



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 AM UTC

PDB ID : 4FFJ / pdb_00004ffj
Title : The crystal structure of spDHBP from S.pneumoniae
Authors : Wang, D.
Deposited on : 2012-06-01
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
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

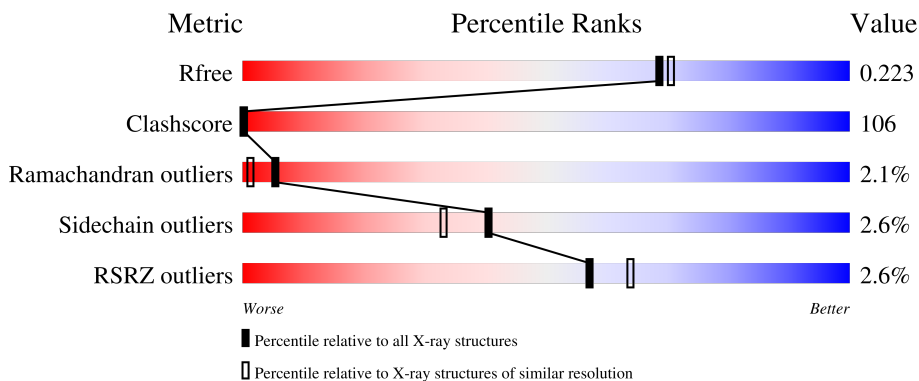
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	302	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	303	-	X	-	-
3	GOL	A	304	-	X	X	-
3	GOL	A	305	-	X	X	-
3	GOL	A	306	-	X	X	-
3	GOL	A	307	-	X	X	-
3	GOL	A	308	-	X	X	-

2 Entry composition [i](#)

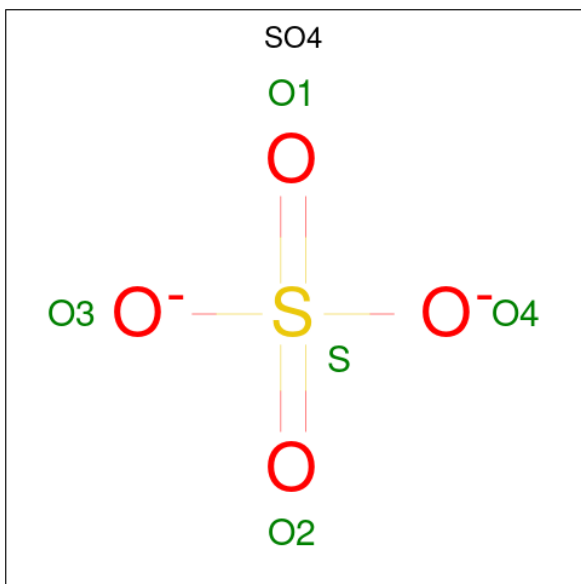
There are 4 unique types of molecules in this entry. The entry contains 1636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Riboflavin biosynthesis protein ribBA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1470	919	249	285	17	7	1	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.01Å 78.01Å 87.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.20 – 1.95 38.20 – 1.95	Depositor EDS
% Data completeness (in resolution range)	84.4 (38.20-1.95) 84.5 (38.20-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.244 (Not available) , 0.223	Depositor DCC
R_{free} test set	1037 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtrriage
Anisotropy	0.119	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1636	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, 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	7.98	644/1485 (43.4%)	3.74	321/1998 (16.1%)

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	10

All (644) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	ASP	C-N	43.14	1.94	1.33
1	A	4	ARG	C-O	40.87	2.05	1.23
1	A	5	LYS	CA-C	40.69	2.09	1.52
1	A	4	ARG	NE-CZ	33.67	1.70	1.33
1	A	198	ARG	CD-NE	-32.21	1.01	1.46
1	A	3	TYR	C-N	-32.20	0.88	1.33
1	A	115	ILE	CA-C	30.68	1.90	1.52
1	A	24	ASP	N-CA	-30.24	1.07	1.46
1	A	3	TYR	CA-C	29.69	1.92	1.52
1	A	75	GLU	CA-CB	-29.46	0.94	1.53
1	A	25	LYS	CA-C	29.29	1.92	1.52
1	A	167	HIS	CG-CD2	28.38	1.67	1.35
1	A	72	PRO	N-CD	28.35	1.87	1.47
1	A	113	GLU	C-O	27.22	1.55	1.24
1	A	161[A]	CYS	CA-C	-26.67	1.20	1.52
1	A	161[B]	CYS	CA-C	-26.67	1.20	1.52
1	A	175	ASP	CA-CB	25.85	1.96	1.53
1	A	203	GLN	CA-C	25.83	1.88	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	ASP	CA-C	25.82	1.87	1.52
1	A	175	ASP	CA-C	-25.79	1.17	1.52
1	A	6	ILE	N-CA	-25.70	1.16	1.46
1	A	182	LYS	N-CA	25.47	1.77	1.46
1	A	115	ILE	N-CA	24.61	1.76	1.46
1	A	186	ILE	CA-CB	23.48	1.84	1.54
1	A	199	LYS	CA-C	-23.20	1.22	1.52
1	A	114	ASP	CA-CB	22.69	1.90	1.53
1	A	114	ASP	C-O	22.47	1.52	1.23
1	A	114	ASP	C-N	-21.93	1.05	1.33
1	A	180	PHE	CA-CB	21.79	1.88	1.53
1	A	149	LEU	N-CA	21.78	1.72	1.46
1	A	8	GLU	CA-C	21.74	1.81	1.52
1	A	184	HIS	CA-C	-21.37	1.25	1.52
1	A	2	GLU	N-CA	21.05	1.73	1.46
1	A	150	LEU	CA-C	-20.91	1.25	1.52
1	A	5	LYS	CA-CB	-20.44	1.25	1.53
1	A	176	ASP	C-N	20.42	1.60	1.33
1	A	71	SER	CA-C	20.37	1.78	1.53
1	A	74	VAL	C-N	20.25	1.61	1.33
1	A	167	HIS	CA-C	-20.09	1.25	1.52
1	A	31	GLY	CA-C	19.94	1.66	1.52
1	A	176	ASP	CA-CB	-19.93	1.22	1.53
1	A	72	PRO	N-CA	19.81	1.70	1.47
1	A	9	ALA	N-CA	19.55	1.69	1.46
1	A	2	GLU	C-N	19.29	1.60	1.33
1	A	8	GLU	CD-OE1	19.12	1.61	1.25
1	A	45	VAL	CA-C	-18.91	1.28	1.52
1	A	36	SER	CA-C	18.89	1.78	1.53
1	A	62	GLU	CA-CB	18.85	1.84	1.53
1	A	72	PRO	CA-C	18.84	1.75	1.52
1	A	48	MET	CA-C	-18.77	1.28	1.52
1	A	193	GLU	CA-C	-18.74	1.28	1.52
1	A	75	GLU	C-O	18.57	1.60	1.23
1	A	178	ILE	N-CA	18.48	1.68	1.46
1	A	165	MET	CA-C	18.28	1.76	1.52
1	A	84	ALA	CA-CB	-17.94	1.29	1.52
1	A	200	VAL	C-O	17.82	1.42	1.24
1	A	131	ALA	CA-C	17.75	1.75	1.52
1	A	70	LEU	CA-C	17.72	1.74	1.52
1	A	167	HIS	CD2-NE2	17.50	1.57	1.37
1	A	199	LYS	N-CA	17.40	1.67	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	ASN	C-N	-17.31	1.10	1.33
1	A	121	ARG	NE-CZ	17.26	1.52	1.33
1	A	177	LEU	C-O	17.14	1.44	1.24
1	A	23	ASP	CG-OD1	17.03	1.57	1.25
1	A	71	SER	CB-OG	17.02	1.76	1.42
1	A	159	GLY	CA-C	-17.00	1.34	1.52
1	A	193	GLU	C-N	16.90	1.59	1.33
1	A	157	GLU	C-N	16.88	1.54	1.33
1	A	167	HIS	ND1-CE1	16.84	1.49	1.32
1	A	22	ILE	C-N	-16.71	1.09	1.33
1	A	167	HIS	CE1-NE2	16.59	1.49	1.32
1	A	93	GLU	C-O	16.56	1.45	1.24
1	A	132	LYS	CA-C	-16.52	1.31	1.52
1	A	4	ARG	CZ-NH2	16.46	1.54	1.33
1	A	195	GLN	N-CA	16.35	1.66	1.46
1	A	202	ASP	CA-CB	16.32	1.81	1.53
1	A	136	VAL	CA-C	16.29	1.77	1.52
1	A	43	GLU	CA-CB	16.25	1.79	1.53
1	A	115	ILE	CA-CB	16.14	1.79	1.54
1	A	108	ARG	CZ-NH2	16.10	1.54	1.33
1	A	4	ARG	CA-C	15.91	1.86	1.52
1	A	45	VAL	CA-CB	15.87	1.74	1.54
1	A	23	ASP	C-O	-15.86	1.04	1.24
1	A	92	LYS	CA-C	-15.82	1.30	1.52
1	A	176	ASP	N-CA	15.70	1.65	1.46
1	A	8	GLU	N-CA	-15.64	1.26	1.46
1	A	197	TYR	C-O	15.59	1.42	1.24
1	A	196	GLU	C-N	15.57	1.54	1.33
1	A	165	MET	N-CA	-15.55	1.27	1.45
1	A	145	ALA	N-CA	15.54	1.65	1.46
1	A	146	THR	CA-C	-15.48	1.33	1.52
1	A	161[A]	CYS	C-O	15.45	1.43	1.23
1	A	161[B]	CYS	C-O	15.45	1.43	1.23
1	A	142	HIS	CE1-NE2	15.41	1.48	1.32
1	A	30	GLU	CD-OE2	15.37	1.54	1.25
1	A	29	ASN	CA-C	15.37	1.85	1.52
1	A	112	ALA	N-CA	-15.30	1.27	1.46
1	A	45	VAL	C-O	15.24	1.42	1.24
1	A	173	ARG	N-CA	15.05	1.64	1.45
1	A	193	GLU	CG-CD	15.04	1.89	1.52
1	A	65	ALA	N-CA	-14.94	1.27	1.46
1	A	55	LEU	C-O	14.87	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ASN	CA-C	-14.85	1.34	1.53
1	A	184	HIS	ND1-CE1	14.77	1.47	1.32
1	A	22	ILE	CA-C	14.73	1.70	1.52
1	A	204	LEU	CG-CD2	14.59	2.00	1.52
1	A	200	VAL	C-N	14.51	1.55	1.33
1	A	146	THR	N-CA	14.34	1.63	1.46
1	A	17	ARG	CA-CB	14.27	1.74	1.53
1	A	167	HIS	CG-ND1	14.27	1.53	1.38
1	A	19	VAL	C-O	14.27	1.38	1.24
1	A	176	ASP	C-O	14.23	1.40	1.24
1	A	194	LEU	CA-CB	14.21	1.77	1.53
1	A	1	MET	N-CA	14.19	1.73	1.46
1	A	41	THR	CA-C	-14.18	1.33	1.53
1	A	185	ASN	C-N	14.10	1.49	1.33
1	A	187	PRO	N-CA	-14.06	1.30	1.47
1	A	99	SER	C-O	14.03	1.43	1.23
1	A	97	GLY	CA-C	14.03	1.72	1.51
1	A	198	ARG	N-CA	14.01	1.64	1.46
1	A	69	MET	CA-CB	14.00	1.75	1.53
1	A	89	ILE	N-CA	-13.94	1.29	1.46
1	A	181	SER	C-O	13.91	1.40	1.24
1	A	83	THR	C-N	13.88	1.51	1.33
1	A	146	THR	C-N	13.87	1.51	1.33
1	A	70	LEU	N-CA	-13.78	1.28	1.46
1	A	34	ILE	C-O	13.72	1.38	1.23
1	A	74	VAL	CA-CB	13.55	1.71	1.54
1	A	98	ILE	C-N	13.55	1.51	1.33
1	A	47	PHE	N-CA	13.54	1.62	1.46
1	A	83	THR	N-CA	13.50	1.71	1.46
1	A	105	LEU	CA-C	13.45	1.70	1.52
1	A	195	GLN	CA-C	-13.44	1.35	1.52
1	A	75	GLU	CA-C	13.30	1.80	1.52
1	A	179	GLN	C-N	13.30	1.52	1.33
1	A	30	GLU	CG-CD	13.29	1.85	1.52
1	A	150	LEU	C-O	13.19	1.39	1.24
1	A	161[A]	CYS	CA-CB	13.14	1.81	1.54
1	A	161[B]	CYS	CA-CB	13.14	1.81	1.54
1	A	59	PRO	CA-CB	13.12	1.71	1.53
1	A	67	GLN	CG-CD	13.11	1.84	1.52
1	A	67	GLN	CD-NE2	-13.07	1.05	1.33
1	A	54	GLY	C-N	13.06	1.51	1.33
1	A	19	VAL	CA-C	-13.04	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ILE	N-CA	-13.04	1.32	1.46
1	A	184	HIS	CG-CD2	13.00	1.50	1.35
1	A	49	ALA	CA-CB	12.97	1.75	1.53
1	A	177	LEU	N-CA	-12.88	1.30	1.46
1	A	121	ARG	N-CA	-12.85	1.29	1.46
1	A	50	THR	N-CA	12.83	1.62	1.46
1	A	47	PHE	CG-CD1	12.78	1.65	1.38
1	A	95	THR	CA-CB	12.77	1.75	1.53
1	A	87	VAL	CA-CB	12.64	1.66	1.54
1	A	8	GLU	C-N	-12.64	1.18	1.33
1	A	84	ALA	CA-C	12.55	1.67	1.53
1	A	200	VAL	CA-CB	12.45	1.70	1.54
1	A	49	ALA	N-CA	-12.43	1.29	1.46
1	A	149	LEU	CA-C	-12.39	1.36	1.52
1	A	204	LEU	C-O	12.38	1.48	1.23
1	A	99	SER	CA-C	-12.35	1.36	1.53
1	A	34	ILE	N-CA	-12.25	1.32	1.46
1	A	202	ASP	CG-OD2	-12.24	1.02	1.25
1	A	150	LEU	C-N	12.20	1.50	1.33
1	A	42	THR	C-O	12.18	1.38	1.24
1	A	187	PRO	C-O	12.14	1.38	1.23
1	A	168	ASP	CA-C	12.05	1.71	1.52
1	A	101	GLU	CG-CD	12.03	1.82	1.52
1	A	50	THR	CA-CB	12.01	1.72	1.53
1	A	196	GLU	CA-C	-11.96	1.37	1.52
1	A	143	THR	CA-C	-11.90	1.37	1.52
1	A	52	ALA	C-O	11.88	1.37	1.23
1	A	167	HIS	CA-CB	11.88	1.72	1.53
1	A	15	LYS	N-CA	11.82	1.61	1.46
1	A	170	LYS	CA-C	-11.75	1.38	1.52
1	A	198	ARG	NE-CZ	11.72	1.46	1.33
1	A	48	MET	N-CA	11.61	1.60	1.46
1	A	113	GLU	CD-OE1	-11.57	1.03	1.25
1	A	53	LYS	CD-CE	-11.56	1.17	1.52
1	A	167	HIS	N-CA	-11.56	1.31	1.46
1	A	180	PHE	CA-C	-11.52	1.38	1.52
1	A	109	MET	CA-C	11.46	1.68	1.52
1	A	202	ASP	C-N	11.45	1.49	1.33
1	A	59	PRO	C-O	11.45	1.37	1.23
1	A	2	GLU	CA-C	11.43	1.68	1.52
1	A	103	ARG	CA-C	-11.42	1.37	1.52
1	A	185	ASN	CG-OD1	11.41	1.45	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	PRO	CA-CB	11.37	1.69	1.53
1	A	203	GLN	CB-CG	-11.34	1.18	1.52
1	A	72	PRO	CA-CB	-11.28	1.38	1.53
1	A	112	ALA	CA-C	-11.24	1.38	1.52
1	A	71	SER	N-CA	11.22	1.62	1.45
1	A	83	THR	CB-OG1	11.20	1.61	1.43
1	A	72	PRO	CB-CG	11.16	2.05	1.49
1	A	190	THR	CA-CB	11.14	1.73	1.53
1	A	3	TYR	N-CA	11.11	1.60	1.46
1	A	96	THR	CA-C	11.09	1.68	1.52
1	A	123	PRO	N-CA	-11.01	1.28	1.47
1	A	176	ASP	CG-OD1	10.98	1.46	1.25
1	A	168	ASP	CG-OD2	-10.97	1.04	1.25
1	A	12	ALA	C-O	10.92	1.36	1.24
1	A	74	VAL	CB-CG1	10.86	1.88	1.52
1	A	130	ILE	CA-C	10.83	1.65	1.52
1	A	26	ASP	C-O	10.82	1.45	1.23
1	A	195	GLN	C-N	10.73	1.48	1.33
1	A	196	GLU	CD-OE2	-10.66	1.05	1.25
1	A	190	THR	N-CA	-10.65	1.33	1.45
1	A	58	MET	N-CA	-10.65	1.34	1.46
1	A	61	SER	CA-CB	-10.64	1.35	1.53
1	A	182	LYS	C-N	-10.63	1.20	1.33
1	A	152	LEU	N-CA	10.58	1.59	1.46
1	A	39	ALA	CA-C	-10.58	1.39	1.53
1	A	91	TYR	CA-C	10.55	1.66	1.52
1	A	141	GLY	N-CA	10.46	1.58	1.45
1	A	90	ASP	C-N	10.46	1.47	1.33
1	A	149	LEU	C-N	10.39	1.48	1.33
1	A	182	LYS	CA-C	10.36	1.66	1.52
1	A	15	LYS	C-N	10.33	1.46	1.33
1	A	117	PRO	N-CA	-10.32	1.33	1.47
1	A	52	ALA	CA-C	-10.31	1.42	1.53
1	A	91	TYR	N-CA	-10.30	1.33	1.46
1	A	104	GLY	C-N	10.22	1.48	1.34
1	A	138	GLU	CA-C	-10.14	1.41	1.52
1	A	177	LEU	CB-CG	10.14	1.73	1.53
1	A	120	PHE	CG-CD2	10.13	1.60	1.38
1	A	184	HIS	CG-ND1	-10.12	1.27	1.38
1	A	184	HIS	CA-CB	10.12	1.69	1.53
1	A	101	GLU	CA-C	10.11	1.66	1.52
1	A	11	GLU	CG-CD	10.07	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	MET	C-N	10.06	1.48	1.33
1	A	98	ILE	CA-CB	-10.06	1.40	1.54
1	A	142	HIS	ND1-CE1	10.05	1.42	1.32
1	A	43	GLU	C-O	10.01	1.36	1.24
1	A	155	LEU	CA-C	10.01	1.67	1.53
1	A	29	ASN	N-CA	10.00	1.65	1.46
1	A	193	GLU	N-CA	9.99	1.58	1.46
1	A	192	LYS	CA-C	-9.96	1.39	1.52
1	A	59	PRO	CA-C	-9.95	1.40	1.52
1	A	53	LYS	CG-CD	9.93	1.82	1.52
1	A	10	LEU	C-O	9.90	1.35	1.24
1	A	2	GLU	CB-CG	-9.88	1.22	1.52
1	A	115	ILE	C-O	-9.86	1.12	1.23
1	A	93	GLU	N-CA	9.83	1.58	1.46
1	A	75	GLU	N-CA	9.82	1.65	1.46
1	A	97	GLY	C-N	-9.82	1.21	1.33
1	A	56	ILE	CB-CG1	9.81	1.73	1.53
1	A	45	VAL	C-N	9.77	1.47	1.34
1	A	85	PHE	CG-CD1	9.76	1.59	1.38
1	A	184	HIS	N-CA	9.76	1.58	1.46
1	A	31	GLY	C-O	-9.75	1.10	1.23
1	A	202	ASP	C-O	9.73	1.36	1.24
1	A	175	ASP	CG-OD2	9.71	1.43	1.25
1	A	11	GLU	C-O	-9.69	1.12	1.24
1	A	160	LEU	CB-CG	9.66	1.72	1.53
1	A	135	GLY	C-N	9.65	1.44	1.34
1	A	2	GLU	C-O	-9.61	1.11	1.24
1	A	186	ILE	N-CA	9.60	1.58	1.46
1	A	48	MET	CA-CB	9.60	1.68	1.53
1	A	105	LEU	C-O	-9.59	1.11	1.24
1	A	120	PHE	CA-CB	9.57	1.71	1.53
1	A	7	GLN	C-N	-9.55	1.20	1.33
1	A	96	THR	CA-CB	-9.55	1.38	1.53
1	A	1	MET	C-N	9.54	1.47	1.33
1	A	126	MET	CA-C	9.51	1.64	1.52
1	A	198	ARG	CZ-NH2	-9.51	1.21	1.33
1	A	62	GLU	CA-C	-9.50	1.40	1.52
1	A	4	ARG	CZ-NH1	9.46	1.46	1.32
1	A	174	THR	CA-C	9.45	1.65	1.52
1	A	130	ILE	CA-CB	9.44	1.65	1.54
1	A	69	MET	N-CA	-9.42	1.32	1.46
1	A	176	ASP	CG-OD2	-9.41	1.07	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	GLU	CA-C	9.39	1.65	1.52
1	A	149	LEU	CG-CD2	9.37	1.83	1.52
1	A	109	MET	C-O	-9.35	1.11	1.24
1	A	184	HIS	C-N	9.34	1.47	1.33
1	A	73	MET	N-CA	9.30	1.57	1.46
1	A	188	LEU	C-O	9.30	1.34	1.23
1	A	158	CYS	N-CA	-9.25	1.35	1.46
1	A	183	LYS	CA-C	9.24	1.65	1.52
1	A	40	ALA	CA-CB	9.15	1.64	1.52
1	A	158	CYS	CA-CB	9.15	1.71	1.53
1	A	92	LYS	CG-CD	9.14	1.79	1.52
1	A	25	LYS	C-N	9.10	1.46	1.33
1	A	188	LEU	CA-CB	-9.10	1.39	1.53
1	A	9	ALA	CA-C	-9.10	1.41	1.52
1	A	98	ILE	CG1-CD1	9.10	1.87	1.51
1	A	182	LYS	CB-CG	9.10	1.79	1.52
1	A	74	VAL	CB-CG2	-9.07	1.22	1.52
1	A	144	GLU	CA-CB	9.05	1.68	1.53
1	A	172	MET	CA-CB	-9.02	1.39	1.53
1	A	52	ALA	N-CA	9.01	1.57	1.46
1	A	157	GLU	CD-OE2	-8.99	1.08	1.25
1	A	170	LYS	C-N	8.99	1.45	1.33
1	A	4	ARG	CA-CB	8.96	1.71	1.53
1	A	157	GLU	CA-C	-8.94	1.43	1.53
1	A	122	ARG	NE-CZ	8.93	1.42	1.33
1	A	21	VAL	N-CA	8.93	1.57	1.46
1	A	191	ILE	CB-CG1	8.92	1.71	1.53
1	A	21	VAL	CA-CB	8.90	1.64	1.54
1	A	98	ILE	CA-C	8.89	1.67	1.52
1	A	11	GLU	CA-CB	8.88	1.67	1.53
1	A	103	ARG	N-CA	8.87	1.57	1.46
1	A	139	ARG	CZ-NH1	8.85	1.45	1.32
1	A	123	PRO	C-N	8.83	1.46	1.33
1	A	10	LEU	CB-CG	8.82	1.71	1.53
1	A	151	LYS	CA-C	8.81	1.64	1.52
1	A	8	GLU	CG-CD	-8.80	1.30	1.52
1	A	7	GLN	N-CA	-8.79	1.35	1.46
1	A	151	LYS	CG-CD	8.76	1.78	1.52
1	A	192	LYS	N-CA	8.76	1.57	1.46
1	A	135	GLY	CA-C	-8.75	1.40	1.52
1	A	183	LYS	N-CA	8.74	1.57	1.46
1	A	7	GLN	CD-NE2	8.74	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	MET	CG-SD	8.72	2.02	1.80
1	A	63	SER	C-O	8.71	1.34	1.24
1	A	120	PHE	CA-C	8.70	1.62	1.52
1	A	14	GLN	C-O	8.70	1.35	1.24
1	A	11	GLU	N-CA	8.67	1.57	1.46
1	A	4	ARG	C-N	-8.65	1.23	1.33
1	A	86	THR	C-N	8.65	1.43	1.33
1	A	90	ASP	N-CA	8.65	1.57	1.46
1	A	194	LEU	CA-C	8.62	1.64	1.52
1	A	185	ASN	CA-CB	8.57	1.66	1.53
1	A	83	THR	C-O	8.56	1.40	1.23
1	A	170	LYS	CA-CB	8.50	1.67	1.53
1	A	8	GLU	CB-CG	8.49	1.77	1.52
1	A	56	ILE	C-O	8.48	1.32	1.24
1	A	204	LEU	CB-CG	-8.45	1.36	1.53
1	A	30	GLU	CB-CG	-8.44	1.27	1.52
1	A	13	LEU	N-CA	8.44	1.56	1.46
1	A	49	ALA	CA-C	8.43	1.64	1.52
1	A	159	GLY	C-O	8.42	1.34	1.23
1	A	199	LYS	C-N	8.41	1.44	1.33
1	A	107	ALA	C-O	8.40	1.33	1.24
1	A	47	PHE	C-N	8.40	1.44	1.33
1	A	133	LYS	CA-C	8.40	1.64	1.52
1	A	7	GLN	CA-C	8.34	1.63	1.52
1	A	197	TYR	CA-C	-8.34	1.42	1.52
1	A	147	VAL	N-CA	-8.34	1.36	1.46
1	A	173	ARG	CA-C	-8.33	1.41	1.53
1	A	134	GLY	C-N	8.32	1.44	1.33
1	A	129	LEU	C-O	8.31	1.33	1.23
1	A	131	ALA	N-CA	8.28	1.56	1.46
1	A	5	LYS	N-CA	8.27	1.55	1.46
1	A	4	ARG	CB-CG	-8.24	1.27	1.52
1	A	101	GLU	N-CA	-8.21	1.35	1.46
1	A	166	ASN	C-O	8.18	1.33	1.23
1	A	46	ASN	C-O	-8.16	1.13	1.24
1	A	152	LEU	CA-CB	8.16	1.66	1.53
1	A	26	ASP	CA-C	8.16	1.70	1.52
1	A	160	LEU	CA-CB	8.15	1.66	1.53
1	A	35	CYS	C-N	8.13	1.44	1.33
1	A	43	GLU	C-N	-8.13	1.23	1.33
1	A	43	GLU	N-CA	8.13	1.56	1.46
1	A	38	GLN	CG-CD	8.12	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	HIS	CE1-NE2	8.12	1.40	1.32
1	A	149	LEU	CB-CG	-8.11	1.37	1.53
1	A	192	LYS	C-N	8.11	1.44	1.33
1	A	23	ASP	CB-CG	-8.09	1.31	1.52
1	A	122	ARG	CD-NE	8.09	1.57	1.46
1	A	168	ASP	CG-OD1	8.08	1.40	1.25
1	A	16	GLY	CA-C	-8.04	1.39	1.51
1	A	164	ILE	CA-CB	8.04	1.64	1.54
1	A	149	LEU	C-O	8.01	1.33	1.24
1	A	119	ASP	CA-CB	7.99	1.66	1.53
1	A	163	GLU	N-CA	-7.99	1.36	1.46
1	A	102	GLU	CA-CB	7.98	1.66	1.53
1	A	72	PRO	CG-CD	7.97	1.77	1.50
1	A	90	ASP	CA-C	-7.97	1.42	1.52
1	A	39	ALA	N-CA	-7.97	1.36	1.46
1	A	94	THR	CA-CB	7.97	1.66	1.53
1	A	168	ASP	C-N	7.93	1.44	1.33
1	A	157	GLU	CA-CB	7.90	1.63	1.52
1	A	129	LEU	C-N	7.90	1.42	1.33
1	A	35	CYS	N-CA	-7.86	1.36	1.45
1	A	99	SER	C-N	7.84	1.44	1.34
1	A	14	GLN	CA-C	7.83	1.63	1.52
1	A	117	PRO	C-O	7.83	1.34	1.24
1	A	20	LEU	CA-C	7.81	1.62	1.52
1	A	149	LEU	CA-CB	7.80	1.65	1.53
1	A	157	GLU	CG-CD	7.80	1.71	1.52
1	A	184	HIS	CB-CG	-7.77	1.39	1.50
1	A	160	LEU	C-O	7.75	1.33	1.23
1	A	108	ARG	N-CA	-7.74	1.36	1.46
1	A	14	GLN	C-N	-7.73	1.21	1.33
1	A	178	ILE	C-O	7.73	1.33	1.24
1	A	121	ARG	CZ-NH2	7.72	1.43	1.33
1	A	86	THR	N-CA	7.71	1.55	1.45
1	A	142	HIS	CG-CD2	7.71	1.44	1.35
1	A	185	ASN	N-CA	-7.67	1.35	1.46
1	A	179	GLN	CB-CG	7.67	1.75	1.52
1	A	162	CYS	C-O	7.66	1.33	1.23
1	A	33	LEU	CA-C	-7.63	1.42	1.52
1	A	54	GLY	N-CA	7.61	1.56	1.45
1	A	37	ALA	N-CA	7.59	1.56	1.46
1	A	144	GLU	CA-C	7.59	1.63	1.52
1	A	150	LEU	CA-CB	7.58	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	THR	C-O	-7.58	1.15	1.24
1	A	43	GLU	CG-CD	7.55	1.71	1.52
1	A	35	CYS	CA-C	-7.53	1.43	1.52
1	A	130	ILE	CB-CG1	7.51	1.68	1.53
1	A	22	ILE	C-O	7.51	1.32	1.24
1	A	198	ARG	CG-CD	7.50	1.75	1.52
1	A	129	LEU	CG-CD1	7.50	1.77	1.52
1	A	69	MET	CB-CG	-7.49	1.29	1.52
1	A	60	MET	C-N	-7.47	1.23	1.33
1	A	62	GLU	CD-OE1	7.46	1.39	1.25
1	A	6	ILE	C-O	7.45	1.32	1.24
1	A	138	GLU	C-N	7.45	1.43	1.33
1	A	148	ASP	N-CA	7.39	1.55	1.46
1	A	113	GLU	N-CA	7.39	1.55	1.46
1	A	153	ALA	N-CA	7.38	1.56	1.46
1	A	73	MET	CA-C	-7.35	1.43	1.52
1	A	16	GLY	N-CA	7.29	1.56	1.45
1	A	143	THR	C-N	7.28	1.44	1.33
1	A	140	ASN	CA-CB	7.28	1.63	1.52
1	A	16	GLY	C-N	7.27	1.43	1.33
1	A	89	ILE	CA-C	7.26	1.61	1.52
1	A	137	LEU	CB-CG	7.26	1.68	1.53
1	A	29	ASN	C-O	7.24	1.38	1.23
1	A	132	LYS	CD-CE	7.24	1.74	1.52
1	A	170	LYS	CB-CG	7.23	1.74	1.52
1	A	60	MET	CA-CB	-7.22	1.41	1.53
1	A	175	ASP	C-O	7.21	1.33	1.24
1	A	10	LEU	CA-C	7.20	1.63	1.52
1	A	73	MET	C-O	-7.20	1.15	1.24
1	A	18	LEU	C-O	7.14	1.32	1.23
1	A	167	HIS	C-O	7.14	1.33	1.24
1	A	63	SER	N-CA	-7.12	1.37	1.46
1	A	188	LEU	C-N	7.10	1.43	1.33
1	A	152	LEU	C-N	7.09	1.43	1.33
1	A	203	GLN	CG-CD	7.07	1.69	1.52
1	A	104	GLY	CA-C	-7.06	1.44	1.52
1	A	146	THR	C-O	-7.06	1.16	1.24
1	A	193	GLU	CD-OE1	7.04	1.38	1.25
1	A	194	LEU	N-CA	7.03	1.55	1.46
1	A	46	ASN	CG-ND2	7.03	1.48	1.33
1	A	33	LEU	CA-CB	-7.02	1.42	1.53
1	A	51	TYR	CB-CG	7.02	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLY	C-O	7.02	1.34	1.24
1	A	52	ALA	C-N	7.01	1.43	1.33
1	A	53	LYS	CA-CB	-7.01	1.45	1.54
1	A	171	MET	CB-CG	7.01	1.73	1.52
1	A	189	ILE	C-O	6.98	1.31	1.24
1	A	177	LEU	CA-C	-6.98	1.43	1.52
1	A	51	TYR	CE2-CZ	6.97	1.54	1.38
1	A	189	ILE	CA-C	6.95	1.61	1.52
1	A	166	ASN	N-CA	6.94	1.53	1.45
1	A	46	ASN	CA-CB	6.93	1.64	1.53
1	A	191	ILE	CB-CG2	6.91	1.75	1.52
1	A	183	LYS	C-O	-6.91	1.16	1.24
1	A	11	GLU	CD-OE2	-6.90	1.12	1.25
1	A	86	THR	CA-C	-6.89	1.44	1.53
1	A	106	THR	CB-OG1	6.89	1.54	1.43
1	A	8	GLU	CD-OE2	6.88	1.38	1.25
1	A	88	SER	C-N	6.88	1.42	1.33
1	A	189	ILE	CB-CG2	6.88	1.75	1.52
1	A	98	ILE	CB-CG1	6.87	1.67	1.53
1	A	125	HIS	N-CA	-6.87	1.37	1.46
1	A	109	MET	SD-CE	-6.82	1.62	1.79
1	A	144	GLU	N-CA	6.82	1.55	1.46
1	A	175	ASP	N-CA	-6.80	1.37	1.46
1	A	123	PRO	CA-C	6.80	1.66	1.52
1	A	3	TYR	C-O	-6.80	1.15	1.24
1	A	113	GLU	CG-CD	6.79	1.69	1.52
1	A	116	THR	C-N	6.79	1.43	1.33
1	A	19	VAL	C-N	6.78	1.43	1.33
1	A	86	THR	C-O	6.77	1.32	1.23
1	A	136	VAL	CA-CB	6.77	1.64	1.54
1	A	166	ASN	CA-CB	6.76	1.63	1.53
1	A	134	GLY	CA-C	6.74	1.60	1.51
1	A	42	THR	N-CA	-6.74	1.38	1.46
1	A	177	LEU	CG-CD2	6.72	1.74	1.52
1	A	29	ASN	CG-OD1	6.70	1.36	1.23
1	A	181	SER	N-CA	-6.68	1.38	1.46
1	A	195	GLN	C-O	6.68	1.31	1.24
1	A	44	ASN	C-N	6.68	1.42	1.33
1	A	23	ASP	CG-OD2	-6.66	1.12	1.25
1	A	61	SER	N-CA	6.65	1.54	1.45
1	A	103	ARG	CZ-NH1	6.60	1.42	1.32
1	A	51	TYR	N-CA	6.60	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	ASN	CA-C	-6.59	1.44	1.52
1	A	202	ASP	CB-CG	6.59	1.68	1.52
1	A	83	THR	CA-C	6.58	1.66	1.52
1	A	169	GLY	C-O	6.58	1.32	1.24
1	A	19	VAL	N-CA	6.58	1.53	1.46
1	A	190	THR	CA-C	-6.58	1.45	1.52
1	A	203	GLN	C-N	-6.57	1.24	1.33
1	A	93	GLU	CA-C	-6.56	1.43	1.52
1	A	167	HIS	C-N	6.55	1.43	1.33
1	A	109	MET	CA-CB	-6.54	1.42	1.53
1	A	175	ASP	CG-OD1	6.51	1.37	1.25
1	A	153	ALA	CA-C	-6.48	1.43	1.52
1	A	191	ILE	CA-C	6.48	1.61	1.52
1	A	171	MET	CA-C	6.47	1.61	1.52
1	A	42	THR	CA-C	-6.47	1.44	1.52
1	A	102	GLU	N-CA	-6.42	1.38	1.46
1	A	139	ARG	C-N	-6.41	1.25	1.33
1	A	130	ILE	C-O	-6.38	1.17	1.24
1	A	180	PHE	CD1-CE1	6.38	1.57	1.38
1	A	142	HIS	N-CA	6.38	1.54	1.46
1	A	142	HIS	C-N	6.37	1.42	1.33
1	A	100	ALA	CA-CB	6.34	1.63	1.53
1	A	84	ALA	C-N	-6.33	1.24	1.33
1	A	145	ALA	CA-C	-6.33	1.44	1.52
1	A	120	PHE	C-O	-6.32	1.16	1.24
1	A	6	ILE	CB-CG2	6.31	1.73	1.52
1	A	10	LEU	N-CA	-6.31	1.38	1.46
1	A	2	GLU	CA-CB	6.29	1.64	1.53
1	A	156	LYS	C-N	6.29	1.41	1.33
1	A	163	GLU	C-O	6.28	1.31	1.23
1	A	139	ARG	CA-C	6.27	1.60	1.52
1	A	68	LEU	CA-C	6.27	1.61	1.52
1	A	152	LEU	CB-CG	6.26	1.66	1.53
1	A	62	GLU	N-CA	6.25	1.54	1.46
1	A	116	THR	CB-CG2	6.24	1.73	1.52
1	A	16	GLY	C-O	6.24	1.32	1.24
1	A	197	TYR	CG-CD2	6.21	1.52	1.39
1	A	129	LEU	N-CA	6.21	1.53	1.46
1	A	147	VAL	CA-C	6.20	1.60	1.52
1	A	18	LEU	CB-CG	6.19	1.65	1.53
1	A	180	PHE	CG-CD1	-6.18	1.25	1.38
1	A	65	ALA	CA-C	6.16	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ARG	CZ-NH2	-6.15	1.25	1.33
1	A	19	VAL	CB-CG2	-6.11	1.32	1.52
1	A	183	LYS	CE-NZ	6.10	1.67	1.49
1	A	203	GLN	CA-CB	6.09	1.63	1.53
1	A	13	LEU	CA-C	-6.07	1.45	1.52
1	A	101	GLU	CA-CB	6.07	1.63	1.53
1	A	190	THR	C-N	6.07	1.41	1.33
1	A	201	TYR	CA-C	6.04	1.60	1.52
1	A	151	LYS	CA-CB	6.03	1.62	1.53
1	A	94	THR	C-N	-6.01	1.25	1.33
1	A	91	TYR	C-O	-6.01	1.16	1.23
1	A	56	ILE	CA-CB	5.98	1.61	1.54
1	A	163	GLU	CD-OE1	5.98	1.36	1.25
1	A	13	LEU	C-N	5.96	1.42	1.33
1	A	178	ILE	CA-CB	5.96	1.62	1.54
1	A	203	GLN	CD-NE2	-5.95	1.20	1.33
1	A	162	CYS	CA-CB	5.95	1.65	1.53
1	A	15	LYS	CB-CG	5.93	1.70	1.52
1	A	19	VAL	CB-CG1	5.92	1.72	1.52
1	A	60	MET	CA-C	5.91	1.59	1.52
1	A	32	ASP	C-O	-5.91	1.16	1.24
1	A	4	ARG	CD-NE	5.90	1.54	1.46
1	A	71	SER	C-N	-5.90	1.26	1.33
1	A	29	ASN	CA-CB	-5.89	1.41	1.53
1	A	198	ARG	CA-C	5.88	1.60	1.52
1	A	66	ASN	C-N	5.86	1.41	1.34
1	A	148	ASP	CA-C	5.86	1.60	1.52
1	A	155	LEU	CB-CG	5.84	1.65	1.53
1	A	35	CYS	CA-CB	5.84	1.64	1.53
1	A	42	THR	CB-OG1	5.84	1.53	1.43
1	A	141	GLY	C-O	5.81	1.32	1.23
1	A	102	GLU	CD-OE1	-5.79	1.14	1.25
1	A	189	ILE	CB-CG1	-5.78	1.41	1.53
1	A	7	GLN	CG-CD	5.78	1.66	1.52
1	A	177	LEU	CA-CB	5.76	1.62	1.53
1	A	126	MET	C-N	5.76	1.41	1.33
1	A	186	ILE	CG1-CD1	5.74	1.74	1.51
1	A	116	THR	CB-OG1	-5.73	1.34	1.43
1	A	92	LYS	CD-CE	5.71	1.69	1.52
1	A	195	GLN	CD-OE1	5.71	1.34	1.23
1	A	40	ALA	C-N	5.70	1.41	1.33
1	A	62	GLU	CD-OE2	5.70	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLN	C-N	5.70	1.42	1.33
1	A	136	VAL	C-O	-5.70	1.16	1.24
1	A	30	GLU	C-O	5.69	1.30	1.23
1	A	48	MET	C-N	5.68	1.41	1.33
1	A	165	MET	SD-CE	5.67	1.93	1.79
1	A	22	ILE	CB-CG2	-5.67	1.33	1.52
1	A	66	ASN	C-O	5.66	1.30	1.24
1	A	144	GLU	C-N	-5.66	1.26	1.33
1	A	7	GLN	C-O	5.65	1.30	1.24
1	A	121	ARG	CB-CG	-5.64	1.35	1.52
1	A	71	SER	CA-CB	-5.64	1.43	1.53
1	A	193	GLU	CB-CG	-5.63	1.35	1.52
1	A	163	GLU	C-N	5.62	1.42	1.33
1	A	179	GLN	CA-C	5.62	1.59	1.52
1	A	17	ARG	CD-NE	5.60	1.54	1.46
1	A	39	ALA	C-N	5.58	1.40	1.33
1	A	108	ARG	CD-NE	5.58	1.54	1.46
1	A	41	THR	CA-CB	5.58	1.62	1.53
1	A	168	ASP	CB-CG	5.56	1.66	1.52
1	A	18	LEU	N-CA	-5.54	1.38	1.45
1	A	190	THR	C-O	-5.54	1.17	1.23
1	A	140	ASN	C-N	5.54	1.46	1.33
1	A	189	ILE	N-CA	-5.54	1.39	1.46
1	A	99	SER	N-CA	5.52	1.53	1.45
1	A	160	LEU	C-N	5.51	1.41	1.33
1	A	168	ASP	C-O	-5.51	1.16	1.24
1	A	106	THR	C-N	5.51	1.40	1.33
1	A	12	ALA	CA-CB	-5.50	1.44	1.53
1	A	37	ALA	C-O	-5.49	1.17	1.24
1	A	132	LYS	CE-NZ	5.49	1.65	1.49
1	A	150	LEU	CG-CD1	5.48	1.70	1.52
1	A	117	PRO	N-CD	5.48	1.55	1.47
1	A	55	LEU	N-CA	-5.47	1.39	1.46
1	A	95	THR	CB-CG2	-5.45	1.34	1.52
1	A	187	PRO	CA-C	-5.43	1.46	1.52
1	A	203	GLN	CD-OE1	5.42	1.33	1.23
1	A	114	ASP	CG-OD2	5.40	1.35	1.25
1	A	17	ARG	NE-CZ	5.40	1.39	1.33
1	A	100	ALA	N-CA	5.40	1.53	1.46
1	A	138	GLU	CB-CG	5.38	1.68	1.52
1	A	181	SER	C-N	-5.38	1.26	1.33
1	A	156	LYS	C-O	-5.37	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ASP	CA-C	-5.37	1.43	1.52
1	A	185	ASN	C-O	5.36	1.30	1.23
1	A	164	ILE	CA-C	5.36	1.59	1.52
1	A	100	ALA	C-N	5.36	1.41	1.33
1	A	67	GLN	CA-CB	5.34	1.62	1.53
1	A	112	ALA	C-N	-5.33	1.26	1.33
1	A	141	GLY	CA-C	5.31	1.62	1.52
1	A	201	TYR	CA-CB	-5.31	1.46	1.53
1	A	6	ILE	C-N	5.30	1.40	1.33
1	A	154	GLY	N-CA	-5.29	1.36	1.45
1	A	151	LYS	C-N	-5.29	1.26	1.34
1	A	73	MET	CA-CB	5.27	1.61	1.53
1	A	188	LEU	N-CA	5.25	1.52	1.46
1	A	102	GLU	C-O	-5.25	1.17	1.24
1	A	155	LEU	N-CA	-5.24	1.39	1.45
1	A	197	TYR	CA-CB	5.22	1.61	1.53
1	A	32	ASP	CG-OD1	5.21	1.35	1.25
1	A	196	GLU	CA-CB	5.21	1.61	1.53
1	A	124	GLY	N-CA	-5.21	1.37	1.45
1	A	116	THR	N-CA	-5.21	1.37	1.45
1	A	180	PHE	CG-CD2	-5.21	1.27	1.38
1	A	32	ASP	C-N	5.21	1.40	1.33
1	A	53	LYS	CE-NZ	5.17	1.64	1.49
1	A	143	THR	CA-CB	5.16	1.61	1.53
1	A	25	LYS	N-CA	-5.15	1.39	1.46
1	A	141	GLY	C-N	-5.14	1.26	1.34
1	A	86	THR	CB-OG1	5.14	1.51	1.43
1	A	171	MET	SD-CE	5.13	1.92	1.79
1	A	175	ASP	C-N	5.12	1.40	1.33
1	A	201	TYR	CG-CD1	-5.08	1.28	1.39
1	A	163	GLU	CG-CD	5.08	1.64	1.52
1	A	125	HIS	CG-ND1	5.07	1.43	1.38
1	A	93	GLU	CG-CD	-5.05	1.39	1.52
1	A	139	ARG	C-O	5.05	1.29	1.23
1	A	122	ARG	CG-CD	-5.04	1.37	1.52
1	A	143	THR	CB-OG1	-5.03	1.35	1.43
1	A	44	ASN	N-CA	5.01	1.52	1.46
1	A	98	ILE	C-O	5.00	1.30	1.24

All (321) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CA-C-O	20.01	141.99	120.58
1	A	185	ASN	OD1-CG-ND2	-17.00	105.60	122.60
1	A	203	GLN	O-C-N	16.89	143.43	122.65
1	A	3	TYR	O-C-N	15.20	142.81	122.59
1	A	193	GLU	CA-C-O	14.44	135.85	120.55
1	A	4	ARG	CA-C-N	13.90	144.23	122.83
1	A	4	ARG	C-N-CA	13.90	144.23	122.83
1	A	5	LYS	CB-CA-C	-13.31	90.43	111.06
1	A	182	LYS	N-CA-C	-13.23	95.26	111.40
1	A	182	LYS	CA-C-O	-12.98	106.66	120.55
1	A	193	GLU	O-C-N	-12.78	108.58	122.12
1	A	2	GLU	N-CA-CB	12.67	131.90	110.49
1	A	25	LYS	N-CA-C	-12.56	84.04	110.80
1	A	5	LYS	N-CA-C	-12.51	98.44	112.57
1	A	114	ASP	CB-CA-C	-12.38	93.58	110.79
1	A	113	GLU	CA-C-N	-12.27	103.23	121.76
1	A	113	GLU	C-N-CA	-12.27	103.23	121.76
1	A	203	GLN	CA-C-O	-12.17	107.95	121.94
1	A	96	THR	N-CA-CB	12.04	128.39	110.33
1	A	115	ILE	N-CA-C	-11.93	91.38	108.80
1	A	24	ASP	CA-C-O	11.87	137.48	120.51
1	A	198	ARG	NE-CZ-NH2	-11.73	108.64	119.20
1	A	113	GLU	CA-C-O	-11.16	108.72	120.55
1	A	184	HIS	ND1-CE1-NE2	-11.06	97.34	108.40
1	A	24	ASP	N-CA-C	11.03	134.29	110.80
1	A	3	TYR	CA-C-O	-10.99	104.80	120.51
1	A	114	ASP	N-CA-CB	-10.90	94.04	110.71
1	A	176	ASP	CA-C-O	10.51	132.15	120.90
1	A	175	ASP	CA-CB-CG	-10.48	102.12	112.60
1	A	5	LYS	CA-CB-CG	10.47	135.04	114.10
1	A	71	SER	N-CA-C	-10.23	96.17	110.29
1	A	150	LEU	O-C-N	-10.03	110.72	122.15
1	A	7	GLN	CA-CB-CG	-9.99	94.13	114.10
1	A	112	ALA	CA-C-N	9.73	133.32	120.28
1	A	112	ALA	C-N-CA	9.73	133.32	120.28
1	A	185	ASN	CA-C-O	9.72	133.03	121.65
1	A	203	GLN	CB-CG-CD	-9.63	96.22	112.60
1	A	29	ASN	CA-C-O	-9.61	104.46	120.80
1	A	4	ARG	NE-CZ-NH1	-9.59	111.91	121.50
1	A	186	ILE	N-CA-CB	-9.36	98.10	111.21
1	A	193	GLU	N-CA-C	9.29	121.40	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ALA	O-C-N	9.26	133.94	123.01
1	A	113	GLU	CB-CA-C	-9.25	95.44	110.79
1	A	74	VAL	CA-C-O	9.06	129.81	120.39
1	A	184	HIS	N-CA-C	-9.06	100.17	112.94
1	A	115	ILE	CA-CB-CG1	-8.96	95.16	110.40
1	A	48	MET	O-C-N	-8.92	112.88	122.07
1	A	178	ILE	CA-C-O	-8.90	111.41	120.85
1	A	112	ALA	N-CA-C	8.89	123.12	110.23
1	A	3	TYR	N-CA-C	-8.87	91.92	110.80
1	A	101	GLU	CB-CG-CD	-8.86	97.54	112.60
1	A	172	MET	N-CA-C	-8.84	95.71	109.76
1	A	19	VAL	O-C-N	-8.79	113.60	123.00
1	A	200	VAL	CG1-CB-CG2	-8.78	91.48	110.80
1	A	196	GLU	CA-C-O	8.70	129.64	120.42
1	A	9	ALA	O-C-N	-8.69	113.00	122.03
1	A	167	HIS	O-C-N	-8.67	112.08	122.22
1	A	180	PHE	N-CA-CB	-8.65	97.36	110.16
1	A	7	GLN	CA-C-O	-8.63	111.40	120.55
1	A	63	SER	O-C-N	-8.61	113.00	122.12
1	A	167	HIS	CA-CB-CG	-8.59	105.21	113.80
1	A	11	GLU	CA-C-O	-8.56	110.73	120.24
1	A	161[A]	CYS	O-C-N	-8.56	113.34	123.27
1	A	161[B]	CYS	O-C-N	-8.56	113.34	123.27
1	A	184	HIS	O-C-N	-8.53	111.87	122.19
1	A	200	VAL	O-C-N	-8.52	113.88	122.23
1	A	93	GLU	O-C-N	-8.47	110.06	122.43
1	A	25	LYS	CA-C-N	-8.36	106.66	121.70
1	A	25	LYS	C-N-CA	-8.36	106.66	121.70
1	A	175	ASP	N-CA-C	8.31	123.54	113.23
1	A	6	ILE	N-CA-C	8.14	118.92	110.62
1	A	72	PRO	CB-CA-C	-8.11	101.34	111.64
1	A	23	ASP	N-CA-C	-8.09	95.39	108.41
1	A	179	GLN	CA-C-O	8.05	129.27	120.82
1	A	105	LEU	O-C-N	8.01	132.13	122.27
1	A	66	ASN	CA-CB-CG	-7.93	104.67	112.60
1	A	195	GLN	O-C-N	-7.91	113.73	122.12
1	A	29	ASN	N-CA-CB	7.86	123.86	110.50
1	A	62	GLU	CA-CB-CG	-7.84	98.42	114.10
1	A	26	ASP	CA-C-O	-7.83	107.49	120.80
1	A	43	GLU	CA-C-O	-7.82	110.56	119.79
1	A	7	GLN	O-C-N	7.80	130.38	122.12
1	A	174	THR	CA-C-N	-7.77	107.99	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	THR	C-N-CA	-7.77	107.99	121.66
1	A	45	VAL	O-C-N	-7.65	113.95	121.83
1	A	189	ILE	CB-CG1-CD1	-7.64	97.76	113.80
1	A	182	LYS	CB-CA-C	-7.63	97.97	110.79
1	A	200	VAL	CA-C-O	7.61	126.50	119.20
1	A	8	GLU	CB-CA-C	-7.59	96.81	110.70
1	A	172	MET	CA-C-O	7.57	129.32	120.69
1	A	115	ILE	CB-CA-C	-7.56	99.63	110.82
1	A	29	ASN	CB-CA-C	-7.46	95.92	110.10
1	A	193	GLU	N-CA-CB	-7.46	99.16	110.12
1	A	112	ALA	CA-C-O	-7.45	113.00	121.19
1	A	151	LYS	CA-CB-CG	-7.43	99.24	114.10
1	A	114	ASP	CA-CB-CG	-7.43	105.17	112.60
1	A	9	ALA	N-CA-C	-7.42	102.88	110.97
1	A	75	GLU	N-CA-CB	7.39	123.07	110.50
1	A	12	ALA	N-CA-C	-7.39	103.23	111.28
1	A	167	HIS	CG-CD2-NE2	-7.36	99.84	107.20
1	A	98	ILE	CA-CB-CG2	7.33	122.96	110.50
1	A	204	LEU	CA-C-O	-7.33	108.35	120.80
1	A	115	ILE	O-C-N	7.32	131.06	123.00
1	A	113	GLU	N-CA-CB	7.30	120.85	110.12
1	A	8	GLU	CB-CG-CD	-7.28	100.22	112.60
1	A	182	LYS	O-C-N	7.28	130.98	122.17
1	A	83	THR	OG1-CB-CG2	-7.25	94.81	109.30
1	A	132	LYS	CD-CE-NZ	-7.23	88.76	111.90
1	A	99	SER	O-C-N	-7.21	113.85	122.65
1	A	45	VAL	N-CA-C	7.21	118.00	110.72
1	A	96	THR	N-CA-C	-7.18	103.49	112.90
1	A	115	ILE	CG1-CB-CG2	7.16	132.19	110.70
1	A	97	GLY	CA-C-O	-7.14	111.47	119.04
1	A	189	ILE	CG1-CB-CG2	-7.12	89.33	110.70
1	A	4	ARG	N-CA-C	-7.11	91.11	111.00
1	A	193	GLU	CA-CB-CG	-7.10	99.89	114.10
1	A	143	THR	CA-C-O	7.10	128.27	120.82
1	A	132	LYS	CG-CD-CE	-7.09	94.99	111.30
1	A	50	THR	CA-CB-OG1	-7.04	99.04	109.60
1	A	184	HIS	CG-ND1-CE1	7.03	121.25	109.30
1	A	7	GLN	OE1-CD-NE2	6.99	129.59	122.60
1	A	146	THR	O-C-N	-6.98	114.88	122.07
1	A	183	LYS	CA-C-O	-6.96	113.11	120.63
1	A	16	GLY	N-CA-C	-6.96	105.22	115.72
1	A	159	GLY	N-CA-C	6.93	121.44	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	GLU	OE1-CD-OE2	6.91	139.48	122.90
1	A	21	VAL	CA-C-O	6.90	127.92	120.53
1	A	104	GLY	O-C-N	-6.89	115.50	122.19
1	A	168	ASP	CA-C-N	-6.89	111.47	121.26
1	A	168	ASP	C-N-CA	-6.89	111.47	121.26
1	A	11	GLU	CA-CB-CG	-6.88	100.33	114.10
1	A	41	THR	O-C-N	-6.86	115.03	122.85
1	A	185	ASN	CB-CG-ND2	6.83	126.64	116.40
1	A	159	GLY	O-C-N	-6.81	117.74	123.73
1	A	136	VAL	O-C-N	6.79	130.94	122.05
1	A	193	GLU	CA-C-N	-6.78	109.28	121.14
1	A	193	GLU	C-N-CA	-6.78	109.28	121.14
1	A	46	ASN	CA-CB-CG	-6.77	105.83	112.60
1	A	196	GLU	O-C-N	-6.75	114.45	122.15
1	A	17	ARG	CG-CD-NE	-6.74	97.16	112.00
1	A	67	GLN	CA-CB-CG	-6.74	100.62	114.10
1	A	61	SER	CA-C-N	-6.73	110.08	120.31
1	A	61	SER	C-N-CA	-6.73	110.08	120.31
1	A	98	ILE	CG1-CB-CG2	-6.71	90.56	110.70
1	A	131	ALA	N-CA-C	-6.69	99.63	110.20
1	A	195	GLN	N-CA-CB	-6.69	100.29	110.12
1	A	114	ASP	N-CA-C	-6.68	95.98	107.61
1	A	149	LEU	O-C-N	-6.68	115.04	122.12
1	A	63	SER	N-CA-CB	-6.67	100.31	110.12
1	A	138	GLU	CB-CA-C	6.66	121.37	110.24
1	A	201	TYR	CA-C-O	-6.59	111.40	119.18
1	A	173	ARG	N-CA-CB	-6.58	99.91	110.51
1	A	193	GLU	CB-CG-CD	-6.57	101.43	112.60
1	A	72	PRO	CA-C-N	-6.56	111.49	120.28
1	A	72	PRO	C-N-CA	-6.56	111.49	120.28
1	A	117	PRO	CA-N-CD	6.51	121.12	112.00
1	A	117	PRO	N-CD-CG	-6.49	93.46	103.20
1	A	122	ARG	CD-NE-CZ	-6.49	115.32	124.40
1	A	194	LEU	N-CA-CB	-6.48	99.83	110.40
1	A	121	ARG	CD-NE-CZ	-6.42	115.41	124.40
1	A	62	GLU	CB-CG-CD	-6.39	101.73	112.60
1	A	85	PHE	CB-CA-C	-6.38	99.44	109.84
1	A	199	LYS	O-C-N	-6.38	115.36	122.12
1	A	119	ASP	CA-CB-CG	-6.35	106.25	112.60
1	A	97	GLY	O-C-N	6.34	130.46	122.28
1	A	7	GLN	N-CA-CB	6.34	119.44	110.12
1	A	185	ASN	O-C-N	-6.34	114.97	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	PHE	CA-CB-CG	-6.31	107.49	113.80
1	A	126	MET	N-CA-C	-6.31	99.53	109.50
1	A	175	ASP	CB-CA-C	-6.29	96.78	109.55
1	A	49	ALA	CA-C-N	-6.27	110.49	122.53
1	A	49	ALA	C-N-CA	-6.27	110.49	122.53
1	A	24	ASP	CB-CA-C	-6.25	97.98	110.42
1	A	121	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	A	38	GLN	CA-C-N	6.22	132.94	122.79
1	A	38	GLN	C-N-CA	6.22	132.94	122.79
1	A	4	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	A	163	GLU	N-CA-CB	6.22	119.12	109.97
1	A	37	ALA	N-CA-C	-6.20	104.42	112.23
1	A	130	ILE	O-C-N	6.19	129.77	122.83
1	A	47	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	119	ASP	CB-CA-C	-6.18	98.92	110.36
1	A	115	ILE	CB-CG1-CD1	-6.17	100.84	113.80
1	A	69	MET	N-CA-CB	-6.16	102.58	111.70
1	A	114	ASP	CA-C-N	-6.15	114.06	122.92
1	A	114	ASP	C-N-CA	-6.15	114.06	122.92
1	A	2	GLU	CA-C-N	6.12	133.23	121.54
1	A	2	GLU	C-N-CA	6.12	133.23	121.54
1	A	112	ALA	O-C-N	-6.11	115.36	122.87
1	A	197	TYR	CA-CB-CG	-6.10	102.92	113.90
1	A	176	ASP	CB-CA-C	6.09	120.56	110.81
1	A	22	ILE	CB-CA-C	-6.09	101.76	110.83
1	A	148	ASP	N-CA-CB	-6.08	101.16	110.16
1	A	146	THR	CA-C-O	6.08	127.20	120.82
1	A	130	ILE	CB-CA-C	-6.07	103.98	111.08
1	A	204	LEU	N-CA-C	6.07	127.98	111.00
1	A	180	PHE	N-CA-C	6.06	117.97	111.36
1	A	151	LYS	N-CA-CB	-6.05	101.23	110.12
1	A	199	LYS	CA-C-N	-6.05	112.97	121.55
1	A	199	LYS	C-N-CA	-6.05	112.97	121.55
1	A	203	GLN	CG-CD-NE2	-6.04	107.34	116.40
1	A	100	ALA	O-C-N	-6.04	115.15	122.22
1	A	156	LYS	O-C-N	-6.03	115.62	122.97
1	A	157	GLU	CA-C-O	6.02	130.17	122.64
1	A	107	ALA	N-CA-C	6.01	118.33	111.11
1	A	174	THR	N-CA-C	6.00	118.60	111.33
1	A	20	LEU	N-CA-C	-5.99	98.76	108.52
1	A	187	PRO	CA-C-N	5.97	131.54	122.65
1	A	187	PRO	C-N-CA	5.97	131.54	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLU	CA-C-N	-5.93	110.59	120.68
1	A	101	GLU	C-N-CA	-5.93	110.59	120.68
1	A	105	LEU	CA-C-O	-5.93	113.15	119.97
1	A	114	ASP	OD1-CG-OD2	-5.92	108.68	122.90
1	A	7	GLN	CB-CA-C	-5.92	100.96	110.79
1	A	35	CYS	O-C-N	-5.92	116.29	123.10
1	A	154	GLY	CA-C-O	5.92	125.59	119.02
1	A	5	LYS	CB-CG-CD	5.90	124.87	111.30
1	A	48	MET	CA-C-O	5.90	127.02	120.82
1	A	176	ASP	O-C-N	-5.89	115.96	122.09
1	A	178	ILE	N-CA-C	-5.85	104.81	110.72
1	A	92	LYS	CA-CB-CG	-5.84	102.42	114.10
1	A	55	LEU	O-C-N	-5.83	116.68	123.27
1	A	97	GLY	N-CA-C	-5.83	107.71	115.40
1	A	159	GLY	CA-C-O	-5.82	114.97	121.31
1	A	202	ASP	CA-CB-CG	-5.80	106.80	112.60
1	A	168	ASP	CB-CA-C	-5.79	100.06	110.37
1	A	43	GLU	CB-CA-C	-5.78	98.58	110.38
1	A	42	THR	CA-CB-OG1	-5.78	100.93	109.60
1	A	72	PRO	N-CD-CG	-5.74	94.59	103.20
1	A	121	ARG	N-CA-CB	5.74	118.48	110.04
1	A	36	SER	N-CA-CB	5.74	118.56	110.36
1	A	174	THR	CA-CB-CG2	5.70	120.19	110.50
1	A	19	VAL	CA-CB-CG2	5.70	120.09	110.40
1	A	59	PRO	N-CA-CB	-5.68	98.26	103.31
1	A	201	TYR	O-C-N	5.64	128.86	122.20
1	A	62	GLU	N-CA-CB	-5.64	101.53	110.28
1	A	193	GLU	OE1-CD-OE2	5.64	136.43	122.90
1	A	100	ALA	CA-C-O	5.63	126.46	120.10
1	A	89	ILE	CA-C-O	-5.60	115.42	121.19
1	A	111	VAL	CA-C-O	-5.60	114.10	120.26
1	A	185	ASN	N-CA-C	5.60	119.36	111.52
1	A	103	ARG	O-C-N	-5.59	115.68	122.22
1	A	189	ILE	CB-CA-C	5.58	120.37	110.71
1	A	48	MET	N-CA-CB	-5.58	101.92	110.01
1	A	180	PHE	O-C-N	-5.58	115.79	122.15
1	A	75	GLU	CA-C-O	-5.58	111.31	120.80
1	A	63	SER	CA-C-O	5.58	126.46	120.55
1	A	48	MET	N-CA-C	5.53	116.98	111.07
1	A	17	ARG	NE-CZ-NH2	-5.53	114.23	119.20
1	A	11	GLU	N-CA-C	-5.52	104.90	111.69
1	A	50	THR	N-CA-CB	-5.52	101.98	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	THR	CA-CB-OG1	-5.51	101.33	109.60
1	A	6	ILE	CA-C-N	5.50	127.65	120.28
1	A	6	ILE	C-N-CA	5.50	127.65	120.28
1	A	60	MET	O-C-N	5.49	129.51	123.25
1	A	61	SER	N-CA-C	-5.49	103.14	110.55
1	A	138	GLU	CA-CB-CG	-5.48	103.14	114.10
1	A	169	GLY	CA-C-O	-5.48	113.00	119.46
1	A	17	ARG	CA-CB-CG	-5.46	103.18	114.10
1	A	20	LEU	CA-C-N	-5.45	116.03	123.12
1	A	20	LEU	C-N-CA	-5.45	116.03	123.12
1	A	151	LYS	N-CA-C	5.45	117.22	111.28
1	A	139	ARG	CA-C-N	-5.43	112.96	122.62
1	A	139	ARG	C-N-CA	-5.43	112.96	122.62
1	A	46	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	84	ALA	CA-C-O	-5.42	115.64	122.63
1	A	167	HIS	CB-CA-C	5.42	120.65	110.63
1	A	153	ALA	O-C-N	-5.42	114.99	122.46
1	A	184	HIS	N-CA-CB	-5.42	102.04	110.98
1	A	196	GLU	N-CA-CB	-5.39	102.19	110.16
1	A	20	LEU	CB-CG-CD2	5.36	126.78	110.70
1	A	4	ARG	CG-CD-NE	-5.33	100.26	112.00
1	A	129	LEU	N-CA-C	-5.32	99.43	108.26
1	A	201	TYR	CA-C-N	-5.30	111.42	121.54
1	A	201	TYR	C-N-CA	-5.30	111.42	121.54
1	A	150	LEU	CA-C-O	5.29	126.03	120.42
1	A	13	LEU	N-CA-C	-5.28	105.61	111.36
1	A	201	TYR	CD1-CG-CD2	5.28	126.02	118.10
1	A	156	LYS	CA-C-O	5.27	126.95	121.15
1	A	198	ARG	NH1-CZ-NH2	5.27	126.16	119.30
1	A	16	GLY	O-C-N	-5.27	116.65	122.55
1	A	54	GLY	O-C-N	-5.27	115.86	122.70
1	A	5	LYS	N-CA-CB	-5.26	102.60	110.91
1	A	166	ASN	CB-CG-OD1	5.25	131.31	120.80
1	A	8	GLU	O-C-N	5.24	129.04	122.23
1	A	53	LYS	CB-CG-CD	-5.24	99.25	111.30
1	A	73	MET	O-C-N	-5.22	116.58	122.12
1	A	122	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	A	67	GLN	CG-CD-OE1	-5.20	110.40	120.80
1	A	47	PHE	CA-C-N	-5.20	113.68	120.44
1	A	47	PHE	C-N-CA	-5.20	113.68	120.44
1	A	104	GLY	CA-C-O	5.19	126.16	120.66
1	A	9	ALA	CB-CA-C	5.19	118.95	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	LYS	O-C-N	-5.18	114.72	122.39
1	A	92	LYS	O-C-N	-5.18	115.50	122.43
1	A	148	ASP	N-CA-C	-5.17	105.73	111.36
1	A	130	ILE	N-CA-C	5.17	116.19	108.54
1	A	136	VAL	N-CA-C	-5.16	104.81	112.04
1	A	50	THR	CA-C-N	-5.16	113.00	121.92
1	A	50	THR	C-N-CA	-5.16	113.00	121.92
1	A	171	MET	CA-C-N	5.14	128.85	121.50
1	A	171	MET	C-N-CA	5.14	128.85	121.50
1	A	30	GLU	N-CA-C	5.12	117.76	108.69
1	A	170	LYS	N-CA-C	-5.12	101.97	109.81
1	A	187	PRO	N-CA-CB	5.12	107.88	103.27
1	A	187	PRO	N-CA-C	5.10	118.89	111.03
1	A	137	LEU	CA-C-N	5.09	132.17	122.60
1	A	137	LEU	C-N-CA	5.09	132.17	122.60
1	A	98	ILE	N-CA-CB	5.08	120.56	110.95
1	A	43	GLU	N-CA-C	-5.08	105.83	112.23
1	A	188	LEU	O-C-N	-5.06	117.27	123.19
1	A	72	PRO	N-CA-C	-5.04	103.04	111.26
1	A	92	LYS	CG-CD-CE	-5.04	99.70	111.30
1	A	130	ILE	CA-CB-CG1	-5.03	101.84	110.40
1	A	17	ARG	CA-C-O	-5.03	115.52	121.60
1	A	84	ALA	O-C-N	5.03	128.99	122.71
1	A	136	VAL	CA-C-O	-5.02	113.62	119.85
1	A	201	TYR	N-CA-C	-5.01	106.10	113.61
1	A	195	GLN	CA-C-O	5.00	125.86	120.55
1	A	66	ASN	CB-CA-C	-5.00	102.35	110.85
1	A	171	MET	N-CA-C	-5.00	102.88	110.28

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ALA	Mainchain
1	A	161[A]	CYS	Mainchain
1	A	175	ASP	Mainchain
1	A	195	GLN	Mainchain
1	A	2	GLU	Mainchain
1	A	203	GLN	Sidechain
1	A	4	ARG	Sidechain
1	A	5	LYS	Peptide,Mainchain
1	A	67	GLN	Sidechain

5.2 Too-close contacts

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	1470	0	1437	294	0
2	A	15	0	0	0	0
3	A	30	0	36	31	0
4	A	121	0	0	15	2
All	All	1636	0	1473	316	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 106.

All (316) 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:95:THR:CA	1:A:95:THR:CB	1.75	1.64
1:A:189:ILE:CG2	1:A:189:ILE:CB	1.75	1.63
1:A:49:ALA:CA	1:A:49:ALA:CB	1.75	1.63
1:A:194:LEU:CB	1:A:194:LEU:CA	1.77	1.63
1:A:45:VAL:CB	1:A:45:VAL:CA	1.74	1.62
1:A:191:ILE:CG2	1:A:191:ILE:CB	1.75	1.61
1:A:8:GLU:CG	1:A:8:GLU:CB	1.77	1.60
3:A:304:GOL:C2	3:A:304:GOL:C1	1.74	1.60
1:A:198:ARG:CD	1:A:198:ARG:CG	1.74	1.60
1:A:92:LYS:CG	1:A:92:LYS:CD	1.79	1.59
1:A:202:ASP:CB	1:A:202:ASP:CA	1.81	1.59
1:A:131:ALA:C	1:A:131:ALA:CA	1.75	1.59
1:A:129:LEU:CD1	1:A:129:LEU:CG	1.77	1.58
1:A:136:VAL:CA	1:A:136:VAL:C	1.77	1.58
1:A:161[B]:CYS:CB	1:A:161[B]:CYS:CA	1.81	1.58
1:A:69:MET:CB	1:A:69:MET:CA	1.75	1.58
1:A:182:LYS:CB	1:A:182:LYS:CG	1.79	1.58
1:A:177:LEU:CD2	1:A:177:LEU:CG	1.74	1.57
1:A:53:LYS:CD	1:A:53:LYS:CG	1.82	1.57
1:A:72:PRO:CD	1:A:72:PRO:CG	1.77	1.57
1:A:179:GLN:CG	1:A:179:GLN:CB	1.75	1.57
1:A:165:MET:C	1:A:165:MET:CA	1.76	1.57
1:A:151:LYS:CD	1:A:151:LYS:CG	1.78	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:SER:C	1:A:36:SER:CA	1.78	1.56
3:A:308:GOL:C2	3:A:308:GOL:C3	1.80	1.56
1:A:71:SER:C	1:A:71:SER:CA	1.78	1.55
1:A:72:PRO:C	1:A:72:PRO:CA	1.75	1.55
1:A:115:ILE:CB	1:A:115:ILE:CA	1.79	1.55
1:A:149:LEU:CG	1:A:149:LEU:CD2	1.83	1.55
1:A:43:GLU:CB	1:A:43:GLU:CA	1.79	1.55
1:A:11:GLU:CD	1:A:11:GLU:CG	1.77	1.54
1:A:72:PRO:CA	1:A:72:PRO:N	1.70	1.54
1:A:70:LEU:C	1:A:70:LEU:CA	1.74	1.53
1:A:8:GLU:C	1:A:8:GLU:CA	1.81	1.53
1:A:62:GLU:CA	1:A:62:GLU:CB	1.84	1.52
1:A:74:VAL:CB	1:A:74:VAL:CG1	1.88	1.52
1:A:83:THR:N	1:A:83:THR:CA	1.71	1.52
1:A:183:LYS:NZ	1:A:183:LYS:CE	1.67	1.51
1:A:186:ILE:CB	1:A:186:ILE:CA	1.84	1.51
1:A:9:ALA:N	1:A:9:ALA:CA	1.69	1.51
1:A:178:ILE:CA	1:A:178:ILE:N	1.68	1.50
1:A:4:ARG:CZ	1:A:4:ARG:NE	1.70	1.50
1:A:161[A]:CYS:CB	1:A:161[A]:CYS:CA	1.85	1.50
1:A:30:GLU:CD	1:A:30:GLU:CG	1.85	1.50
1:A:149:LEU:CA	1:A:149:LEU:N	1.72	1.49
1:A:180:PHE:CB	1:A:180:PHE:CA	1.87	1.49
1:A:1:MET:N	1:A:1:MET:CA	1.73	1.49
1:A:2:GLU:CA	1:A:2:GLU:N	1.73	1.49
1:A:4:ARG:C	1:A:4:ARG:CA	1.86	1.49
1:A:67:GLN:CG	1:A:67:GLN:CD	1.84	1.49
1:A:114:ASP:CB	1:A:114:ASP:CA	1.90	1.49
1:A:75:GLU:C	1:A:75:GLU:CA	1.80	1.48
1:A:98:ILE:CD1	1:A:98:ILE:CG1	1.87	1.48
1:A:101:GLU:CD	1:A:101:GLU:CG	1.82	1.48
1:A:24:ASP:C	1:A:24:ASP:CA	1.87	1.47
1:A:182:LYS:N	1:A:182:LYS:CA	1.77	1.46
1:A:203:GLN:C	1:A:203:GLN:CA	1.88	1.46
1:A:29:ASN:C	1:A:29:ASN:CA	1.85	1.46
1:A:115:ILE:CA	1:A:115:ILE:C	1.90	1.45
1:A:171:MET:CG	1:A:171:MET:SD	2.02	1.45
1:A:115:ILE:CA	1:A:115:ILE:N	1.76	1.45
1:A:193:GLU:CD	1:A:193:GLU:CG	1.89	1.44
3:A:304:GOL:O3	3:A:304:GOL:C3	1.66	1.43
1:A:3:TYR:C	1:A:3:TYR:CA	1.92	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:307:GOL:C1	3:A:307:GOL:O1	1.67	1.42
1:A:175:ASP:CB	1:A:175:ASP:CA	1.96	1.42
1:A:25:LYS:CA	1:A:25:LYS:C	1.92	1.41
3:A:304:GOL:C1	3:A:304:GOL:O1	1.70	1.39
3:A:307:GOL:C2	3:A:307:GOL:O2	1.70	1.39
1:A:204:LEU:CD2	1:A:204:LEU:CG	2.00	1.39
3:A:306:GOL:O3	3:A:306:GOL:C3	1.70	1.38
3:A:305:GOL:O1	3:A:305:GOL:C1	1.72	1.37
1:A:72:PRO:CD	1:A:72:PRO:N	1.87	1.37
1:A:72:PRO:CG	1:A:72:PRO:CB	2.05	1.34
1:A:71:SER:OG	1:A:71:SER:CB	1.76	1.31
1:A:5:LYS:C	1:A:5:LYS:CA	2.09	1.26
1:A:24:ASP:C	1:A:25:LYS:N	1.94	1.26
1:A:5:LYS:HA	4:A:514:HOH:O	1.08	1.19
3:A:306:GOL:C3	3:A:306:GOL:C2	2.22	1.18
1:A:189:ILE:CG2	1:A:189:ILE:CG1	2.24	1.16
1:A:23:ASP:C	1:A:24:ASP:N	2.09	1.10
1:A:187:PRO:CD	3:A:305:GOL:H32	1.81	1.10
1:A:53:LYS:CG	1:A:53:LYS:CE	2.35	1.05
1:A:5:LYS:CA	4:A:514:HOH:O	1.70	1.03
1:A:187:PRO:HD2	3:A:305:GOL:H32	1.41	1.02
3:A:304:GOL:C1	3:A:304:GOL:H2	1.89	0.99
1:A:71:SER:CA	1:A:72:PRO:CD	2.41	0.99
1:A:4:ARG:C	1:A:4:ARG:O	2.05	0.98
1:A:8:GLU:CB	1:A:8:GLU:CD	2.38	0.97
1:A:115:ILE:CA	1:A:115:ILE:CG1	2.42	0.97
1:A:25:LYS:C	1:A:25:LYS:N	2.25	0.95
1:A:198:ARG:CG	1:A:198:ARG:NE	2.27	0.95
1:A:114:ASP:C	1:A:115:ILE:CA	2.39	0.94
1:A:175:ASP:CB	1:A:175:ASP:C	2.40	0.94
1:A:69:MET:CA	1:A:69:MET:CG	2.46	0.92
1:A:8:GLU:C	1:A:9:ALA:CA	2.42	0.92
1:A:5:LYS:C	1:A:5:LYS:CB	2.44	0.91
1:A:177:LEU:CD2	1:A:177:LEU:CD1	2.49	0.91
1:A:71:SER:HA	1:A:72:PRO:CD	2.01	0.91
1:A:161[B]:CYS:CB	1:A:161[B]:CYS:C	2.44	0.90
1:A:72:PRO:C	1:A:72:PRO:CB	2.43	0.90
1:A:29:ASN:C	1:A:29:ASN:CB	2.44	0.90
1:A:3:TYR:CA	1:A:4:ARG:CA	2.51	0.89
1:A:45:VAL:CB	1:A:45:VAL:C	2.46	0.88
1:A:129:LEU:CD1	1:A:129:LEU:CD2	2.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LYS:NZ	4:A:508:HOH:O	1.96	0.86
1:A:4:ARG:C	1:A:4:ARG:N	2.33	0.86
1:A:62:GLU:CA	1:A:62:GLU:CG	2.54	0.86
1:A:95:THR:CA	1:A:95:THR:CG2	2.53	0.86
1:A:189:ILE:CG2	1:A:189:ILE:CA	2.55	0.84
1:A:71:SER:C	1:A:72:PRO:CD	2.51	0.83
1:A:3:TYR:CA	1:A:4:ARG:N	2.37	0.82
1:A:8:GLU:CB	1:A:8:GLU:C	2.52	0.82
1:A:69:MET:CB	1:A:69:MET:N	2.41	0.82
1:A:24:ASP:C	1:A:24:ASP:CB	2.52	0.81
1:A:129:LEU:CD1	1:A:129:LEU:CB	2.57	0.81
1:A:114:ASP:CB	1:A:114:ASP:C	2.53	0.81
1:A:193:GLU:CD	1:A:193:GLU:CB	2.53	0.81
1:A:45:VAL:CA	1:A:45:VAL:CG1	2.60	0.80
1:A:187:PRO:HD3	3:A:305:GOL:H32	1.63	0.79
1:A:161[A]:CYS:CB	1:A:161[A]:CYS:C	2.53	0.78
1:A:114:ASP:CB	1:A:114:ASP:N	2.45	0.78
1:A:72:PRO:CB	4:A:519:HOH:O	2.32	0.78
1:A:3:TYR:CA	1:A:4:ARG:HB2	2.13	0.77
1:A:45:VAL:CA	1:A:45:VAL:CG2	2.62	0.77
1:A:53:LYS:CD	1:A:53:LYS:CB	2.62	0.77
1:A:9:ALA:N	1:A:9:ALA:C	2.43	0.77
1:A:101:GLU:CD	1:A:101:GLU:CB	2.58	0.76
1:A:198:ARG:CD	1:A:198:ARG:CB	2.63	0.75
1:A:72:PRO:HB3	4:A:519:HOH:O	1.85	0.75
1:A:36:SER:C	1:A:36:SER:CB	2.59	0.75
1:A:191:ILE:CG2	1:A:191:ILE:CA	2.65	0.75
1:A:131:ALA:CA	1:A:132:LYS:N	2.49	0.74
1:A:43:GLU:CA	1:A:43:GLU:CG	2.65	0.74
1:A:165:MET:C	1:A:165:MET:N	2.42	0.74
1:A:62:GLU:CB	1:A:62:GLU:C	2.60	0.74
1:A:161[B]:CYS:CB	1:A:161[B]:CYS:N	2.51	0.74
1:A:71:SER:CA	1:A:72:PRO:HD2	2.17	0.74
1:A:177:LEU:C	1:A:178:ILE:CA	2.61	0.74
1:A:148:ASP:C	1:A:149:LEU:CA	2.59	0.73
1:A:12:ALA:HB1	3:A:305:GOL:H31	1.70	0.73
1:A:72:PRO:N	1:A:72:PRO:CB	2.49	0.73
1:A:92:LYS:CG	1:A:92:LYS:CE	2.67	0.73
1:A:165:MET:C	1:A:165:MET:CB	2.60	0.73
1:A:72:PRO:CA	1:A:73:MET:N	2.50	0.73
1:A:8:GLU:CG	1:A:8:GLU:CA	2.66	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:C	1:A:70:LEU:N	2.42	0.73
1:A:72:PRO:CA	4:A:519:HOH:O	2.37	0.73
1:A:183:LYS:NZ	1:A:183:LYS:CD	2.52	0.72
1:A:43:GLU:CB	1:A:43:GLU:C	2.61	0.72
1:A:70:LEU:C	1:A:70:LEU:CB	2.62	0.72
1:A:115:ILE:CA	1:A:115:ILE:HG13	2.20	0.72
1:A:180:PHE:CB	1:A:180:PHE:N	2.52	0.72
1:A:71:SER:CB	1:A:72:PRO:HD2	2.20	0.71
1:A:3:TYR:CA	1:A:4:ARG:CB	2.68	0.71
1:A:194:LEU:CA	1:A:194:LEU:CG	2.66	0.71
1:A:74:VAL:CG1	1:A:74:VAL:CG2	2.63	0.71
1:A:204:LEU:CD2	1:A:204:LEU:CB	2.68	0.71
1:A:70:LEU:CA	1:A:71:SER:N	2.51	0.71
1:A:30:GLU:CD	1:A:30:GLU:CB	2.58	0.70
1:A:115:ILE:CA	1:A:116:THR:N	2.53	0.70
1:A:71:SER:HB2	1:A:72:PRO:HD2	1.73	0.70
1:A:10:LEU:O	1:A:14:GLN:HG3	1.92	0.70
1:A:194:LEU:CB	1:A:194:LEU:N	2.54	0.70
1:A:114:ASP:CA	1:A:114:ASP:CG	2.63	0.69
1:A:71:SER:CA	1:A:72:PRO:N	2.50	0.69
1:A:149:LEU:CD2	1:A:149:LEU:CB	2.66	0.69
1:A:125:HIS:NE2	3:A:308:GOL:H12	2.08	0.69
1:A:49:ALA:CB	1:A:49:ALA:N	2.53	0.68
3:A:304:GOL:C2	3:A:304:GOL:O1	2.42	0.68
1:A:11:GLU:CD	1:A:11:GLU:CB	2.64	0.68
1:A:175:ASP:HA	1:A:178:ILE:HD12	1.74	0.68
1:A:180:PHE:CA	1:A:180:PHE:CG	2.77	0.67
1:A:108:ARG:NE	3:A:304:GOL:O2	2.22	0.67
1:A:131:ALA:C	1:A:131:ALA:CB	2.67	0.67
1:A:24:ASP:CB	1:A:192:LYS:HB2	2.24	0.67
1:A:71:SER:C	1:A:72:PRO:CA	2.61	0.67
3:A:308:GOL:C3	3:A:308:GOL:H2	2.15	0.67
1:A:1:MET:N	1:A:1:MET:C	2.52	0.67
1:A:161[A]:CYS:CB	1:A:161[A]:CYS:N	2.58	0.67
1:A:151:LYS:CD	1:A:151:LYS:CB	2.73	0.66
1:A:95:THR:CB	1:A:95:THR:C	2.65	0.66
1:A:161[B]:CYS:CA	1:A:161[B]:CYS:SG	2.82	0.66
1:A:186:ILE:CB	1:A:186:ILE:N	2.59	0.66
1:A:71:SER:C	1:A:71:SER:CB	2.66	0.66
1:A:83:THR:N	1:A:83:THR:C	2.53	0.66
1:A:4:ARG:CZ	1:A:4:ARG:CD	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:SER:C	1:A:71:SER:N	2.53	0.65
1:A:179:GLN:CG	1:A:179:GLN:CA	2.68	0.65
1:A:182:LYS:N	1:A:182:LYS:C	2.54	0.65
1:A:49:ALA:CB	1:A:49:ALA:C	2.68	0.65
1:A:136:VAL:C	1:A:136:VAL:N	2.52	0.65
1:A:203:GLN:CA	1:A:204:LEU:N	2.56	0.65
1:A:3:TYR:C	1:A:3:TYR:N	2.54	0.65
1:A:71:SER:HA	1:A:72:PRO:HD3	1.79	0.65
1:A:204:LEU:CD2	1:A:204:LEU:CA	2.75	0.65
1:A:131:ALA:C	1:A:131:ALA:N	2.54	0.65
1:A:178:ILE:N	1:A:178:ILE:C	2.51	0.65
1:A:9:ALA:N	1:A:9:ALA:CB	2.57	0.64
1:A:186:ILE:CA	1:A:186:ILE:CG2	2.74	0.64
1:A:24:ASP:CB	1:A:192:LYS:H	2.10	0.64
1:A:151:LYS:CG	1:A:151:LYS:CE	2.74	0.64
1:A:189:ILE:CG2	1:A:189:ILE:HG12	2.24	0.63
1:A:136:VAL:C	1:A:136:VAL:CB	2.71	0.63
1:A:8:GLU:CA	1:A:9:ALA:N	2.53	0.63
1:A:186:ILE:CA	1:A:186:ILE:CG1	2.75	0.63
1:A:62:GLU:CB	1:A:62:GLU:N	2.62	0.62
1:A:4:ARG:O	4:A:485:HOH:O	2.16	0.62
1:A:4:ARG:N	4:A:486:HOH:O	2.33	0.62
1:A:149:LEU:N	1:A:149:LEU:C	2.52	0.62
1:A:204:LEU:CD2	1:A:204:LEU:HA	2.29	0.62
1:A:92:LYS:CD	1:A:92:LYS:CB	2.77	0.62
1:A:67:GLN:CD	1:A:67:GLN:CB	2.72	0.61
1:A:194:LEU:CB	1:A:194:LEU:C	2.73	0.61
1:A:202:ASP:CB	1:A:202:ASP:N	2.60	0.60
1:A:8:GLU:C	1:A:8:GLU:N	2.50	0.60
1:A:149:LEU:N	1:A:149:LEU:CB	2.64	0.60
1:A:197:TYR:OH	4:A:492:HOH:O	2.15	0.60
1:A:98:ILE:CD1	1:A:98:ILE:CB	2.78	0.60
1:A:5:LYS:C	1:A:5:LYS:HB2	2.26	0.59
1:A:160:LEU:HD12	1:A:160:LEU:N	2.16	0.59
1:A:114:ASP:O	1:A:115:ILE:CA	2.50	0.59
1:A:45:VAL:CB	1:A:45:VAL:N	2.62	0.58
1:A:64:LEU:HD23	1:A:158:CYS:HB2	1.85	0.58
1:A:171:MET:SD	1:A:171:MET:CB	2.91	0.58
1:A:181:SER:C	1:A:182:LYS:CA	2.66	0.58
1:A:23:ASP:C	1:A:24:ASP:CA	2.72	0.58
1:A:177:LEU:CD2	1:A:177:LEU:CB	2.78	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:307:GOL:C1	3:A:307:GOL:HO1	2.10	0.57
1:A:115:ILE:C	1:A:115:ILE:N	2.62	0.57
1:A:72:PRO:CG	1:A:72:PRO:N	2.68	0.57
3:A:304:GOL:C2	3:A:304:GOL:HO1	2.18	0.57
1:A:17:ARG:HD3	3:A:305:GOL:H2	1.88	0.56
1:A:11:GLU:CG	1:A:11:GLU:OE2	2.41	0.56
1:A:72:PRO:N	4:A:519:HOH:O	2.39	0.56
1:A:109:MET:O	1:A:115:ILE:HD13	2.05	0.56
1:A:45:VAL:C	1:A:45:VAL:CG1	2.78	0.56
1:A:203:GLN:C	1:A:203:GLN:CB	2.77	0.55
1:A:175:ASP:CA	1:A:175:ASP:CG	2.78	0.55
3:A:308:GOL:O1	4:A:520:HOH:O	2.18	0.55
1:A:174:THR:O	1:A:178:ILE:HD12	2.06	0.54
1:A:92:LYS:HD3	1:A:119:ASP:HA	1.88	0.54
3:A:304:GOL:C3	3:A:304:GOL:HO3	2.09	0.54
1:A:23:ASP:HB2	1:A:142:HIS:CE1	2.43	0.54
1:A:149:LEU:CD2	1:A:149:LEU:CD1	2.79	0.54
1:A:62:GLU:CA	1:A:62:GLU:HG3	2.36	0.54
1:A:69:MET:CB	1:A:69:MET:C	2.74	0.53
1:A:72:PRO:CG	1:A:72:PRO:CA	2.81	0.53
1:A:2:GLU:N	1:A:2:GLU:C	2.64	0.53
1:A:3:TYR:C	4:A:486:HOH:O	2.50	0.53
1:A:64:LEU:CD2	1:A:158:CYS:HB2	2.38	0.53
1:A:115:ILE:CB	1:A:115:ILE:C	2.82	0.53
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.91	0.53
1:A:159:GLY:C	1:A:160:LEU:HD12	2.34	0.52
1:A:202:ASP:CA	1:A:202:ASP:CG	2.80	0.52
3:A:306:GOL:C3	3:A:306:GOL:C1	2.87	0.52
1:A:95:THR:CB	1:A:95:THR:N	2.62	0.52
1:A:23:ASP:CA	1:A:24:ASP:N	2.72	0.52
1:A:182:LYS:CG	1:A:182:LYS:CA	2.84	0.52
3:A:306:GOL:O3	3:A:306:GOL:C2	2.58	0.51
1:A:163:GLU:HB3	1:A:171:MET:HE1	1.91	0.51
1:A:171:MET:SD	1:A:171:MET:HA	2.51	0.51
1:A:136:VAL:CA	1:A:137:LEU:N	2.61	0.51
1:A:25:LYS:CA	1:A:26:ASP:N	2.69	0.51
1:A:178:ILE:N	1:A:178:ILE:CB	2.65	0.51
3:A:304:GOL:C1	3:A:304:GOL:HO1	2.13	0.50
1:A:36:SER:CA	1:A:37:ALA:N	2.62	0.50
1:A:202:ASP:CB	1:A:202:ASP:C	2.78	0.50
1:A:165:MET:CA	1:A:166:ASN:N	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:C	1:A:9:ALA:C	2.76	0.50
1:A:33:LEU:O	1:A:161[A]:CYS:HA	2.12	0.50
1:A:26:ASP:N	1:A:29:ASN:HB2	2.27	0.49
1:A:3:TYR:CA	1:A:3:TYR:O	2.48	0.49
1:A:53:LYS:CD	1:A:53:LYS:HB2	2.43	0.49
1:A:182:LYS:CB	1:A:182:LYS:N	2.68	0.48
1:A:43:GLU:CB	1:A:43:GLU:N	2.72	0.48
1:A:161[A]:CYS:C	1:A:161[A]:CYS:SG	2.96	0.48
1:A:167:HIS:HB2	4:A:496:HOH:O	2.13	0.48
1:A:180:PHE:CB	1:A:180:PHE:C	2.74	0.47
1:A:72:PRO:C	1:A:72:PRO:N	2.70	0.47
1:A:161[A]:CYS:CA	1:A:161[A]:CYS:SG	3.01	0.47
1:A:198:ARG:CD	1:A:198:ARG:HB3	2.45	0.47
1:A:41:THR:O	1:A:42:THR:C	2.56	0.47
3:A:306:GOL:C3	3:A:306:GOL:HO3	2.13	0.47
3:A:307:GOL:C2	3:A:307:GOL:HO2	2.13	0.47
1:A:29:ASN:C	1:A:29:ASN:CG	2.83	0.46
1:A:4:ARG:HD3	1:A:4:ARG:HH11	1.80	0.46
1:A:72:PRO:C	1:A:72:PRO:HB2	2.36	0.45
3:A:304:GOL:C2	3:A:304:GOL:O3	2.58	0.45
1:A:186:ILE:CB	1:A:186:ILE:C	2.79	0.45
1:A:171:MET:SD	1:A:171:MET:CA	3.04	0.45
1:A:115:ILE:HG13	1:A:115:ILE:HA	1.96	0.44
1:A:8:GLU:CB	1:A:8:GLU:OE1	2.65	0.44
1:A:29:ASN:CA	1:A:29:ASN:O	2.56	0.44
1:A:95:THR:CA	1:A:95:THR:OG1	2.56	0.44
1:A:192:LYS:O	1:A:195:GLN:HB2	2.17	0.44
1:A:125:HIS:NE2	3:A:308:GOL:C1	2.79	0.43
1:A:136:VAL:HA	1:A:139:ARG:O	2.19	0.43
1:A:36:SER:C	1:A:36:SER:N	2.62	0.43
1:A:191:ILE:CG2	1:A:191:ILE:CG1	2.89	0.43
1:A:189:ILE:HD12	1:A:189:ILE:HA	1.89	0.43
1:A:12:ALA:CB	3:A:305:GOL:H31	2.45	0.42
1:A:114:ASP:O	1:A:115:ILE:HA	2.18	0.42
1:A:163:GLU:HB3	1:A:171:MET:CE	2.49	0.42
1:A:167:HIS:HD2	1:A:168:ASP:OD1	2.03	0.42
1:A:116:THR:O	1:A:117:PRO:C	2.62	0.42
1:A:175:ASP:CB	1:A:175:ASP:N	2.69	0.41
1:A:189:ILE:CG1	1:A:189:ILE:HG23	2.37	0.41
1:A:23:ASP:C	1:A:24:ASP:HA	2.45	0.41
1:A:3:TYR:CA	1:A:4:ARG:HA	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:CYS:HA	4:A:406:HOH:O	2.20	0.41
1:A:109:MET:CE	4:A:477:HOH:O	2.67	0.41
1:A:174:THR:HG22	1:A:178:ILE:HD11	2.02	0.40
1:A:26:ASP:H	1:A:29:ASN:HB2	1.86	0.40
1:A:198:ARG:CG	1:A:198:ARG:HE	2.24	0.40
1:A:136:VAL:CA	1:A:136:VAL:O	2.47	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)
4:A:418:HOH:O	4:A:495:HOH:O[7_555]	0.57	1.63
4:A:410:HOH:O	4:A:497:HOH:O[7_555]	0.94	1.26

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	188/210 (90%)	177 (94%)	7 (4%)	4 (2%)	5 1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	25	LYS
1	A	2	GLU
1	A	4	ARG

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	154/183 (84%)	150 (97%)	4 (3%)	40 33

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	83	THR
1	A	115	ILE
1	A	203	GLN

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	7	GLN
1	A	142	HIS
1	A	167	HIS
1	A	203	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

8 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
2	SO4	A	301	-	4,4,4	1.35	1 (25%)	6,6,6	1.57	2 (33%)
3	GOL	A	307	-	5,5,5	5.27	4 (80%)	5,5,5	1.30	1 (20%)
2	SO4	A	303	-	4,4,4	4.65	3 (75%)	6,6,6	1.77	2 (33%)
3	GOL	A	308	-	5,5,5	5.65	4 (80%)	5,5,5	1.92	2 (40%)
3	GOL	A	305	-	5,5,5	3.69	2 (40%)	5,5,5	2.29	3 (60%)
3	GOL	A	306	-	5,5,5	9.26	3 (60%)	5,5,5	4.34	5 (100%)
3	GOL	A	304	-	5,5,5	5.60	5 (100%)	5,5,5	3.24	3 (60%)
2	SO4	A	302	-	4,4,4	2.04	2 (50%)	6,6,6	3.68	4 (66%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	307	-	-	2/4/4/4	-
3	GOL	A	308	-	-	2/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	A	306	-	-	0/4/4/4	-
3	GOL	A	304	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	306	GOL	C3-C2	18.65	2.22	1.51
3	A	307	GOL	O2-C2	9.21	1.70	1.43
3	A	308	GOL	C3-C2	7.61	1.80	1.51
2	A	303	SO4	O2-S	7.47	1.89	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	305	GOL	O1-C1	7.06	1.72	1.42
3	A	306	GOL	O3-C3	6.68	1.70	1.42
3	A	304	GOL	O1-C1	6.63	1.70	1.42
3	A	308	GOL	O1-C1	-6.52	1.15	1.42
3	A	304	GOL	C1-C2	6.05	1.74	1.51
3	A	307	GOL	O1-C1	5.94	1.67	1.42
3	A	306	GOL	O2-C2	-5.69	1.26	1.43
3	A	304	GOL	O3-C3	5.68	1.66	1.42
3	A	308	GOL	C1-C2	-5.68	1.30	1.51
3	A	308	GOL	O2-C2	4.97	1.57	1.43
3	A	304	GOL	C3-C2	4.81	1.70	1.51
2	A	303	SO4	O1-S	-4.68	1.17	1.44
3	A	304	GOL	O2-C2	-4.58	1.30	1.43
3	A	305	GOL	C3-C2	4.01	1.67	1.51
3	A	307	GOL	O3-C3	-3.31	1.28	1.42
2	A	302	SO4	O1-S	3.24	1.64	1.44
2	A	303	SO4	O4-S	2.84	1.71	1.48
3	A	307	GOL	C3-C2	-2.61	1.41	1.51
2	A	301	SO4	O3-S	2.52	1.68	1.48
2	A	302	SO4	O2-S	2.17	1.57	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	SO4	O3-S-O2	-6.89	73.56	109.56
3	A	306	GOL	O3-C3-C2	-6.54	80.95	110.38
3	A	304	GOL	C3-C2-C1	4.87	129.65	111.80
3	A	304	GOL	O1-C1-C2	-4.72	89.12	110.38
3	A	306	GOL	C3-C2-C1	-4.17	96.49	111.80
3	A	306	GOL	O1-C1-C2	-4.01	92.31	110.38
2	A	302	SO4	O4-S-O3	3.49	127.78	108.54
3	A	305	GOL	O3-C3-C2	3.32	125.31	110.38
2	A	303	SO4	O3-S-O2	3.31	126.86	109.56
3	A	306	GOL	O2-C2-C1	3.25	122.63	109.18
2	A	302	SO4	O2-S-O1	3.20	131.62	109.06
3	A	308	GOL	C3-C2-C1	3.13	123.28	111.80
2	A	302	SO4	O4-S-O1	-2.82	94.79	109.56
3	A	305	GOL	C3-C2-C1	2.80	122.07	111.80
3	A	306	GOL	O2-C2-C3	-2.70	97.99	109.18
2	A	301	SO4	O4-S-O3	2.22	120.75	108.54
3	A	304	GOL	O3-C3-C2	-2.21	100.42	110.38
3	A	305	GOL	O1-C1-C2	2.20	120.27	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308	GOL	O2-C2-C1	-2.13	100.36	109.18
2	A	301	SO4	O4-S-O1	-2.08	98.67	109.56
3	A	307	GOL	O2-C2-C1	2.08	117.80	109.18
2	A	303	SO4	O2-S-O1	-2.06	94.53	109.06

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	307	GOL	O1-C1-C2-C3
3	A	308	GOL	O1-C1-C2-C3
3	A	305	GOL	O1-C1-C2-C3
3	A	305	GOL	O1-C1-C2-O2
3	A	307	GOL	O1-C1-C2-O2
3	A	308	GOL	O1-C1-C2-O2
3	A	304	GOL	O1-C1-C2-O2
3	A	304	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	307	GOL	4	0
3	A	308	GOL	5	0
3	A	305	GOL	7	0
3	A	306	GOL	5	0
3	A	304	GOL	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	23:ASP	C	24:ASP	N	2.09
1	A	24:ASP	C	25:LYS	N	1.94
1	A	74:VAL	C	75:GLU	N	1.61
1	A	2:GLU	C	3:TYR	N	1.60
1	A	176:ASP	C	177:LEU	N	1.60
1	A	7:GLN	C	8:GLU	N	1.20
1	A	182:LYS	C	183:LYS	N	1.20
1	A	8:GLU	C	9:ALA	N	1.18
1	A	29:ASN	C	30:GLU	N	1.10
1	A	22:ILE	C	23:ASP	N	1.09
1	A	114:ASP	C	115:ILE	N	1.05
1	A	3:TYR	C	4:ARG	N	0.88

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, 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	195/210 (92%)	-0.39	5 (2%) 57 64	14, 29, 48, 76	6 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ASP	4.0
1	A	24	ASP	3.2
1	A	114	ASP	2.8
1	A	3	TYR	2.1
1	A	75	GLU	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
2	SO4	A	303	5/5	0.58	0.13	128,132,150,159	0
3	GOL	A	306	6/6	0.76	0.18	65,72,81,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	307	6/6	0.84	0.15	60,65,78,79	0
3	GOL	A	304	6/6	0.89	0.15	46,48,55,56	0
2	SO4	A	302	5/5	0.91	0.10	67,74,87,91	0
3	GOL	A	305	6/6	0.91	0.13	38,49,55,60	0
3	GOL	A	308	6/6	0.91	0.11	50,53,63,77	0
2	SO4	A	301	5/5	0.98	0.05	38,45,49,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.