Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:45 am BST

PDB ID	:	4FFJ
Title	:	The crystal structure of spDHBPs 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 following versions of software and data (see references ①) were used in the production of this report:

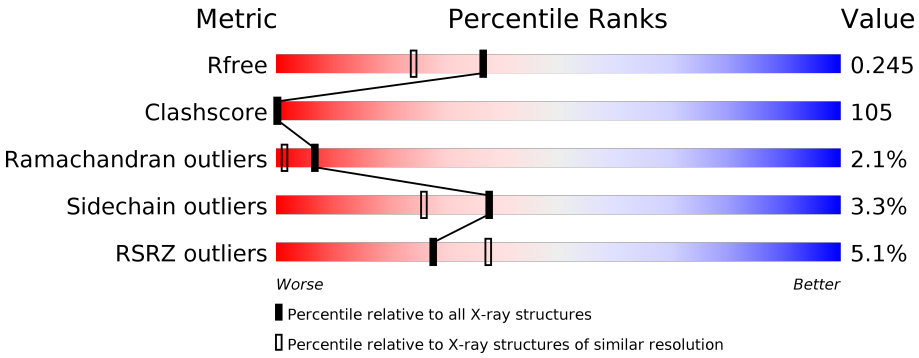
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	210	5% 7% 45% 35% 6% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	302	-	X	-	-
2	SO4	A	303	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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

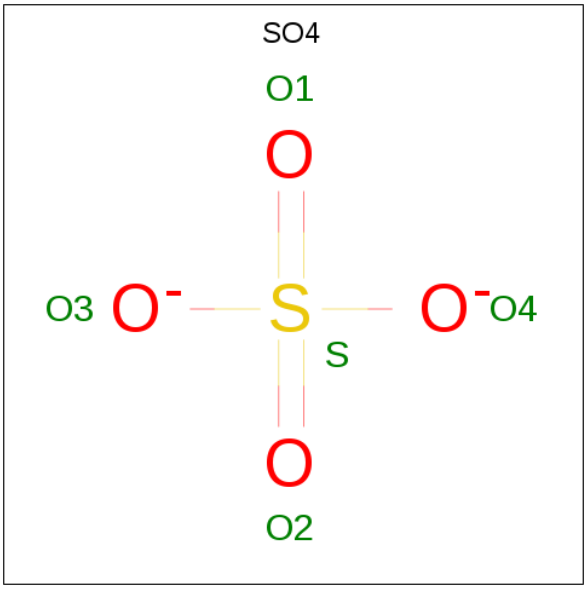
There are 4 unique types of molecules in this entry. The entry contains 1636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

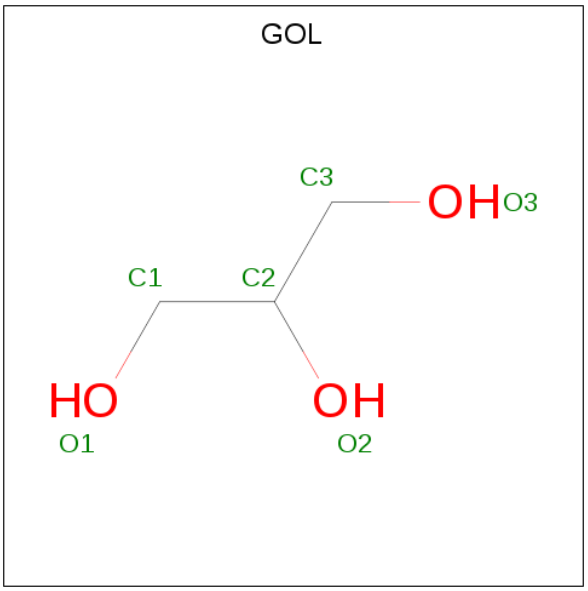
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	7	1	0
			1470	919	249	285	17			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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.

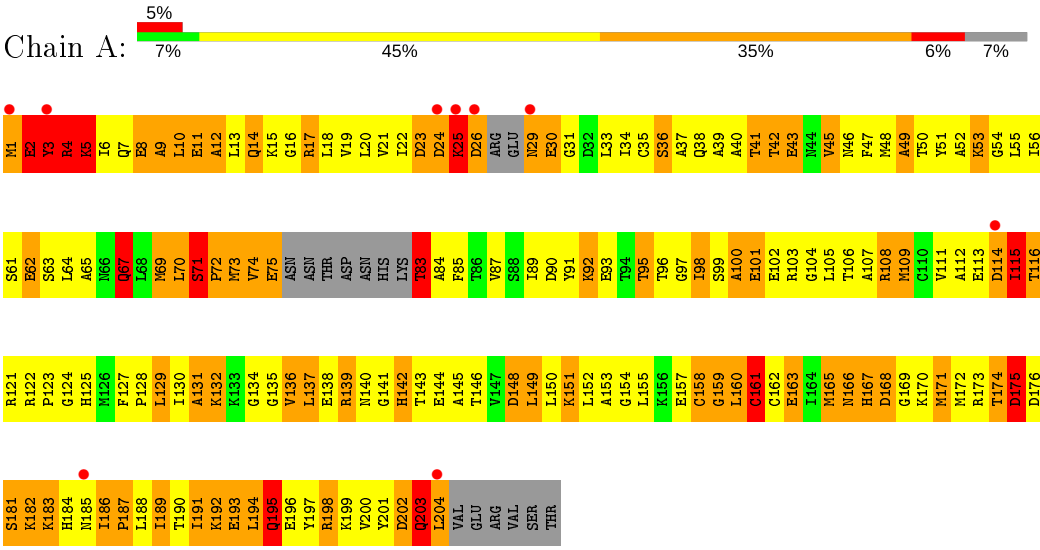
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Riboflavin biosynthesis protein ribBA

Chain A:



4 Data and refinement statistics (i)

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) 84.6 (38.20-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.244 0.182 , 0.245	Depositor DCC
R_{free} test set	870 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	6.00	464/1485 (31.2%)	3.15	198/1998 (9.9%)

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 (464) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ARG	C-O	43.13	2.05	1.23
1	A	8	GLU	CD-OE1	32.75	1.61	1.25
1	A	4	ARG	NE-CZ	28.49	1.70	1.33
1	A	72	PRO	N-CD	28.28	1.87	1.47
1	A	75	GLU	CA-CB	-27.01	0.94	1.53
1	A	198	ARG	CD-NE	-26.64	1.01	1.46
1	A	30	GLU	CD-OE2	26.28	1.54	1.25
1	A	71	SER	CB-OG	26.11	1.76	1.42
1	A	24	ASP	C-N	26.11	1.94	1.34
1	A	193	GLU	CG-CD	25.14	1.89	1.51
1	A	30	GLU	CG-CD	22.22	1.85	1.51
1	A	5	LYS	CA-C	21.59	2.09	1.52
1	A	113	GLU	CD-OE1	-20.25	1.03	1.25
1	A	101	GLU	CG-CD	20.12	1.82	1.51
1	A	3	TYR	C-N	-19.91	0.88	1.34
1	A	75	GLU	C-O	19.65	1.60	1.23
1	A	24	ASP	N-CA	-19.59	1.07	1.46
1	A	175	ASP	CA-CB	19.24	1.96	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLU	CD-OE2	-18.69	1.05	1.25
1	A	167	HIS	CG-CD2	18.42	1.67	1.35
1	A	47	PHE	CG-CD1	17.96	1.65	1.38
1	A	113	GLU	C-O	17.16	1.55	1.23
1	A	74	VAL	CB-CG1	16.92	1.88	1.52
1	A	11	GLU	CG-CD	16.85	1.77	1.51
1	A	4	ARG	CZ-NH2	16.77	1.54	1.33
1	A	114	ASP	CA-CB	16.65	1.90	1.53
1	A	108	ARG	CZ-NH2	16.41	1.54	1.33
1	A	157	GLU	CD-OE2	-15.81	1.08	1.25
1	A	182	LYS	N-CA	15.78	1.77	1.46
1	A	180	PHE	CA-CB	15.44	1.88	1.53
1	A	2	GLU	CB-CG	-15.44	1.22	1.52
1	A	3	TYR	CA-C	15.23	1.92	1.52
1	A	6	ILE	N-CA	-15.21	1.16	1.46
1	A	114	ASP	C-O	15.20	1.52	1.23
1	A	25	LYS	CA-C	15.03	1.92	1.52
1	A	115	ILE	N-CA	14.97	1.76	1.46
1	A	67	GLN	CG-CD	14.69	1.84	1.51
1	A	8	GLU	CG-CD	-14.60	1.30	1.51
1	A	121	ARG	NE-CZ	14.60	1.52	1.33
1	A	161[A]	CYS	CA-CB	14.52	1.85	1.53
1	A	161[B]	CYS	CA-CB	14.52	1.85	1.53
1	A	74	VAL	CB-CG2	-14.40	1.22	1.52
1	A	176	ASP	CA-CB	-14.38	1.22	1.53
1	A	115	ILE	CA-C	14.36	1.90	1.52
1	A	120	PHE	CG-CD2	14.25	1.60	1.38
1	A	23	ASP	CG-OD1	14.07	1.57	1.25
1	A	62	GLU	CA-CB	13.92	1.84	1.53
1	A	85	PHE	CG-CD1	13.73	1.59	1.38
1	A	175	ASP	CA-C	-13.72	1.17	1.52
1	A	203	GLN	CA-C	13.71	1.88	1.52
1	A	72	PRO	N-CA	13.57	1.70	1.47
1	A	8	GLU	CB-CG	13.57	1.77	1.52
1	A	2	GLU	N-CA	13.50	1.73	1.46
1	A	1	MET	N-CA	13.43	1.73	1.46
1	A	53	LYS	CD-CE	-13.40	1.17	1.51
1	A	24	ASP	CA-C	13.24	1.87	1.52
1	A	204	LEU	CG-CD2	13.20	2.00	1.51
1	A	149	LEU	N-CA	13.18	1.72	1.46
1	A	30	GLU	CB-CG	-13.17	1.27	1.52
1	A	204	LEU	C-O	13.14	1.48	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLU	CG-CD	13.06	1.71	1.51
1	A	5	LYS	CA-CB	-13.04	1.25	1.53
1	A	97	GLY	CA-C	12.94	1.72	1.51
1	A	186	ILE	CA-CB	12.87	1.84	1.54
1	A	4	ARG	CA-C	12.85	1.86	1.52
1	A	83	THR	N-CA	12.77	1.71	1.46
1	A	43	GLU	CG-CD	12.64	1.71	1.51
1	A	51	TYR	CE2-CZ	12.63	1.54	1.38
1	A	203	GLN	CB-CG	-12.63	1.18	1.52
1	A	62	GLU	CD-OE1	12.61	1.39	1.25
1	A	161[A]	CYS	CA-C	-12.48	1.20	1.52
1	A	161[B]	CYS	CA-C	-12.48	1.20	1.52
1	A	29	ASN	CA-C	12.41	1.85	1.52
1	A	202	ASP	CA-CB	12.32	1.81	1.53
1	A	114	ASP	C-N	-12.25	1.05	1.34
1	A	11	GLU	CD-OE2	-12.19	1.12	1.25
1	A	74	VAL	C-N	12.03	1.61	1.34
1	A	193	GLU	CD-OE1	11.89	1.38	1.25
1	A	43	GLU	CA-CB	11.78	1.79	1.53
1	A	93	GLU	C-O	11.78	1.45	1.23
1	A	199	LYS	CA-C	-11.67	1.22	1.52
1	A	8	GLU	CD-OE2	11.62	1.38	1.25
1	A	176	ASP	C-N	11.59	1.60	1.34
1	A	2	GLU	C-N	11.58	1.60	1.34
1	A	61	SER	CA-CB	-11.51	1.35	1.52
1	A	26	ASP	C-O	11.49	1.45	1.23
1	A	9	ALA	N-CA	11.44	1.69	1.46
1	A	113	GLU	CG-CD	11.39	1.69	1.51
1	A	72	PRO	CA-C	11.26	1.75	1.52
1	A	178	ILE	N-CA	11.21	1.68	1.46
1	A	49	ALA	CA-CB	11.18	1.75	1.52
1	A	72	PRO	CB-CG	11.10	2.05	1.50
1	A	123	PRO	N-CA	-11.01	1.28	1.47
1	A	8	GLU	CA-C	10.99	1.81	1.52
1	A	177	LEU	C-O	10.96	1.44	1.23
1	A	159	GLY	CA-C	-10.93	1.34	1.51
1	A	193	GLU	C-N	10.87	1.59	1.34
1	A	67	GLN	CD-NE2	-10.82	1.05	1.32
1	A	75	GLU	CA-C	10.74	1.80	1.52
1	A	84	ALA	CA-CB	-10.70	1.29	1.52
1	A	99	SER	C-O	10.62	1.43	1.23
1	A	22	ILE	C-N	-10.62	1.09	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	HIS	CA-C	-10.60	1.25	1.52
1	A	184	HIS	CA-C	-10.60	1.25	1.52
1	A	199	LYS	N-CA	10.53	1.67	1.46
1	A	115	ILE	CA-CB	10.51	1.79	1.54
1	A	161[A]	CYS	C-O	10.46	1.43	1.23
1	A	161[B]	CYS	C-O	10.46	1.43	1.23
1	A	150	LEU	CA-C	-10.43	1.25	1.52
1	A	51	TYR	CB-CG	10.30	1.67	1.51
1	A	102	GLU	CD-OE1	-10.28	1.14	1.25
1	A	200	VAL	C-O	10.27	1.42	1.23
1	A	194	LEU	CA-CB	10.25	1.77	1.53
1	A	29	ASN	C-N	-10.21	1.10	1.34
1	A	197	TYR	CG-CD2	10.19	1.52	1.39
1	A	202	ASP	CG-OD2	-10.11	1.02	1.25
1	A	182	LYS	CB-CG	10.07	1.79	1.52
1	A	163	GLU	CD-OE1	10.05	1.36	1.25
1	A	197	TYR	C-O	10.01	1.42	1.23
1	A	45	VAL	C-O	9.96	1.42	1.23
1	A	4	ARG	CZ-NH1	9.96	1.46	1.33
1	A	23	ASP	C-O	-9.93	1.04	1.23
1	A	187	PRO	N-CA	-9.92	1.30	1.47
1	A	198	ARG	NE-CZ	9.92	1.46	1.33
1	A	195	GLN	N-CA	9.90	1.66	1.46
1	A	8	GLU	N-CA	-9.88	1.26	1.46
1	A	36	SER	CA-C	9.88	1.78	1.52
1	A	71	SER	CA-C	9.82	1.78	1.52
1	A	55	LEU	C-O	9.81	1.42	1.23
1	A	69	MET	CA-CB	9.78	1.75	1.53
1	A	19	VAL	CB-CG2	-9.74	1.32	1.52
1	A	185	ASN	CG-OD1	9.68	1.45	1.24
1	A	45	VAL	CA-CB	9.58	1.74	1.54
1	A	62	GLU	CD-OE2	9.57	1.36	1.25
1	A	145	ALA	N-CA	9.56	1.65	1.46
1	A	112	ALA	N-CA	-9.56	1.27	1.46
1	A	45	VAL	CA-C	-9.51	1.28	1.52
1	A	23	ASP	CB-CG	-9.49	1.31	1.51
1	A	29	ASN	N-CA	9.45	1.65	1.46
1	A	193	GLU	CA-C	-9.44	1.28	1.52
1	A	176	ASP	N-CA	9.43	1.65	1.46
1	A	200	VAL	C-N	9.39	1.55	1.34
1	A	31	GLY	CA-C	9.38	1.66	1.51
1	A	139	ARG	CZ-NH1	9.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	VAL	CA-C	9.29	1.77	1.52
1	A	75	GLU	N-CA	9.28	1.65	1.46
1	A	180	PHE	CD1-CE1	9.27	1.57	1.39
1	A	38	GLN	CG-CD	9.26	1.72	1.51
1	A	17	ARG	CA-CB	9.26	1.74	1.53
1	A	48	MET	CA-C	-9.22	1.28	1.52
1	A	83	THR	CB-OG1	9.21	1.61	1.43
1	A	198	ARG	CZ-NH2	-9.20	1.21	1.33
1	A	198	ARG	CG-CD	9.20	1.75	1.51
1	A	165	MET	CA-C	9.19	1.76	1.52
1	A	4	ARG	CB-CG	-9.19	1.27	1.52
1	A	65	ALA	N-CA	-9.19	1.27	1.46
1	A	165	MET	N-CA	-9.18	1.27	1.46
1	A	132	LYS	CD-CE	9.16	1.74	1.51
1	A	19	VAL	CB-CG1	9.15	1.72	1.52
1	A	83	THR	C-O	9.12	1.40	1.23
1	A	176	ASP	CG-OD1	9.07	1.46	1.25
1	A	168	ASP	CG-OD2	-9.06	1.04	1.25
1	A	70	LEU	N-CA	-9.03	1.28	1.46
1	A	176	ASP	C-O	8.99	1.40	1.23
1	A	157	GLU	C-N	8.99	1.54	1.34
1	A	181	SER	C-O	8.97	1.40	1.23
1	A	198	ARG	N-CA	8.95	1.64	1.46
1	A	173	ARG	N-CA	8.86	1.64	1.46
1	A	59	PRO	CA-CB	8.84	1.71	1.53
1	A	196	GLU	C-N	8.82	1.54	1.34
1	A	131	ALA	CA-C	8.80	1.75	1.52
1	A	53	LYS	CG-CD	8.76	1.82	1.52
1	A	193	GLU	CB-CG	-8.73	1.35	1.52
1	A	150	LEU	C-O	8.66	1.39	1.23
1	A	138	GLU	CB-CG	8.65	1.68	1.52
1	A	92	LYS	CA-C	-8.62	1.30	1.52
1	A	180	PHE	CG-CD1	-8.58	1.25	1.38
1	A	167	HIS	CA-CB	8.57	1.72	1.53
1	A	146	THR	N-CA	8.55	1.63	1.46
1	A	43	GLU	CD-OE2	-8.54	1.16	1.25
1	A	149	LEU	CG-CD2	8.54	1.83	1.51
1	A	163	GLU	CG-CD	8.53	1.64	1.51
1	A	179	GLN	CB-CG	8.48	1.75	1.52
1	A	184	HIS	CG-CD2	8.47	1.50	1.35
1	A	141	GLY	N-CA	8.39	1.58	1.46
1	A	70	LEU	CA-C	8.39	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	GLU	CG-CD	-8.35	1.39	1.51
1	A	95	THR	CA-CB	8.35	1.75	1.53
1	A	49	ALA	N-CA	-8.34	1.29	1.46
1	A	51	TYR	CD2-CE2	-8.27	1.26	1.39
1	A	72	PRO	CG-CD	8.25	1.77	1.50
1	A	171	MET	CG-SD	8.23	2.02	1.81
1	A	89	ILE	N-CA	-8.21	1.29	1.46
1	A	121	ARG	N-CA	-8.20	1.29	1.46
1	A	132	LYS	CA-C	-8.15	1.31	1.52
1	A	50	THR	N-CA	8.14	1.62	1.46
1	A	203	GLN	CG-CD	8.12	1.69	1.51
1	A	47	PHE	N-CA	8.07	1.62	1.46
1	A	92	LYS	CG-CD	8.07	1.79	1.52
1	A	138	GLU	CG-CD	8.06	1.64	1.51
1	A	201	TYR	CG-CD1	-8.05	1.28	1.39
1	A	31	GLY	C-O	-8.03	1.10	1.23
1	A	121	ARG	CZ-NH2	8.03	1.43	1.33
1	A	175	ASP	CG-OD2	8.02	1.43	1.25
1	A	34	ILE	C-O	8.01	1.38	1.23
1	A	170	LYS	CB-CG	8.00	1.74	1.52
1	A	202	ASP	CB-CG	7.99	1.68	1.51
1	A	42	THR	C-O	7.96	1.38	1.23
1	A	4	ARG	CA-CB	7.92	1.71	1.53
1	A	74	VAL	CA-CB	7.86	1.71	1.54
1	A	71	SER	N-CA	7.83	1.62	1.46
1	A	179	GLN	C-N	7.81	1.52	1.34
1	A	117	PRO	N-CA	-7.80	1.33	1.47
1	A	158	CYS	CA-CB	7.79	1.71	1.53
1	A	177	LEU	N-CA	-7.78	1.30	1.46
1	A	176	ASP	CG-OD2	-7.77	1.07	1.25
1	A	120	PHE	CA-CB	7.77	1.71	1.53
1	A	201	TYR	CD1-CE1	7.76	1.50	1.39
1	A	19	VAL	C-O	7.75	1.38	1.23
1	A	128	PRO	CA-CB	7.75	1.69	1.53
1	A	151	LYS	CG-CD	7.73	1.78	1.52
1	A	29	ASN	C-O	7.72	1.38	1.23
1	A	187	PRO	C-O	7.72	1.38	1.23
1	A	15	LYS	N-CA	7.69	1.61	1.46
1	A	16	GLY	CA-C	-7.64	1.39	1.51
1	A	72	PRO	CA-CB	-7.64	1.38	1.53
1	A	54	GLY	C-N	7.62	1.51	1.34
1	A	146	THR	CA-C	-7.61	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	ALA	C-O	7.61	1.37	1.23
1	A	83	THR	C-N	7.58	1.51	1.34
1	A	190	THR	CA-CB	7.57	1.73	1.53
1	A	122	ARG	NE-CZ	7.56	1.42	1.33
1	A	43	GLU	CD-OE1	7.55	1.33	1.25
1	A	146	THR	C-N	7.54	1.51	1.34
1	A	200	VAL	CA-CB	7.53	1.70	1.54
1	A	7	GLN	CD-NE2	7.50	1.51	1.32
1	A	183	LYS	CE-NZ	7.44	1.67	1.49
1	A	41	THR	CA-C	-7.42	1.33	1.52
1	A	98	ILE	C-N	7.42	1.51	1.34
1	A	123	PRO	C-N	7.41	1.46	1.33
1	A	127	PHE	CE1-CZ	7.38	1.51	1.37
1	A	50	THR	CA-CB	7.36	1.72	1.53
1	A	140	ASN	C-N	7.36	1.46	1.33
1	A	92	LYS	CD-CE	7.33	1.69	1.51
1	A	15	LYS	C-N	7.31	1.46	1.33
1	A	177	LEU	CB-CG	7.30	1.73	1.52
1	A	91	TYR	CG-CD2	7.30	1.48	1.39
1	A	191	ILE	CB-CG2	7.26	1.75	1.52
1	A	167	HIS	N-CA	-7.24	1.31	1.46
1	A	180	PHE	CG-CD2	-7.23	1.27	1.38
1	A	189	ILE	CB-CG2	7.22	1.75	1.52
1	A	167	HIS	CD2-NE2	7.22	1.57	1.42
1	A	91	TYR	CE1-CZ	7.21	1.48	1.38
1	A	167	HIS	CE1-NE2	7.17	1.49	1.32
1	A	43	GLU	C-O	7.17	1.36	1.23
1	A	168	ASP	CA-C	7.17	1.71	1.52
1	A	130	ILE	N-CA	-7.14	1.32	1.46
1	A	196	GLU	CB-CG	-7.13	1.38	1.52
1	A	12	ALA	C-O	7.13	1.36	1.23
1	A	180	PHE	CD2-CE2	7.09	1.53	1.39
1	A	3	TYR	N-CA	7.09	1.60	1.46
1	A	69	MET	N-CA	-7.04	1.32	1.46
1	A	185	ASN	CA-C	-7.03	1.34	1.52
1	A	160	LEU	CB-CG	6.97	1.72	1.52
1	A	135	GLY	CA-C	-6.97	1.40	1.51
1	A	34	ILE	N-CA	-6.96	1.32	1.46
1	A	48	MET	N-CA	6.92	1.60	1.46
1	A	171	MET	CB-CG	6.91	1.73	1.51
1	A	167	HIS	CG-ND1	6.91	1.53	1.38
1	A	105	LEU	CA-C	6.90	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	LEU	C-N	6.90	1.50	1.34
1	A	54	GLY	N-CA	6.90	1.56	1.46
1	A	103	ARG	CZ-NH1	6.88	1.42	1.33
1	A	59	PRO	C-O	6.88	1.37	1.23
1	A	129	LEU	CG-CD1	6.88	1.77	1.51
1	A	8	GLU	C-N	-6.85	1.18	1.34
1	A	102	GLU	CD-OE2	6.83	1.33	1.25
1	A	184	HIS	CA-CB	6.83	1.69	1.53
1	A	123	PRO	CA-C	6.80	1.66	1.52
1	A	56	ILE	CB-CG1	6.79	1.73	1.54
1	A	195	GLN	CA-C	-6.79	1.35	1.52
1	A	202	ASP	C-O	6.79	1.36	1.23
1	A	138	GLU	CD-OE1	6.76	1.33	1.25
1	A	113	GLU	CD-OE2	6.76	1.33	1.25
1	A	159	GLY	C-O	6.76	1.34	1.23
1	A	168	ASP	CB-CG	6.76	1.66	1.51
1	A	152	LEU	N-CA	6.75	1.59	1.46
1	A	97	GLY	C-O	6.73	1.34	1.23
1	A	7	GLN	CG-CD	6.71	1.66	1.51
1	A	132	LYS	CE-NZ	6.70	1.65	1.49
1	A	141	GLY	CA-C	6.70	1.62	1.51
1	A	168	ASP	CG-OD1	6.68	1.40	1.25
1	A	69	MET	CB-CG	-6.68	1.29	1.51
1	A	16	GLY	N-CA	6.67	1.56	1.46
1	A	142	HIS	CE1-NE2	6.66	1.48	1.32
1	A	185	ASN	C-N	6.63	1.49	1.34
1	A	22	ILE	CA-C	6.63	1.70	1.52
1	A	6	ILE	CB-CG2	6.62	1.73	1.52
1	A	202	ASP	C-N	6.61	1.49	1.34
1	A	85	PHE	CE1-CZ	6.60	1.49	1.37
1	A	26	ASP	CA-C	6.59	1.70	1.52
1	A	190	THR	N-CA	-6.59	1.33	1.46
1	A	15	LYS	CB-CG	6.56	1.70	1.52
1	A	122	ARG	CD-NE	6.54	1.57	1.46
1	A	10	LEU	C-O	6.50	1.35	1.23
1	A	48	MET	CA-CB	6.49	1.68	1.53
1	A	91	TYR	N-CA	-6.49	1.33	1.46
1	A	59	PRO	CA-C	-6.46	1.40	1.52
1	A	144	GLU	CA-CB	6.45	1.68	1.53
1	A	99	SER	CA-C	-6.42	1.36	1.52
1	A	71	SER	CA-CB	-6.42	1.43	1.52
1	A	172	MET	C-N	6.42	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	MET	CA-CB	-6.41	1.39	1.53
1	A	10	LEU	CB-CG	6.39	1.71	1.52
1	A	197	TYR	CB-CG	6.37	1.61	1.51
1	A	134	GLY	C-N	6.37	1.44	1.33
1	A	53	LYS	CE-NZ	6.33	1.64	1.49
1	A	183	LYS	CD-CE	6.32	1.67	1.51
1	A	93	GLU	N-CA	6.31	1.58	1.46
1	A	121	ARG	CB-CG	-6.31	1.35	1.52
1	A	116	THR	CB-CG2	6.30	1.73	1.52
1	A	195	GLN	C-N	6.29	1.48	1.34
1	A	11	GLU	CA-CB	6.26	1.67	1.53
1	A	149	LEU	CA-C	-6.26	1.36	1.52
1	A	188	LEU	CA-CB	-6.26	1.39	1.53
1	A	14	GLN	C-O	6.25	1.35	1.23
1	A	98	ILE	CA-CB	-6.25	1.40	1.54
1	A	157	GLU	CD-OE1	-6.22	1.18	1.25
1	A	47	PHE	CD2-CE2	6.22	1.51	1.39
1	A	177	LEU	CG-CD2	6.18	1.74	1.51
1	A	170	LYS	CA-CB	6.16	1.67	1.53
1	A	191	ILE	CB-CG1	6.16	1.71	1.54
1	A	127	PHE	CG-CD2	6.14	1.48	1.38
1	A	22	ILE	CB-CG2	-6.13	1.33	1.52
1	A	139	ARG	CG-CD	6.10	1.67	1.51
1	A	19	VAL	CA-C	-6.10	1.37	1.52
1	A	104	GLY	C-N	6.09	1.48	1.34
1	A	149	LEU	C-N	6.09	1.48	1.34
1	A	168	ASP	C-N	6.09	1.44	1.33
1	A	103	ARG	CA-C	-6.07	1.37	1.52
1	A	109	MET	CA-C	6.07	1.68	1.52
1	A	188	LEU	C-O	6.07	1.34	1.23
1	A	154	GLY	N-CA	-6.07	1.36	1.46
1	A	46	ASN	CG-ND2	6.06	1.48	1.32
1	A	193	GLU	N-CA	6.05	1.58	1.46
1	A	182	LYS	C-N	-6.05	1.20	1.34
1	A	2	GLU	C-O	-6.04	1.11	1.23
1	A	186	ILE	N-CA	6.02	1.58	1.46
1	A	7	GLN	C-N	-6.01	1.20	1.34
1	A	109	MET	C-O	-6.00	1.11	1.23
1	A	184	HIS	CB-CG	-5.99	1.39	1.50
1	A	196	GLU	CA-C	-5.99	1.37	1.52
1	A	105	LEU	C-O	-5.98	1.11	1.23
1	A	58	MET	N-CA	-5.97	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	GLU	CD-OE2	-5.97	1.19	1.25
1	A	115	ILE	C-O	-5.94	1.12	1.23
1	A	47	PHE	CE2-CZ	5.92	1.48	1.37
1	A	99	SER	CB-OG	-5.88	1.34	1.42
1	A	184	HIS	N-CA	5.88	1.58	1.46
1	A	143	THR	CA-C	-5.86	1.37	1.52
1	A	122	ARG	CG-CD	-5.85	1.37	1.51
1	A	167	HIS	ND1-CE1	5.85	1.49	1.34
1	A	11	GLU	C-O	-5.85	1.12	1.23
1	A	122	ARG	CZ-NH2	-5.85	1.25	1.33
1	A	96	THR	CA-C	5.84	1.68	1.52
1	A	60	MET	CA-CB	-5.83	1.41	1.53
1	A	2	GLU	CA-C	5.82	1.68	1.52
1	A	45	VAL	C-N	5.82	1.47	1.34
1	A	90	ASP	C-N	5.82	1.47	1.34
1	A	52	ALA	N-CA	5.78	1.57	1.46
1	A	63	SER	C-O	5.77	1.34	1.23
1	A	180	PHE	CA-C	-5.77	1.38	1.52
1	A	117	PRO	C-O	5.76	1.34	1.23
1	A	106	THR	CB-OG1	5.76	1.54	1.43
1	A	114	ASP	CB-CG	-5.72	1.39	1.51
1	A	119	ASP	CA-CB	5.69	1.66	1.53
1	A	40	ALA	CA-CB	5.69	1.64	1.52
1	A	152	LEU	CA-CB	5.69	1.66	1.53
1	A	87	VAL	CA-CB	5.68	1.66	1.54
1	A	160	LEU	CA-CB	5.67	1.66	1.53
1	A	170	LYS	CA-C	-5.66	1.38	1.52
1	A	134	GLY	CA-C	5.66	1.60	1.51
1	A	102	GLU	CA-CB	5.65	1.66	1.53
1	A	1	MET	C-N	5.65	1.47	1.34
1	A	96	THR	CA-CB	-5.65	1.38	1.53
1	A	200	VAL	CB-CG1	5.64	1.64	1.52
1	A	73	MET	N-CA	5.63	1.57	1.46
1	A	184	HIS	C-N	5.63	1.47	1.34
1	A	4	ARG	CG-CD	5.61	1.66	1.51
1	A	29	ASN	CG-OD1	5.60	1.36	1.24
1	A	16	GLY	C-O	5.57	1.32	1.23
1	A	85	PHE	CE2-CZ	5.56	1.48	1.37
1	A	21	VAL	N-CA	5.54	1.57	1.46
1	A	84	ALA	CA-C	5.53	1.67	1.52
1	A	103	ARG	N-CA	5.53	1.57	1.46
1	A	204	LEU	CB-CG	-5.51	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	GLY	C-O	5.51	1.32	1.23
1	A	23	ASP	CG-OD2	-5.50	1.12	1.25
1	A	198	ARG	CB-CG	5.50	1.67	1.52
1	A	112	ALA	CA-C	-5.50	1.38	1.52
1	A	160	LEU	C-O	5.49	1.33	1.23
1	A	124	GLY	N-CA	-5.49	1.37	1.46
1	A	155	LEU	CA-C	5.49	1.67	1.52
1	A	185	ASN	N-CA	-5.47	1.35	1.46
1	A	107	ALA	C-O	5.46	1.33	1.23
1	A	109	MET	CA-CB	-5.44	1.42	1.53
1	A	11	GLU	N-CA	5.44	1.57	1.46
1	A	158	CYS	N-CA	-5.44	1.35	1.46
1	A	127	PHE	CD1-CE1	5.42	1.50	1.39
1	A	98	ILE	CA-C	5.42	1.67	1.52
1	A	15	LYS	CE-NZ	-5.41	1.35	1.49
1	A	117	PRO	N-CD	5.41	1.55	1.47
1	A	97	GLY	C-N	-5.40	1.21	1.34
1	A	175	ASP	C-O	5.40	1.33	1.23
1	A	192	LYS	N-CA	5.39	1.57	1.46
1	A	95	THR	CB-CG2	-5.39	1.34	1.52
1	A	183	LYS	N-CA	5.38	1.57	1.46
1	A	175	ASP	CG-OD1	5.38	1.37	1.25
1	A	111	VAL	CB-CG1	-5.37	1.41	1.52
1	A	100	ALA	CA-CB	5.36	1.63	1.52
1	A	197	TYR	CD1-CE1	5.34	1.47	1.39
1	A	149	LEU	C-O	5.34	1.33	1.23
1	A	162	CYS	C-O	5.34	1.33	1.23
1	A	87	VAL	CB-CG1	5.33	1.64	1.52
1	A	90	ASP	N-CA	5.33	1.57	1.46
1	A	98	ILE	CG1-CD1	5.33	1.87	1.50
1	A	83	THR	CA-C	5.32	1.66	1.52
1	A	137	LEU	CB-CG	5.32	1.68	1.52
1	A	7	GLN	N-CA	-5.31	1.35	1.46
1	A	87	VAL	CB-CG2	-5.31	1.41	1.52
1	A	14	GLN	C-N	-5.29	1.21	1.34
1	A	184	HIS	CG-ND1	-5.29	1.27	1.38
1	A	149	LEU	CB-CG	-5.28	1.37	1.52
1	A	141	GLY	C-O	5.26	1.32	1.23
1	A	178	ILE	C-O	5.25	1.33	1.23
1	A	166	ASN	C-O	5.25	1.33	1.23
1	A	192	LYS	CA-C	-5.25	1.39	1.52
1	A	129	LEU	C-O	5.24	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	LYS	C-N	5.24	1.46	1.34
1	A	43	GLU	N-CA	5.23	1.56	1.46
1	A	120	PHE	CE1-CZ	5.21	1.47	1.37
1	A	101	GLU	N-CA	-5.20	1.35	1.46
1	A	131	ALA	N-CA	5.20	1.56	1.46
1	A	13	LEU	N-CA	5.19	1.56	1.46
1	A	7	GLN	CB-CG	5.19	1.66	1.52
1	A	39	ALA	CA-C	-5.16	1.39	1.52
1	A	130	ILE	CB-CG1	5.15	1.68	1.54
1	A	35	CYS	N-CA	-5.12	1.36	1.46
1	A	182	LYS	CA-C	5.11	1.66	1.52
1	A	157	GLU	CB-CG	5.10	1.61	1.52
1	A	149	LEU	CA-CB	5.10	1.65	1.53
1	A	101	GLU	CA-C	5.08	1.66	1.52
1	A	167	HIS	C-O	5.08	1.33	1.23
1	A	150	LEU	CG-CD1	5.08	1.70	1.51
1	A	91	TYR	CA-C	5.06	1.66	1.52
1	A	142	HIS	CG-CD2	5.05	1.44	1.35
1	A	162	CYS	CA-CB	5.05	1.65	1.53
1	A	163	GLU	N-CA	-5.04	1.36	1.46
1	A	150	LEU	CA-CB	5.04	1.65	1.53
1	A	46	ASN	C-O	-5.03	1.13	1.23
1	A	184	HIS	ND1-CE1	5.03	1.47	1.34
1	A	6	ILE	C-O	5.02	1.32	1.23
1	A	62	GLU	CA-C	-5.01	1.40	1.52
1	A	185	ASN	CA-CB	5.00	1.66	1.53

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	ARG	NE-CZ-NH2	-23.32	108.64	120.30
1	A	4	ARG	NE-CZ-NH1	-16.77	111.91	120.30
1	A	30	GLU	OE1-CD-OE2	13.48	139.48	123.30
1	A	121	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	A	203	GLN	O-C-N	12.96	143.43	122.70
1	A	3	TYR	O-C-N	12.57	142.81	122.70
1	A	17	ARG	NE-CZ-NH2	-12.15	114.23	120.30
1	A	200	VAL	CG1-CB-CG2	-12.14	91.48	110.90
1	A	175	ASP	CB-CG-OD1	-12.13	107.38	118.30
1	A	175	ASP	CB-CG-OD2	11.86	128.98	118.30
1	A	2	GLU	N-CA-CB	11.83	131.90	110.60
1	A	122	ARG	NE-CZ-NH2	-11.57	114.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	GLU	OE1-CD-OE2	10.94	136.43	123.30
1	A	23	ASP	CA-C-O	10.42	141.99	120.10
1	A	180	PHE	CB-CG-CD1	-10.29	113.59	120.80
1	A	189	ILE	CG1-CB-CG2	-10.03	89.33	111.40
1	A	25	LYS	N-CA-C	-9.99	84.04	111.00
1	A	5	LYS	CB-CA-C	-9.98	90.43	110.40
1	A	132	LYS	CD-CE-NZ	-9.97	88.76	111.70
1	A	8	GLU	OE1-CD-OE2	-9.93	111.38	123.30
1	A	5	LYS	CA-CB-CG	9.84	135.04	113.40
1	A	198	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	96	THR	N-CA-CB	9.52	128.39	110.30
1	A	98	ILE	CG1-CB-CG2	-9.47	90.56	111.40
1	A	115	ILE	CG1-CB-CG2	9.45	132.19	111.40
1	A	91	TYR	CG-CD2-CE2	-9.37	113.80	121.30
1	A	184	HIS	CG-ND1-CE1	9.32	121.25	108.20
1	A	20	LEU	CB-CG-CD2	9.28	126.78	111.00
1	A	114	ASP	N-CA-CB	-9.20	94.04	110.60
1	A	114	ASP	CB-CG-OD2	9.04	126.43	118.30
1	A	4	ARG	C-N-CA	9.01	144.23	121.70
1	A	160	LEU	CB-CG-CD2	-8.97	95.76	111.00
1	A	193	GLU	O-C-N	-8.83	108.58	122.70
1	A	7	GLN	CA-CB-CG	-8.76	94.13	113.40
1	A	24	ASP	N-CA-C	8.63	134.29	111.00
1	A	114	ASP	CB-CA-C	-8.41	93.58	110.40
1	A	24	ASP	CA-C-N	-8.40	98.72	117.20
1	A	115	ILE	CA-CB-CG1	-8.34	95.16	111.00
1	A	24	ASP	CA-C-O	8.28	137.48	120.10
1	A	108	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	91	TYR	CD1-CE1-CZ	-8.08	112.52	119.80
1	A	85	PHE	CB-CG-CD1	-8.08	115.15	120.80
1	A	11	GLU	OE1-CD-OE2	7.92	132.80	123.30
1	A	93	GLU	O-C-N	-7.90	110.06	122.70
1	A	114	ASP	OD1-CG-OD2	-7.69	108.68	123.30
1	A	101	GLU	OE1-CD-OE2	7.64	132.46	123.30
1	A	201	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	193	GLU	CA-C-O	7.50	135.85	120.10
1	A	150	LEU	O-C-N	-7.49	110.72	122.70
1	A	113	GLU	CB-CA-C	-7.48	95.44	110.40
1	A	29	ASN	CA-C-O	-7.45	104.46	120.10
1	A	91	TYR	CB-CG-CD2	-7.39	116.57	121.00
1	A	113	GLU	C-N-CA	-7.39	103.23	121.70
1	A	201	TYR	CD1-CG-CD2	7.38	126.02	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	ARG	N-CA-C	-7.37	91.11	111.00
1	A	29	ASN	N-CA-CB	7.37	123.86	110.60
1	A	180	PHE	N-CA-CB	-7.36	97.36	110.60
1	A	114	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	3	TYR	CA-C-O	-7.29	104.80	120.10
1	A	115	ILE	N-CA-C	-7.27	91.38	111.00
1	A	204	LEU	CB-CG-CD1	7.26	123.34	111.00
1	A	29	ASN	CB-CA-C	-7.24	95.92	110.40
1	A	71	SER	C-N-CD	-7.24	104.68	120.60
1	A	51	TYR	CB-CG-CD1	-7.11	116.73	121.00
1	A	185	ASN	OD1-CG-ND2	-7.09	105.60	121.90
1	A	3	TYR	N-CA-C	-7.07	91.92	111.00
1	A	131	ALA	O-C-N	7.02	133.94	122.70
1	A	17	ARG	CG-CD-NE	-6.97	97.16	111.80
1	A	109	MET	CG-SD-CE	6.94	111.30	100.20
1	A	75	GLU	N-CA-CB	6.93	123.07	110.60
1	A	197	TYR	CB-CG-CD1	-6.86	116.88	121.00
1	A	120	PHE	CB-CG-CD2	-6.86	116.00	120.80
1	A	50	THR	CA-CB-CG2	-6.84	102.82	112.40
1	A	194	LEU	CB-CG-CD2	-6.82	99.41	111.00
1	A	175	ASP	CB-CA-C	-6.81	96.78	110.40
1	A	62	GLU	CA-CB-CG	-6.81	98.42	113.40
1	A	8	GLU	CB-CA-C	-6.79	96.81	110.40
1	A	63	SER	N-CA-CB	-6.79	100.31	110.50
1	A	184	HIS	O-C-N	-6.77	111.87	122.70
1	A	115	ILE	CA-C-N	-6.73	102.40	117.20
1	A	117	PRO	CA-N-CD	6.73	121.12	111.70
1	A	190	THR	CA-CB-CG2	-6.71	103.00	112.40
1	A	167	HIS	O-C-N	-6.64	112.08	122.70
1	A	83	THR	OG1-CB-CG2	-6.61	94.81	110.00
1	A	112	ALA	CA-C-N	6.55	131.62	117.20
1	A	117	PRO	N-CD-CG	-6.49	93.46	103.20
1	A	122	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	151	LYS	CA-CB-CG	-6.44	99.24	113.40
1	A	116	THR	CA-CB-CG2	-6.43	103.39	112.40
1	A	182	LYS	CA-C-O	-6.40	106.66	120.10
1	A	193	GLU	N-CA-CB	-6.36	99.16	110.60
1	A	204	LEU	N-CA-C	6.29	127.98	111.00
1	A	182	LYS	CB-CA-C	-6.21	97.97	110.40
1	A	47	PHE	CB-CG-CD2	6.21	125.15	120.80
1	A	24	ASP	CB-CA-C	-6.21	97.98	110.40
1	A	101	GLU	CB-CG-CD	-6.17	97.54	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ASN	CA-C-O	6.16	133.03	120.10
1	A	198	ARG	NH1-CZ-NH2	6.14	126.16	119.40
1	A	193	GLU	CA-CB-CG	-6.14	99.89	113.40
1	A	48	MET	O-C-N	-6.14	112.88	122.70
1	A	19	VAL	CA-CB-CG2	6.12	120.09	110.90
1	A	9	ALA	O-C-N	-6.07	113.00	122.70
1	A	63	SER	O-C-N	-6.07	113.00	122.70
1	A	98	ILE	CA-CB-CG2	6.03	122.96	110.90
1	A	25	LYS	C-N-CA	-6.01	106.66	121.70
1	A	26	ASP	CA-C-O	-6.01	107.49	120.10
1	A	113	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	A	183	LYS	CD-CE-NZ	-6.00	97.91	111.70
1	A	73	MET	CG-SD-CE	5.99	109.78	100.20
1	A	115	ILE	CB-CA-C	-5.99	99.63	111.60
1	A	11	GLU	CA-CB-CG	-5.94	100.33	113.40
1	A	173	ARG	N-CA-CB	-5.94	99.91	110.60
1	A	201	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	122	ARG	CD-NE-CZ	-5.92	115.32	123.60
1	A	18	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	A	203	GLN	CB-CG-CD	-5.91	96.22	111.60
1	A	43	GLU	CB-CA-C	-5.91	98.58	110.40
1	A	9	ALA	CB-CA-C	5.90	118.95	110.10
1	A	127	PHE	CZ-CE2-CD2	5.90	127.18	120.10
1	A	105	LEU	O-C-N	5.89	132.13	122.70
1	A	160	LEU	CA-CB-CG	-5.88	101.78	115.30
1	A	161[A]	CYS	O-C-N	-5.88	113.29	122.70
1	A	161[B]	CYS	O-C-N	-5.88	113.29	122.70
1	A	121	ARG	CD-NE-CZ	-5.85	115.41	123.60
1	A	182	LYS	N-CA-C	-5.83	95.26	111.00
1	A	67	GLN	CA-CB-CG	-5.81	100.62	113.40
1	A	203	GLN	CA-C-O	-5.79	107.95	120.10
1	A	23	ASP	N-CA-C	-5.78	95.39	111.00
1	A	70	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	A	189	ILE	CB-CG1-CD1	-5.76	97.76	113.90
1	A	72	PRO	N-CD-CG	-5.74	94.59	103.20
1	A	119	ASP	CB-CA-C	-5.74	98.92	110.40
1	A	176	ASP	CA-C-O	5.74	132.15	120.10
1	A	195	GLN	N-CA-CB	-5.73	100.29	110.60
1	A	149	LEU	CB-CG-CD1	5.71	120.72	111.00
1	A	184	HIS	ND1-CE1-NE2	-5.71	97.34	109.90
1	A	90	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	113	GLU	N-CA-CB	5.69	120.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	VAL	O-C-N	-5.69	113.60	122.70
1	A	172	MET	N-CA-C	-5.66	95.71	111.00
1	A	91	TYR	CD1-CG-CD2	5.65	124.12	117.90
1	A	4	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	A	132	LYS	CG-CD-CE	-5.64	94.99	111.90
1	A	195	GLN	O-C-N	-5.60	113.73	122.70
1	A	67	GLN	CG-CD-OE1	-5.60	110.40	121.60
1	A	204	LEU	CA-C-O	-5.60	108.35	120.10
1	A	180	PHE	CD1-CG-CD2	5.58	125.56	118.30
1	A	174	THR	CA-CB-CG2	5.56	120.19	112.40
1	A	114	ASP	N-CA-C	-5.56	95.98	111.00
1	A	202	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	A	25	LYS	CA-C-N	-5.54	105.02	117.20
1	A	99	SER	O-C-N	-5.53	113.85	122.70
1	A	186	ILE	N-CA-CB	-5.52	98.10	110.80
1	A	197	TYR	CA-CB-CG	-5.51	102.92	113.40
1	A	51	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
1	A	200	VAL	O-C-N	-5.51	113.88	122.70
1	A	4	ARG	CG-CD-NE	-5.49	100.26	111.80
1	A	71	SER	N-CA-C	-5.49	96.17	111.00
1	A	174	THR	C-N-CA	-5.49	107.99	121.70
1	A	138	GLU	CB-CA-C	5.48	121.37	110.40
1	A	85	PHE	CB-CA-C	-5.48	99.44	110.40
1	A	45	VAL	O-C-N	-5.47	113.95	122.70
1	A	51	TYR	CD1-CE1-CZ	-5.47	114.88	119.80
1	A	85	PHE	CG-CD1-CE1	-5.42	114.83	120.80
1	A	113	GLU	CA-C-O	-5.42	108.72	120.10
1	A	36	SER	N-CA-CB	5.38	118.56	110.50
1	A	119	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	102	GLU	CG-CD-OE1	5.35	129.01	118.30
1	A	92	LYS	CA-C-N	5.33	128.93	117.20
1	A	47	PHE	CB-CG-CD1	-5.30	117.09	120.80
1	A	194	LEU	N-CA-CB	-5.28	99.83	110.40
1	A	203	GLN	CG-CD-OE1	-5.27	111.05	121.60
1	A	180	PHE	CD1-CE1-CZ	-5.25	113.80	120.10
1	A	148	ASP	N-CA-CB	-5.25	101.16	110.60
1	A	85	PHE	CD1-CG-CD2	5.23	125.10	118.30
1	A	115	ILE	O-C-N	5.22	131.06	122.70
1	A	161[A]	CYS	N-CA-CB	-5.21	101.22	110.60
1	A	161[B]	CYS	N-CA-CB	-5.21	101.22	110.60
1	A	151	LYS	N-CA-CB	-5.20	101.23	110.60
1	A	102	GLU	CG-CD-OE2	-5.19	107.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	GLU	CB-CG-CD	-5.18	100.22	114.20
1	A	182	LYS	O-C-N	5.17	130.98	122.70
1	A	168	ASP	CB-CA-C	-5.17	100.06	110.40
1	A	83	THR	N-CA-C	-5.16	97.07	111.00
1	A	168	ASP	C-N-CA	-5.16	111.47	122.30
1	A	196	GLU	O-C-N	-5.16	114.45	122.70
1	A	136	VAL	O-C-N	5.15	130.94	122.70
1	A	167	HIS	CB-CA-C	5.13	120.65	110.40
1	A	175	ASP	CA-CB-CG	-5.13	102.12	113.40
1	A	12	ALA	N-CA-CB	5.12	117.27	110.10
1	A	198	ARG	CD-NE-CZ	5.12	130.76	123.60
1	A	5	LYS	CB-CG-CD	5.10	124.87	111.60
1	A	153	ALA	N-CA-CB	-5.08	102.98	110.10
1	A	176	ASP	CB-CA-C	5.08	120.56	110.40
1	A	97	GLY	CA-C-O	-5.07	111.47	120.60
1	A	201	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	A	93	GLU	CA-C-N	5.05	128.30	117.20
1	A	62	GLU	N-CA-CB	-5.04	101.53	110.60

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	Mainchain,Peptide
1	A	67	GLN	Sidechain

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	1470	0	1436	290	0
2	A	15	0	0	0	0
3	A	30	0	36	31	0
4	A	121	0	0	14	2
All	All	1636	0	1472	312	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 105.

All (312) 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:CB	1:A:189:ILE:CG2	1.75	1.63
1:A:49:ALA:CB	1:A:49:ALA:CA	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:CB	1:A:191:ILE:CG2	1.75	1.61
1:A:8:GLU:CG	1:A:8:GLU:CB	1.77	1.60
3:A:304:GOL:C1	3:A:304:GOL:C2	1.74	1.60
1:A:198:ARG:CG	1:A:198:ARG:CD	1.74	1.60
1:A:92:LYS:CD	1:A:92:LYS:CG	1.79	1.59
1:A:202:ASP:CB	1:A:202:ASP:CA	1.81	1.59
1:A:129:LEU:CG	1:A:129:LEU:CD1	1.77	1.58
1:A:161[B]:CYS:CB	1:A:161[B]:CYS:CA	1.81	1.58
1:A:182:LYS:CG	1:A:182:LYS:CB	1.79	1.58
1:A:69:MET:CA	1:A:69:MET:CB	1.75	1.58
1:A:177:LEU:CG	1:A:177:LEU:CD2	1.74	1.57
1:A:53:LYS:CG	1:A:53:LYS:CD	1.82	1.57
1:A:179:GLN:CG	1:A:179:GLN:CB	1.75	1.57
1:A:72:PRO:CG	1:A:72:PRO:CD	1.77	1.57
1:A:151:LYS:CD	1:A:151:LYS:CG	1.78	1.56
3:A:308:GOL:C2	3:A:308:GOL:C3	1.80	1.56
1:A:115:ILE:CA	1:A:115:ILE:CB	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:72:PRO:CA	1:A:72:PRO:N	1.70	1.54
1:A:136:VAL:C	1:A:136:VAL:CA	1.77	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:CE	1:A:183:LYS:NZ	1.67	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ALA:C	1:A:131:ALA:CA	1.75	1.51
1:A:186:ILE:CA	1:A:186:ILE:CB	1.84	1.51
1:A:36:SER:C	1:A:36:SER:CA	1.78	1.51
1:A:9:ALA:CA	1:A:9:ALA:N	1.69	1.51
1:A:165:MET:C	1:A:165:MET:CA	1.76	1.51
1:A:70:LEU:C	1:A:70:LEU:CA	1.74	1.50
1:A:71:SER:CA	1:A:71:SER:C	1.78	1.50
1:A:72:PRO:CA	1:A:72:PRO:C	1.75	1.50
1:A:178:ILE:CA	1:A:178:ILE:N	1.68	1.50
1:A:161[A]:CYS:CA	1:A:161[A]:CYS:CB	1.85	1.50
1:A:4:ARG:NE	1:A:4:ARG:CZ	1.70	1.50
1:A:149:LEU:CA	1:A:149:LEU:N	1.72	1.49
1:A:180:PHE:CA	1:A:180:PHE:CB	1.87	1.49
1:A:1:MET:CA	1:A:1:MET:N	1.73	1.49
1:A:11:GLU:CG	1:A:11:GLU:CD	1.77	1.49
1:A:2:GLU:CA	1:A:2:GLU:N	1.73	1.49
1:A:114:ASP:CB	1:A:114:ASP:CA	1.90	1.49
1:A:8:GLU:CA	1:A:8:GLU:C	1.81	1.48
1:A:98:ILE:CG1	1:A:98:ILE:CD1	1.87	1.48
1:A:75:GLU:CA	1:A:75:GLU:C	1.80	1.47
1:A:182:LYS:N	1:A:182:LYS:CA	1.77	1.46
1:A:171:MET:SD	1:A:171:MET:CG	2.02	1.45
1:A:115:ILE:CA	1:A:115:ILE:N	1.76	1.45
1:A:67:GLN:CG	1:A:67:GLN:CD	1.84	1.44
1:A:101:GLU:CD	1:A:101:GLU:CG	1.82	1.44
1:A:4:ARG:CA	1:A:4:ARG:C	1.86	1.44
1:A:30:GLU:CD	1:A:30:GLU:CG	1.85	1.44
3:A:304:GOL:C3	3:A:304:GOL:O3	1.66	1.43
1:A:29:ASN:C	1:A:29:ASN:CA	1.85	1.43
1:A:24:ASP:CA	1:A:24:ASP:C	1.87	1.43
3:A:307:GOL:C1	3:A:307:GOL:O1	1.67	1.42
1:A:175:ASP:CA	1:A:175:ASP:CB	1.96	1.42
1:A:203:GLN:C	1:A:203:GLN:CA	1.88	1.42
1:A:193:GLU:CD	1:A:193:GLU:CG	1.89	1.40
3:A:304:GOL:C1	3:A:304:GOL:O1	1.70	1.39
3:A:307:GOL:O2	3:A:307:GOL:C2	1.70	1.39
1:A:204:LEU:CG	1:A:204:LEU:CD2	2.00	1.39
1:A:115:ILE:C	1:A:115:ILE:CA	1.90	1.38
1:A:3:TYR:CA	1:A:3:TYR:C	1.92	1.38
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:N	1:A:72:PRO:CD	1.87	1.37
1:A:25:LYS:CA	1:A:25:LYS:C	1.92	1.36
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	1.21
1:A:24:ASP:C	1:A:25:LYS:N	1.94	1.21
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:187:PRO:CD	3:A:305:GOL:H32	1.81	1.10
1:A:23:ASP:C	1:A:24:ASP:N	2.09	1.05
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:115:ILE:CG1	1:A:115:ILE:CA	2.42	0.97
1:A:198:ARG:NE	1:A:198:ARG:CG	2.27	0.95
1:A:4:ARG:C	1:A:4:ARG:O	2.05	0.94
1:A:8:GLU:CD	1:A:8:GLU:CB	2.38	0.93
1:A:69:MET:CA	1:A:69:MET:CG	2.46	0.92
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:25:LYS:C	1:A:25:LYS:N	2.25	0.90
1:A:175:ASP:C	1:A:175:ASP:CB	2.40	0.89
1:A:3:TYR:CA	1:A:4:ARG:CA	2.51	0.89
1:A:114:ASP:C	1:A:115:ILE:CA	2.39	0.88
1:A:129:LEU:CD2	1:A:129:LEU:CD1	2.52	0.87
1:A:8:GLU:C	1:A:9:ALA:CA	2.42	0.87
1:A:3:TYR:CA	1:A:4:ARG:N	2.37	0.86
1:A:5:LYS:CB	1:A:5:LYS:C	2.44	0.86
1:A:62:GLU:CA	1:A:62:GLU:CG	2.54	0.86
1:A:161[B]:CYS:CB	1:A:161[B]:CYS:C	2.44	0.86
1:A:95:THR:CG2	1:A:95:THR:CA	2.53	0.86
1:A:72:PRO:CB	1:A:72:PRO:C	2.43	0.85
1:A:29:ASN:CB	1:A:29:ASN:C	2.44	0.85
1:A:189:ILE:CA	1:A:189:ILE:CG2	2.55	0.84
1:A:45:VAL:C	1:A:45:VAL:CB	2.46	0.83
1:A:69:MET:N	1:A:69:MET:CB	2.41	0.82
1:A:4:ARG:N	1:A:4:ARG:C	2.33	0.82
1:A:129:LEU:CB	1:A:129:LEU:CD1	2.57	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:SER:C	1:A:72:PRO:CD	2.51	0.78
1:A:8:GLU:C	1:A:8:GLU:CB	2.52	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:45:VAL:CG2	1:A:45:VAL:CA	2.62	0.77
1:A:3:TYR:CA	1:A:4:ARG:HB2	2.13	0.77
1:A:53:LYS:CB	1:A:53:LYS:CD	2.62	0.77
1:A:24:ASP:CB	1:A:24:ASP:C	2.52	0.77
1:A:114:ASP:C	1:A:114:ASP:CB	2.53	0.76
1:A:193:GLU:CD	1:A:193:GLU:CB	2.53	0.76
1:A:198:ARG:CB	1:A:198:ARG:CD	2.63	0.75
1:A:71:SER:CA	1:A:72:PRO:N	2.50	0.75
1:A:72:PRO:HB3	4:A:519:HOH:O	1.85	0.75
1:A:191:ILE:CA	1:A:191:ILE:CG2	2.65	0.75
1:A:131:ALA:CA	1:A:132:LYS:N	2.49	0.74
1:A:43:GLU:CG	1:A:43:GLU:CA	2.65	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:12:ALA:HB1	3:A:305:GOL:H31	1.70	0.73
1:A:72:PRO:CA	1:A:73:MET:N	2.50	0.73
1:A:72:PRO:CB	1:A:72:PRO:N	2.49	0.73
1:A:161[A]:CYS:CB	1:A:161[A]:CYS:C	2.53	0.73
1:A:92:LYS:CG	1:A:92:LYS:CE	2.67	0.73
1:A:8:GLU:CG	1:A:8:GLU:CA	2.66	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:115:ILE:HG13	1:A:115:ILE:CA	2.20	0.72
1:A:180:PHE:N	1:A:180:PHE:CB	2.52	0.72
1:A:9:ALA:N	1:A:9:ALA:C	2.43	0.72
1:A:101:GLU:CD	1:A:101:GLU:CB	2.58	0.72
1:A:71:SER:CB	1:A:72:PRO:HD2	2.20	0.71
1:A:194:LEU:CG	1:A:194:LEU:CA	2.66	0.71
1:A:3:TYR:CA	1:A:4:ARG:CB	2.68	0.71
1:A:74:VAL:CG2	1:A:74:VAL:CG1	2.63	0.71
1:A:204:LEU:CB	1:A:204:LEU:CD2	2.68	0.71
1:A:70:LEU:CA	1:A:71:SER:N	2.51	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:MET:N	1:A:165:MET:C	2.42	0.70
1:A:194:LEU:CB	1:A:194:LEU:N	2.54	0.70
1:A:62:GLU:CB	1:A:62:GLU:C	2.60	0.69
1:A:149:LEU:CB	1:A:149:LEU:CD2	2.66	0.69
1:A:165:MET:C	1:A:165:MET:CB	2.60	0.69
1:A:125:HIS:NE2	3:A:308:GOL:H12	2.08	0.69
1:A:148:ASP:C	1:A:149:LEU:CA	2.59	0.68
1:A:49:ALA:CB	1:A:49:ALA:N	2.53	0.68
1:A:70:LEU:C	1:A:70:LEU:N	2.42	0.68
3:A:304:GOL:O1	3:A:304:GOL:C2	2.42	0.68
1:A:30:GLU:CD	1:A:30:GLU:CB	2.58	0.68
1:A:36:SER:C	1:A:36:SER:CB	2.59	0.68
1:A:175:ASP:HA	1:A:178:ILE:HD12	1.74	0.68
1:A:43:GLU:C	1:A:43:GLU:CB	2.61	0.68
1:A:70:LEU:C	1:A:70:LEU:CB	2.62	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:177:LEU:C	1:A:178:ILE:CA	2.61	0.67
1:A:24:ASP:CB	1:A:192:LYS:HB2	2.24	0.67
3:A:308:GOL:H2	3:A:308:GOL:C3	2.15	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:161[B]:CYS:CA	1:A:161[B]:CYS:SG	2.82	0.66
1:A:186:ILE:N	1:A:186:ILE:CB	2.59	0.66
1:A:179:GLN:CA	1:A:179:GLN:CG	2.68	0.65
1:A:4:ARG:CD	1:A:4:ARG:CZ	2.74	0.65
1:A:203:GLN:CA	1:A:204:LEU:N	2.56	0.65
1:A:71:SER:HA	1:A:72:PRO:HD3	1.79	0.65
1:A:204:LEU:CA	1:A:204:LEU:CD2	2.75	0.65
1:A:114:ASP:CA	1:A:114:ASP:CG	2.63	0.65
1:A:186:ILE:CA	1:A:186:ILE:CG2	2.74	0.64
1:A:9:ALA:N	1:A:9:ALA:CB	2.57	0.64
1:A:8:GLU:CA	1:A:9:ALA:N	2.53	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:186:ILE:CG1	1:A:186:ILE:CA	2.75	0.63
1:A:62:GLU:N	1:A:62:GLU:CB	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:71:SER:C	1:A:72:PRO:CA	2.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HA	1:A:204:LEU:CD2	2.29	0.62
1:A:92:LYS:CB	1:A:92:LYS:CD	2.77	0.62
1:A:131:ALA:C	1:A:131:ALA:N	2.54	0.61
1:A:95:THR:C	1:A:95:THR:CB	2.65	0.61
1:A:11:GLU:CB	1:A:11:GLU:CD	2.64	0.61
1:A:83:THR:N	1:A:83:THR:C	2.53	0.61
1:A:136:VAL:C	1:A:136:VAL:N	2.52	0.61
1:A:71:SER:C	1:A:71:SER:N	2.53	0.61
1:A:182:LYS:N	1:A:182:LYS:C	2.54	0.61
1:A:49:ALA:CB	1:A:49:ALA:C	2.68	0.61
1:A:3:TYR:N	1:A:3:TYR:C	2.54	0.60
1:A:202:ASP:CB	1:A:202:ASP:N	2.60	0.60
1:A:131:ALA:C	1:A:131:ALA:CB	2.67	0.60
1:A:149:LEU:N	1:A:149:LEU:CB	2.64	0.60
1:A:1:MET:C	1:A:1:MET:N	2.52	0.60
1:A:178:ILE:N	1:A:178:ILE:C	2.51	0.60
1:A:71:SER:CB	1:A:71:SER:C	2.66	0.60
1:A:98:ILE:CD1	1:A:98:ILE:CB	2.78	0.60
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:171:MET:SD	1:A:171:MET:CB	2.91	0.58
1:A:45:VAL:N	1:A:45:VAL:CB	2.62	0.58
1:A:64:LEU:HD23	1:A:158:CYS:HB2	1.85	0.58
1:A:177:LEU:CD2	1:A:177:LEU:CB	2.78	0.58
1:A:3:TYR:CA	1:A:3:TYR:O	2.48	0.58
1:A:149:LEU:N	1:A:149:LEU:C	2.52	0.57
1:A:11:GLU:OE2	1:A:11:GLU:CG	2.41	0.57
1:A:67:GLN:CB	1:A:67:GLN:CD	2.72	0.57
1:A:72:PRO:CG	1:A:72:PRO:N	2.68	0.57
1:A:136:VAL:C	1:A:136:VAL:CB	2.71	0.56
1:A:8:GLU:C	1:A:8:GLU:N	2.50	0.56
1:A:17:ARG:HD3	3:A:305:GOL:H2	1.88	0.56
1:A:194:LEU:CB	1:A:194:LEU:C	2.73	0.56
1:A:109:MET:O	1:A:115:ILE:HD13	2.05	0.56
1:A:72:PRO:N	4:A:519:HOH:O	2.39	0.56
3:A:307:GOL:C1	3:A:307:GOL:HO1	2.10	0.55
3:A:304:GOL:HO1	3:A:304:GOL:C2	2.20	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:25:LYS:CA	1:A:26:ASP:N	2.69	0.54
1:A:92:LYS:HD3	1:A:119:ASP:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:101:GLU:CG	1:A:101:GLU:OE1	2.50	0.54
1:A:149:LEU:CD1	1:A:149:LEU:CD2	2.79	0.54
1:A:181:SER:C	1:A:182:LYS:CA	2.66	0.54
1:A:62:GLU:CA	1:A:62:GLU:HG3	2.36	0.54
1:A:23:ASP:C	1:A:24:ASP:CA	2.72	0.53
1:A:72:PRO:CA	1:A:72:PRO:CG	2.81	0.53
1:A:64:LEU:CD2	1:A:158:CYS:HB2	2.38	0.53
1:A:115:ILE:C	1:A:115:ILE:N	2.62	0.53
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.91	0.53
1:A:203:GLN:CA	1:A:203:GLN:O	2.51	0.52
3:A:307:GOL:HO2	3:A:307:GOL:C2	2.13	0.52
3:A:306:GOL:C1	3:A:306:GOL:C3	2.87	0.52
1:A:5:LYS:C	1:A:5:LYS:HB2	2.26	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: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:203:GLN:CB	1:A:203:GLN:C	2.77	0.51
1:A:178:ILE:N	1:A:178:ILE:CB	2.65	0.51
1:A:45:VAL:C	1:A:45:VAL:CG1	2.78	0.51
1:A:175:ASP:CA	1:A:175:ASP:CG	2.78	0.50
1:A:165:MET:CA	1:A:166:ASN:N	2.60	0.50
1:A:36:SER:CA	1:A:37:ALA:N	2.62	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:136:VAL:CA	1:A:136:VAL:O	2.47	0.49
1:A:53:LYS:HB2	1:A:53:LYS:CD	2.43	0.49
1:A:182:LYS:N	1:A:182:LYS:CB	2.68	0.48
1:A:2:GLU:C	1:A:2:GLU:N	2.64	0.48
1:A:3:TYR:C	4:A:486:HOH:O	2.50	0.48
1:A:43:GLU:N	1:A:43:GLU:CB	2.72	0.48
1:A:167:HIS:HB2	4:A:496:HOH:O	2.13	0.48
1:A:171:MET:HB3	1:A:171:MET:HE3	1.96	0.47
1:A:202:ASP:CA	1:A:202:ASP:CG	2.80	0.47
1:A:198:ARG:HB3	1:A:198:ARG:CD	2.45	0.47
1:A:159:GLY:C	1:A:160:LEU:HD12	2.34	0.47
1:A:161[A]:CYS:CA	1:A:161[A]:CYS:SG	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:306:GOL:C3	3:A:306:GOL:HO3	2.13	0.47
1:A:109:MET:HE3	4:A:477:HOH:O	2.14	0.46
1:A:115:ILE:C	1:A:115:ILE:CB	2.82	0.46
1:A:4:ARG:HD3	1:A:4:ARG:HH11	1.80	0.46
3:A:304:GOL:O3	3:A:304:GOL:C2	2.58	0.45
1:A:171:MET:CA	1:A:171:MET:SD	3.04	0.45
1:A:115:ILE:HG13	1:A:115:ILE:HA	1.96	0.44
3:A:304:GOL:C1	3:A:304:GOL:HO1	2.13	0.44
1:A:8:GLU:OE1	1:A:8:GLU:CB	2.65	0.44
1:A:29:ASN:O	1:A:29:ASN:CA	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:161[A]:CYS:SG	1:A:161[A]:CYS:C	2.96	0.43
1:A:136:VAL:HA	1:A:139:ARG:O	2.19	0.43
1:A:69:MET:C	1:A:69:MET:CB	2.74	0.43
1:A:191:ILE:CG1	1:A:191:ILE:CG2	2.89	0.43
1:A:180:PHE:C	1:A:180:PHE:CB	2.74	0.43
1:A:189:ILE:HD12	1:A:189:ILE:HA	1.89	0.43
1:A:114:ASP:O	1:A:115:ILE:HA	2.18	0.42
1:A:12:ALA:CB	3:A:305:GOL:H31	2.45	0.42
1:A:163:GLU:HB3	1:A:171:MET:CE	2.49	0.42
1:A:41:THR:O	1:A:42:THR:C	2.56	0.42
1:A:167:HIS:HD2	1:A:168:ASP:OD1	2.03	0.42
1:A:175:ASP:N	1:A:175:ASP:CB	2.69	0.41
1:A:189:ILE:HG23	1:A:189:ILE:CG1	2.37	0.41
1:A:72:PRO:C	1:A:72:PRO:HB2	2.36	0.41
1:A:3:TYR:CA	1:A:4:ARG:HA	2.44	0.41
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:186:ILE:C	1:A:186:ILE:CB	2.79	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:8:GLU:C	1:A:9:ALA:C	2.76	0.40
1:A:30:GLU:OE1	1:A:30:GLU:CG	2.60	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%)	7 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%)	148 (96%)	6 (4%)	32 19

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER

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Mol	Chain	Res	Type
1	A	83	THR
1	A	115	ILE
1	A	161[A]	CYS
1	A	161[B]	CYS
1	A	203	GLN

Some 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
3	GOL	A	306	-	5,5,5	8.69	3 (60%)	5,5,5	4.06	5 (100%)
2	SO4	A	303	-	4,4,4	5.01	3 (75%)	6,6,6	1.80	2 (33%)
3	GOL	A	305	-	5,5,5	3.62	2 (40%)	5,5,5	2.18	3 (60%)
3	GOL	A	308	-	5,5,5	5.38	4 (80%)	5,5,5	1.80	1 (20%)
2	SO4	A	302	-	4,4,4	2.08	2 (50%)	6,6,6	3.80	4 (66%)
3	GOL	A	304	-	5,5,5	5.42	5 (100%)	5,5,5	3.05	3 (60%)
3	GOL	A	307	-	5,5,5	5.15	4 (80%)	5,5,5	1.22	0
2	SO4	A	301	-	4,4,4	1.35	1 (25%)	6,6,6	1.66	2 (33%)

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
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	A	306	-	-	0/4/4/4	-
3	GOL	A	304	-	-	2/4/4/4	-
3	GOL	A	307	-	-	2/4/4/4	-
3	GOL	A	308	-	-	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	17.29	2.22	1.51
3	A	307	GOL	O2-C2	8.95	1.70	1.43
2	A	303	SO4	O2-S	7.96	1.89	1.46
3	A	308	GOL	C3-C2	7.06	1.80	1.51
3	A	305	GOL	O1-C1	7.03	1.72	1.42
3	A	306	GOL	O3-C3	6.65	1.70	1.42
3	A	304	GOL	O1-C1	6.59	1.70	1.42
3	A	308	GOL	O1-C1	-6.48	1.15	1.42
3	A	307	GOL	O1-C1	5.92	1.67	1.42
3	A	304	GOL	O3-C3	5.66	1.66	1.42
3	A	304	GOL	C1-C2	5.62	1.74	1.51
3	A	306	GOL	O2-C2	-5.55	1.26	1.43
2	A	303	SO4	O1-S	-5.31	1.17	1.46
3	A	308	GOL	C1-C2	-5.25	1.30	1.51
3	A	308	GOL	O2-C2	4.83	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	304	GOL	C3-C2	4.47	1.70	1.51
3	A	304	GOL	O2-C2	-4.47	1.30	1.43
3	A	305	GOL	C3-C2	3.73	1.67	1.51
2	A	302	SO4	O1-S	3.33	1.64	1.46
3	A	307	GOL	O3-C3	-3.29	1.28	1.42
2	A	303	SO4	O4-S	2.85	1.71	1.47
2	A	301	SO4	O3-S	2.53	1.68	1.47
3	A	307	GOL	C3-C2	-2.40	1.41	1.51
2	A	302	SO4	O2-S	2.17	1.57	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	SO4	O3-S-O2	-6.85	73.56	109.31
3	A	306	GOL	O3-C3-C2	-6.10	80.95	110.20
3	A	304	GOL	C3-C2-C1	4.61	129.65	111.70
3	A	304	GOL	O1-C1-C2	-4.40	89.12	110.20
2	A	302	SO4	O4-S-O3	4.39	127.78	109.06
3	A	306	GOL	C3-C2-C1	-3.91	96.49	111.70
3	A	306	GOL	O1-C1-C2	-3.73	92.31	110.20
2	A	303	SO4	O3-S-O2	3.36	126.86	109.31
3	A	305	GOL	O3-C3-C2	3.15	125.31	110.20
3	A	306	GOL	O2-C2-C1	3.07	122.63	109.12
2	A	302	SO4	O2-S-O1	3.00	131.62	109.43
3	A	308	GOL	C3-C2-C1	2.98	123.28	111.70
2	A	302	SO4	O4-S-O1	-2.78	94.79	109.31
2	A	301	SO4	O4-S-O3	2.74	120.75	109.06
3	A	305	GOL	C3-C2-C1	2.67	122.07	111.70
3	A	306	GOL	O2-C2-C3	-2.53	97.99	109.12
3	A	305	GOL	O1-C1-C2	2.10	120.27	110.20
3	A	304	GOL	O3-C3-C2	-2.04	100.42	110.20
2	A	301	SO4	O4-S-O1	-2.04	98.67	109.31
2	A	303	SO4	O2-S-O1	-2.02	94.53	109.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	A	308	GOL	O1-C1-C2-O2
3	A	307	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	306	GOL	5	0
3	A	305	GOL	7	0
3	A	308	GOL	5	0
3	A	304	GOL	10	0
3	A	307	GOL	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3:TYR	C	4:ARG	N	0.88

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	195/210 (92%)	0.09	10 (5%) 28 37	20, 29, 53, 76	5 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	LEU	4.5
1	A	24	ASP	3.1
1	A	1	MET	2.7
1	A	178	ILE	2.6
1	A	3	TYR	2.5
1	A	29	ASN	2.3
1	A	114	ASP	2.2
1	A	26	ASP	2.1
1	A	25	LYS	2.1
1	A	185	ASN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	307	6/6	0.68	0.21	60,65,78,79	0
2	SO4	A	303	5/5	0.71	0.30	128,132,150,159	0
3	GOL	A	306	6/6	0.76	0.22	65,72,81,85	0
3	GOL	A	305	6/6	0.80	0.29	38,49,55,60	0
3	GOL	A	304	6/6	0.86	0.29	46,48,55,56	0
3	GOL	A	308	6/6	0.91	0.20	50,53,63,77	0
2	SO4	A	302	5/5	0.95	0.09	67,74,87,91	0
2	SO4	A	301	5/5	0.98	0.08	38,45,49,57	0

6.5 Other polymers (i)

There are no such residues in this entry.