3	1:C:189:PRO:HD2	1.95	0.48
5:C:2800:B12:H353	5:C:2800:B12:C30	2.40	0.47
5:A:1800:B12:H372	5:A:1800:B12:H351	1.97	0.47
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.97	0.47
2:B:331:LEU:HD13	2:B:365:GLN:HB3	1.97	0.47
1:C:597:ARG:HG2	1:C:597:ARG:HH11	1.80	0.47
5:A:1800:B12:O7R	5:A:1800:B12:C2B	2.63	0.46
4:C:2802[B]:MCD:NP2	4:C:2802[B]:MCD:HP92	2.28	0.46
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.97	0.46
1:A:597:ARG:HH11	1:A:597:ARG:HG2	1.81	0.46
1:A:514:LYS:HD3	1:A:534:LEU:HD22	1.98	0.46
1:A:665:VAL:N	1:A:666:PRO:CD	2.79	0.46
2:D:339:ASN:HA	2:D:342:ARG:HB2	1.97	0.46
5:C:2800:B12:C42	5:C:2800:B12:H363	2.47	0.45
2:B:518:LEU:HD21	2:B:581:VAL:HG11	1.98	0.45
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.98	0.45
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.98	0.45
2:B:274:THR:HA	2:B:313:VAL:HG13	1.97	0.45
5:C:2800:B12:H2B	5:C:2800:B12:O2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:PRO:O	2:D:93:PHE:HB2	2.17	0.45
2:B:281:ASN:ND2	2:B:323:ASN:HD21	2.14	0.44
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.99	0.44
1:A:264:VAL:HG12	1:A:268:ARG:HH21	1.81	0.44
1:A:357:GLN:HE22	2:B:290:GLN:NE2	2.03	0.44
1:A:310:LYS:HE2	2:B:21:LEU:HD11	2.00	0.44
2:B:532:SER:CB	2:B:533:PRO:HD3	2.47	0.44
1:A:188:LYS:HB3	1:A:189:PRO:HD2	1.98	0.44
1:A:665:VAL:N	1:A:666:PRO:HD2	2.34	0.43
2:D:579:LEU:HG	2:D:583:LYS:HE3	2.01	0.43
1:C:444:MET:HE2	1:C:564:ARG:HD3	1.99	0.43
5:C:2800:B12:HM51	5:C:2800:B12:HM63	1.85	0.43
1:A:139:ALA:HB1	5:A:1800:B12:H362	2.01	0.43
1:C:203:GLU:OE2	1:C:207:ARG:HD3	2.19	0.43
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.54	0.43
2:B:515:LEU:HD23	2:B:566:ASP:HB3	2.01	0.42
2:B:579:LEU:HG	2:B:583:LYS:HE3	2.00	0.42
2:B:425:LYS:HZ3	2:B:425:LYS:HB2	1.83	0.42
1:A:492:GLN:HE22	1:A:495:LYS:NZ	2.17	0.42
2:B:246:ALA:HB1	2:B:250:ALA:HB3	2.00	0.42
1:C:197:GLN:HA	1:C:239:SER:HB3	2.02	0.42
1:A:138:MET:SD	1:A:485:ASN:HB2	2.59	0.42
1:C:215:GLN:HB3	1:C:216:PRO:CD	2.46	0.42
1:C:636:THR:HB	1:C:637:PRO:HD2	2.01	0.42
2:D:334:GLU:O	2:D:335:ASP:C	2.63	0.42
1:A:541:ALA:O	1:A:542:MET:HB2	2.19	0.42
1:C:605:MET:HE3	1:C:664:LEU:HB3	2.01	0.42
5:A:1800:B12:H2B	5:A:1800:B12:O2	2.19	0.42
1:C:23:ARG:CD	7:C:4304:HOH:O	2.62	0.42
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.55	0.42
1:C:252:ALA:O	1:C:256:MET:HG3	2.20	0.42
5:C:2800:B12:H363	5:C:2800:B12:H421	2.02	0.42
2:D:267:VAL:HA	2:D:271:PHE:O	2.20	0.42
1:A:571:SER:HB3	1:A:623:ASP:HB3	2.02	0.42
1:C:171:VAL:HG23	1:C:196:ILE:HG12	2.01	0.42
1:C:521:ASN:O	1:C:529:ARG:HD3	2.19	0.42
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.85	0.41
1:A:521:ASN:O	1:A:529:ARG:HD3	2.21	0.41
1:C:579:GLU:HB3	1:C:712:PRO:HB2	2.01	0.41
5:A:1800:B12:HM63	5:A:1800:B12:HM51	1.74	0.41
2:D:107:TRP:CD1	2:D:358:ILE:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:HB3	2:B:459:PRO:HG2	2.02	0.41
5:A:1800:B12:H262	5:A:1800:B12:H91	1.97	0.41
2:D:331:LEU:HD13	2:D:365:GLN:HB3	2.03	0.41
2:D:518:LEU:HD21	2:D:581:VAL:HG11	2.02	0.41
1:A:256:MET:HE2	1:A:256:MET:HB3	1.92	0.41
1:A:89:PHE:CE2	3:A:1801[A]:SCD:HS21	2.55	0.41
1:A:683:THR:HG21	1:A:718:LEU:HD13	2.02	0.41
2:B:267:VAL:HA	2:B:271:PHE:O	2.21	0.41
5:C:2800:B12:C61	5:C:2800:B12:H551	2.50	0.41
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.50	0.41
1:A:374:LEU:HB2	1:A:481:LEU:HD23	2.03	0.41
1:C:503:ARG:HD2	1:C:508:VAL:HG21	2.03	0.41
1:A:606:GLY:O	1:A:634:PHE:HA	2.20	0.40
5:A:1800:B12:H601	5:A:1800:B12:H252	2.03	0.40
1:C:201:LEU:HG	1:C:218:MET:HE1	2.03	0.40
1:A:89:PHE:CE2	4:A:1802[B]:MCD:HS2	2.57	0.40
1:C:613:GLY:HA2	5:C:2800:B12:H3P1	2.03	0.40
2:D:197:LEU:HD12	2:D:233:ALA:HB1	2.03	0.40
2:B:460:ILE:HD13	2:B:494:SER:HB3	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LYS:NZ	2:D:20:THR:OG1[2_646]	1.69	0.51
1:A:670:LYS:CD	2:D:20:THR:O[2_646]	2.02	0.18

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	723/727 (99%)	695 (96%)	27 (4%)	1 (0%)	48 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	723/727 (99%)	693 (96%)	29 (4%)	1 (0%)	48	57
2	B	617/637 (97%)	594 (96%)	21 (3%)	2 (0%)	36	42
2	D	617/637 (97%)	596 (97%)	19 (3%)	2 (0%)	36	42
All	All	2680/2728 (98%)	2578 (96%)	96 (4%)	6 (0%)	43	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	576	ASN
2	D	171	ASP
1	A	576	ASN
2	B	171	ASP
2	D	228	SER
2	B	228	SER

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	573/590 (97%)	558 (97%)	15 (3%)	40	55
1	C	573/590 (97%)	559 (98%)	14 (2%)	43	58
2	B	481/509 (94%)	461 (96%)	20 (4%)	26	36
2	D	481/509 (94%)	457 (95%)	24 (5%)	22	28
All	All	2108/2198 (96%)	2035 (96%)	73 (4%)	32	43

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	96	LYS
1	A	123	ARG
1	A	202	LYS
1	A	430	VAL

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Mol	Chain	Res	Type
1	A	480	VAL
1	A	514	LYS
1	A	525	LYS
1	A	533	LYS
1	A	577	THR
1	A	592	GLN
1	A	597	ARG
1	A	656	SER
1	A	668	LEU
1	A	721	LYS
2	B	22	SER
2	B	77	ARG
2	B	186	SER
2	B	188	LYS
2	B	191	LYS
2	B	193	LEU
2	B	216	VAL
2	B	224	LEU
2	B	226	LYS
2	B	228	SER
2	B	300	LEU
2	B	334	GLU
2	B	410	ARG
2	B	425	LYS
2	B	435	THR
2	B	477	LYS
2	B	512	LYS
2	B	532	SER
2	B	619	MET
2	B	638	LYS
1	C	23	ARG
1	C	24	ARG
1	C	67	ILE
1	C	96	LYS
1	C	202	LYS
1	C	218	MET
1	C	365	THR
1	C	473	GLU
1	C	533	LYS
1	C	567	SER
1	C	592	GLN
1	C	597	ARG

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Mol	Chain	Res	Type
1	C	668	LEU
1	C	721	LYS
2	D	60	LYS
2	D	77	ARG
2	D	141	ASP
2	D	159	LEU
2	D	186	SER
2	D	188	LYS
2	D	191	LYS
2	D	193	LEU
2	D	216	VAL
2	D	224	LEU
2	D	228	SER
2	D	297	LEU
2	D	300	LEU
2	D	334	GLU
2	D	410	ARG
2	D	425	LYS
2	D	435	THR
2	D	477	LYS
2	D	512	LYS
2	D	522	ARG
2	D	532	SER
2	D	617	LEU
2	D	619	MET
2	D	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	191	GLN
1	A	198	ASN
1	A	246	GLN
1	A	385	ASN
1	A	492	GLN
1	A	521	ASN
1	A	562	GLN
1	A	635	GLN
1	A	643	GLN
2	B	290	GLN
2	B	322	GLN

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Mol	Chain	Res	Type
2	B	323	ASN
2	B	391	ASN
2	B	421	GLN
2	B	577	GLN
1	C	191	GLN
1	C	198	ASN
1	C	246	GLN
1	C	359	HIS
1	C	385	ASN
1	C	492	GLN
1	C	521	ASN
1	C	643	GLN
2	D	290	GLN
2	D	322	GLN
2	D	323	ASN
2	D	391	ASN

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

10 ligands are modelled in this entry.

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	$\#\|Z\|>2$
6	GOL	B	3001	-	5,5,5	0.23	0	5,5,5	0.33	0
3	SCD	C	2801[A]	-	55,57,57	1.13	4 (7%)	79,84,84	1.31	10 (12%)
5	B12	C	2800	1	94,101,101	0.99	5 (5%)	149,166,166	1.56	26 (17%)
5	B12	A	1800	1	94,101,101	0.96	3 (3%)	149,166,166	1.62	30 (20%)
4	MCD	C	2802[B]	-	54,57,57	1.18	5 (9%)	78,85,85	1.25	10 (12%)
6	GOL	B	3002	-	5,5,5	0.29	0	5,5,5	0.97	0
6	GOL	D	3004	-	5,5,5	0.29	0	5,5,5	0.67	0
4	MCD	A	1802[B]	-	54,57,57	1.20	5 (9%)	78,85,85	1.26	8 (10%)
3	SCD	A	1801[A]	-	55,57,57	1.17	6 (10%)	79,84,84	1.36	9 (11%)
6	GOL	D	3003	-	5,5,5	0.22	0	5,5,5	0.41	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
6	GOL	B	3001	-	-	4/4/4/4	-
3	SCD	C	2801[A]	-	-	5/56/72/72	0/3/3/3
5	B12	C	2800	1	-	10/56/223/223	0/3/11/11
5	B12	A	1800	1	-	9/56/223/223	0/3/11/11
4	MCD	C	2802[B]	-	-	2/59/75/75	0/3/3/3
6	GOL	B	3002	-	-	2/4/4/4	-
6	GOL	D	3004	-	-	2/4/4/4	-
4	MCD	A	1802[B]	-	-	3/59/75/75	0/3/3/3
3	SCD	A	1801[A]	-	-	4/56/72/72	0/3/3/3
6	GOL	D	3003	-	-	4/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1802[B]	MCD	CP2-NP1	3.67	1.54	1.46
3	A	1801[A]	SCD	CP2-NP1	3.63	1.54	1.46
4	A	1802[B]	MCD	CP5-NP2	3.51	1.54	1.46
4	C	2802[B]	MCD	CP5-NP2	3.44	1.53	1.46
4	C	2802[B]	MCD	CP2-NP1	3.31	1.53	1.46
3	A	1801[A]	SCD	CP5-NP2	3.29	1.53	1.46
3	C	2801[A]	SCD	CP2-NP1	3.14	1.53	1.46
3	A	1801[A]	SCD	P2-O7	-3.12	1.47	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2801[A]	SCD	CP5-NP2	3.10	1.53	1.46
4	A	1802[B]	MCD	P2-O7	-2.97	1.47	1.59
3	C	2801[A]	SCD	P2-O7	-2.92	1.48	1.59
5	A	1800	B12	C14-N23	2.89	1.39	1.35
4	C	2802[B]	MCD	P2-O7	-2.82	1.48	1.59
5	A	1800	B12	C2B-N1B	-2.48	1.33	1.37
5	C	2800	B12	C14-N23	2.45	1.38	1.35
4	A	1802[B]	MCD	P2-O6	2.43	1.62	1.59
5	C	2800	B12	P-O2	2.37	1.66	1.59
5	C	2800	B12	C19-N24	-2.33	1.46	1.49
4	A	1802[B]	MCD	OS4-CS4	2.25	1.28	1.22
5	C	2800	B12	C30-C3	2.21	1.59	1.54
3	A	1801[A]	SCD	P2-O6	2.20	1.61	1.59
5	C	2800	B12	C35-C5	2.18	1.55	1.50
3	A	1801[A]	SCD	OS4-CS4	2.15	1.29	1.22
5	A	1800	B12	P-O2	2.15	1.65	1.59
4	C	2802[B]	MCD	OS4-CS4	2.15	1.28	1.22
3	C	2801[A]	SCD	C2-N1	2.14	1.37	1.33
3	A	1801[A]	SCD	C2-N1	2.03	1.37	1.33
4	C	2802[B]	MCD	P2-O6	2.01	1.61	1.59

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1800	B12	C16-C15-C14	-4.85	113.86	121.26
5	C	2800	B12	C19-N24-C16	4.82	112.56	107.29
3	C	2801[A]	SCD	CP8-CPA-CPB	4.68	115.95	108.22
4	A	1802[B]	MCD	CP5-NP2-CP6	-4.66	114.17	122.55
3	A	1801[A]	SCD	CP8-CPA-CPB	4.39	115.47	108.22
4	C	2802[B]	MCD	CP5-NP2-CP6	-4.36	114.70	122.55
3	C	2801[A]	SCD	CP5-NP2-CP6	-4.23	114.95	122.55
3	A	1801[A]	SCD	CP5-NP2-CP6	-4.20	115.01	122.55
5	C	2800	B12	C20-C1-C19	4.17	113.36	109.35
5	C	2800	B12	C16-C15-C14	-4.00	115.16	121.26
4	C	2802[B]	MCD	CP8-CPA-CPB	3.93	114.71	108.22
5	A	1800	B12	C54-C17-C16	-3.89	92.26	112.41
5	C	2800	B12	C54-C17-C16	-3.81	92.66	112.41
5	C	2800	B12	C9B-C8B-N1B	3.78	106.98	105.30
3	A	1801[A]	SCD	O7-CPB-CPA	-3.67	104.65	110.55
4	A	1802[B]	MCD	CP8-CPA-CPB	3.65	114.25	108.22
5	A	1800	B12	C19-N24-C16	3.65	111.28	107.29
5	A	1800	B12	C55-C17-C18	3.63	118.05	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2802[B]	MCD	O7-CPB-CPA	-3.60	104.75	110.55
5	A	1800	B12	C13-C14-C15	-3.56	118.90	124.32
5	C	2800	B12	C55-C17-C16	3.55	123.54	116.59
4	A	1802[B]	MCD	O7-CPB-CPA	-3.54	104.85	110.55
5	C	2800	B12	C9-N22-C6	3.54	109.54	105.28
5	A	1800	B12	C12-C11-C10	-3.41	119.01	123.40
5	A	1800	B12	C9B-C8B-N1B	3.36	106.79	105.30
3	C	2801[A]	SCD	O7-CPB-CPA	-3.35	105.16	110.55
5	C	2800	B12	C55-C17-C18	3.06	116.95	111.12
3	A	1801[A]	SCD	CP2-NP1-CP3	-3.06	117.13	122.82
3	C	2801[A]	SCD	CP9-CPA-CPB	3.06	113.27	108.22
5	A	1800	B12	C7B-C8B-C9B	3.05	126.13	122.47
3	C	2801[A]	SCD	CS3-CS2-CS1	-3.02	109.22	113.49
3	A	1801[A]	SCD	OS5-CS4-CS3	3.02	123.54	114.00
4	C	2802[B]	MCD	CP9-CPA-CPB	3.01	113.19	108.22
5	A	1800	B12	C55-C56-C57	-2.93	104.72	111.25
4	A	1802[B]	MCD	CP1-CP2-NP1	-2.91	104.03	112.20
5	A	1800	B12	C13-C14-N23	2.88	113.00	109.09
5	C	2800	B12	O51-C50-C49	-2.88	112.36	121.04
4	C	2802[B]	MCD	CP9-CPA-CP7	-2.87	103.87	108.77
5	A	1800	B12	C5-C6-N22	-2.75	119.72	123.88
5	A	1800	B12	C5M-C5B-C6B	-2.73	115.18	120.76
5	A	1800	B12	C9-N22-C6	2.71	108.54	105.28
5	A	1800	B12	C10-C11-N23	2.69	128.97	124.42
5	A	1800	B12	O5-P-O4	2.67	124.89	112.44
3	C	2801[A]	SCD	OS5-CS4-CS3	2.63	122.31	114.00
5	A	1800	B12	O51-C50-C49	-2.62	113.12	121.04
5	A	1800	B12	C20-C1-C2	-2.62	108.96	113.28
5	C	2800	B12	C18-C19-N24	2.62	106.27	102.33
5	C	2800	B12	C2P-C1P-N59	-2.59	109.11	112.92
5	A	1800	B12	C4B-C5B-C6B	2.57	123.46	119.69
3	C	2801[A]	SCD	CP1-CP2-NP1	-2.55	105.04	112.20
5	A	1800	B12	C55-C17-C16	2.52	121.53	116.59
4	C	2802[B]	MCD	CP1-CP2-NP1	-2.52	105.13	112.20
5	C	2800	B12	C7B-C8B-C9B	2.51	125.48	122.47
3	A	1801[A]	SCD	CP1-CP2-NP1	-2.48	105.23	112.20
4	C	2802[B]	MCD	OS1-CS1-CPS	2.48	125.88	121.68
5	C	2800	B12	C3-C4-C5	-2.47	119.68	123.82
5	A	1800	B12	C18-C19-N24	2.47	106.04	102.33
3	A	1801[A]	SCD	OP2-CP6-NP2	2.41	128.08	122.98
5	C	2800	B12	C35-C5-C4	-2.40	111.93	116.79
5	C	2800	B12	C54-C17-C55	-2.40	105.28	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1800	B12	C1P-N59-C57	-2.39	117.56	122.69
5	C	2800	B12	C1P-N59-C57	-2.38	117.59	122.69
5	A	1800	B12	C53-C15-C16	2.37	124.39	120.36
4	A	1802[B]	MCD	CP2-NP1-CP3	-2.37	118.41	122.82
5	C	2800	B12	C1-C2-C3	-2.37	98.62	101.60
5	C	2800	B12	C2-C1-C19	-2.35	114.96	118.61
5	A	1800	B12	C3-C4-C5	-2.35	119.89	123.82
5	C	2800	B12	C15-C16-N24	2.32	125.73	122.42
3	C	2801[A]	SCD	OS5-CS4-OS4	-2.32	117.38	123.33
3	C	2801[A]	SCD	OP2-CP6-NP2	2.29	127.82	122.98
5	A	1800	B12	C2-C1-N21	2.28	104.95	101.78
4	A	1802[B]	MCD	OP2-CP6-CP7	-2.28	114.53	120.89
4	A	1802[B]	MCD	C2'-C3'-C4'	-2.28	99.25	103.24
5	C	2800	B12	C2-C1-N21	2.27	104.94	101.78
5	C	2800	B12	O5-P-O4	2.27	123.01	112.44
5	A	1800	B12	C1-C2-C3	-2.27	98.75	101.60
5	A	1800	B12	C42-C43-N45	2.27	123.76	116.49
4	C	2802[B]	MCD	C2'-C3'-C4'	-2.24	99.33	103.24
5	A	1800	B12	C54-C17-C18	-2.21	109.81	112.99
5	A	1800	B12	C41-C8-C9	-2.21	107.33	111.19
4	A	1802[B]	MCD	CP9-CPA-CP7	-2.20	105.01	108.77
3	C	2801[A]	SCD	C2'-C3'-C4'	-2.20	99.38	103.24
5	C	2800	B12	C55-C56-C57	-2.20	106.35	111.25
5	C	2800	B12	C13-C14-C15	-2.19	120.98	124.32
5	A	1800	B12	C7B-C8B-N1B	-2.18	127.08	131.39
5	C	2800	B12	C8B-C9B-N3B	-2.17	107.65	110.00
5	C	2800	B12	C4B-C5B-C6B	2.16	122.85	119.69
5	A	1800	B12	C2P-C1P-N59	-2.15	109.76	112.92
3	A	1801[A]	SCD	C2'-C3'-C4'	-2.15	99.48	103.24
4	C	2802[B]	MCD	OP2-CP6-CP7	-2.12	114.97	120.89
4	C	2802[B]	MCD	CPS-CS1-CS2	-2.09	114.28	117.36
3	A	1801[A]	SCD	CP9-CPA-CPB	2.08	111.66	108.22
5	C	2800	B12	C30-C31-C32	2.06	119.56	112.55

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2801[A]	SCD	P1-O6-P2-O7
4	A	1802[B]	MCD	P1-O6-P2-O7
4	C	2802[B]	MCD	P1-O6-P2-O7
5	A	1800	B12	C2R-C1R-N1B-C2B

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Mol	Chain	Res	Type	Atoms
5	C	2800	B12	C2R-C1R-N1B-C2B
6	B	3001	GOL	O1-C1-C2-C3
6	B	3001	GOL	C1-C2-C3-O3
6	B	3002	GOL	C1-C2-C3-O3
6	D	3003	GOL	O1-C1-C2-C3
6	D	3003	GOL	C1-C2-C3-O3
6	D	3004	GOL	C1-C2-C3-O3
5	C	2800	B12	C42-C41-C8-C9
6	B	3001	GOL	O1-C1-C2-O2
6	B	3002	GOL	O2-C2-C3-O3
5	A	1800	B12	C16-C17-C55-C56
5	A	1800	B12	C2R-C1R-N1B-C8B
5	C	2800	B12	C2R-C1R-N1B-C8B
6	B	3001	GOL	O2-C2-C3-O3
6	D	3003	GOL	O1-C1-C2-O2
6	D	3004	GOL	O2-C2-C3-O3
6	D	3003	GOL	O2-C2-C3-O3
5	A	1800	B12	C41-C42-C43-O44
5	A	1800	B12	C41-C42-C43-N45
3	A	1801[A]	SCD	P1-O6-P2-O7
5	A	1800	B12	O6R-C1R-N1B-C8B
5	C	2800	B12	O6R-C1R-N1B-C8B
3	A	1801[A]	SCD	P2-O6-P1-O12
3	C	2801[A]	SCD	P2-O6-P1-O12
4	C	2802[B]	MCD	P2-O6-P1-O12
3	A	1801[A]	SCD	CP8-CPA-CPB-O7
3	C	2801[A]	SCD	CP8-CPA-CPB-O7
4	A	1802[B]	MCD	P2-O6-P1-O12
5	C	2800	B12	C55-C56-C57-O58
4	A	1802[B]	MCD	CPS-CS1-CS2-CS4
3	C	2801[A]	SCD	P2-O6-P1-O11
5	A	1800	B12	C2P-O3-P-O4
5	A	1800	B12	C2P-O3-P-O5
5	C	2800	B12	C2P-O3-P-O4
5	C	2800	B12	C2P-O3-P-O5
5	C	2800	B12	C55-C56-C57-N59
5	C	2800	B12	C30-C31-C32-N33
5	A	1800	B12	C30-C31-C32-N33
3	A	1801[A]	SCD	CS2-CS3-CS4-OS4
5	C	2800	B12	C30-C31-C32-O34
3	C	2801[A]	SCD	CS2-CS3-CS4-OS5

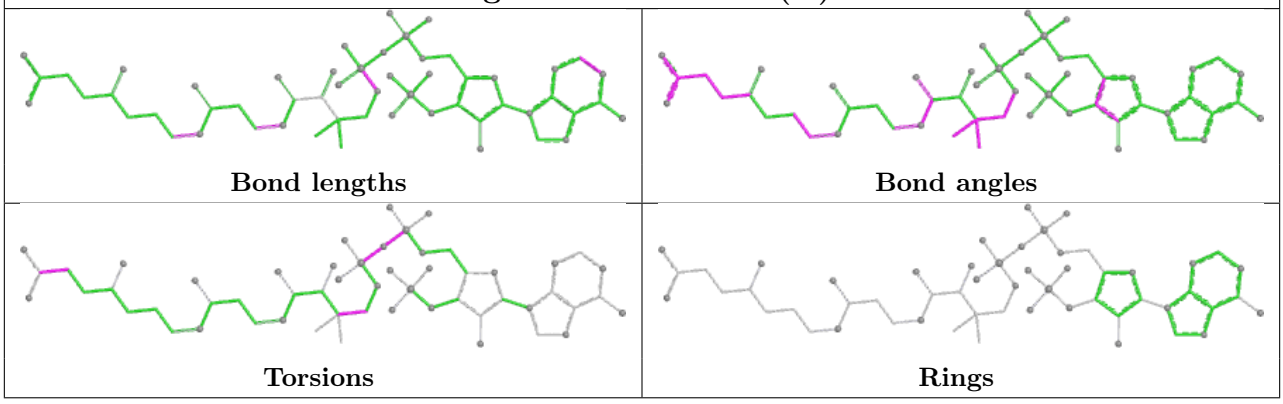
There are no ring outliers.

8 monomers are involved in 44 short contacts:

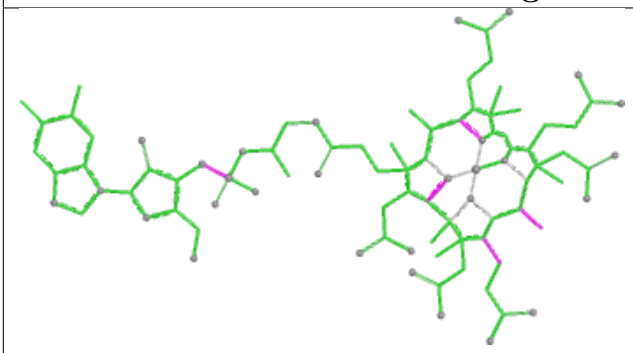
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2801[A]	SCD	1	0
5	C	2800	B12	16	0
5	A	1800	B12	17	0
4	C	2802[B]	MCD	2	0
6	B	3002	GOL	1	0
6	D	3004	GOL	2	0
4	A	1802[B]	MCD	3	0
3	A	1801[A]	SCD	2	0

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.

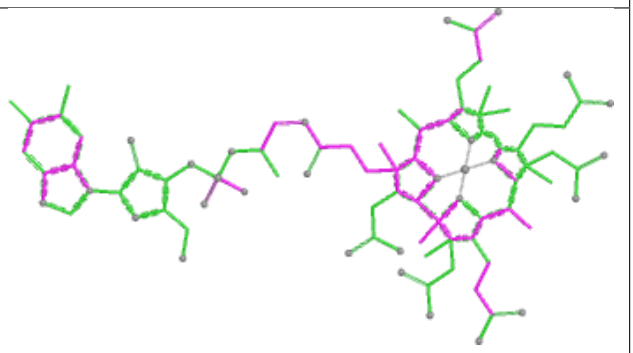
Ligand SCD C 2801 (A)



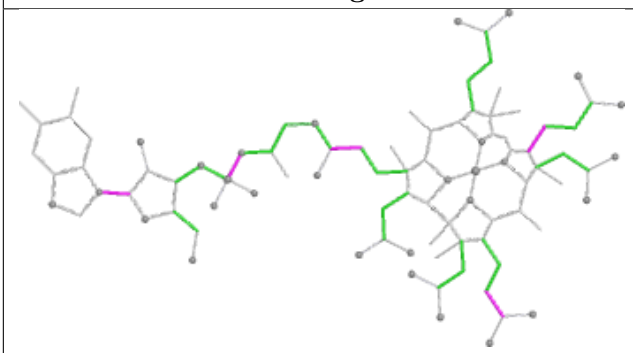
Ligand B12 C 2800



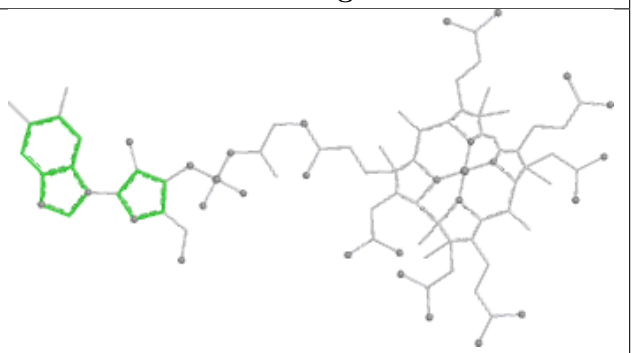
Bond lengths



Bond angles

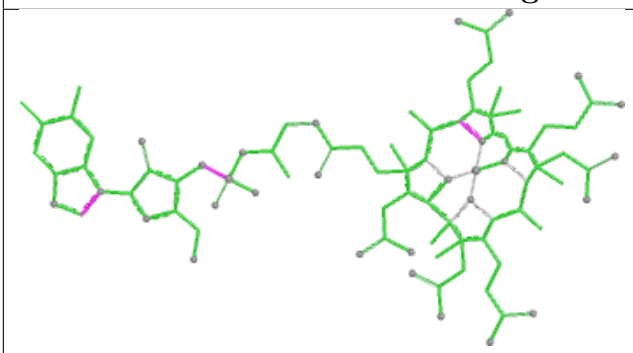


Torsions

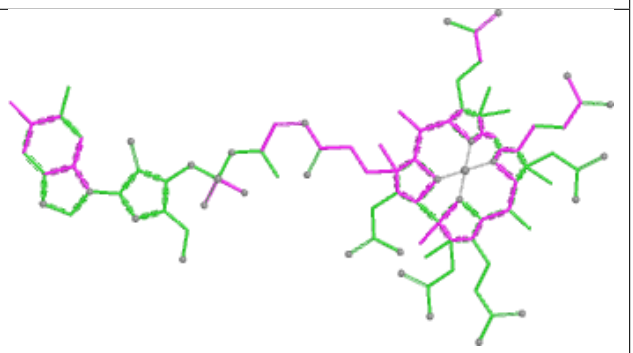


Rings

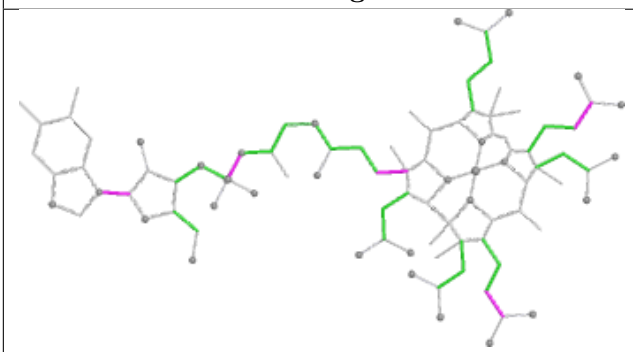
Ligand B12 A 1800



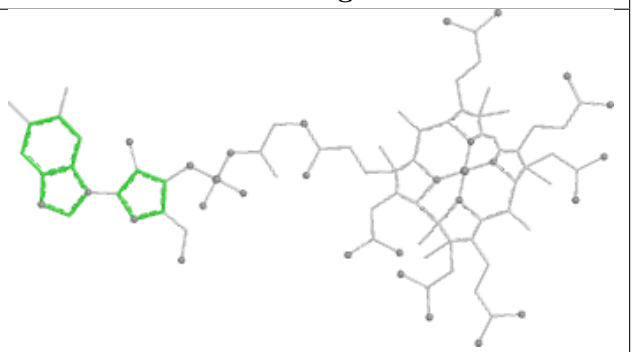
Bond lengths



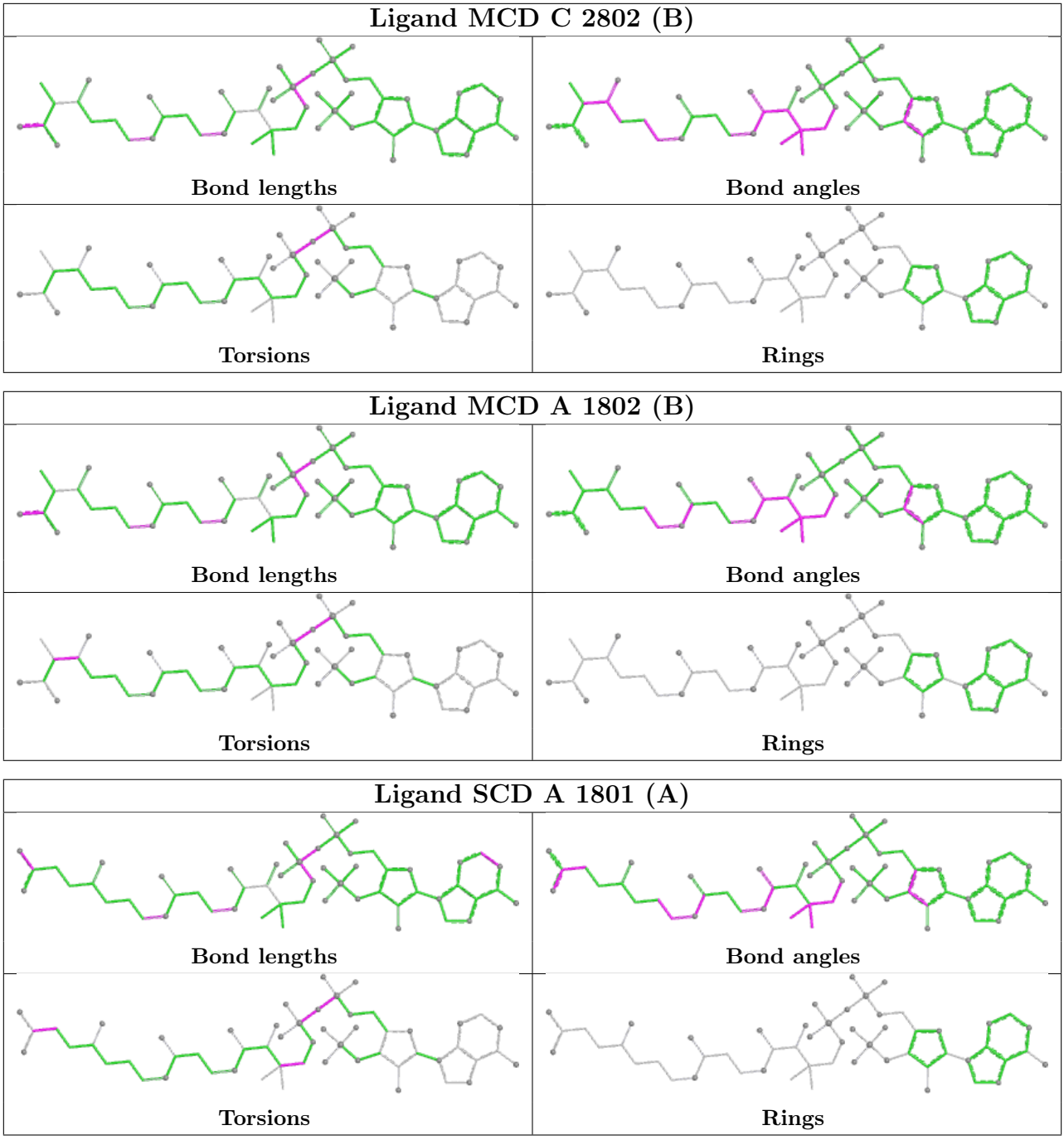
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	A	725/727 (99%)	0.14	12 (1%) 69 66	17, 36, 60, 80	0
1	C	725/727 (99%)	0.34	29 (4%) 42 39	17, 36, 60, 81	0
2	B	619/637 (97%)	0.69	46 (7%) 20 18	24, 49, 73, 89	0
2	D	619/637 (97%)	0.90	74 (11%) 9 6	26, 50, 73, 89	0
All	All	2688/2728 (98%)	0.50	161 (5%) 27 24	17, 42, 70, 89	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	20	THR	5.1
1	C	23	ARG	4.6
2	B	170	TYR	4.0
1	C	576	ASN	3.9
2	D	146	ALA	3.7
1	C	501	ALA	3.6
2	D	183	TYR	3.5
2	B	635	GLY	3.5
1	C	728	ALA	3.5
1	C	9	SER	3.4
1	C	25	PHE	3.3
2	D	182	VAL	3.3
2	D	638	LYS	3.3
1	C	16	PRO	3.1
2	B	183	TYR	3.1
2	D	126	LEU	3.1
2	B	179	LEU	3.0
2	D	637	ALA	3.0
1	C	7	PHE	2.9
2	D	140	VAL	2.9
1	C	27	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	20	THR	2.9
2	D	25	GLY	2.8
2	D	170	TYR	2.8
2	B	106	ALA	2.8
2	D	227	PHE	2.8
2	B	155	SER	2.8
2	B	195	LEU	2.8
2	B	612	LEU	2.8
1	C	21	ALA	2.8
2	D	190	ALA	2.8
2	D	145	ILE	2.7
1	C	486	SER	2.7
2	D	427	GLY	2.7
2	D	195	LEU	2.7
2	B	423	VAL	2.7
1	C	14	ASN	2.7
2	B	487	GLY	2.7
2	D	180	VAL	2.7
2	D	272	THR	2.7
2	D	164	VAL	2.7
2	D	217	LEU	2.7
2	D	220	TRP	2.7
2	B	194	ALA	2.6
2	B	638	LYS	2.6
2	D	151	ASP	2.6
2	D	218	GLY	2.6
2	D	193	LEU	2.6
1	C	19	ALA	2.6
1	A	576	ASN	2.6
2	D	192	ASP	2.6
1	A	595	GLY	2.6
1	A	726	LEU	2.6
2	D	312	GLY	2.6
2	D	307	ILE	2.6
2	D	276	ALA	2.5
2	B	427	GLY	2.5
2	B	182	VAL	2.5
2	D	93	PHE	2.5
2	B	118	GLU	2.5
1	C	726	LEU	2.5
2	B	207	LEU	2.5
2	D	179	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	305	ALA	2.5
2	B	197	LEU	2.5
1	C	543	ALA	2.5
2	B	432	ALA	2.5
2	B	602	PHE	2.4
2	B	124	ALA	2.4
2	D	487	GLY	2.4
2	D	507	VAL	2.4
2	D	191	LYS	2.4
2	D	202	ILE	2.4
2	B	147	PRO	2.4
2	B	609	ALA	2.4
2	D	89	GLY	2.4
2	D	260	ALA	2.4
2	B	311	PHE	2.4
2	B	149	HIS	2.4
2	D	230	ASP	2.3
2	B	161	MET	2.3
2	B	636	VAL	2.3
2	D	209	GLY	2.3
2	D	194	ALA	2.3
1	A	92	PHE	2.3
1	C	574	VAL	2.3
2	D	150	LEU	2.3
2	D	188	LYS	2.3
1	C	274	GLY	2.3
2	D	161	MET	2.3
2	D	184	GLU	2.3
2	D	310	VAL	2.3
2	D	433	VAL	2.3
2	B	190	ALA	2.3
2	B	447	ALA	2.3
2	D	253	ALA	2.3
2	D	273	ALA	2.3
2	D	318	ARG	2.2
2	D	176	ALA	2.2
2	D	606	ALA	2.2
1	C	430	VAL	2.2
2	D	216	VAL	2.2
2	D	426	LEU	2.2
2	D	438	VAL	2.2
2	D	96	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	438	GLU	2.2
1	C	30	ALA	2.2
2	B	176	ALA	2.2
2	D	124	ALA	2.2
2	D	357	SER	2.2
2	D	634	LEU	2.2
2	D	313	VAL	2.2
2	B	373	ASP	2.2
1	C	671	GLU	2.2
2	B	576	GLN	2.2
1	C	29	ALA	2.2
2	B	241	TYR	2.2
2	B	227	PHE	2.2
2	D	311	PHE	2.2
1	A	474	HIS	2.2
1	C	592	GLN	2.2
1	A	9	SER	2.2
2	B	175	ALA	2.2
2	D	91	ALA	2.2
1	C	517	TRP	2.1
2	D	158	LEU	2.1
1	C	694	ASP	2.1
2	D	157	VAL	2.1
2	D	147	PRO	2.1
2	D	354	GLY	2.1
1	A	728	ALA	2.1
2	B	274	THR	2.1
2	B	171	ASP	2.1
2	D	201	PRO	2.1
2	D	267	VAL	2.1
2	B	264	ARG	2.1
2	D	274	THR	2.1
2	B	174	ALA	2.1
1	C	502	GLU	2.1
2	D	323	ASN	2.1
2	D	153	VAL	2.1
1	A	155	GLY	2.1
2	B	186	SER	2.1
2	D	121	THR	2.1
1	A	4	LEU	2.1
1	C	474	HIS	2.1
2	D	224	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	187	ASP	2.1
1	C	17	VAL	2.1
2	B	185	ARG	2.1
2	B	230	ASP	2.0
2	B	189	PRO	2.0
1	C	35	GLY	2.0
1	A	575	LYS	2.0
1	C	491	GLU	2.0
2	B	434	MET	2.0
2	B	587	ALA	2.0
2	B	606	ALA	2.0
2	D	320	ALA	2.0
2	D	197	LEU	2.0
1	A	5	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, 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
6	GOL	D	3004	6/6	0.48	0.29	84,84,85,86	0
6	GOL	D	3003	6/6	0.51	0.25	94,95,95,95	0
6	GOL	B	3001	6/6	0.74	0.23	95,95,95,95	0
6	GOL	B	3002	6/6	0.79	0.36	82,83,84,84	0
4	MCD	C	2802[B]	55/55	0.95	0.08	19,24,35,37	55
5	B12	A	1800	91/91	0.95	0.07	16,27,34,37	0
3	SCD	A	1801[A]	55/55	0.96	0.07	15,22,26,27	55
3	SCD	C	2801[A]	55/55	0.96	0.07	15,21,27,28	55
4	MCD	A	1802[B]	55/55	0.96	0.07	21,24,36,39	55

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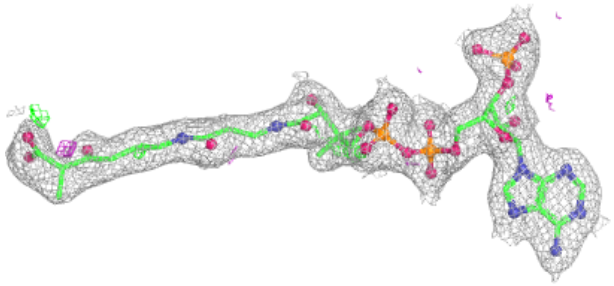
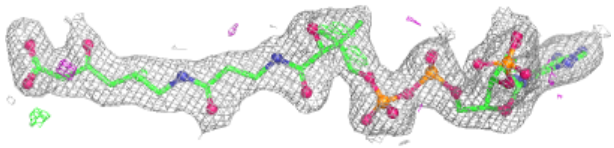
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	B12	C	2800	91/91	0.97	0.07	18,26,32,36	0

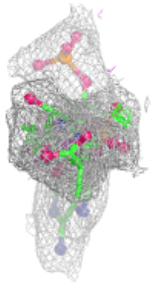
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MCD C 2802 (B):

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

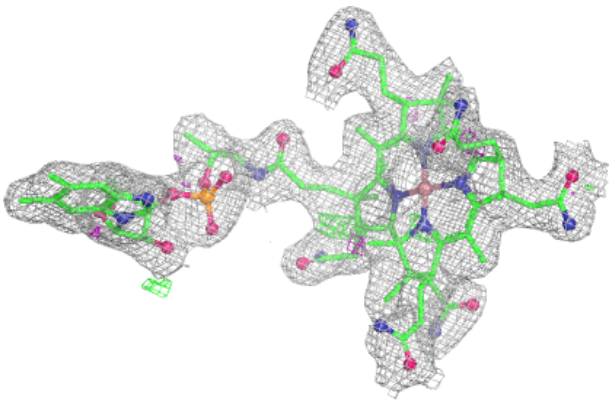


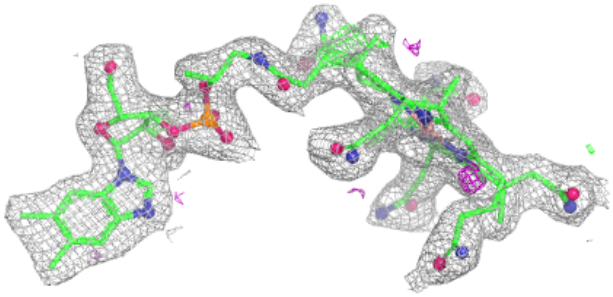


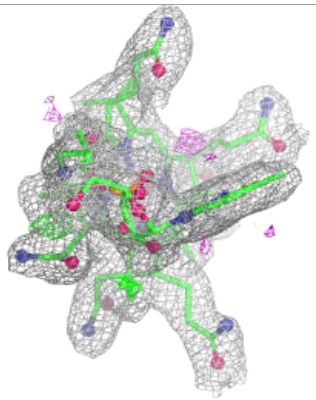


Electron density around B12 A 1800:

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

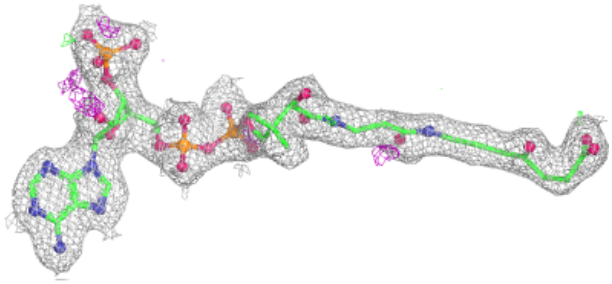


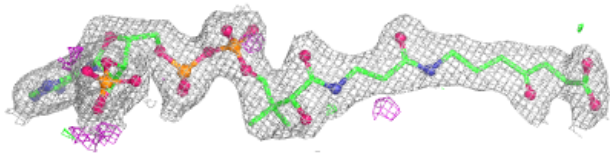




Electron density around SCD A 1801 (A):

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

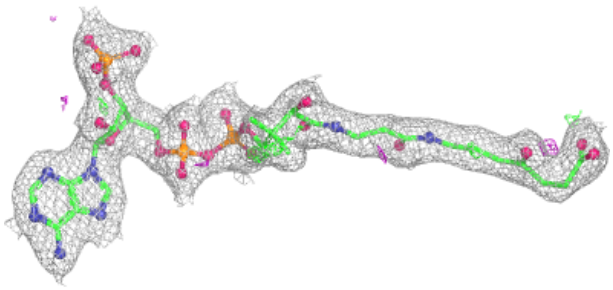


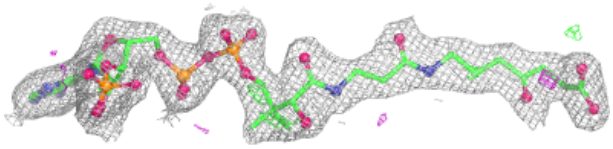


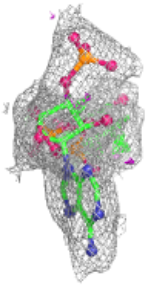


Electron density around SCD C 2801 (A):

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

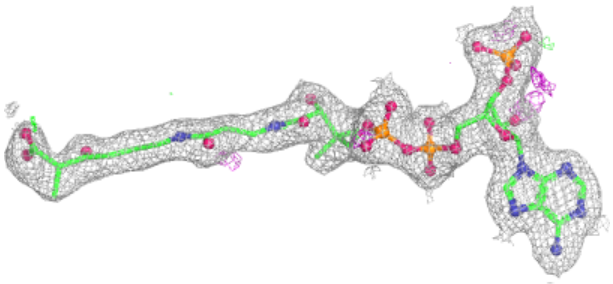


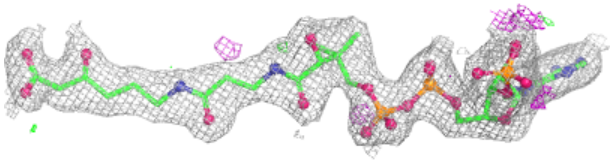


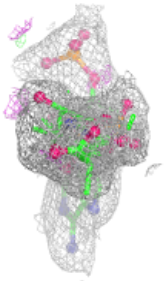


Electron density around MCD A 1802 (B):

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

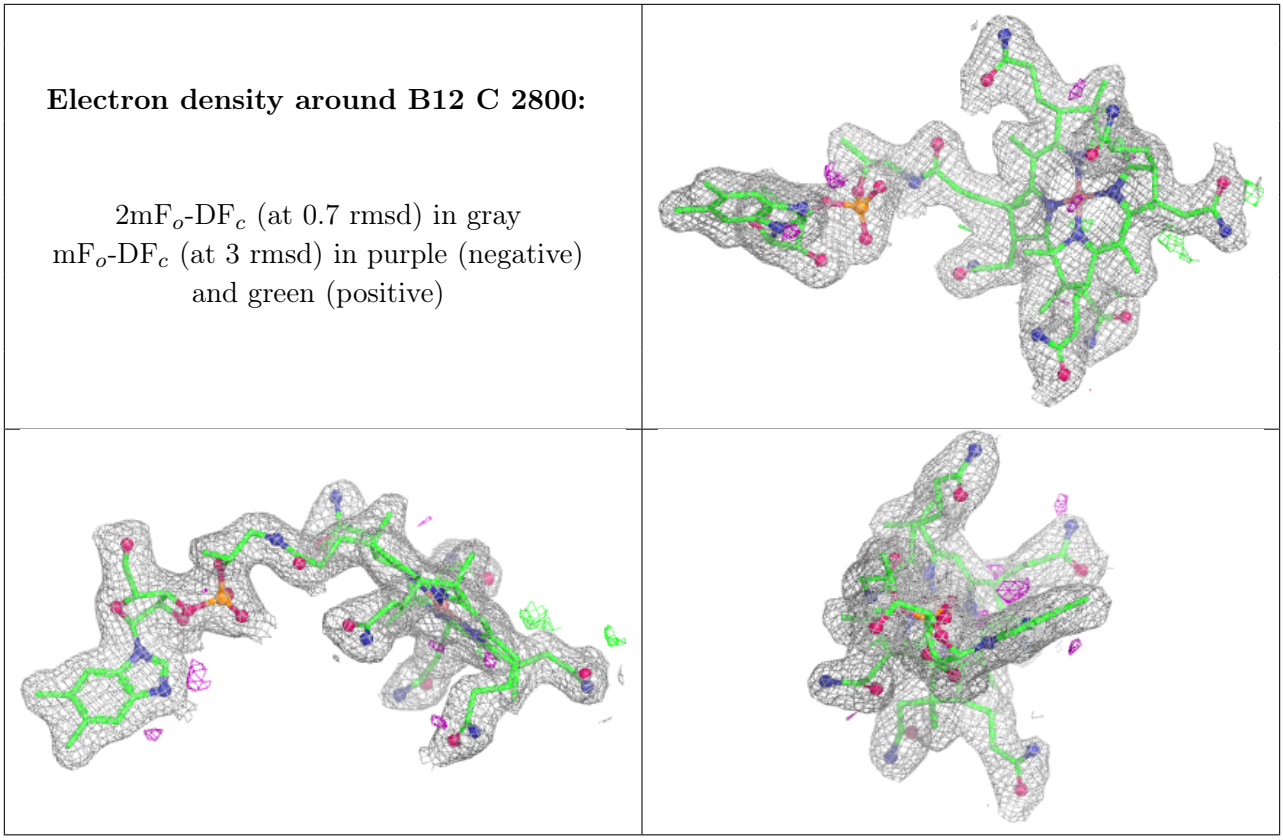






Electron density around B12 C 2800:

$2mF_o$-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 (i)

There are no such residues in this entry.