



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:08 AM UTC

PDB ID : 2CBF / pdb\_00002cbf  
Title : THE X-RAY STRUCTURE OF A COBALAMIN BIOSYNTHETIC ENZYME, COBALT PRECORRIN-4 METHYLTRANSFERASE, CBIF, FROM BACILLUS MEGATERIUM, WITH THE HIS-TAG CLEAVED OFF  
Authors : Schubert, H.L.; Raux, E.; Woodcock, S.C.; Warren, M.J.; Wilson, K.S.  
Deposited on : 1998-05-01  
Resolution : 3.10 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](mailto: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>.

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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)  
Xtrriage (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

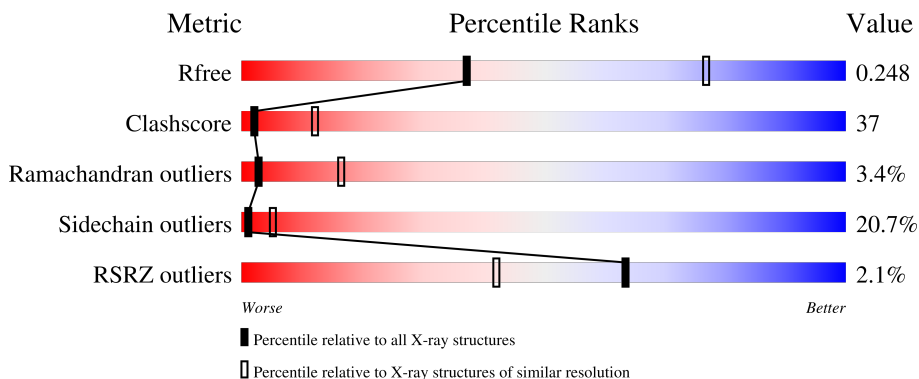
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	234	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1807 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.

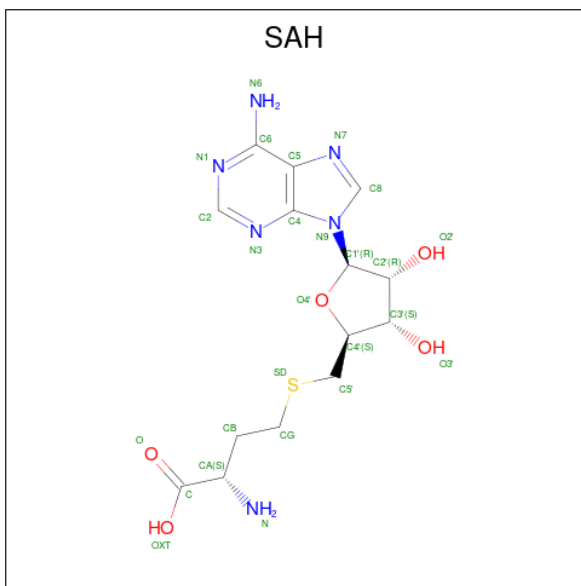
- Molecule 1 is a protein called COBALT-PRECORRIN-4 TRANSMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1781	1135	298	335	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	ALA	conflict	UNP O87696

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).

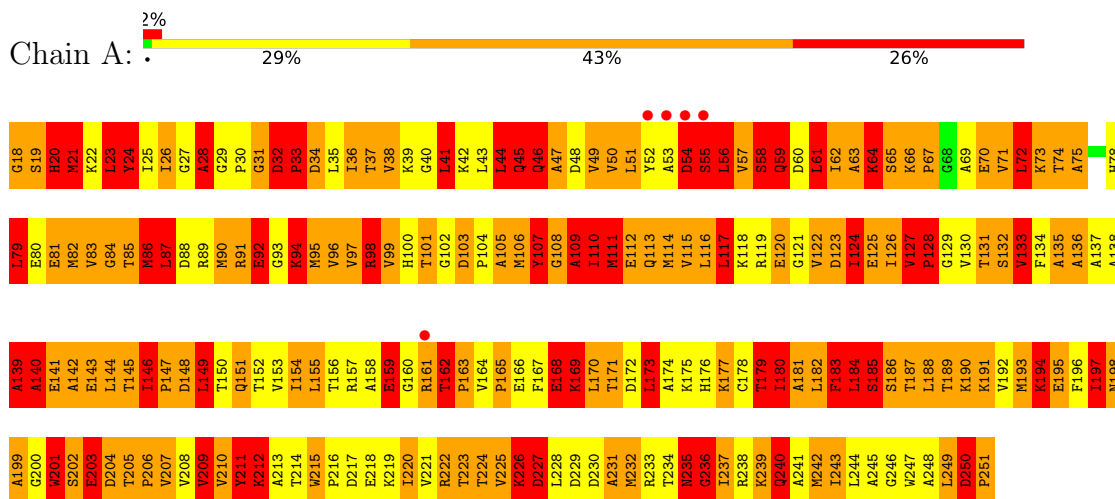


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	26	14	6	5	1	0	0

### 3 Residue-property plots

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: COBALT-PRECORRIN-4 TRANSMETHYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.04Å 80.04Å 77.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-3.10) 92.7 (20.00-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.10Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.281 0.181 , 0.248	Depositor DCC
$R_{free}$ test set	225 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtrriage
Anisotropy	0.308	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 77.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SAH

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	3.27	223/1809 (12.3%)	6.41	878/2451 (35.8%)

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	59

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	ARG	C-O	16.27	1.44	1.24
1	A	109	ALA	CA-CB	-14.49	1.32	1.53
1	A	129	GLY	C-N	13.44	1.48	1.33
1	A	177	LYS	C-O	13.11	1.40	1.23
1	A	71	VAL	C-O	-12.29	1.10	1.24
1	A	43	LEU	CA-C	-12.00	1.36	1.52
1	A	216	PRO	CA-CB	-11.71	1.32	1.53
1	A	213	ALA	CA-CB	-11.49	1.35	1.53
1	A	142	ALA	CA-CB	-11.41	1.37	1.53
1	A	139	ALA	C-O	-11.26	1.11	1.24
1	A	91	ARG	C-O	-11.16	1.09	1.24
1	A	36	ILE	N-CA	10.80	1.60	1.46
1	A	20	HIS	CD2-NE2	10.37	1.49	1.37
1	A	157	ARG	CA-C	-10.15	1.40	1.52
1	A	180	ILE	CA-CB	-9.99	1.42	1.54
1	A	127	VAL	CA-C	-9.73	1.45	1.53
1	A	110	ILE	N-CA	-9.71	1.35	1.46
1	A	121	GLY	N-CA	-9.61	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	ILE	C-N	-9.60	1.21	1.33
1	A	119	ARG	C-O	-9.59	1.11	1.24
1	A	71	VAL	N-CA	-9.48	1.35	1.46
1	A	20	HIS	ND1-CE1	9.37	1.42	1.32
1	A	61	LEU	N-CA	-9.19	1.34	1.46
1	A	23	LEU	N-CA	-9.17	1.35	1.46
1	A	158	ALA	N-CA	9.14	1.57	1.46
1	A	44	LEU	C-N	-9.09	1.21	1.34
1	A	250	ASP	CA-C	-9.04	1.41	1.52
1	A	163	PRO	C-N	9.02	1.42	1.33
1	A	19	SER	CB-OG	8.81	1.59	1.42
1	A	81	GLU	CD-OE2	8.80	1.42	1.25
1	A	116	LEU	C-O	-8.80	1.13	1.24
1	A	188	LEU	N-CA	-8.79	1.37	1.46
1	A	156	THR	C-O	8.75	1.32	1.24
1	A	20	HIS	N-CA	8.74	1.57	1.46
1	A	69	ALA	C-N	-8.73	1.21	1.33
1	A	189	THR	CA-C	-8.73	1.41	1.52
1	A	97	VAL	C-N	-8.72	1.21	1.33
1	A	43	LEU	C-O	-8.70	1.13	1.24
1	A	237	ILE	N-CA	-8.69	1.37	1.46
1	A	140	ALA	CA-C	-8.60	1.40	1.52
1	A	50	VAL	N-CA	8.42	1.56	1.46
1	A	123	ASP	CA-CB	-8.42	1.41	1.53
1	A	190	LYS	C-N	-8.19	1.23	1.33
1	A	83	VAL	C-N	-8.07	1.23	1.33
1	A	64	LYS	CA-CB	-8.06	1.41	1.53
1	A	170	LEU	C-O	8.06	1.33	1.24
1	A	98	ARG	CZ-NH1	8.05	1.44	1.32
1	A	95	MET	SD-CE	-8.02	1.59	1.79
1	A	207	VAL	C-O	-7.98	1.15	1.24
1	A	236	GLY	N-CA	-7.97	1.33	1.45
1	A	27	GLY	C-O	7.94	1.32	1.24
1	A	93	GLY	CA-C	-7.82	1.40	1.51
1	A	43	LEU	CB-CG	7.81	1.69	1.53
1	A	219	LYS	C-O	-7.75	1.14	1.23
1	A	153	VAL	CA-CB	-7.75	1.45	1.54
1	A	130	VAL	CA-CB	-7.72	1.45	1.53
1	A	227	ASP	CA-C	-7.72	1.41	1.52
1	A	123	ASP	N-CA	-7.70	1.35	1.46
1	A	180	ILE	C-O	7.69	1.32	1.24
1	A	21	MET	CA-CB	-7.64	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	PHE	C-N	-7.61	1.24	1.33
1	A	163	PRO	C-O	7.57	1.32	1.23
1	A	205	THR	CA-C	-7.55	1.44	1.53
1	A	103	ASP	C-N	-7.50	1.26	1.34
1	A	44	LEU	C-O	-7.49	1.14	1.24
1	A	246	GLY	C-O	-7.49	1.17	1.23
1	A	18	GLY	N-CA	7.47	1.57	1.45
1	A	109	ALA	CA-C	7.47	1.62	1.53
1	A	71	VAL	C-N	-7.47	1.23	1.33
1	A	100	HIS	CB-CG	-7.40	1.39	1.50
1	A	82	MET	C-O	7.37	1.32	1.24
1	A	214	THR	CB-OG1	-7.37	1.31	1.43
1	A	243	ILE	CA-CB	7.32	1.63	1.53
1	A	251	PRO	N-CD	7.26	1.57	1.47
1	A	176	HIS	CG-CD2	7.22	1.43	1.35
1	A	240	GLN	CA-CB	-7.18	1.42	1.53
1	A	24	TYR	C-O	-7.16	1.15	1.23
1	A	50	VAL	C-O	-7.12	1.16	1.24
1	A	127	VAL	C-N	-7.09	1.25	1.33
1	A	69	ALA	CA-CB	-7.08	1.42	1.53
1	A	234	THR	CA-C	-7.07	1.43	1.52
1	A	192	VAL	CA-CB	-7.03	1.46	1.54
1	A	91	ARG	C-N	7.02	1.44	1.33
1	A	139	ALA	C-N	-7.01	1.24	1.33
1	A	106	MET	C-N	6.99	1.43	1.33
1	A	134	PHE	CA-C	-6.97	1.43	1.52
1	A	124	ILE	N-CA	-6.97	1.34	1.45
1	A	19	SER	C-O	6.96	1.33	1.24
1	A	85	THR	C-O	-6.91	1.16	1.24
1	A	205	THR	C-N	-6.91	1.24	1.33
1	A	56	LEU	CA-CB	-6.89	1.41	1.53
1	A	37	THR	CA-C	6.89	1.62	1.52
1	A	101	THR	C-N	-6.85	1.23	1.33
1	A	195	GLU	C-O	6.83	1.32	1.24
1	A	44	LEU	N-CA	6.83	1.55	1.46
1	A	89	ARG	CA-CB	-6.83	1.42	1.53
1	A	119	ARG	C-N	-6.81	1.24	1.33
1	A	191	LYS	C-N	6.78	1.42	1.33
1	A	106	MET	SD-CE	-6.77	1.62	1.79
1	A	244	LEU	CA-CB	6.76	1.63	1.53
1	A	211	TYR	N-CA	-6.66	1.38	1.46
1	A	229	ASP	C-N	6.64	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	LEU	N-CA	-6.62	1.37	1.46
1	A	131	THR	CB-OG1	-6.59	1.33	1.43
1	A	123	ASP	C-O	-6.55	1.15	1.23
1	A	134	PHE	CE2-CZ	-6.54	1.19	1.38
1	A	45	GLN	C-O	-6.53	1.15	1.24
1	A	203	GLU	C-N	-6.49	1.24	1.33
1	A	157	ARG	C-O	6.46	1.31	1.23
1	A	100	HIS	CA-CB	-6.43	1.43	1.53
1	A	55	SER	C-N	-6.41	1.24	1.33
1	A	155	LEU	CA-CB	-6.40	1.44	1.53
1	A	189	THR	C-N	-6.39	1.24	1.33
1	A	134	PHE	N-CA	-6.38	1.38	1.46
1	A	104	PRO	C-N	-6.38	1.23	1.33
1	A	93	GLY	N-CA	-6.38	1.35	1.45
1	A	151	GLN	CA-C	-6.38	1.44	1.52
1	A	249	LEU	C-O	6.37	1.33	1.24
1	A	212	LYS	C-O	-6.37	1.15	1.23
1	A	72	LEU	CB-CG	-6.37	1.40	1.53
1	A	121	GLY	C-O	-6.33	1.15	1.23
1	A	71	VAL	CA-C	-6.32	1.45	1.52
1	A	150	THR	CA-CB	-6.32	1.42	1.53
1	A	214	THR	N-CA	-6.32	1.37	1.46
1	A	59	GLN	C-O	6.28	1.31	1.24
1	A	61	LEU	C-O	6.26	1.31	1.24
1	A	36	ILE	CB-CG1	-6.23	1.41	1.53
1	A	128	PRO	N-CD	-6.20	1.39	1.47
1	A	234	THR	CB-OG1	6.13	1.53	1.43
1	A	183	PHE	C-O	-6.12	1.15	1.23
1	A	215	TRP	CD2-CE3	-6.11	1.30	1.40
1	A	166	GLU	C-N	6.11	1.40	1.33
1	A	49	VAL	CA-C	-6.09	1.45	1.52
1	A	113	GLN	C-O	-6.06	1.17	1.24
1	A	126	ILE	CA-CB	6.06	1.62	1.54
1	A	80	GLU	CA-CB	-6.05	1.43	1.53
1	A	35	LEU	CA-C	-6.05	1.44	1.52
1	A	64	LYS	C-O	-6.04	1.14	1.24
1	A	104	PRO	N-CD	-6.04	1.39	1.47
1	A	69	ALA	CA-C	-6.03	1.45	1.52
1	A	92	GLU	C-O	-6.03	1.16	1.24
1	A	98	ARG	N-CA	-6.03	1.38	1.46
1	A	242	MET	SD-CE	-6.01	1.64	1.79
1	A	160	GLY	C-O	6.00	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	TYR	C-O	-5.94	1.17	1.24
1	A	93	GLY	C-N	-5.93	1.25	1.33
1	A	150	THR	C-O	5.92	1.31	1.23
1	A	131	THR	C-O	5.89	1.31	1.23
1	A	94	LYS	CA-CB	5.87	1.63	1.53
1	A	125	GLU	N-CA	-5.87	1.39	1.46
1	A	93	GLY	C-O	-5.87	1.16	1.24
1	A	136	ALA	N-CA	-5.87	1.39	1.46
1	A	220	ILE	C-O	-5.80	1.18	1.24
1	A	190	LYS	C-O	-5.77	1.17	1.24
1	A	215	TRP	CD2-CE2	-5.77	1.31	1.41
1	A	131	THR	N-CA	-5.76	1.38	1.45
1	A	212	LYS	CA-C	-5.74	1.45	1.53
1	A	49	VAL	CA-CB	-5.73	1.46	1.53
1	A	22	LYS	C-O	5.72	1.31	1.23
1	A	243	ILE	CB-CG1	5.69	1.64	1.53
1	A	204	ASP	CA-CB	5.69	1.63	1.53
1	A	199	ALA	N-CA	5.68	1.53	1.46
1	A	26	ILE	CA-CB	-5.67	1.47	1.54
1	A	72	LEU	N-CA	-5.65	1.39	1.46
1	A	83	VAL	CA-CB	-5.61	1.47	1.54
1	A	60	ASP	CA-CB	-5.60	1.43	1.53
1	A	232	MET	C-O	5.59	1.30	1.24
1	A	70	GLU	CD-OE1	5.59	1.35	1.25
1	A	156	THR	N-CA	5.56	1.54	1.46
1	A	147	PRO	C-O	5.56	1.30	1.23
1	A	251	PRO	N-CA	5.55	1.55	1.47
1	A	31	GLY	CA-C	-5.54	1.44	1.51
1	A	83	VAL	N-CA	-5.52	1.40	1.46
1	A	38	VAL	C-O	-5.51	1.18	1.24
1	A	102	GLY	C-O	5.50	1.31	1.24
1	A	33	PRO	CA-CB	-5.49	1.46	1.53
1	A	242	MET	CG-SD	5.48	1.94	1.80
1	A	121	GLY	CA-C	-5.48	1.44	1.51
1	A	240	GLN	C-O	5.48	1.30	1.23
1	A	219	LYS	N-CA	-5.46	1.39	1.46
1	A	251	PRO	C-O	5.45	1.34	1.23
1	A	27	GLY	CA-C	5.44	1.60	1.52
1	A	39	LYS	N-CA	-5.43	1.39	1.46
1	A	19	SER	C-N	5.43	1.42	1.33
1	A	56	LEU	C-O	-5.43	1.17	1.24
1	A	135	ALA	N-CA	5.40	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	LEU	C-N	-5.39	1.26	1.33
1	A	98	ARG	CA-CB	-5.39	1.43	1.53
1	A	238	ARG	C-O	5.38	1.31	1.24
1	A	45	GLN	CD-OE1	5.38	1.33	1.23
1	A	50	VAL	CB-CG2	-5.37	1.34	1.52
1	A	219	LYS	C-N	-5.37	1.26	1.33
1	A	33	PRO	CA-C	-5.35	1.44	1.52
1	A	158	ALA	C-N	-5.35	1.26	1.33
1	A	234	THR	N-CA	-5.30	1.39	1.46
1	A	87	LEU	CA-CB	-5.29	1.45	1.53
1	A	155	LEU	C-O	5.29	1.30	1.24
1	A	92	GLU	C-N	-5.25	1.25	1.33
1	A	157	ARG	N-CA	5.25	1.52	1.45
1	A	69	ALA	C-O	-5.23	1.17	1.23
1	A	241	ALA	C-O	5.22	1.30	1.23
1	A	120	GLU	C-O	5.20	1.30	1.24
1	A	250	ASP	C-O	-5.18	1.17	1.24
1	A	226	LYS	C-O	5.18	1.30	1.24
1	A	215	TRP	CA-CB	-5.18	1.45	1.53
1	A	28	ALA	CA-CB	-5.16	1.44	1.53
1	A	166	GLU	C-O	5.14	1.30	1.24
1	A	222	ARG	CZ-NH1	5.14	1.40	1.32
1	A	170	LEU	N-CA	5.13	1.52	1.46
1	A	39	LYS	C-O	5.12	1.30	1.24
1	A	185	SER	CA-C	-5.12	1.46	1.52
1	A	188	LEU	C-O	5.11	1.31	1.24
1	A	79	LEU	C-O	-5.11	1.17	1.24
1	A	223	THR	C-N	-5.09	1.26	1.33
1	A	214	THR	CA-C	-5.08	1.45	1.52
1	A	220	ILE	N-CA	-5.08	1.39	1.46
1	A	83	VAL	CA-C	-5.07	1.46	1.52
1	A	232	MET	N-CA	-5.06	1.40	1.46
1	A	89	ARG	CD-NE	5.06	1.53	1.46
1	A	242	MET	C-O	-5.05	1.17	1.24
1	A	112	GLU	CA-CB	-5.03	1.45	1.53
1	A	213	ALA	C-O	-5.01	1.18	1.24
1	A	216	PRO	C-O	-5.00	1.18	1.24

All (878) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ILE	CA-C-O	-50.22	93.83	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASN	OD1-CG-ND2	42.52	165.12	122.60
1	A	45	GLN	OE1-CD-NE2	34.69	157.29	122.60
1	A	98	ARG	NE-CZ-NH1	31.91	153.41	121.50
1	A	71	VAL	O-C-N	-31.04	85.07	122.94
1	A	139	ALA	CA-C-O	-28.88	90.95	120.70
1	A	100	HIS	O-C-N	-27.38	91.40	123.16
1	A	222	ARG	NE-CZ-NH2	-26.91	94.98	119.20
1	A	221	VAL	CA-C-O	-26.27	93.06	120.39
1	A	222	ARG	NH1-CZ-NH2	24.40	151.02	119.30
1	A	217	ASP	CB-CG-OD2	-23.61	64.08	118.40
1	A	93	GLY	O-C-N	-22.76	95.82	122.45
1	A	98	ARG	NE-CZ-NH2	-22.55	98.91	119.20
1	A	73	LYS	O-C-N	-22.18	98.21	123.27
1	A	139	ALA	N-CA-CB	-21.72	78.58	110.07
1	A	22	LYS	CA-C-O	-21.47	96.05	120.31
1	A	129	GLY	N-CA-C	21.43	142.42	111.14
1	A	121	GLY	O-C-N	-21.34	94.96	122.70
1	A	22	LYS	O-C-N	21.25	146.89	123.52
1	A	177	LYS	CA-C-O	-20.95	96.34	121.28
1	A	251	PRO	CA-N-CD	-20.88	82.77	112.00
1	A	61	LEU	N-CA-CB	20.66	140.71	110.13
1	A	123	ASP	CA-CB-CG	19.88	132.48	112.60
1	A	94	LYS	O-C-N	-19.85	100.22	122.85
1	A	100	HIS	CA-C-O	19.54	143.39	120.92
1	A	73	LYS	CA-C-O	19.39	141.57	120.43
1	A	107	TYR	O-C-N	-19.27	99.45	122.58
1	A	168	GLU	CB-CG-CD	19.08	145.04	112.60
1	A	91	ARG	CA-C-O	19.07	142.57	119.49
1	A	89	ARG	NE-CZ-NH2	-19.03	102.07	119.20
1	A	164	VAL	O-C-N	19.01	137.18	121.40
1	A	36	ILE	CA-C-O	-18.82	100.44	120.57
1	A	106	MET	CA-C-O	18.49	141.78	120.70
1	A	32	ASP	O-C-N	-18.18	103.64	121.27
1	A	82	MET	CA-C-O	18.01	139.73	120.82
1	A	101	THR	CA-C-O	-17.99	102.48	121.55
1	A	101	THR	CA-CB-OG1	-17.87	82.80	109.60
1	A	64	LYS	CA-C-O	-17.84	87.06	119.36
1	A	47	ALA	N-CA-CB	-17.60	84.09	109.97
1	A	189	THR	O-C-N	-17.57	99.22	122.59
1	A	105	ALA	N-CA-CB	-17.53	82.94	110.46
1	A	65	SER	CA-C-O	-17.52	101.05	121.72
1	A	151	GLN	O-C-N	-17.25	101.84	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	LYS	N-CA-CB	17.25	135.66	110.13
1	A	238	ARG	NE-CZ-NH1	17.12	138.62	121.50
1	A	129	GLY	CA-C-N	-17.04	100.96	122.43
1	A	129	GLY	C-N-CA	-17.04	100.96	122.43
1	A	209	VAL	CA-C-O	-17.02	101.10	120.84
1	A	128	PRO	CA-C-N	16.96	136.07	121.82
1	A	128	PRO	C-N-CA	16.96	136.07	121.82
1	A	217	ASP	OD1-CG-OD2	16.92	163.51	122.90
1	A	190	LYS	CG-CD-CE	16.85	150.06	111.30
1	A	23	LEU	CA-C-O	-16.59	102.08	120.32
1	A	155	LEU	N-CA-CB	-16.42	83.21	110.47
1	A	139	ALA	O-C-N	16.35	139.75	122.09
1	A	146	ILE	O-C-N	16.32	136.58	120.59
1	A	60	ASP	N-CA-C	16.22	132.33	112.87
1	A	26	ILE	CA-C-O	-16.20	101.70	120.65
1	A	104	PRO	CA-C-O	-16.08	97.76	118.99
1	A	215	TRP	O-C-N	-16.02	104.62	121.60
1	A	84	GLY	O-C-N	-16.01	106.82	122.19
1	A	233	ARG	CA-C-O	-16.00	100.91	119.79
1	A	165	PRO	CA-C-N	15.89	142.85	120.29
1	A	165	PRO	C-N-CA	15.89	142.85	120.29
1	A	26	ILE	CA-C-N	15.88	135.28	120.98
1	A	26	ILE	C-N-CA	15.88	135.28	120.98
1	A	63	ALA	CB-CA-C	-15.88	81.43	110.01
1	A	122	VAL	CB-CA-C	15.64	128.79	111.59
1	A	173	LEU	O-C-N	-15.45	105.75	122.12
1	A	134	PHE	CG-CD2-CE2	15.41	146.90	120.70
1	A	222	ARG	CD-NE-CZ	-15.36	102.90	124.40
1	A	59	GLN	N-CA-C	-15.33	92.70	111.40
1	A	240	GLN	CG-CD-NE2	15.25	139.27	116.40
1	A	219	LYS	CA-C-O	-15.03	103.37	120.66
1	A	65	SER	O-C-N	14.96	139.69	122.94
1	A	94	LYS	N-CA-CB	-14.89	87.81	110.45
1	A	37	THR	CA-C-O	14.81	141.69	120.51
1	A	129	GLY	O-C-N	-14.77	110.75	123.60
1	A	64	LYS	CG-CD-CE	14.73	145.18	111.30
1	A	47	ALA	CA-C-N	14.70	140.43	120.44
1	A	47	ALA	C-N-CA	14.70	140.43	120.44
1	A	131	THR	CA-CB-CG2	14.66	135.43	110.50
1	A	92	GLU	CA-C-O	-14.60	100.43	119.11
1	A	96	VAL	O-C-N	-14.47	107.72	122.76
1	A	106	MET	N-CA-CB	14.47	134.91	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NH1-CZ-NH2	14.36	137.97	119.30
1	A	221	VAL	CA-CB-CG1	14.36	134.81	110.40
1	A	154	ILE	CA-C-O	-14.26	104.19	120.74
1	A	195	GLU	CA-CB-CG	14.18	142.46	114.10
1	A	36	ILE	N-CA-CB	14.15	127.97	110.99
1	A	79	LEU	O-C-N	14.15	141.41	122.59
1	A	201	TRP	CA-C-O	-14.11	105.17	121.81
1	A	243	ILE	O-C-N	14.10	138.07	122.99
1	A	42	LYS	N-CA-C	-14.09	96.22	113.41
1	A	139	ALA	N-CA-C	-14.07	95.94	111.14
1	A	62	ILE	CA-C-O	13.98	135.88	120.64
1	A	110	ILE	N-CA-C	-13.90	98.28	113.43
1	A	191	LYS	CA-CB-CG	13.84	141.78	114.10
1	A	180	ILE	CA-CB-CG1	13.82	133.90	110.40
1	A	207	VAL	CA-C-N	-13.76	106.13	123.19
1	A	207	VAL	C-N-CA	-13.76	106.13	123.19
1	A	108	GLY	O-C-N	-13.72	104.86	122.70
1	A	71	VAL	CA-C-N	13.71	142.81	122.93
1	A	71	VAL	C-N-CA	13.71	142.81	122.93
1	A	212	LYS	N-CA-CB	-13.69	91.44	111.70
1	A	213	ALA	CB-CA-C	-13.59	90.59	110.16
1	A	183	PHE	O-C-N	-13.32	107.61	122.79
1	A	190	LYS	CB-CG-CD	13.28	141.85	111.30
1	A	180	ILE	O-C-N	-13.23	107.62	123.10
1	A	102	GLY	CA-C-O	-13.21	104.07	121.51
1	A	50	VAL	CA-C-N	13.20	141.20	122.85
1	A	50	VAL	C-N-CA	13.20	141.20	122.85
1	A	166	GLU	CA-C-N	-13.14	99.24	122.62
1	A	166	GLU	C-N-CA	-13.14	99.24	122.62
1	A	109	ALA	CA-C-O	-13.09	105.67	122.03
1	A	108	GLY	CA-C-O	12.99	143.17	120.57
1	A	217	ASP	CA-CB-CG	-12.93	99.67	112.60
1	A	212	LYS	CA-C-N	12.87	140.07	121.02
1	A	212	LYS	C-N-CA	12.87	140.07	121.02
1	A	61	LEU	N-CA-C	-12.84	95.73	111.40
1	A	220	ILE	CA-C-O	-12.75	105.74	120.66
1	A	235	ASN	CB-CG-ND2	-12.72	97.31	116.40
1	A	58	SER	CA-CB-OG	-12.72	85.66	111.10
1	A	230	ASP	CA-CB-CG	-12.68	99.92	112.60
1	A	59	GLN	N-CA-CB	12.67	128.88	110.13
1	A	229	ASP	CB-CG-OD2	12.67	147.53	118.40
1	A	198	ASN	O-C-N	-12.64	107.44	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	LYS	CG-CD-CE	12.63	140.35	111.30
1	A	120	GLU	CA-C-N	12.61	146.13	121.41
1	A	120	GLU	C-N-CA	12.61	146.13	121.41
1	A	237	ILE	O-C-N	-12.53	108.60	122.64
1	A	46	GLN	CB-CG-CD	-12.52	91.31	112.60
1	A	195	GLU	N-CA-CB	-12.49	90.41	110.14
1	A	151	GLN	CA-C-O	12.48	133.91	119.18
1	A	47	ALA	O-C-N	-12.48	107.67	122.89
1	A	79	LEU	CA-C-N	-12.43	102.23	120.38
1	A	79	LEU	C-N-CA	-12.43	102.23	120.38
1	A	207	VAL	N-CA-C	12.40	125.78	107.80
1	A	173	LEU	CA-C-O	-12.36	107.28	120.63
1	A	230	ASP	CA-C-N	12.35	136.50	120.44
1	A	230	ASP	C-N-CA	12.35	136.50	120.44
1	A	38	VAL	CA-C-O	12.34	135.49	121.18
1	A	21	MET	CA-C-O	-12.30	107.27	121.66
1	A	49	VAL	N-CA-CB	-12.26	96.22	111.67
1	A	204	ASP	CB-CG-OD2	12.25	146.58	118.40
1	A	113	GLN	CG-CD-OE1	-12.17	96.46	120.80
1	A	123	ASP	CB-CG-OD2	-12.15	90.46	118.40
1	A	211	TYR	CB-CG-CD1	12.13	139.00	120.80
1	A	39	LYS	CA-C-O	-12.12	106.62	120.20
1	A	26	ILE	N-CA-C	12.12	126.77	108.23
1	A	47	ALA	CB-CA-C	12.12	130.37	109.65
1	A	67	PRO	CA-C-O	-12.07	107.28	121.03
1	A	45	GLN	CG-CD-NE2	-12.05	98.33	116.40
1	A	138	ALA	CA-C-O	12.03	133.30	120.55
1	A	105	ALA	N-CA-C	-12.03	98.60	113.28
1	A	48	ASP	CA-CB-CG	-12.02	100.58	112.60
1	A	235	ASN	CA-CB-CG	-12.01	100.59	112.60
1	A	172	ASP	N-CA-C	11.99	125.49	111.11
1	A	20	HIS	CA-CB-CG	-11.98	101.82	113.80
1	A	99	VAL	CA-C-O	-11.87	107.42	120.48
1	A	25	ILE	O-C-N	11.84	139.19	122.62
1	A	198	ASN	N-CA-CB	11.81	128.41	110.22
1	A	89	ARG	CA-C-O	11.80	132.93	120.42
1	A	133	VAL	CA-CB-CG2	-11.80	90.33	110.40
1	A	70	GLU	CA-C-O	-11.79	107.25	120.69
1	A	113	GLN	OE1-CD-NE2	11.79	134.39	122.60
1	A	171	THR	CA-C-O	-11.78	107.24	121.02
1	A	212	LYS	O-C-N	-11.77	107.95	122.55
1	A	242	MET	N-CA-C	-11.77	90.21	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	HIS	O-C-N	11.77	138.59	122.46
1	A	126	ILE	CA-C-O	-11.77	107.19	120.84
1	A	25	ILE	CA-C-O	-11.76	105.22	120.86
1	A	134	PHE	CD1-CG-CD2	-11.74	100.98	118.60
1	A	235	ASN	CB-CG-OD1	-11.71	97.37	120.80
1	A	165	PRO	O-C-N	-11.70	108.50	123.01
1	A	207	VAL	CA-C-O	-11.67	108.05	120.53
1	A	96	VAL	CA-C-N	11.63	140.94	122.33
1	A	96	VAL	C-N-CA	11.63	140.94	122.33
1	A	135	ALA	CA-C-O	-11.61	108.63	120.82
1	A	69	ALA	CA-C-O	-11.58	108.42	121.15
1	A	106	MET	O-C-N	-11.57	107.97	123.01
1	A	178	CYS	CA-C-O	-11.54	107.01	121.78
1	A	59	GLN	CB-CG-CD	11.44	132.04	112.60
1	A	73	LYS	N-CA-CB	11.40	129.02	110.43
1	A	238	ARG	O-C-N	-11.35	108.75	122.25
1	A	133	VAL	CA-C-O	11.34	134.95	120.78
1	A	118	LYS	O-C-N	-11.31	108.36	122.27
1	A	221	VAL	CG1-CB-CG2	-11.22	86.12	110.80
1	A	161	ARG	CA-C-O	11.21	136.53	120.51
1	A	20	HIS	CA-C-O	-11.19	106.17	119.27
1	A	229	ASP	CA-CB-CG	-11.15	101.45	112.60
1	A	62	ILE	O-C-N	-11.15	110.64	121.90
1	A	72	LEU	O-C-N	-11.15	109.05	123.21
1	A	209	VAL	CA-CB-CG2	11.13	129.32	110.40
1	A	183	PHE	CB-CG-CD1	11.11	139.59	120.70
1	A	57	VAL	CG1-CB-CG2	-11.09	86.41	110.80
1	A	64	LYS	N-CA-C	-11.07	100.48	113.21
1	A	132	SER	CA-C-O	-11.05	105.61	119.31
1	A	147	PRO	CB-CA-C	-11.05	97.53	111.56
1	A	176	HIS	CA-CB-CG	-11.04	102.75	113.80
1	A	111	MET	O-C-N	-11.04	110.42	122.12
1	A	211	TYR	CA-C-N	-11.01	106.72	122.36
1	A	211	TYR	C-N-CA	-11.01	106.72	122.36
1	A	202	SER	O-C-N	-11.01	109.87	122.75
1	A	67	PRO	O-C-N	10.99	135.41	123.10
1	A	131	THR	CA-CB-OG1	-10.93	93.20	109.60
1	A	223	THR	OG1-CB-CG2	-10.92	87.46	109.30
1	A	250	ASP	CB-CA-C	-10.82	88.85	110.17
1	A	83	VAL	O-C-N	-10.81	111.32	121.91
1	A	204	ASP	O-C-N	-10.80	108.27	122.42
1	A	32	ASP	OD1-CG-OD2	-10.80	96.99	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ALA	N-CA-CB	10.75	127.34	110.46
1	A	180	ILE	CG1-CB-CG2	-10.73	78.52	110.70
1	A	97	VAL	CA-C-O	-10.72	109.17	120.64
1	A	205	THR	N-CA-C	-10.70	95.31	110.08
1	A	158	ALA	O-C-N	-10.70	109.84	122.89
1	A	93	GLY	CA-C-O	10.65	131.31	119.06
1	A	102	GLY	O-C-N	10.63	137.22	122.55
1	A	237	ILE	N-CA-CB	-10.61	100.11	111.46
1	A	85	THR	O-C-N	10.57	132.96	122.07
1	A	222	ARG	CA-C-O	-10.56	109.07	120.80
1	A	40	GLY	O-C-N	10.55	132.43	122.19
1	A	146	ILE	CA-C-N	10.54	130.65	119.90
1	A	146	ILE	C-N-CA	10.54	130.65	119.90
1	A	184	LEU	N-CA-CB	-10.52	92.71	110.49
1	A	148	ASP	O-C-N	-10.52	108.60	122.59
1	A	86	MET	N-CA-CB	-10.49	94.31	109.94
1	A	164	VAL	CA-C-O	-10.48	107.59	120.90
1	A	186	SER	CA-CB-OG	-10.48	90.14	111.10
1	A	211	TYR	CA-C-O	-10.48	109.25	120.46
1	A	163	PRO	O-C-N	10.45	135.55	122.91
1	A	49	VAL	O-C-N	-10.39	109.27	122.88
1	A	95	MET	N-CA-CB	10.39	127.51	110.37
1	A	20	HIS	CA-C-N	-10.36	104.09	122.32
1	A	20	HIS	C-N-CA	-10.36	104.09	122.32
1	A	60	ASP	CB-CG-OD2	-10.33	94.64	118.40
1	A	203	GLU	CA-C-O	10.32	131.77	119.28
1	A	142	ALA	O-C-N	-10.29	110.17	123.13
1	A	206	PRO	CA-C-O	10.27	132.96	121.36
1	A	166	GLU	CB-CG-CD	10.20	129.95	112.60
1	A	218	GLU	CA-C-O	-10.18	109.96	121.15
1	A	197	ILE	CB-CG1-CD1	10.14	135.09	113.80
1	A	128	PRO	N-CA-C	-10.13	96.84	111.33
1	A	73	LYS	CB-CG-CD	10.09	134.51	111.30
1	A	224	THR	CA-C-O	-10.08	110.67	121.36
1	A	163	PRO	CA-C-O	-10.08	109.35	121.95
1	A	120	GLU	O-C-N	-10.04	109.23	122.59
1	A	163	PRO	N-CA-CB	10.04	112.83	103.39
1	A	106	MET	CB-CA-C	-9.98	94.06	111.22
1	A	112	GLU	N-CA-C	-9.97	99.24	111.40
1	A	112	GLU	CB-CG-CD	9.92	129.46	112.60
1	A	103	ASP	OD1-CG-OD2	9.91	146.68	122.90
1	A	236	GLY	O-C-N	-9.88	109.85	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	GLU	N-CA-CB	9.85	125.51	110.44
1	A	235	ASN	N-CA-CB	-9.84	94.48	110.42
1	A	208	VAL	CA-C-N	-9.80	108.89	122.91
1	A	208	VAL	C-N-CA	-9.80	108.89	122.91
1	A	141	GLU	CB-CG-CD	9.80	129.26	112.60
1	A	152	THR	CA-C-N	-9.78	110.33	123.14
1	A	152	THR	C-N-CA	-9.78	110.33	123.14
1	A	168	GLU	CG-CD-OE1	-9.77	95.94	118.40
1	A	38	VAL	CG1-CB-CG2	-9.74	89.37	110.80
1	A	126	ILE	CA-CB-CG1	-9.73	93.86	110.40
1	A	119	ARG	CA-C-N	9.71	140.09	121.54
1	A	119	ARG	C-N-CA	9.71	140.09	121.54
1	A	240	GLN	CA-C-N	-9.70	107.49	122.62
1	A	240	GLN	C-N-CA	-9.70	107.49	122.62
1	A	202	SER	CA-CB-OG	-9.69	91.73	111.10
1	A	96	VAL	N-CA-CB	-9.66	94.65	112.43
1	A	111	MET	CA-C-O	9.66	130.79	120.55
1	A	151	GLN	CA-C-N	9.64	136.31	123.00
1	A	151	GLN	C-N-CA	9.64	136.31	123.00
1	A	240	GLN	CA-CB-CG	9.57	133.24	114.10
1	A	140	ALA	N-CA-CB	-9.57	94.51	110.39
1	A	94	LYS	CD-CE-NZ	9.52	142.35	111.90
1	A	144	LEU	CA-C-O	-9.52	107.77	119.28
1	A	205	THR	N-CA-CB	-9.51	96.22	110.11
1	A	230	ASP	N-CA-C	9.50	121.63	111.28
1	A	30	PRO	CB-CA-C	-9.49	96.03	111.31
1	A	236	GLY	CA-C-N	9.48	137.66	121.63
1	A	236	GLY	C-N-CA	9.48	137.66	121.63
1	A	215	TRP	CA-C-O	9.48	131.30	120.87
1	A	216	PRO	N-CA-CB	-9.47	94.20	103.20
1	A	239	LYS	CA-CB-CG	9.45	133.00	114.10
1	A	171	THR	CA-CB-OG1	-9.44	95.44	109.60
1	A	115	VAL	CA-CB-CG1	-9.41	94.41	110.40
1	A	206	PRO	O-C-N	-9.36	111.01	122.89
1	A	20	HIS	CE1-NE2-CD2	-9.35	99.65	109.00
1	A	83	VAL	N-CA-CB	9.33	121.47	110.55
1	A	161	ARG	O-C-N	-9.33	110.19	122.59
1	A	123	ASP	CB-CG-OD1	9.32	139.85	118.40
1	A	164	VAL	N-CA-C	-9.27	97.55	107.84
1	A	87	LEU	CB-CG-CD2	-9.26	82.91	110.70
1	A	132	SER	O-C-N	9.26	135.24	122.46
1	A	83	VAL	CB-CA-C	-9.25	100.12	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	THR	O-C-N	-9.24	110.30	122.59
1	A	59	GLN	OE1-CD-NE2	9.22	131.82	122.60
1	A	165	PRO	CA-C-O	9.19	132.22	121.56
1	A	251	PRO	N-CD-CG	-9.18	89.42	103.20
1	A	218	GLU	N-CA-C	9.16	123.16	110.24
1	A	150	THR	CA-C-O	9.15	131.24	120.99
1	A	211	TYR	CB-CG-CD2	-9.13	107.10	120.80
1	A	19	SER	N-CA-CB	-9.12	95.64	110.42
1	A	36	ILE	N-CA-C	-9.12	95.31	108.36
1	A	101	THR	O-C-N	9.12	134.03	122.81
1	A	112	GLU	CB-CA-C	9.11	126.09	110.79
1	A	185	SER	O-C-N	-9.11	110.38	122.22
1	A	94	LYS	CA-C-O	9.11	132.56	121.81
1	A	237	ILE	N-CA-C	-9.09	95.95	108.12
1	A	171	THR	CB-CA-C	-9.08	95.77	110.84
1	A	32	ASP	CA-C-O	9.07	128.82	120.02
1	A	66	LYS	CA-C-O	9.06	132.57	120.16
1	A	215	TRP	N-CA-C	9.04	123.22	110.20
1	A	181	ALA	O-C-N	-9.04	112.79	123.27
1	A	20	HIS	CG-CD2-NE2	9.02	116.22	107.20
1	A	215	TRP	CB-CG-CD1	-9.02	113.37	126.90
1	A	193	MET	CG-SD-CE	-9.02	81.07	100.90
1	A	229	ASP	CA-C-N	-9.00	108.22	120.28
1	A	229	ASP	C-N-CA	-9.00	108.22	120.28
1	A	210	VAL	N-CA-C	8.96	120.72	108.17
1	A	171	THR	O-C-N	8.96	133.04	122.20
1	A	33	PRO	CB-CA-C	-8.95	96.80	111.56
1	A	98	ARG	NH1-CZ-NH2	-8.95	107.67	119.30
1	A	48	ASP	O-C-N	-8.93	112.44	122.09
1	A	85	THR	CA-C-O	-8.90	111.47	120.82
1	A	231	ALA	O-C-N	8.89	131.23	122.07
1	A	59	GLN	O-C-N	-8.89	111.42	122.17
1	A	83	VAL	CA-CB-CG2	-8.88	95.31	110.40
1	A	112	GLU	CA-CB-CG	8.87	131.84	114.10
1	A	86	MET	O-C-N	-8.86	112.87	122.09
1	A	99	VAL	N-CA-CB	8.86	123.07	111.90
1	A	98	ARG	CA-C-O	-8.85	110.80	120.36
1	A	91	ARG	CA-C-N	-8.83	104.36	121.58
1	A	91	ARG	C-N-CA	-8.83	104.36	121.58
1	A	241	ALA	CA-C-N	-8.81	109.73	122.94
1	A	241	ALA	C-N-CA	-8.81	109.73	122.94
1	A	43	LEU	N-CA-C	-8.79	100.88	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	LYS	O-C-N	-8.79	110.90	122.59
1	A	50	VAL	CA-C-O	-8.79	110.37	120.65
1	A	58	SER	CA-C-N	8.79	135.39	120.71
1	A	58	SER	C-N-CA	8.79	135.39	120.71
1	A	221	VAL	N-CA-C	-8.78	94.93	107.75
1	A	243	ILE	CB-CG1-CD1	-8.75	95.42	113.80
1	A	238	ARG	NH1-CZ-NH2	-8.75	107.93	119.30
1	A	239	LYS	CB-CA-C	-8.74	95.75	110.43
1	A	98	ARG	CB-CG-CD	8.72	131.36	111.30
1	A	127	VAL	O-C-N	-8.72	112.90	120.92
1	A	140	ALA	O-C-N	-8.68	110.81	122.43
1	A	231	ALA	CA-C-N	-8.67	109.17	120.44
1	A	231	ALA	C-N-CA	-8.67	109.17	120.44
1	A	119	ARG	CA-C-O	-8.67	108.11	120.51
1	A	32	ASP	CB-CA-C	-8.66	95.36	109.56
1	A	189	THR	CA-CB-CG2	-8.66	95.78	110.50
1	A	238	ARG	CG-CD-NE	8.65	131.02	112.00
1	A	107	TYR	N-CA-CB	8.63	125.03	111.91
1	A	153	VAL	N-CA-CB	-8.63	99.50	111.41
1	A	138	ALA	N-CA-CB	8.62	122.79	110.12
1	A	251	PRO	N-CA-CB	-8.62	93.52	103.00
1	A	142	ALA	CA-C-O	-8.62	111.24	120.46
1	A	87	LEU	N-CA-C	8.61	121.75	111.33
1	A	45	GLN	CG-CD-OE1	-8.58	103.64	120.80
1	A	141	GLU	N-CA-CB	-8.57	98.88	111.91
1	A	44	LEU	O-C-N	-8.56	111.74	122.27
1	A	204	ASP	OD1-CG-OD2	-8.55	102.37	122.90
1	A	168	GLU	CA-C-N	-8.54	108.27	120.82
1	A	168	GLU	C-N-CA	-8.54	108.27	120.82
1	A	235	ASN	CA-C-N	8.54	138.15	121.41
1	A	235	ASN	C-N-CA	8.54	138.15	121.41
1	A	225	VAL	N-CA-C	8.53	119.32	110.36
1	A	32	ASP	CB-CG-OD2	8.53	138.01	118.40
1	A	179	THR	O-C-N	-8.50	112.34	122.89
1	A	133	VAL	CG1-CB-CG2	-8.49	92.11	110.80
1	A	133	VAL	CA-C-N	8.45	134.82	120.71
1	A	133	VAL	C-N-CA	8.45	134.82	120.71
1	A	238	ARG	CA-C-N	8.44	139.05	121.91
1	A	238	ARG	C-N-CA	8.44	139.05	121.91
1	A	225	VAL	CA-CB-CG2	-8.44	96.05	110.40
1	A	107	TYR	CD1-CG-CD2	-8.44	105.44	118.10
1	A	174	ALA	N-CA-C	8.41	123.11	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	N-CA-C	-8.39	96.55	109.64
1	A	115	VAL	O-C-N	-8.38	113.68	121.89
1	A	203	GLU	OE1-CD-OE2	8.38	143.01	122.90
1	A	55	SER	O-C-N	-8.36	110.49	122.87
1	A	113	GLN	CG-CD-NE2	8.31	128.86	116.40
1	A	117	LEU	N-CA-C	-8.30	101.47	111.69
1	A	123	ASP	CA-C-O	-8.30	111.37	120.92
1	A	220	ILE	N-CA-CB	8.30	122.13	111.67
1	A	250	ASP	CA-CB-CG	-8.30	104.30	112.60
1	A	98	ARG	CD-NE-CZ	8.30	136.02	124.40
1	A	25	ILE	CB-CA-C	8.29	122.31	111.53
1	A	190	LYS	CB-CA-C	-8.28	96.88	110.79
1	A	33	PRO	CA-C-O	8.27	135.66	120.60
1	A	61	LEU	CB-CA-C	-8.27	96.90	110.79
1	A	218	GLU	CA-CB-CG	8.26	130.63	114.10
1	A	111	MET	N-CA-C	8.26	120.28	111.28
1	A	33	PRO	CA-CB-CG	-8.25	88.83	104.50
1	A	122	VAL	N-CA-CB	-8.24	97.71	111.38
1	A	203	GLU	O-C-N	-8.23	111.01	122.37
1	A	175	LYS	O-C-N	-8.23	111.41	122.43
1	A	213	ALA	CA-C-O	8.22	130.15	120.70
1	A	141	GLU	CA-C-O	8.20	131.25	121.65
1	A	185	SER	CA-C-O	8.19	129.85	119.95
1	A	237	ILE	CA-CB-CG1	-8.19	96.48	110.40
1	A	95	MET	CA-C-N	-8.18	110.67	122.45
1	A	95	MET	C-N-CA	-8.18	110.67	122.45
1	A	103	ASP	N-CA-CB	8.18	123.84	109.94
1	A	140	ALA	CA-C-N	8.15	133.66	122.34
1	A	140	ALA	C-N-CA	8.15	133.66	122.34
1	A	113	GLN	CB-CA-C	8.14	123.84	110.81
1	A	210	VAL	CA-C-N	8.13	134.66	123.11
1	A	210	VAL	C-N-CA	8.13	134.66	123.11
1	A	249	LEU	N-CA-CB	-8.13	97.94	110.46
1	A	194	LYS	CA-C-O	-8.12	108.89	120.51
1	A	173	LEU	N-CA-CB	8.12	122.23	110.06
1	A	18	GLY	O-C-N	-8.11	110.02	123.00
1	A	199	ALA	CB-CA-C	-8.09	94.74	110.11
1	A	80	GLU	O-C-N	-8.08	112.99	122.20
1	A	73	LYS	CA-CB-CG	8.07	130.25	114.10
1	A	229	ASP	OD1-CG-OD2	-8.07	103.53	122.90
1	A	94	LYS	CA-C-N	8.05	133.31	122.84
1	A	94	LYS	C-N-CA	8.05	133.31	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	GLY	CA-C-N	8.03	138.19	121.32
1	A	93	GLY	C-N-CA	8.03	138.19	121.32
1	A	162	THR	OG1-CB-CG2	8.02	125.33	109.30
1	A	167	PHE	CB-CG-CD1	-8.01	107.08	120.70
1	A	40	GLY	CA-C-O	-8.01	112.17	120.66
1	A	222	ARG	NE-CZ-NH1	-8.01	113.50	121.50
1	A	43	LEU	CA-C-O	7.99	129.11	120.24
1	A	195	GLU	O-C-N	-7.98	113.10	122.20
1	A	87	LEU	CB-CG-CD1	7.97	134.62	110.70
1	A	142	ALA	N-CA-CB	-7.97	97.24	110.47
1	A	218	GLU	CA-C-N	-7.97	109.82	122.73
1	A	218	GLU	C-N-CA	-7.97	109.82	122.73
1	A	109	ALA	CB-CA-C	-7.97	100.48	112.11
1	A	183	PHE	CA-C-O	7.96	131.10	121.87
1	A	156	THR	N-CA-C	7.95	119.04	108.07
1	A	191	LYS	CB-CA-C	-7.92	97.64	110.79
1	A	44	LEU	CA-C-N	7.90	132.31	120.31
1	A	44	LEU	C-N-CA	7.90	132.31	120.31
1	A	240	GLN	CG-CD-OE1	-7.90	105.01	120.80
1	A	185	SER	N-CA-C	7.89	122.67	112.41
1	A	61	LEU	CD1-CG-CD2	7.88	128.13	110.80
1	A	131	THR	O-C-N	-7.85	113.59	122.86
1	A	183	PHE	N-CA-CB	7.84	121.58	110.36
1	A	35	LEU	N-CA-CB	-7.84	97.25	110.49
1	A	19	SER	N-CA-C	-7.81	103.75	113.20
1	A	124	ILE	CB-CG1-CD1	-7.81	97.40	113.80
1	A	81	GLU	OE1-CD-OE2	7.80	141.63	122.90
1	A	143	GLU	O-C-N	-7.80	112.84	122.82
1	A	242	MET	CA-C-N	7.79	133.57	123.13
1	A	242	MET	C-N-CA	7.79	133.57	123.13
1	A	188	LEU	O-C-N	7.77	132.72	122.15
1	A	219	LYS	CA-C-N	7.77	133.67	123.11
1	A	219	LYS	C-N-CA	7.77	133.67	123.11
1	A	100	HIS	CA-CB-CG	7.76	121.56	113.80
1	A	123	ASP	O-C-N	-7.76	114.16	123.16
1	A	191	LYS	CA-C-O	-7.75	112.34	120.55
1	A	97	VAL	CA-C-N	7.73	133.89	122.99
1	A	97	VAL	C-N-CA	7.73	133.89	122.99
1	A	139	ALA	CB-CA-C	-7.72	98.70	110.90
1	A	194	LYS	CD-CE-NZ	7.72	136.60	111.90
1	A	240	GLN	OE1-CD-NE2	-7.69	114.91	122.60
1	A	130	VAL	CA-CB-CG1	7.68	123.46	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	N-CA-C	7.67	119.96	108.23
1	A	151	GLN	N-CA-CB	-7.66	99.39	110.80
1	A	159	GLU	O-C-N	7.65	132.34	122.93
1	A	60	ASP	OD1-CG-OD2	7.63	141.21	122.90
1	A	114	MET	N-CA-CB	7.63	123.38	110.49
1	A	174	ALA	CA-C-O	-7.62	109.14	119.05
1	A	183	PHE	CB-CG-CD2	-7.61	107.77	120.70
1	A	19	SER	CA-C-O	-7.60	109.16	119.12
1	A	30	PRO	CA-C-N	-7.59	106.53	121.41
1	A	30	PRO	C-N-CA	-7.59	106.53	121.41
1	A	227	ASP	OD1-CG-OD2	-7.57	104.73	122.90
1	A	250	ASP	O-C-N	-7.56	112.62	121.32
1	A	243	ILE	CB-CA-C	-7.56	101.17	110.99
1	A	165	PRO	CA-CB-CG	7.55	118.84	104.50
1	A	213	ALA	N-CA-CB	7.52	121.39	109.51
1	A	115	VAL	CB-CA-C	-7.51	102.20	112.04
1	A	83	VAL	CA-CB-CG1	7.49	123.13	110.40
1	A	183	PHE	CG-CD1-CE1	7.47	133.40	120.70
1	A	126	ILE	CB-CG1-CD1	-7.46	98.13	113.80
1	A	145	THR	OG1-CB-CG2	7.45	124.21	109.30
1	A	248	ALA	N-CA-CB	-7.44	98.27	110.40
1	A	187	THR	OG1-CB-CG2	-7.42	94.46	109.30
1	A	233	ARG	O-C-N	7.42	132.27	122.33
1	A	183	PHE	CA-C-N	7.40	135.68	121.54
1	A	183	PHE	C-N-CA	7.40	135.68	121.54
1	A	97	VAL	N-CA-C	7.39	118.39	108.27
1	A	59	GLN	CB-CA-C	7.39	123.20	110.79
1	A	156	THR	CA-CB-CG2	7.38	123.04	110.50
1	A	125	GLU	CB-CG-CD	7.37	125.13	112.60
1	A	33	PRO	CA-N-CD	-7.36	101.70	112.00
1	A	215	TRP	N-CA-CB	-7.35	99.47	110.05
1	A	218	GLU	OE1-CD-OE2	7.33	140.50	122.90
1	A	233	ARG	CA-C-N	7.33	130.70	120.29
1	A	233	ARG	C-N-CA	7.33	130.70	120.29
1	A	215	TRP	CZ3-CH2-CZ2	-7.31	111.99	121.50
1	A	134	PHE	CZ-CE2-CD2	-7.31	106.84	120.00
1	A	44	LEU	N-CA-CB	7.31	121.61	110.28
1	A	67	PRO	CA-C-N	-7.30	107.10	121.41
1	A	67	PRO	C-N-CA	-7.30	107.10	121.41
1	A	238	ARG	CB-CG-CD	7.29	128.07	111.30
1	A	197	ILE	O-C-N	-7.28	112.44	121.90
1	A	123	ASP	CA-C-N	7.28	132.45	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASP	C-N-CA	7.28	132.45	122.34
1	A	135	ALA	N-CA-CB	-7.28	99.46	110.01
1	A	28	ALA	CA-C-O	7.26	127.82	119.18
1	A	222	ARG	O-C-N	-7.25	114.71	123.19
1	A	50	VAL	O-C-N	-7.25	114.09	122.94
1	A	27	GLY	O-C-N	7.25	127.77	122.62
1	A	97	VAL	CA-CB-CG1	7.24	122.70	110.40
1	A	127	VAL	CA-CB-CG1	-7.23	98.11	110.40
1	A	165	PRO	N-CA-CB	-7.22	97.07	103.35
1	A	190	LYS	CA-C-O	-7.22	112.83	120.55
1	A	227	ASP	CA-C-O	-7.22	110.90	119.35
1	A	170	LEU	O-C-N	-7.22	114.64	122.07
1	A	224	THR	CA-C-N	-7.21	111.30	120.60
1	A	224	THR	C-N-CA	-7.21	111.30	120.60
1	A	140	ALA	CA-C-O	-7.21	110.52	119.38
1	A	169	LYS	O-C-N	-7.20	113.61	122.82
1	A	243	ILE	CA-C-O	-7.20	112.57	120.48
1	A	118	LYS	CA-C-N	7.19	135.27	121.54
1	A	118	LYS	C-N-CA	7.19	135.27	121.54
1	A	188	LEU	CA-C-O	-7.18	112.04	119.51
1	A	99	VAL	N-CA-C	-7.17	95.88	107.28
1	A	72	LEU	CB-CG-CD2	-7.17	89.20	110.70
1	A	192	VAL	CG1-CB-CG2	-7.15	95.07	110.80
1	A	107	TYR	CA-C-O	7.15	130.01	121.65
1	A	45	GLN	CA-CB-CG	-7.13	99.83	114.10
1	A	223	THR	CA-CB-OG1	-7.13	98.90	109.60
1	A	205	THR	CA-C-N	7.13	127.17	119.90
1	A	205	THR	C-N-CA	7.13	127.17	119.90
1	A	18	GLY	CA-C-O	7.12	135.75	120.80
1	A	162	THR	CA-C-N	7.12	127.54	119.92
1	A	162	THR	C-N-CA	7.12	127.54	119.92
1	A	231	ALA	CB-CA-C	7.11	122.05	110.88
1	A	172	ASP	N-CA-CB	-7.11	99.35	109.94
1	A	183	PHE	CD1-CE1-CZ	-7.10	107.21	120.00
1	A	70	GLU	N-CA-C	-7.07	98.52	109.76
1	A	146	ILE	CB-CA-C	-7.06	103.03	110.16
1	A	148	ASP	OD1-CG-OD2	-7.06	105.96	122.90
1	A	201	TRP	O-C-N	7.05	130.89	122.85
1	A	36	ILE	CA-CB-CG1	7.05	122.39	110.40
1	A	156	THR	N-CA-CB	-7.04	98.26	110.86
1	A	223	THR	CA-CB-CG2	7.00	122.40	110.50
1	A	181	ALA	CA-C-O	7.00	127.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	VAL	CA-CB-CG2	-6.98	98.53	110.40
1	A	193	MET	CB-CA-C	-6.98	99.21	110.79
1	A	214	THR	CA-CB-CG2	6.98	122.36	110.50
1	A	104	PRO	CA-C-N	-6.96	109.12	122.06
1	A	104	PRO	C-N-CA	-6.96	109.12	122.06
1	A	35	LEU	O-C-N	-6.94	113.36	122.59
1	A	224	THR	OG1-CB-CG2	6.92	123.13	109.30
1	A	219	LYS	O-C-N	6.91	131.70	123.27
1	A	121	GLY	CA-C-O	6.91	132.59	120.57
1	A	118	LYS	CB-CA-C	-6.90	97.42	110.67
1	A	114	MET	CA-C-O	6.90	130.37	120.51
1	A	122	VAL	CA-C-O	-6.89	113.64	121.98
1	A	82	MET	O-C-N	-6.89	114.97	122.07
1	A	172	ASP	CB-CG-OD2	6.88	134.23	118.40
1	A	195	GLU	CG-CD-OE2	-6.86	102.61	118.40
1	A	131	THR	OG1-CB-CG2	-6.86	95.58	109.30
1	A	168	GLU	N-CA-C	-6.86	102.19	113.50
1	A	202	SER	N-CA-CB	-6.83	100.49	110.26
1	A	105	ALA	CA-C-O	-6.82	111.07	119.18
1	A	223	THR	CA-C-O	-6.82	110.76	120.51
1	A	167	PHE	CB-CG-CD2	6.82	132.29	120.70
1	A	137	ALA	CA-C-N	6.81	129.41	120.28
1	A	137	ALA	C-N-CA	6.81	129.41	120.28
1	A	141	GLU	N-CA-C	6.81	121.05	111.52
1	A	232	MET	CA-C-O	6.80	127.97	120.82
1	A	172	ASP	CB-CG-OD1	-6.80	102.75	118.40
1	A	149	LEU	N-CA-C	-6.79	101.22	111.34
1	A	164	VAL	CA-CB-CG2	-6.78	98.87	110.40
1	A	242	MET	CB-CA-C	6.78	122.31	109.37
1	A	60	ASP	CA-C-N	6.77	132.02	120.71
1	A	60	ASP	C-N-CA	6.77	132.02	120.71
1	A	20	HIS	ND1-CG-CD2	-6.75	99.35	106.10
1	A	130	VAL	CA-C-N	6.73	131.51	120.94
1	A	130	VAL	C-N-CA	6.73	131.51	120.94
1	A	211	TYR	N-CA-CB	6.73	121.64	110.47
1	A	80	GLU	CA-C-O	-6.72	112.67	120.20
1	A	162	THR	CB-CA-C	-6.72	96.94	110.17
1	A	154	ILE	N-CA-C	6.71	117.51	107.51
1	A	80	GLU	CA-C-N	6.69	129.25	120.28
1	A	80	GLU	C-N-CA	6.69	129.25	120.28
1	A	177	LYS	O-C-N	6.69	131.38	122.41
1	A	34	ASP	CA-CB-CG	6.69	119.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	LEU	CA-CB-CG	6.69	139.70	116.30
1	A	173	LEU	CB-CG-CD2	-6.68	90.65	110.70
1	A	179	THR	CA-CB-CG2	6.68	121.85	110.50
1	A	226	LYS	CA-CB-CG	6.67	127.43	114.10
1	A	170	LEU	CB-CA-C	6.66	121.34	110.88
1	A	80	GLU	CA-CB-CG	-6.66	100.78	114.10
1	A	58	SER	N-CA-CB	-6.66	100.33	110.45
1	A	201	TRP	N-CA-C	-6.64	101.59	110.55
1	A	92	GLU	CA-C-N	6.62	133.51	121.85
1	A	92	GLU	C-N-CA	6.62	133.51	121.85
1	A	84	GLY	N-CA-C	-6.62	104.79	112.73
1	A	205	THR	OG1-CB-CG2	6.62	122.53	109.30
1	A	80	GLU	CG-CD-OE1	6.61	133.60	118.40
1	A	83	VAL	N-CA-C	6.60	116.76	110.42
1	A	112	GLU	O-C-N	-6.59	114.20	122.17
1	A	212	LYS	CD-CE-NZ	-6.58	90.84	111.90
1	A	130	VAL	CA-C-O	-6.58	112.72	120.75
1	A	230	ASP	O-C-N	-6.58	115.14	122.12
1	A	171	THR	CA-CB-CG2	-6.58	99.32	110.50
1	A	231	ALA	N-CA-CB	-6.56	100.49	110.01
1	A	36	ILE	CB-CG1-CD1	6.55	127.56	113.80
1	A	182	LEU	N-CA-C	6.55	119.94	107.75
1	A	153	VAL	N-CA-C	-6.55	98.94	108.11
1	A	165	PRO	CB-CA-C	6.54	119.60	111.23
1	A	113	GLN	N-CA-C	-6.53	103.27	111.11
1	A	31	GLY	O-C-N	-6.52	114.22	122.70
1	A	196	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	20	HIS	CB-CG-ND1	6.51	132.47	122.70
1	A	196	PHE	O-C-N	6.51	129.57	122.15
1	A	216	PRO	N-CD-CG	-6.50	93.45	103.20
1	A	21	MET	CB-CG-SD	6.50	132.19	112.70
1	A	208	VAL	O-C-N	-6.47	116.38	123.18
1	A	238	ARG	NE-CZ-NH2	-6.46	113.38	119.20
1	A	144	LEU	O-C-N	6.46	131.29	122.37
1	A	44	LEU	CA-C-O	6.45	127.39	119.97
1	A	107	TYR	CG-CD2-CE2	6.45	130.88	121.20
1	A	215	TRP	NE1-CE2-CD2	6.45	115.79	107.40
1	A	168	GLU	O-C-N	6.45	129.45	121.84
1	A	125	GLU	CB-CA-C	6.45	120.07	110.14
1	A	23	LEU	CB-CA-C	6.42	120.72	110.19
1	A	129	GLY	CA-C-O	6.39	128.41	121.57
1	A	179	THR	CA-C-N	6.39	131.43	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	THR	C-N-CA	6.39	131.43	123.12
1	A	167	PHE	CD1-CE1-CZ	-6.38	108.51	120.00
1	A	28	ALA	O-C-N	-6.38	113.35	122.41
1	A	23	LEU	CB-CG-CD1	6.37	129.81	110.70
1	A	234	THR	CA-CB-OG1	-6.37	100.05	109.60
1	A	39	LYS	N-CA-CB	-6.36	100.09	110.14
1	A	188	LEU	N-CA-CB	6.36	124.25	111.60
1	A	107	TYR	CG-CD1-CE1	6.35	130.72	121.20
1	A	97	VAL	CA-CB-CG2	-6.34	99.62	110.40
1	A	89	ARG	N-CA-CB	-6.34	100.78	110.16
1	A	192	VAL	CA-CB-CG1	6.33	121.17	110.40
1	A	57	VAL	CA-C-O	-6.33	113.37	121.40
1	A	71	VAL	CA-C-O	6.31	128.03	120.65
1	A	244	LEU	O-C-N	6.31	130.40	123.27
1	A	29	GLY	CA-C-O	6.30	130.53	121.52
1	A	33	PRO	CA-C-N	-6.30	112.72	122.49
1	A	33	PRO	C-N-CA	-6.30	112.72	122.49
1	A	80	GLU	N-CA-C	6.30	119.81	111.75
1	A	184	LEU	CB-CG-CD1	6.29	129.57	110.70
1	A	118	LYS	CA-C-O	6.29	127.20	119.97
1	A	114	MET	O-C-N	-6.29	114.23	122.59
1	A	225	VAL	CA-C-O	-6.29	114.73	121.27
1	A	186	SER	O-C-N	6.28	128.78	122.12
1	A	152	THR	CA-CB-OG1	-6.28	100.18	109.60
1	A	125	GLU	CA-C-N	-6.27	113.94	122.91
1	A	125	GLU	C-N-CA	-6.27	113.94	122.91
1	A	56	LEU	CA-CB-CG	6.26	138.21	116.30
1	A	20	HIS	N-CA-CB	6.25	120.19	110.44
1	A	134	PHE	CB-CG-CD1	6.25	131.32	120.70
1	A	59	GLN	CG-CD-OE1	-6.24	108.31	120.80
1	A	25	ILE	CA-C-N	-6.22	114.59	122.37
1	A	25	ILE	C-N-CA	-6.22	114.59	122.37
1	A	191	LYS	O-C-N	6.22	128.71	122.12
1	A	24	TYR	N-CA-CB	-6.21	100.68	110.06
1	A	251	PRO	CB-CG-CD	-6.20	86.27	106.10
1	A	167	PHE	CB-CA-C	-6.18	103.43	111.40
1	A	202	SER	N-CA-C	6.18	118.53	110.43
1	A	159	GLU	CA-C-O	-6.17	113.72	120.81
1	A	41	LEU	CB-CG-CD2	-6.17	92.20	110.70
1	A	178	CYS	CA-C-N	6.16	132.63	121.97
1	A	178	CYS	C-N-CA	6.16	132.63	121.97
1	A	141	GLU	CA-C-N	-6.16	114.36	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLU	C-N-CA	-6.16	114.36	123.11
1	A	85	THR	CA-CB-OG1	-6.15	100.37	109.60
1	A	249	LEU	CB-CG-CD2	-6.14	92.27	110.70
1	A	69	ALA	CB-CA-C	-6.14	99.81	109.70
1	A	141	GLU	O-C-N	-6.14	115.22	122.58
1	A	183	PHE	CE1-CZ-CE2	6.13	131.04	120.00
1	A	197	ILE	CA-C-O	6.11	128.23	120.96
1	A	39	LYS	O-C-N	6.10	129.15	122.20
1	A	100	HIS	CA-C-N	6.09	129.95	120.75
1	A	100	HIS	C-N-CA	6.09	129.95	120.75
1	A	194	LYS	CB-CA-C	6.09	122.53	110.42
1	A	217	ASP	CB-CG-OD1	6.09	132.40	118.40
1	A	122	VAL	CA-CB-CG1	-6.08	100.06	110.40
1	A	150	THR	CA-CB-OG1	-6.08	100.47	109.60
1	A	82	MET	CA-C-N	-6.08	112.90	120.56
1	A	82	MET	C-N-CA	-6.08	112.90	120.56
1	A	247	TRP	CA-C-O	-6.08	111.44	119.10
1	A	73	LYS	CG-CD-CE	6.07	125.26	111.30
1	A	189	THR	CA-C-N	6.05	130.82	120.71
1	A	189	THR	C-N-CA	6.05	130.82	120.71
1	A	127	VAL	CA-CB-CG2	6.03	120.64	110.40
1	A	235	ASN	O-C-N	-6.03	113.47	122.39
1	A	219	LYS	N-CA-CB	6.02	121.90	111.00
1	A	35	LEU	CA-C-O	6.01	129.11	120.51
1	A	176	HIS	CA-C-O	-6.01	111.24	119.05
1	A	48	ASP	CB-CG-OD2	-6.00	104.59	118.40
1	A	127	VAL	CG1-CB-CG2	-6.00	97.60	110.80
1	A	193	MET	N-CA-CB	6.00	118.94	110.12
1	A	248	ALA	O-C-N	-6.00	114.19	122.46
1	A	128	PRO	N-CD-CG	-6.00	94.21	103.20
1	A	89	ARG	O-C-N	-5.98	115.34	122.15
1	A	113	GLN	N-CA-CB	-5.98	101.04	109.94
1	A	187	THR	CA-C-N	5.98	132.21	121.15
1	A	187	THR	C-N-CA	5.98	132.21	121.15
1	A	215	TRP	CB-CG-CD2	5.96	135.14	126.80
1	A	224	THR	N-CA-C	5.95	116.96	108.74
1	A	48	ASP	OD1-CG-OD2	5.94	137.16	122.90
1	A	19	SER	CA-C-N	-5.94	111.20	121.66
1	A	19	SER	C-N-CA	-5.94	111.20	121.66
1	A	155	LEU	CB-CG-CD2	5.94	128.52	110.70
1	A	236	GLY	N-CA-C	5.94	127.26	113.18
1	A	136	ALA	N-CA-CB	5.93	118.61	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	CB-CA-C	-5.93	100.69	110.72
1	A	114	MET	CG-SD-CE	5.93	113.95	100.90
1	A	222	ARG	CG-CD-NE	-5.93	98.95	112.00
1	A	24	TYR	CE1-CZ-OH	5.92	137.67	119.90
1	A	227	ASP	CB-CG-OD2	5.91	131.99	118.40
1	A	97	VAL	N-CA-CB	-5.89	101.27	111.63
1	A	216	PRO	CA-C-N	5.88	132.68	122.56
1	A	216	PRO	C-N-CA	5.88	132.68	122.56
1	A	69	ALA	N-CA-C	5.88	118.52	110.24
1	A	133	VAL	CA-CB-CG1	-5.88	100.41	110.40
1	A	122	VAL	CA-C-N	-5.86	113.41	122.09
1	A	122	VAL	C-N-CA	-5.86	113.41	122.09
1	A	187	THR	N-CA-CB	5.86	119.47	110.79
1	A	239	LYS	CG-CD-CE	-5.86	97.81	111.30
1	A	82	MET	CA-CB-CG	-5.86	102.38	114.10
1	A	147	PRO	N-CA-CB	-5.86	98.09	103.25
1	A	56	LEU	O-C-N	-5.85	114.80	122.59
1	A	250	ASP	CB-CG-OD1	-5.85	104.94	118.40
1	A	228	LEU	CA-C-O	5.84	128.86	120.51
1	A	142	ALA	N-CA-C	5.83	118.32	107.99
1	A	247	TRP	CH2-CZ2-CE2	5.83	125.07	117.50
1	A	154	ILE	O-C-N	5.82	131.31	122.76
1	A	94	LYS	CB-CG-CD	5.82	124.67	111.30
1	A	20	HIS	N-CA-C	-5.81	106.03	113.23
1	A	104	PRO	O-C-N	5.81	131.87	122.17
1	A	150	THR	CA-CB-CG2	-5.81	100.62	110.50
1	A	46	GLN	N-CA-C	-5.79	106.08	114.12
1	A	92	GLU	CG-CD-OE2	-5.79	105.09	118.40
1	A	106	MET	CA-C-N	-5.74	114.36	122.34
1	A	106	MET	C-N-CA	-5.74	114.36	122.34
1	A	148	ASP	CB-CG-OD2	5.72	131.55	118.40
1	A	116	LEU	N-CA-C	-5.70	105.16	111.71
1	A	100	HIS	ND1-CE1-NE2	-5.70	102.70	108.40
1	A	152	THR	CA-CB-CG2	-5.70	100.82	110.50
1	A	54	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	98	ARG	N-CA-C	5.68	118.16	108.90
1	A	180	ILE	CB-CA-C	-5.68	102.67	110.96
1	A	183	PHE	CA-CB-CG	-5.68	108.12	113.80
1	A	24	TYR	CA-C-N	5.67	131.04	123.10
1	A	24	TYR	C-N-CA	5.67	131.04	123.10
1	A	176	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	A	225	VAL	O-C-N	5.66	127.60	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	LEU	CA-C-O	-5.65	112.43	119.38
1	A	58	SER	CA-C-O	-5.65	115.14	121.81
1	A	182	LEU	CA-C-O	5.65	126.94	120.84
1	A	60	ASP	CA-C-O	-5.63	112.01	119.10
1	A	182	LEU	CD1-CG-CD2	5.62	123.17	110.80
1	A	90	MET	CG-SD-CE	5.62	113.27	100.90
1	A	190	LYS	CD-CE-NZ	5.62	129.88	111.90
1	A	154	ILE	CG1-CB-CG2	-5.61	93.86	110.70
1	A	172	ASP	CB-CA-C	-5.61	101.84	110.81
1	A	190	LYS	N-CA-C	-5.61	104.56	111.40
1	A	55	SER	CA-C-N	5.60	132.24	121.54
1	A	55	SER	C-N-CA	5.60	132.24	121.54
1	A	59	GLN	CA-C-O	5.59	126.53	120.55
1	A	164	VAL	N-CA-CB	5.58	115.68	111.83
1	A	199	ALA	CA-C-O	5.58	126.43	119.12
1	A	151	GLN	CG-CD-OE1	-5.57	109.65	120.80
1	A	251	PRO	CB-CA-C	5.57	120.68	110.10
1	A	65	SER	N-CA-CB	5.57	119.36	110.46
1	A	147	PRO	CA-C-O	-5.57	115.07	121.36
1	A	203	GLU	CG-CD-OE1	-5.56	105.61	118.40
1	A	175	LYS	CA-CB-CG	-5.55	102.99	114.10
1	A	126	ILE	O-C-N	5.55	128.81	122.93
1	A	67	PRO	N-CA-C	-5.55	102.42	110.80
1	A	209	VAL	CA-C-N	5.53	130.05	123.19
1	A	209	VAL	C-N-CA	5.53	130.05	123.19
1	A	63	ALA	N-CA-C	5.53	120.02	113.16
1	A	173	LEU	CB-CG-CD1	5.52	127.26	110.70
1	A	232	MET	N-CA-CB	5.52	118.01	110.01
1	A	220	ILE	O-C-N	-5.52	115.65	122.88
1	A	36	ILE	CA-CB-CG2	-5.51	101.13	110.50
1	A	99	VAL	CA-C-N	5.51	130.24	122.09
1	A	99	VAL	C-N-CA	5.51	130.24	122.09
1	A	53	ALA	O-C-N	-5.49	116.81	123.13
1	A	31	GLY	CA-C-N	5.49	128.47	120.51
1	A	31	GLY	C-N-CA	5.49	128.47	120.51
1	A	88	ASP	CA-C-O	-5.49	115.06	120.82
1	A	103	ASP	CB-CA-C	5.48	115.94	109.47
1	A	146	ILE	CA-CB-CG1	5.47	119.70	110.40
1	A	66	LYS	CG-CD-CE	5.45	123.84	111.30
1	A	227	ASP	CA-CB-CG	-5.45	107.15	112.60
1	A	186	SER	CB-CA-C	5.44	119.83	110.79
1	A	184	LEU	CA-C-O	-5.44	112.73	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PRO	N-CA-CB	5.43	108.51	103.46
1	A	150	THR	O-C-N	-5.43	117.20	123.33
1	A	70	GLU	CA-CB-CG	5.41	124.92	114.10
1	A	156	THR	CA-C-N	-5.41	113.36	122.29
1	A	156	THR	C-N-CA	-5.41	113.36	122.29
1	A	212	LYS	CG-CD-CE	-5.40	98.88	111.30
1	A	155	LEU	CD1-CG-CD2	-5.40	98.93	110.80
1	A	24	TYR	CB-CA-C	-5.39	100.41	109.53
1	A	153	VAL	CG1-CB-CG2	-5.39	98.94	110.80
1	A	218	GLU	CB-CA-C	-5.38	101.04	109.70
1	A	37	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	28	ALA	CA-C-N	-5.38	113.43	121.87
1	A	28	ALA	C-N-CA	-5.38	113.43	121.87
1	A	230	ASP	CB-CG-OD1	5.38	130.77	118.40
1	A	124	ILE	CA-CB-CG1	5.37	119.53	110.40
1	A	79	LEU	CA-C-O	-5.37	112.83	120.51
1	A	65	SER	CA-CB-OG	-5.34	100.43	111.10
1	A	132	SER	N-CA-CB	-5.33	101.70	110.40
1	A	143	GLU	CB-CA-C	-5.33	100.21	109.64
1	A	190	LYS	CA-CB-CG	-5.33	103.45	114.10
1	A	54	ASP	N-CA-CB	-5.31	101.51	110.49
1	A	167	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	35	LEU	CD1-CG-CD2	-5.30	99.14	110.80
1	A	81	GLU	CG-CD-OE2	-5.30	106.22	118.40
1	A	46	GLN	CB-CA-C	5.29	118.26	109.38
1	A	149	LEU	CB-CA-C	5.29	120.40	112.31
1	A	70	GLU	N-CA-CB	5.28	118.14	109.95
1	A	120	GLU	CA-C-O	5.26	128.04	120.51
1	A	34	ASP	N-CA-CB	5.26	118.55	110.61
1	A	175	LYS	CB-CA-C	-5.25	99.34	110.31
1	A	90	MET	O-C-N	-5.24	116.67	122.07
1	A	148	ASP	CA-CB-CG	-5.24	107.36	112.60
1	A	100	HIS	CB-CG-ND1	-5.23	114.85	122.70
1	A	120	GLU	CG-CD-OE1	5.23	130.43	118.40
1	A	183	PHE	CD1-CG-CD2	-5.22	110.76	118.60
1	A	35	LEU	CA-CB-CG	-5.22	98.03	116.30
1	A	53	ALA	CA-C-N	-5.22	111.58	121.54
1	A	53	ALA	C-N-CA	-5.22	111.58	121.54
1	A	188	LEU	CA-C-N	-5.22	111.58	121.54
1	A	188	LEU	C-N-CA	-5.22	111.58	121.54
1	A	103	ASP	CB-CG-OD2	-5.21	106.41	118.40
1	A	195	GLU	CB-CG-CD	-5.21	103.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLU	CG-CD-OE2	5.19	130.33	118.40
1	A	184	LEU	CA-C-N	-5.18	114.35	122.49
1	A	184	LEU	C-N-CA	-5.18	114.35	122.49
1	A	24	TYR	O-C-N	-5.18	116.90	123.01
1	A	90	MET	CA-C-O	5.17	126.25	120.82
1	A	21	MET	O-C-N	5.17	129.54	122.41
1	A	35	LEU	CB-CG-CD2	5.16	126.19	110.70
1	A	18	GLY	CA-C-N	5.16	132.26	121.94
1	A	18	GLY	C-N-CA	5.16	132.26	121.94
1	A	26	ILE	CB-CA-C	-5.14	104.74	110.96
1	A	103	ASP	CB-CG-OD1	-5.14	106.58	118.40
1	A	166	GLU	CA-C-O	5.14	125.87	120.42
1	A	128	PRO	CA-CB-CG	-5.14	94.74	104.50
1	A	212	LYS	CA-CB-CG	-5.13	103.83	114.10
1	A	152	THR	N-CA-C	5.11	117.30	109.07
1	A	50	VAL	N-CA-CB	-5.11	105.18	111.00
1	A	187	THR	CA-CB-CG2	-5.09	101.84	110.50
1	A	106	MET	CA-CB-CG	-5.09	103.92	114.10
1	A	158	ALA	N-CA-CB	-5.09	102.49	109.97
1	A	144	LEU	CA-C-N	5.09	129.94	122.77
1	A	144	LEU	C-N-CA	5.09	129.94	122.77
1	A	200	GLY	CA-C-N	-5.07	110.67	121.32
1	A	200	GLY	C-N-CA	-5.07	110.67	121.32
1	A	193	MET	CA-C-O	-5.07	115.17	120.55
1	A	204	ASP	CA-C-O	5.07	124.93	119.15
1	A	182	LEU	CB-CG-CD1	-5.06	95.52	110.70
1	A	95	MET	CA-CB-CG	5.05	124.21	114.10
1	A	36	ILE	O-C-N	-5.05	117.42	123.03
1	A	37	THR	CB-CA-C	-5.05	100.37	110.42
1	A	100	HIS	CB-CA-C	5.05	117.86	109.53
1	A	183	PHE	CZ-CE2-CD2	-5.04	110.93	120.00
1	A	24	TYR	CG-CD2-CE2	-5.04	113.64	121.20
1	A	90	MET	N-CA-C	-5.04	105.68	111.07
1	A	60	ASP	CB-CA-C	-5.03	99.19	110.21
1	A	143	GLU	N-CA-C	5.02	116.76	110.24
1	A	170	LEU	N-CA-C	5.01	116.43	111.07
1	A	83	VAL	CA-C-O	5.00	126.47	121.17

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	THR	Mainchain
1	A	107	TYR	Mainchain
1	A	109	ALA	Mainchain
1	A	117	LEU	Mainchain
1	A	120	GLU	Mainchain
1	A	124	ILE	Mainchain
1	A	127	VAL	Mainchain
1	A	128	PRO	Mainchain
1	A	139	ALA	Mainchain
1	A	140	ALA	Mainchain
1	A	141	GLU	Mainchain
1	A	142	ALA	Mainchain
1	A	159	GLU	Mainchain
1	A	169	LYS	Mainchain
1	A	173	LEU	Mainchain
1	A	179	THR	Mainchain
1	A	180	ILE	Mainchain
1	A	181	ALA	Mainchain
1	A	185	SER	Mainchain
1	A	189	THR	Mainchain
1	A	19	SER	Mainchain
1	A	199	ALA	Mainchain
1	A	201	TRP	Mainchain
1	A	202	SER	Mainchain
1	A	209	VAL	Mainchain
1	A	21	MET	Mainchain
1	A	211	TYR	Sidechain
1	A	212	LYS	Mainchain
1	A	220	ILE	Mainchain
1	A	227	ASP	Mainchain
1	A	23	LEU	Mainchain,Peptide
1	A	235	ASN	Mainchain,Peptide
1	A	236	GLY	Mainchain
1	A	24	TYR	Sidechain
1	A	245	ALA	Mainchain
1	A	250	ASP	Mainchain
1	A	28	ALA	Mainchain
1	A	32	ASP	Mainchain
1	A	36	ILE	Mainchain
1	A	41	LEU	Mainchain
1	A	45	GLN	Mainchain
1	A	46	GLN	Mainchain
1	A	49	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	55	SER	Mainchain
1	A	56	LEU	Mainchain
1	A	58	SER	Mainchain
1	A	59	GLN	Mainchain
1	A	61	LEU	Mainchain
1	A	64	LYS	Mainchain
1	A	71	VAL	Mainchain
1	A	72	LEU	Mainchain
1	A	87	LEU	Mainchain
1	A	92	GLU	Mainchain
1	A	94	LYS	Mainchain
1	A	96	VAL	Mainchain
1	A	98	ARG	Mainchain,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	1781	0	1851	137	0
2	A	26	0	19	1	0
All	All	1807	0	1870	137	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 37.

All (137) 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)
1:A:177:LYS:O	1:A:177:LYS:HG2	1.41	1.11
1:A:177:LYS:O	1:A:177:LYS:CG	2.08	0.96
1:A:250:ASP:OD1	1:A:251:PRO:HD3	1.65	0.95
1:A:59:GLN:NE2	1:A:62:ILE:HD12	1.81	0.95
1:A:161:ARG:HG3	1:A:162:THR:H	1.34	0.90
1:A:136:ALA:O	1:A:139:ALA:HB3	1.71	0.89
1:A:50:VAL:HG11	1:A:52:TYR:CE2	2.08	0.88
1:A:161:ARG:CG	1:A:162:THR:H	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:O	1:A:45:GLN:HG3	1.77	0.84
1:A:44:LEU:HD11	1:A:52:TYR:OH	1.77	0.84
1:A:56:LEU:HD21	1:A:240:GLN:HG3	1.59	0.84
1:A:159:GLU:HG3	1:A:163:PRO:HA	1.61	0.82
1:A:250:ASP:OD1	1:A:251:PRO:CD	2.26	0.82
1:A:108:GLY:O	1:A:109:ALA:HB3	1.78	0.82
1:A:54:ASP:OD1	1:A:56:LEU:HB2	1.82	0.79
1:A:98:ARG:HD3	1:A:113:GLN:HE22	1.50	0.75
1:A:143:GLU:HG2	1:A:145:THR:O	1.86	0.75
1:A:231:ALA:O	1:A:235:ASN:HB2	1.85	0.75
1:A:50:VAL:HG11	1:A:52:TYR:CZ	2.23	0.73
1:A:59:GLN:HE21	1:A:62:ILE:HD12	1.54	0.72
1:A:74:THR:O	1:A:75:ALA:CB	2.37	0.72
1:A:44:LEU:CD1	1:A:52:TYR:OH	2.37	0.72
1:A:47:ALA:O	1:A:66:LYS:HE2	1.90	0.72
1:A:161:ARG:HG3	1:A:162:THR:N	2.06	0.71
1:A:168:GLU:O	1:A:173:LEU:HD11	1.91	0.70
1:A:161:ARG:CG	1:A:162:THR:N	2.56	0.69
1:A:187:THR:O	1:A:188:LEU:HD23	1.93	0.69
1:A:212:LYS:O	1:A:215:TRP:HB2	1.93	0.69
1:A:159:GLU:CG	1:A:163:PRO:HA	2.23	0.68
1:A:56:LEU:CD2	1:A:240:GLN:HG3	2.26	0.66
1:A:59:GLN:NE2	1:A:62:ILE:CD1	2.58	0.66
1:A:98:ARG:CD	1:A:113:GLN:HE22	2.08	0.66
1:A:211:TYR:CD2	1:A:212:LYS:HB2	2.31	0.65
1:A:52:TYR:CE1	1:A:99:VAL:HG21	2.31	0.65
1:A:124:ILE:HD13	1:A:124:ILE:N	2.11	0.65
1:A:82:MET:O	1:A:86:MET:HB2	1.98	0.63
1:A:50:VAL:CG1	1:A:52:TYR:CE2	2.78	0.63
1:A:115:VAL:O	1:A:116:LEU:C	2.40	0.63
1:A:78:HIS:CE1	1:A:81:GLU:HB2	2.35	0.62
1:A:184:LEU:HA	2:A:300:SAH:O3'	2.00	0.62
1:A:32:ASP:OD1	1:A:33:PRO:N	2.33	0.61
1:A:144:LEU:HB3	1:A:179:THR:HG21	1.83	0.61
1:A:46:GLN:HG3	1:A:95:MET:SD	2.41	0.60
1:A:74:THR:O	1:A:75:ALA:HB2	2.02	0.60
1:A:182:LEU:HD12	1:A:243:ILE:CG2	2.31	0.60
1:A:112:GLU:O	1:A:113:GLN:C	2.43	0.59
1:A:106:MET:O	1:A:107:TYR:C	2.41	0.59
1:A:204:ASP:O	1:A:205:THR:C	2.38	0.59
1:A:203:GLU:HG3	1:A:226:LYS:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:SER:O	1:A:56:LEU:HG	2.02	0.58
1:A:113:GLN:O	1:A:114:MET:C	2.45	0.58
1:A:111:MET:SD	1:A:114:MET:HE2	2.42	0.58
1:A:66:LYS:HB2	1:A:67:PRO:CD	2.34	0.58
1:A:165:PRO:HG2	1:A:168:GLU:CD	2.29	0.58
1:A:84:GLY:O	1:A:85:THR:C	2.43	0.58
1:A:55:SER:O	1:A:56:LEU:CG	2.52	0.58
1:A:250:ASP:CG	1:A:251:PRO:N	2.61	0.57
1:A:87:LEU:O	1:A:91:ARG:HG3	2.04	0.57
1:A:239:LYS:HE3	1:A:240:GLN:HE21	1.69	0.57
1:A:31:GLY:HA3	1:A:215:TRP:NE1	2.20	0.57
1:A:168:GLU:O	1:A:173:LEU:CD1	2.53	0.56
1:A:209:VAL:O	1:A:209:VAL:HG12	2.06	0.56
1:A:114:MET:O	1:A:115:VAL:C	2.48	0.55
1:A:127:VAL:O	1:A:128:PRO:C	2.48	0.55
1:A:98:ARG:HH11	1:A:113:GLN:CD	2.15	0.54
1:A:58:SER:O	1:A:62:ILE:HG13	2.06	0.54
1:A:223:THR:HG23	1:A:224:THR:N	2.23	0.54
1:A:250:ASP:OD1	1:A:251:PRO:N	2.40	0.54
1:A:170:LEU:O	1:A:171:THR:C	2.49	0.54
1:A:108:GLY:O	1:A:109:ALA:CB	2.44	0.54
1:A:51:LEU:CD2	1:A:72:LEU:HD12	2.38	0.54
1:A:211:TYR:O	1:A:212:LYS:C	2.49	0.53
1:A:133:VAL:HG23	1:A:183:PHE:CZ	2.44	0.53
1:A:250:ASP:CG	1:A:251:PRO:CD	2.82	0.53
1:A:147:PRO:O	1:A:148:ASP:HB2	2.09	0.53
1:A:161:ARG:O	1:A:163:PRO:HD3	2.09	0.53
1:A:136:ALA:O	1:A:139:ALA:CB	2.52	0.52
1:A:37:THR:O	1:A:38:VAL:C	2.51	0.52
1:A:250:ASP:CG	1:A:251:PRO:HD3	2.35	0.52
1:A:223:THR:OG1	1:A:224:THR:N	2.42	0.51
1:A:232:MET:CE	1:A:237:ILE:HG22	2.40	0.50
1:A:20:HIS:ND1	1:A:20:HIS:N	2.58	0.50
1:A:132:SER:O	1:A:135:ALA:HB3	2.12	0.50
1:A:58:SER:OG	1:A:59:GLN:N	2.40	0.49
1:A:82:MET:O	1:A:83:VAL:C	2.55	0.49
1:A:146:ILE:HB	1:A:149:LEU:HB3	1.94	0.49
1:A:209:VAL:HG22	1:A:243:ILE:HG12	1.95	0.49
1:A:78:HIS:O	1:A:79:LEU:C	2.55	0.48
1:A:21:MET:HE3	1:A:122:VAL:HG22	1.95	0.48
1:A:55:SER:O	1:A:56:LEU:CB	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:O	1:A:62:ILE:N	2.46	0.48
1:A:133:VAL:CG2	1:A:183:PHE:CZ	2.97	0.48
1:A:103:ASP:OD1	1:A:105:ALA:HB2	2.14	0.48
1:A:182:LEU:HD12	1:A:243:ILE:HB	1.97	0.47
1:A:78:HIS:O	1:A:81:GLU:N	2.48	0.47
1:A:110:ILE:O	1:A:114:MET:HG3	2.15	0.47
1:A:24:TYR:CD2	1:A:24:TYR:N	2.83	0.46
1:A:98:ARG:NH1	1:A:113:GLN:OE1	2.47	0.46
1:A:139:ALA:HB3	1:A:140:ALA:H	1.63	0.46
1:A:201:TRP:CE3	1:A:205:THR:HG21	2.50	0.46
1:A:226:LYS:HG2	1:A:227:ASP:OD1	2.14	0.46
1:A:133:VAL:HG23	1:A:183:PHE:HZ	1.78	0.46
1:A:52:TYR:CD1	1:A:99:VAL:HB	2.51	0.46
1:A:206:PRO:O	1:A:207:VAL:HG23	2.16	0.46
1:A:90:MET:C	1:A:92:GLU:N	2.72	0.46
1:A:123:ASP:C	1:A:124:ILE:HD13	2.40	0.46
1:A:23:LEU:HB3	1:A:124:ILE:HD12	1.96	0.46
1:A:209:VAL:HG21	1:A:232:MET:SD	2.56	0.46
1:A:168:GLU:O	1:A:169:LYS:C	2.55	0.45
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.55	0.45
1:A:203:GLU:HG3	1:A:226:LYS:CB	2.45	0.45
1:A:61:LEU:O	1:A:63:ALA:N	2.50	0.45
1:A:243:ILE:HD13	1:A:243:ILE:HG21	1.73	0.45
1:A:41:LEU:HD11	1:A:64:LYS:HD2	1.98	0.44
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.64	0.44
1:A:123:ASP:O	1:A:124:ILE:HD13	2.18	0.44
1:A:222:ARG:HH11	1:A:222:ARG:HD3	1.05	0.44
1:A:28:ALA:HB1	1:A:61:LEU:CD1	2.47	0.43
1:A:249:LEU:HA	1:A:249:LEU:HD23	1.87	0.43
1:A:197:ILE:O	1:A:198:ASN:C	2.57	0.43
1:A:154:ILE:HG21	1:A:154:ILE:HD13	1.71	0.42
1:A:32:ASP:O	1:A:34:ASP:N	2.51	0.42
1:A:126:ILE:HG21	1:A:126:ILE:HD13	1.71	0.42
1:A:124:ILE:HG22	1:A:125:GLU:N	2.35	0.42
1:A:212:LYS:HE2	1:A:240:GLN:NE2	2.34	0.42
1:A:18:GLY:O	1:A:21:MET:N	2.49	0.42
1:A:74:THR:O	1:A:75:ALA:HB3	2.18	0.42
1:A:154:ILE:HB	1:A:180:ILE:HD12	2.00	0.42
1:A:26:ILE:HG21	1:A:26:ILE:HD13	1.76	0.42
1:A:206:PRO:C	1:A:207:VAL:HG23	2.45	0.41
1:A:124:ILE:CG2	1:A:125:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HG2	1:A:162:THR:H	1.79	0.41
1:A:83:VAL:O	1:A:84:GLY:C	2.62	0.41
1:A:225:VAL:H	1:A:225:VAL:HG23	1.46	0.41
1:A:194:LYS:O	1:A:195:GLU:C	2.63	0.41
1:A:212:LYS:CE	1:A:240:GLN:NE2	2.83	0.41
1:A:57:VAL:CG1	1:A:58:SER:N	2.82	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	232/234 (99%)	201 (87%)	23 (10%)	8 (3%)	<b>3</b> <b>16</b>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	56	LEU
1	A	79	LEU
1	A	184	LEU
1	A	75	ALA
1	A	236	GLY
1	A	133	VAL
1	A	250	ASP

#### 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	193/193 (100%)	153 (79%)	40 (21%)	<b>1</b> <b>5</b>

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	33	PRO
1	A	44	LEU
1	A	51	LEU
1	A	55	SER
1	A	59	GLN
1	A	64	LYS
1	A	65	SER
1	A	70	GLU
1	A	73	LYS
1	A	74	THR
1	A	86	MET
1	A	87	LEU
1	A	94	LYS
1	A	97	VAL
1	A	110	ILE
1	A	111	MET
1	A	131	THR
1	A	133	VAL
1	A	146	ILE
1	A	149	LEU
1	A	151	GLN
1	A	155	LEU
1	A	162	THR
1	A	168	GLU
1	A	173	LEU
1	A	180	ILE
1	A	183	PHE
1	A	185	SER
1	A	186	SER
1	A	190	LYS
1	A	191	LYS
1	A	193	MET
1	A	194	LYS
1	A	197	ILE

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Mol	Chain	Res	Type
1	A	203	GLU
1	A	210	VAL
1	A	226	LYS
1	A	240	GLN
1	A	242	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	151	GLN
1	A	198	ASN
1	A	240	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
2	SAH	A	300	-	27,28,28	2.15	8 (29%)	36,40,40	3.09	25 (69%)

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
2	SAH	A	300	-	-	3/15/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	SAH	C5-N7	-5.59	1.28	1.39
2	A	300	SAH	C8-N7	3.96	1.39	1.31
2	A	300	SAH	O3'-C3'	3.74	1.52	1.43
2	A	300	SAH	C1'-N9	-3.68	1.36	1.46
2	A	300	SAH	C5-C4	-3.67	1.32	1.39
2	A	300	SAH	C8-N9	-3.08	1.32	1.37
2	A	300	SAH	C5'-SD	2.47	1.90	1.81
2	A	300	SAH	C6-N6	-2.07	1.28	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SAH	C5-C4-N3	-6.11	118.30	126.72
2	A	300	SAH	C5-C4-N9	5.17	111.45	105.81
2	A	300	SAH	C5'-SD-CG	-5.15	86.99	102.26
2	A	300	SAH	C4-N9-C8	-4.80	100.70	105.74
2	A	300	SAH	O3'-C3'-C2'	-4.46	97.50	111.82
2	A	300	SAH	O4'-C1'-C2'	4.24	115.70	106.62
2	A	300	SAH	C2-N1-C6	-4.09	112.01	118.73
2	A	300	SAH	O2'-C2'-C3'	-4.04	98.86	111.82
2	A	300	SAH	CB-CA-C	3.89	120.75	110.45
2	A	300	SAH	N9-C8-N7	-3.77	108.58	113.94
2	A	300	SAH	N3-C2-N1	-3.60	123.14	128.58
2	A	300	SAH	O4'-C4'-C5'	-3.31	100.32	108.83
2	A	300	SAH	C5'-C4'-C3'	3.25	123.17	115.06
2	A	300	SAH	C4-C5-N7	-3.11	107.02	110.58
2	A	300	SAH	C2-N3-C4	3.08	119.36	111.83
2	A	300	SAH	N6-C6-N1	-3.08	111.52	118.38
2	A	300	SAH	CB-CA-N	2.80	117.43	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SAH	O4'-C1'-N9	-2.80	102.71	108.09
2	A	300	SAH	C5-C6-N1	2.72	124.42	117.51
2	A	300	SAH	C3'-C2'-C1'	-2.64	96.46	101.46
2	A	300	SAH	C6-C5-N7	2.57	137.05	132.09
2	A	300	SAH	OXT-C-O	-2.48	118.45	124.08
2	A	300	SAH	C4'-C5'-SD	-2.31	105.52	113.78
2	A	300	SAH	C2'-C1'-N9	2.21	118.80	113.30
2	A	300	SAH	CB-CG-SD	-2.06	108.86	113.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

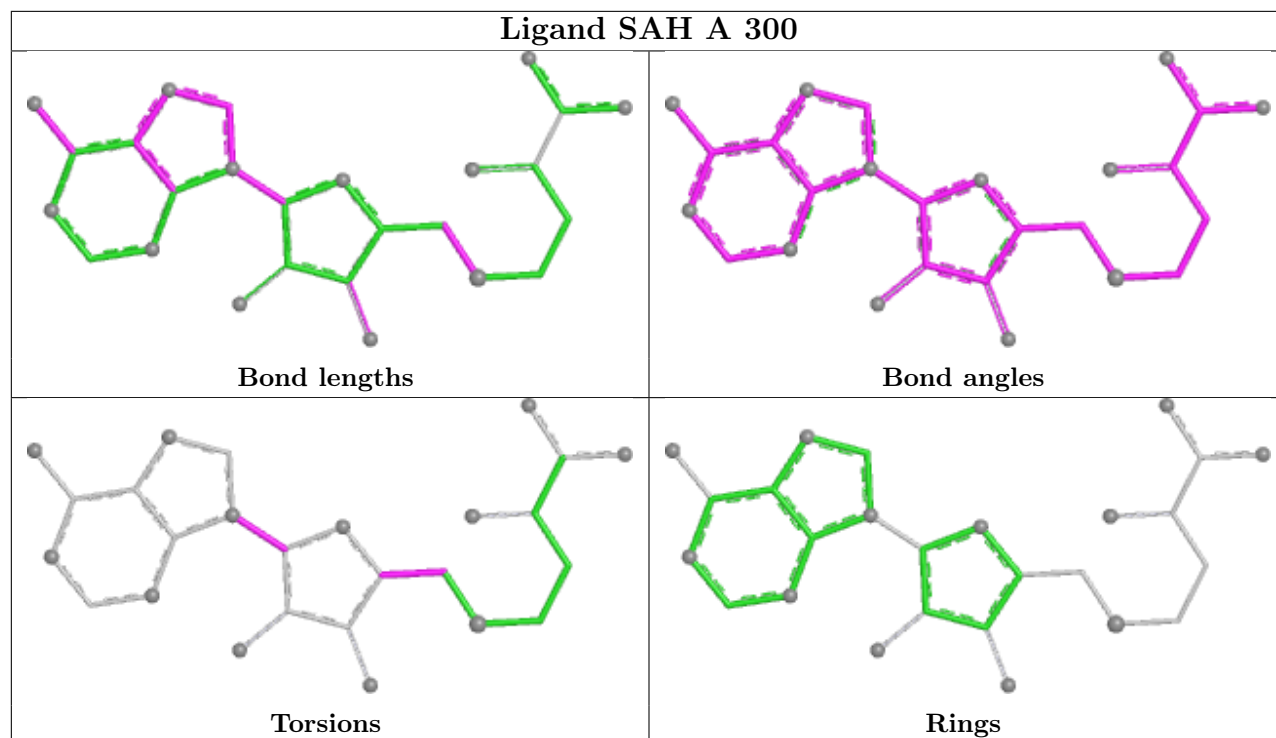
Mol	Chain	Res	Type	Atoms
2	A	300	SAH	C3'-C4'-C5'-SD
2	A	300	SAH	O4'-C4'-C5'-SD
2	A	300	SAH	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	SAH	1	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 than 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	234/234 (100%)	-0.49	5 (2%) 63 42	14, 32, 63, 87	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	ASP	4.0
1	A	53	ALA	3.0
1	A	52	TYR	2.5
1	A	161	ARG	2.3
1	A	55	SER	2.3

### 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.

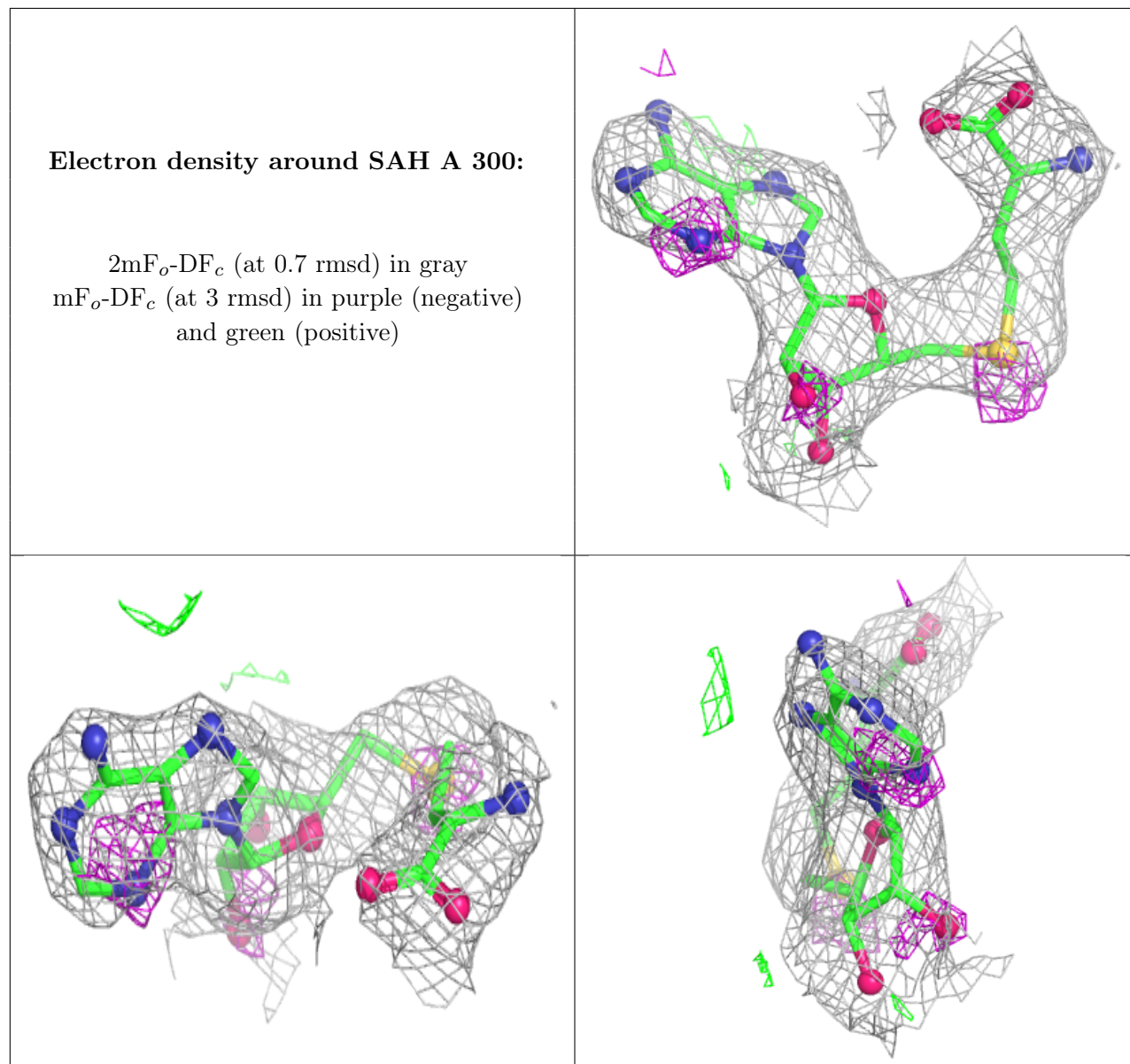
### 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SAH	A	300	26/26	0.94	0.09	17,22,24,27	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.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.