



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:56 pm GMT

PDB ID : 4RDT
Title : Structure of the bacterial Zn-transporter ZnuD from *Neisseria meningitidis*
(flexible conformation bound to a zinc ion)
Authors : Calmettes, C.; El Bakkouri, M.; Moraes, T.F.
Deposited on : 2014-09-19
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

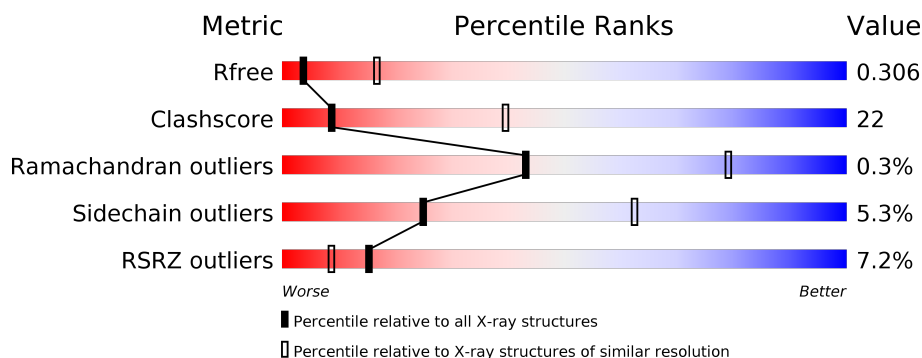
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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. 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	748	<div> <div>5%</div> <div>53%</div> <div>29%</div> <div>•</div> <div>15%</div> </div>
1	B	748	<div> <div>7%</div> <div>54%</div> <div>28%</div> <div>••</div> <div>15%</div> </div>

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
3	GOL	A	802	-	-	-	X
3	GOL	A	803	-	-	-	X
3	GOL	A	804	-	-	-	X
4	C8E	A	806	-	-	X	-
5	SO4	A	807	-	-	X	-
5	SO4	B	802	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10159 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 ZnuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	1	0
			5044	3158	932	945	9			
1	B	635	Total	C	N	O	S	0	0	0
			5032	3150	927	946	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q9JZN9
A	-12	ALA	-	EXPRESSION TAG	UNP Q9JZN9
A	-11	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-10	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-9	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-8	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-7	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-6	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-5	LEU	-	EXPRESSION TAG	UNP Q9JZN9
A	-4	VAL	-	EXPRESSION TAG	UNP Q9JZN9
A	-3	PRO	-	EXPRESSION TAG	UNP Q9JZN9
A	-2	ARG	-	EXPRESSION TAG	UNP Q9JZN9
A	-1	GLY	-	EXPRESSION TAG	UNP Q9JZN9
A	0	SER	-	EXPRESSION TAG	UNP Q9JZN9
B	-13	MET	-	EXPRESSION TAG	UNP Q9JZN9
B	-12	ALA	-	EXPRESSION TAG	UNP Q9JZN9
B	-11	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-10	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-9	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-8	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-7	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-6	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-5	LEU	-	EXPRESSION TAG	UNP Q9JZN9
B	-4	VAL	-	EXPRESSION TAG	UNP Q9JZN9
B	-3	PRO	-	EXPRESSION TAG	UNP Q9JZN9

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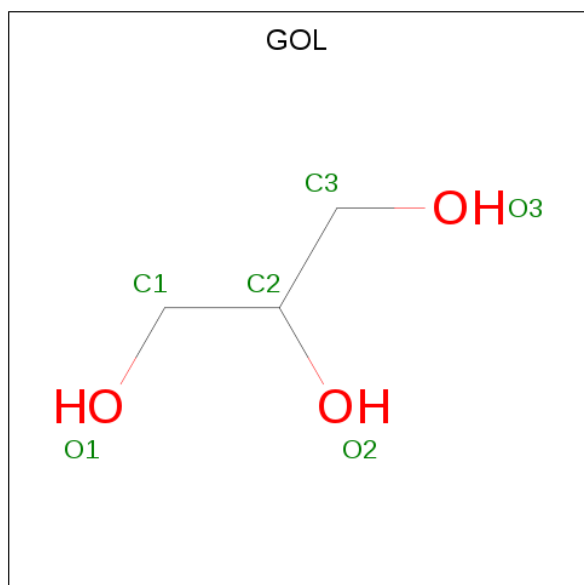
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ARG	-	EXPRESSION TAG	UNP Q9JZN9
B	-1	GLY	-	EXPRESSION TAG	UNP Q9JZN9
B	0	SER	-	EXPRESSION TAG	UNP Q9JZN9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

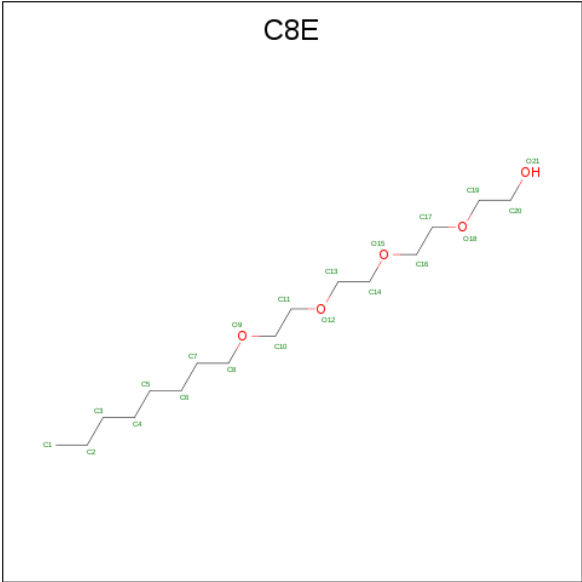
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



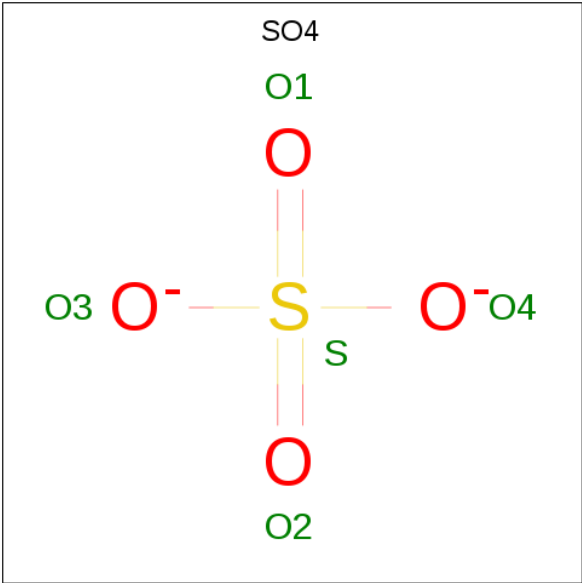
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

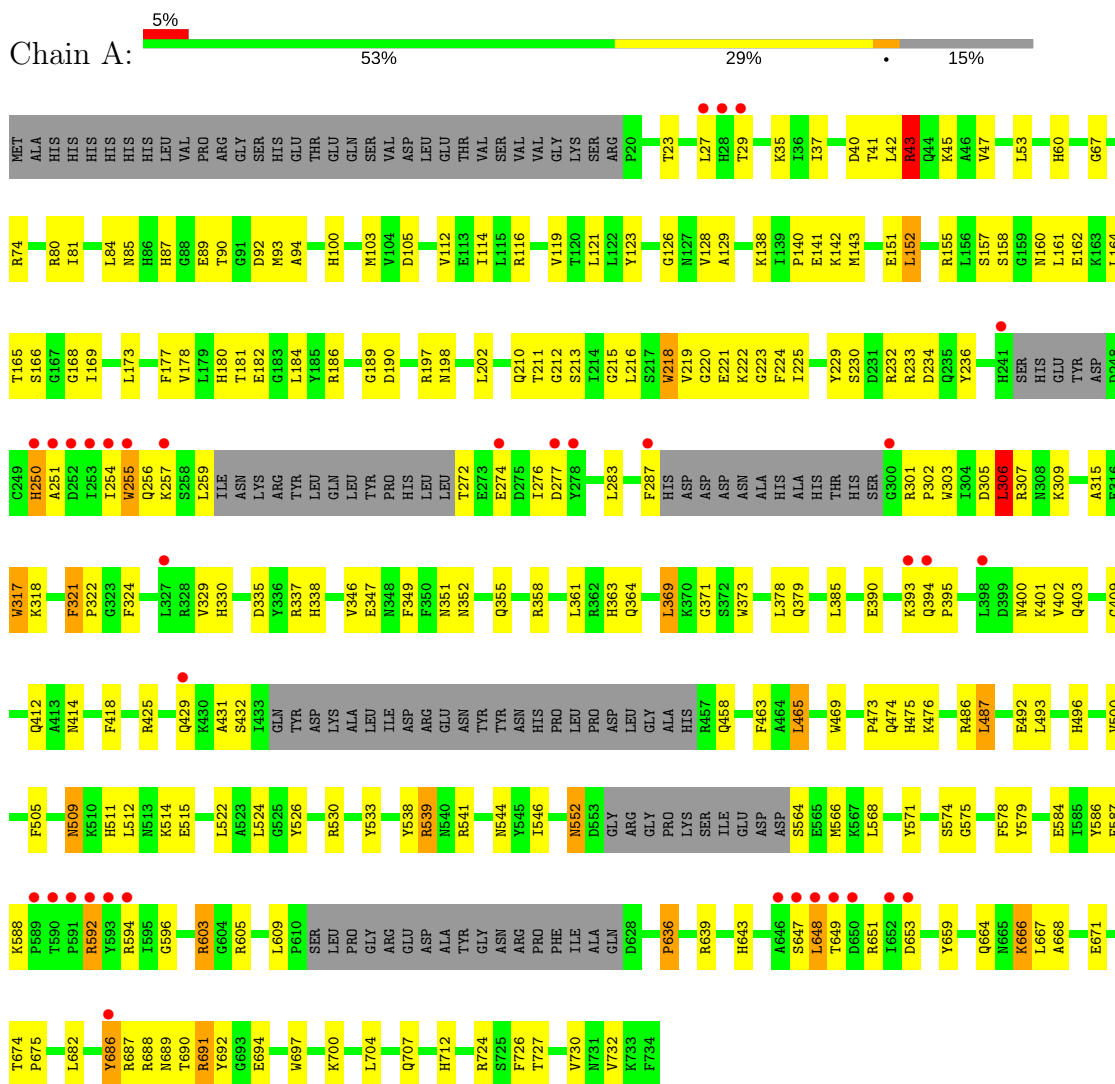
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total 9	O 9	0	0
6	B	2	Total 2	O 2	0	0

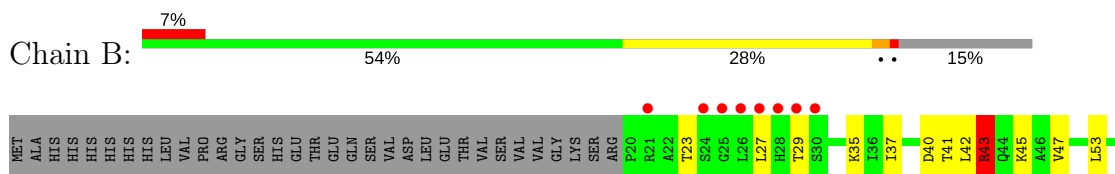
3 Residue-property plots

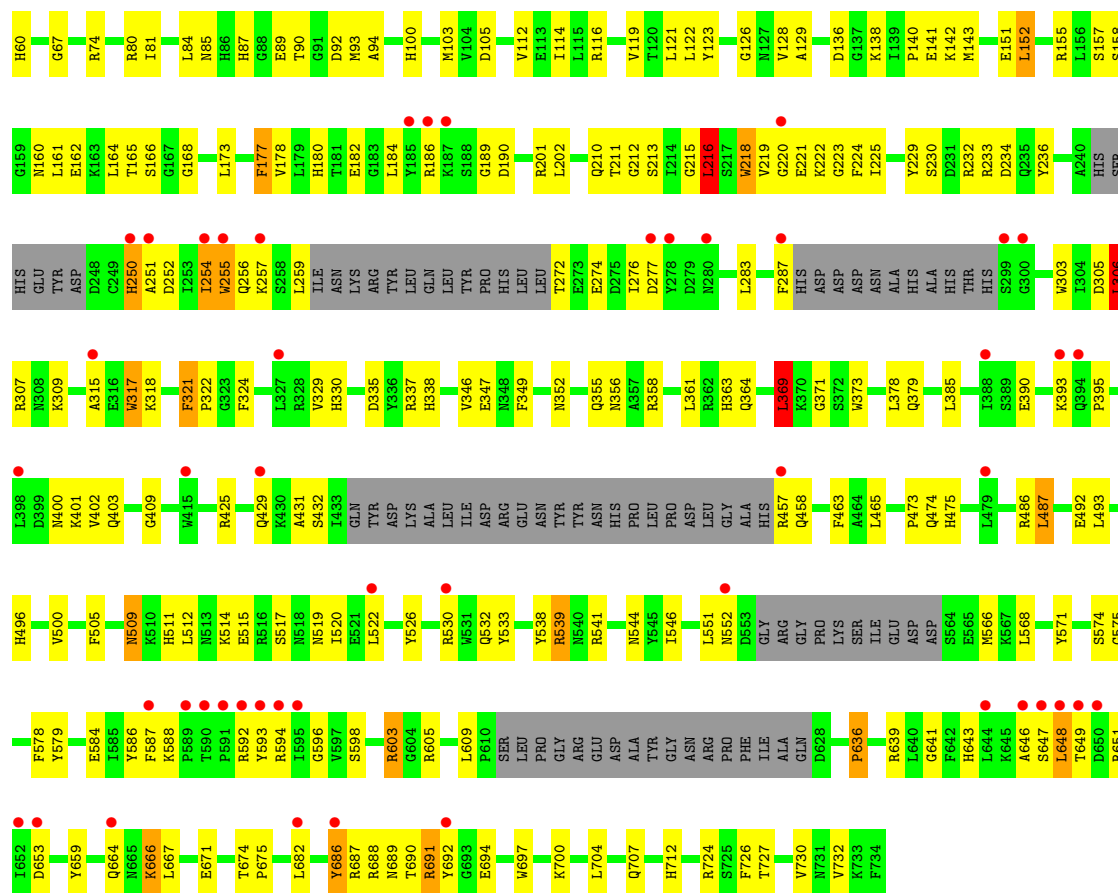
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ZnuD



- Molecule 1: ZnuD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.34Å 156.23Å 158.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.20 49.93 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.93-3.20) 93.4 (49.93-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.270 , 0.305 0.272 , 0.306	Depositor DCC
R_{free} test set	1664 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.040 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10159	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4419e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, C8E, 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	0.41	0/5160	0.76	11/6969 (0.2%)
1	B	0.36	0/5144	0.74	11/6948 (0.2%)
All	All	0.39	0/10304	0.75	22/13917 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	LEU	CA-CB-CG	8.03	133.76	115.30
1	B	369	LEU	CA-CB-CG	7.98	133.66	115.30
1	B	648	LEU	CA-CB-CG	7.76	133.16	115.30
1	A	216	LEU	CB-CG-CD2	7.67	124.04	111.00
1	A	173	LEU	CA-CB-CG	7.23	131.94	115.30
1	A	648	LEU	CA-CB-CG	7.03	131.47	115.30
1	A	43	ARG	CA-CB-CG	6.97	128.73	113.40
1	B	43	ARG	CA-CB-CG	6.86	128.49	113.40
1	B	173	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	539	ARG	CB-CG-CD	6.76	129.16	111.60
1	B	539	ARG	CB-CG-CD	6.57	128.69	111.60
1	B	216	LEU	CB-CG-CD1	6.52	122.09	111.00
1	A	317	TRP	CA-CB-CG	6.43	125.92	113.70
1	B	317	TRP	CA-CB-CG	6.38	125.81	113.70
1	A	306	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	306	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	465	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	465	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	475	HIS	N-CA-C	-5.31	96.67	111.00
1	A	475	HIS	N-CA-C	-5.27	96.76	111.00
1	B	487	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	487	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

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	5044	0	4883	220	0
1	B	5032	0	4868	209	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	24	2	0
4	A	42	0	68	24	0
5	A	5	0	0	3	0
5	B	5	0	0	2	0
6	A	9	0	0	0	0
6	B	2	0	0	1	0
All	All	10159	0	9843	436	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (436) 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:B:143:MET:CG	1:B:219:VAL:HG21	1.65	1.26
1:B:283:LEU:HG	1:B:287:PHE:CE2	1.71	1.25
1:B:283:LEU:CG	1:B:287:PHE:HE2	1.54	1.20
1:A:465:LEU:HD12	4:A:806:C8E:C17	1.72	1.19
1:A:465:LEU:HD12	4:A:806:C8E:H171	1.26	1.12
1:A:143:MET:CG	1:A:219:VAL:HG21	1.80	1.11
1:B:143:MET:HG2	1:B:219:VAL:CG2	1.83	1.08
1:B:255:TRP:CE3	1:B:256:GLN:HG2	1.89	1.06
1:A:143:MET:HG2	1:A:219:VAL:HG21	1.08	1.05
1:B:283:LEU:HG	1:B:287:PHE:HE2	0.92	1.05
1:B:283:LEU:CG	1:B:287:PHE:CE2	2.35	1.03
1:B:283:LEU:O	1:B:287:PHE:HD2	1.42	1.01
1:B:283:LEU:CD1	1:B:287:PHE:CE2	2.44	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MET:HG2	1:B:219:VAL:HG21	1.01	1.00
1:B:593:TYR:CD1	1:B:646:ALA:HB2	1.99	0.97
1:B:593:TYR:CE1	1:B:646:ALA:CB	2.47	0.97
1:A:283:LEU:O	1:A:287:PHE:HD2	1.48	0.96
1:A:256:GLN:HB3	1:A:257:LYS:HB3	1.50	0.94
1:A:493:LEU:HD12	1:A:512:LEU:HD12	1.51	0.92
1:B:593:TYR:CD1	1:B:646:ALA:CB	2.52	0.92
1:B:493:LEU:HD12	1:B:512:LEU:HD12	1.53	0.90
1:B:283:LEU:O	1:B:287:PHE:CD2	2.25	0.90
1:B:60:HIS:CE1	1:B:639:ARG:HH21	1.90	0.90
1:A:143:MET:HG2	1:A:219:VAL:CG2	2.01	0.90
1:B:283:LEU:HD11	1:B:287:PHE:CE2	2.09	0.88
1:A:465:LEU:HD12	4:A:806:C8E:H172	1.51	0.88
1:A:648:LEU:HA	1:A:649:THR:HG22	1.54	0.88
1:A:60:HIS:CE1	1:A:639:ARG:HH21	1.91	0.88
1:B:143:MET:SD	1:B:219:VAL:HG21	2.14	0.87
1:B:648:LEU:HA	1:B:649:THR:HG22	1.55	0.87
1:A:164:LEU:HD11	1:A:184:LEU:HD11	1.57	0.86
1:B:593:TYR:CE1	1:B:646:ALA:HB1	2.10	0.86
1:B:234:ASP:HB2	1:B:306:LEU:HG	1.60	0.83
1:B:47:VAL:HG21	1:B:186:ARG:HD2	1.60	0.83
1:A:530:ARG:HG3	1:A:587:PHE:HE1	1.43	0.82
1:B:283:LEU:HD11	1:B:287:PHE:CZ	2.14	0.82
1:B:493:LEU:CD1	1:B:512:LEU:HD12	2.10	0.82
1:A:648:LEU:HA	1:A:649:THR:CG2	2.09	0.82
1:A:493:LEU:CD1	1:A:512:LEU:HD12	2.09	0.82
1:A:493:LEU:HG	1:A:509:ASN:O	1.79	0.82
1:A:664:GLN:HG2	1:A:712:HIS:HD2	1.45	0.81
1:B:164:LEU:HD11	1:B:184:LEU:HD11	1.61	0.81
1:A:283:LEU:O	1:A:287:PHE:CD2	2.33	0.80
1:B:648:LEU:HA	1:B:649:THR:CG2	2.11	0.80
1:A:234:ASP:HB2	1:A:306:LEU:HG	1.61	0.80
1:B:493:LEU:HG	1:B:509:ASN:O	1.81	0.80
1:B:519:ASN:O	1:B:520:ILE:HG13	1.81	0.80
1:A:158:SER:HB3	1:A:726:PHE:H	1.47	0.79
1:A:47:VAL:HG21	1:A:186:ARG:HD2	1.65	0.77
1:A:168:GLY:O	1:A:169:ILE:HD13	1.85	0.77
1:A:539:ARG:HD3	5:A:807:SO4:O3	1.83	0.77
1:A:42:LEU:HD11	1:A:112:VAL:HG12	1.66	0.77
1:B:593:TYR:HD1	1:B:646:ALA:HB2	1.46	0.77
1:A:469:TRP:HE3	4:A:806:C8E:C4	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASN:HB3	1:A:162:GLU:H	1.51	0.76
1:B:42:LEU:HD11	1:B:112:VAL:HG12	1.66	0.76
1:A:469:TRP:CE3	4:A:806:C8E:H41	2.20	0.76
4:A:806:C8E:H13	4:A:806:C8E:C5	2.15	0.76
1:B:160:ASN:HB3	1:B:162:GLU:H	1.51	0.76
1:B:385:LEU:HD23	1:B:395:PRO:HB3	1.67	0.75
1:A:60:HIS:HD2	1:A:636:PRO:HB3	1.52	0.75
1:A:385:LEU:HD23	1:A:395:PRO:HB3	1.66	0.74
1:A:566:MET:O	1:A:566:MET:HG3	1.88	0.74
1:A:324:PHE:HD1	1:A:363:HIS:HA	1.53	0.74
1:B:324:PHE:HD1	1:B:363:HIS:HA	1.52	0.74
1:A:469:TRP:HE3	4:A:806:C8E:H42	1.54	0.73
1:B:60:HIS:HD2	1:B:636:PRO:HB3	1.54	0.72
1:A:250:HIS:HB2	1:A:254:ILE:HD11	1.71	0.72
1:A:592:ARG:HH21	1:A:649:THR:CG2	2.01	0.72
1:A:60:HIS:CD2	1:A:636:PRO:HB3	2.26	0.71
4:A:806:C8E:H13	4:A:806:C8E:H132	1.70	0.71
1:A:469:TRP:CE3	4:A:806:C8E:C4	2.74	0.71
1:B:158:SER:HB3	1:B:726:PHE:H	1.54	0.71
1:A:143:MET:SD	1:A:219:VAL:HG21	2.31	0.70
1:B:60:HIS:CD2	1:B:636:PRO:HB3	2.26	0.70
1:A:530:ARG:HG3	1:A:587:PHE:CE1	2.27	0.70
1:A:254:ILE:HG21	1:A:393:LYS:NZ	2.08	0.69
1:B:593:TYR:CD1	1:B:646:ALA:HB1	2.27	0.68
1:B:143:MET:SD	1:B:219:VAL:CG2	2.80	0.68
4:A:806:C8E:H13	4:A:806:C8E:H52	1.75	0.68
1:A:210:GLN:NE2	4:A:805:C8E:O12	2.27	0.68
1:B:40:ASP:OD1	1:B:41:THR:N	2.27	0.68
1:A:92:ASP:HB3	1:A:103:MET:HG2	1.76	0.67
1:A:143:MET:SD	1:A:178:VAL:CG2	2.82	0.67
1:A:40:ASP:OD1	1:A:41:THR:N	2.27	0.67
1:B:92:ASP:HB3	1:B:103:MET:HG2	1.77	0.67
1:A:250:HIS:HB2	1:A:254:ILE:CD1	2.26	0.66
1:B:222:LYS:HB2	1:B:317:TRP:HB2	1.76	0.66
1:B:221:GLU:HB3	1:B:222:LYS:HA	1.77	0.66
1:A:324:PHE:CD1	1:A:361:LEU:HD13	2.30	0.66
1:A:255:TRP:CE3	1:A:256:GLN:HG2	2.31	0.66
1:B:143:MET:SD	1:B:178:VAL:CG2	2.84	0.66
1:A:222:LYS:HB2	1:A:317:TRP:HB2	1.76	0.65
1:A:221:GLU:HB3	1:A:222:LYS:HA	1.79	0.65
1:A:105:ASP:OD2	1:A:211:THR:HG21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HG22	1:A:393:LYS:HE3	1.79	0.65
1:B:257:LYS:HE3	1:B:259:LEU:HD11	1.79	0.65
1:B:255:TRP:HE3	1:B:256:GLN:HG2	1.59	0.64
1:B:45:LYS:O	1:B:155:ARG:NH2	2.30	0.64
1:A:257:LYS:HE3	1:A:259:LEU:HD11	1.80	0.64
1:B:324:PHE:CD1	1:B:361:LEU:HD13	2.32	0.64
1:B:505:PHE:HB2	1:B:566:MET:CE	2.28	0.63
1:A:686:TYR:HB3	1:A:697:TRP:HB2	1.80	0.63
1:B:84:LEU:HD13	1:B:87:HIS:HA	1.81	0.63
1:A:256:GLN:CB	1:A:257:LYS:HB3	2.28	0.62
1:A:255:TRP:HB3	1:A:256:GLN:HG3	1.81	0.62
1:A:418:PHE:HE1	4:A:806:C8E:H31	1.65	0.61
1:A:586:TYR:CD1	1:A:596:GLY:HA3	2.35	0.61
1:A:164:LEU:CD1	1:A:184:LEU:HD11	2.29	0.61
1:A:219:VAL:HG12	1:A:220:GLY:N	2.15	0.61
1:B:105:ASP:OD2	1:B:211:THR:HG21	2.01	0.61
1:A:255:TRP:HB2	1:A:393:LYS:HG3	1.82	0.61
1:A:465:LEU:CD1	4:A:806:C8E:H172	2.29	0.61
1:B:80:ARG:NH2	1:B:546:ILE:O	2.34	0.61
1:A:160:ASN:HB3	1:A:162:GLU:N	2.16	0.61
1:A:84:LEU:HD13	1:A:87:HIS:HA	1.81	0.61
1:B:686:TYR:HB3	1:B:697:TRP:HB2	1.81	0.61
1:A:315:ALA:HB3	1:A:329:VAL:HG22	1.83	0.60
1:B:160:ASN:HB3	1:B:162:GLU:N	2.15	0.60
1:B:255:TRP:CE3	1:B:256:GLN:CG	2.77	0.60
1:A:180:HIS:O	1:A:215:GLY:N	2.32	0.60
1:A:80:ARG:NH2	1:A:546:ILE:O	2.35	0.60
1:B:143:MET:CG	1:B:219:VAL:CG2	2.57	0.60
1:B:315:ALA:HB3	1:B:329:VAL:HG22	1.83	0.60
1:B:586:TYR:CD1	1:B:596:GLY:HA3	2.36	0.60
1:B:250:HIS:HB2	1:B:254:ILE:HD11	1.84	0.59
1:B:255:TRP:HB2	1:B:393:LYS:HG3	1.82	0.59
1:A:254:ILE:CG2	1:A:393:LYS:HE3	2.33	0.59
1:A:45:LYS:O	1:A:155:ARG:NH2	2.34	0.59
1:B:143:MET:HG2	1:B:219:VAL:CB	2.32	0.59
1:B:647:SER:HB3	1:B:653:ASP:OD1	2.02	0.59
1:A:233:ARG:HD2	1:A:307:ARG:HG2	1.85	0.58
1:B:157:SER:HB2	1:B:162:GLU:HB3	1.83	0.58
1:B:180:HIS:O	1:B:215:GLY:N	2.32	0.58
1:A:157:SER:HB2	1:A:162:GLU:HB3	1.85	0.58
1:B:225:ILE:HD11	1:B:317:TRP:HZ3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TRP:HB2	4:A:806:C8E:C3	2.34	0.58
1:A:141:GLU:HG2	1:A:224:PHE:CZ	2.38	0.58
1:A:355:GLN:HE21	1:A:379:GLN:HE21	1.52	0.57
1:A:647:SER:HB3	1:A:653:ASP:OD1	2.04	0.57
1:B:219:VAL:HG12	1:B:220:GLY:N	2.18	0.57
4:A:806:C8E:H13	4:A:806:C8E:H51	1.85	0.57
1:B:164:LEU:CD1	1:B:184:LEU:HD11	2.33	0.56
1:A:222:LYS:CB	1:A:317:TRP:HB2	2.36	0.56
1:B:539:ARG:NH1	5:B:802:SO4:O1	2.39	0.56
1:A:539:ARG:HD3	5:A:807:SO4:S	2.46	0.56
1:B:505:PHE:HB2	1:B:566:MET:HE1	1.88	0.56
1:B:168:GLY:HA2	1:B:182:GLU:HA	1.88	0.56
1:B:23:THR:HG23	1:B:87:HIS:HE1	1.70	0.56
1:A:225:ILE:HD11	1:A:317:TRP:HZ3	1.70	0.55
1:B:255:TRP:CD2	1:B:256:GLN:HG2	2.39	0.55
1:B:222:LYS:CB	1:B:317:TRP:HB2	2.35	0.55
1:A:23:THR:HG23	1:A:87:HIS:HE1	1.71	0.55
1:A:168:GLY:HA2	1:A:182:GLU:HA	1.88	0.55
1:A:552:ASN:HD22	1:A:552:ASN:N	2.03	0.55
1:B:141:GLU:HG2	1:B:224:PHE:CZ	2.42	0.55
1:B:355:GLN:HE21	1:B:379:GLN:HE21	1.53	0.55
1:B:664:GLN:HG2	1:B:712:HIS:ND1	2.22	0.55
1:B:539:ARG:HG3	1:B:579:TYR:HB3	1.88	0.55
1:B:283:LEU:CD2	1:B:287:PHE:HE2	2.17	0.54
1:A:165:THR:O	1:A:184:LEU:HD12	2.08	0.54
1:A:469:TRP:HB2	4:A:806:C8E:H32	1.90	0.54
1:A:255:TRP:HE3	1:A:256:GLN:HG2	1.71	0.54
1:A:539:ARG:HG3	1:A:579:TYR:HB3	1.89	0.54
1:A:539:ARG:NH1	5:A:807:SO4:O3	2.38	0.53
1:A:651:ARG:HH12	1:A:689:ASN:H	1.56	0.53
1:B:651:ARG:HH12	1:B:689:ASN:H	1.57	0.53
1:B:321:PHE:HB2	1:B:322:PRO:CD	2.38	0.53
1:A:143:MET:SD	1:A:219:VAL:CG2	2.96	0.53
1:A:321:PHE:HB2	1:A:322:PRO:CD	2.39	0.53
1:A:37:ILE:HB	1:A:112:VAL:HG13	1.90	0.53
1:B:155:ARG:HE	1:B:164:LEU:HD23	1.73	0.53
1:B:218:TRP:HB2	1:B:225:ILE:H	1.74	0.52
1:B:505:PHE:HB2	1:B:566:MET:HE3	1.90	0.52
1:A:155:ARG:HE	1:A:164:LEU:HD23	1.74	0.52
1:A:337[B]:ARG:HG3	1:A:351:ASN:OD1	2.10	0.52
1:B:161:LEU:H	1:B:189:GLY:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:TRP:CE3	1:B:256:GLN:NE2	2.78	0.52
1:B:324:PHE:CD1	1:B:363:HIS:HA	2.38	0.52
1:A:335:ASP:OD2	1:A:337[B]:ARG:NH2	2.43	0.52
1:A:363:HIS:ND1	1:A:364:GLN:O	2.40	0.52
1:B:530:ARG:O	1:B:587:PHE:HD1	1.93	0.52
1:A:225:ILE:HG23	1:A:315:ALA:HB2	1.91	0.52
1:A:161:LEU:H	1:A:189:GLY:H	1.58	0.51
1:B:165:THR:O	1:B:184:LEU:HD12	2.10	0.51
1:B:539:ARG:HA	1:B:578:PHE:O	2.10	0.51
1:A:89:GLU:HG3	1:A:378:LEU:HD12	1.91	0.51
1:B:219:VAL:CG1	1:B:220:GLY:N	2.74	0.51
1:B:89:GLU:HG3	1:B:378:LEU:HD12	1.92	0.51
1:A:465:LEU:CD1	4:A:806:C8E:H171	2.19	0.51
1:B:309:LYS:HB2	1:B:335:ASP:HB3	1.93	0.51
1:A:219:VAL:CG1	1:A:220:GLY:N	2.74	0.51
1:A:67:GLY:HA3	1:A:236:TYR:CD1	2.45	0.51
1:A:74:ARG:HD3	1:A:538:TYR:CE1	2.46	0.51
1:A:592:ARG:HH21	1:A:649:THR:HG22	1.76	0.51
1:A:198:ASN:OD1	3:A:803:GOL:O2	2.27	0.51
1:B:60:HIS:CE1	1:B:639:ARG:NH2	2.71	0.51
1:A:539:ARG:HA	1:A:578:PHE:O	2.11	0.51
1:B:37:ILE:HB	1:B:112:VAL:HG13	1.91	0.51
1:B:588:LYS:HG2	1:B:594:ARG:HB2	1.93	0.51
1:A:373:TRP:CE3	1:A:409:GLY:HA3	2.46	0.50
1:B:363:HIS:ND1	1:B:364:GLN:O	2.38	0.50
1:A:324:PHE:CD1	1:A:363:HIS:HA	2.38	0.50
1:A:255:TRP:CH2	1:A:394:GLN:NE2	2.80	0.50
1:A:259:LEU:HD23	1:A:272:THR:HA	1.93	0.50
1:A:664:GLN:HG2	1:A:712:HIS:CD2	2.36	0.50
1:B:283:LEU:HG	1:B:287:PHE:CD2	2.37	0.50
1:A:166:SER:HB3	1:A:184:LEU:HD13	1.93	0.50
1:A:222:LYS:HD2	1:A:317:TRP:CD1	2.47	0.50
1:A:254:ILE:O	1:A:255:TRP:HD1	1.95	0.50
1:A:648:LEU:O	1:A:648:LEU:HD12	2.12	0.50
1:B:143:MET:HG2	1:B:219:VAL:HG11	1.93	0.50
1:B:355:GLN:NE2	1:B:379:GLN:HE21	2.09	0.50
1:A:588:LYS:HG2	1:A:594:ARG:HB2	1.94	0.50
1:B:574:SER:CB	1:B:609:LEU:HD23	2.42	0.50
1:A:355:GLN:NE2	1:A:379:GLN:HE21	2.08	0.50
1:B:255:TRP:HE3	1:B:256:GLN:HE21	1.55	0.50
1:B:697:TRP:CD1	1:B:730:VAL:HG13	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:TRP:CZ3	1:A:305:ASP:HB2	2.47	0.49
1:A:84:LEU:HD11	1:A:123:TYR:CD1	2.46	0.49
1:B:225:ILE:HG23	1:B:315:ALA:HB2	1.93	0.49
1:B:85:ASN:HB2	1:B:90:THR:HG22	1.94	0.49
4:A:806:C8E:C1	4:A:806:C8E:C5	2.85	0.49
4:A:806:C8E:C1	4:A:806:C8E:H132	2.40	0.49
1:B:143:MET:SD	1:B:178:VAL:HG22	2.53	0.49
1:B:505:PHE:HB3	1:B:568:LEU:HD13	1.93	0.49
1:B:522:LEU:O	1:B:522:LEU:HD12	2.12	0.49
1:B:121:LEU:O	1:B:425:ARG:HD2	2.13	0.49
1:B:166:SER:HB3	1:B:184:LEU:HD13	1.93	0.49
1:A:221:GLU:CB	1:A:222:LYS:HA	2.42	0.49
1:B:539:ARG:CG	1:B:579:TYR:HB3	2.42	0.49
1:A:143:MET:SD	1:A:178:VAL:HG22	2.52	0.49
1:B:84:LEU:HD11	1:B:123:TYR:CD1	2.48	0.49
1:A:539:ARG:CG	1:A:579:TYR:HB3	2.43	0.49
1:A:574:SER:CB	1:A:609:LEU:HD23	2.43	0.49
1:B:373:TRP:CE3	1:B:409:GLY:HA3	2.48	0.49
1:A:505:PHE:HB3	1:A:568:LEU:HD13	1.95	0.49
1:A:667:LEU:HB2	1:A:671:GLU:HB2	1.94	0.49
1:B:103:MET:SD	1:B:232:ARG:HD3	2.53	0.49
1:A:160:ASN:OD1	3:A:804:GOL:H12	2.12	0.49
1:B:574:SER:HB2	1:B:609:LEU:HD23	1.94	0.49
1:A:697:TRP:CD1	1:A:730:VAL:HG13	2.47	0.48
1:A:469:TRP:CE3	4:A:806:C8E:H42	2.41	0.48
1:B:259:LEU:HD23	1:B:272:THR:HA	1.95	0.48
1:B:574:SER:OG	1:B:575:GLY:N	2.45	0.48
1:A:103:MET:SD	1:A:232:ARG:HD3	2.53	0.48
1:A:330:HIS:HB3	1:A:358:ARG:HG3	1.93	0.48
1:A:574:SER:OG	1:A:575:GLY:N	2.45	0.48
1:B:222:LYS:HD2	1:B:317:TRP:CD1	2.47	0.48
1:A:85:ASN:HB2	1:A:90:THR:HG22	1.95	0.48
1:A:486:ARG:HB3	1:A:515:GLU:HB2	1.95	0.48
1:A:574:SER:HB2	1:A:609:LEU:HD23	1.96	0.48
1:A:274:GLU:HA	1:A:276:ILE:HG22	1.95	0.48
1:B:177:PHE:CE1	1:B:216:LEU:HD21	2.49	0.48
1:B:254:ILE:O	1:B:255:TRP:HD1	1.96	0.48
1:A:309:LYS:HB2	1:A:335:ASP:HB3	1.95	0.48
1:B:274:GLU:HA	1:B:276:ILE:HG22	1.95	0.48
1:A:143:MET:SD	1:A:178:VAL:HG23	2.53	0.47
1:A:465:LEU:CD1	4:A:806:C8E:C17	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ARG:HD3	1:B:538:TYR:CE1	2.48	0.47
1:B:303:TRP:CZ3	1:B:305:ASP:HB2	2.49	0.47
1:B:330:HIS:HB3	1:B:358:ARG:HG3	1.95	0.47
1:A:121:LEU:O	1:A:425:ARG:HD2	2.14	0.47
1:B:639:ARG:HD2	1:B:659:TYR:CD1	2.50	0.47
1:A:697:TRP:HD1	1:A:730:VAL:HG13	1.80	0.47
1:B:403:GLN:O	1:B:429:GLN:HA	2.14	0.47
1:B:67:GLY:HA3	1:B:236:TYR:CD1	2.49	0.47
1:B:60:HIS:HE1	1:B:639:ARG:HH21	1.52	0.47
1:A:81:ILE:HG22	1:A:129:ALA:HB3	1.97	0.47
1:A:403:GLN:O	1:A:429:GLN:HA	2.14	0.46
1:A:53:LEU:HD22	1:A:114:ILE:HD11	1.97	0.46
1:A:255:TRP:HA	1:A:256:GLN:HA	1.52	0.46
1:A:390:GLU:HG2	1:A:395:PRO:HG3	1.96	0.46
1:B:143:MET:SD	1:B:178:VAL:HG23	2.55	0.46
1:B:29:THR:OG1	1:B:119:VAL:HG13	2.15	0.46
1:B:93:MET:SD	1:B:352:ASN:HB2	2.56	0.46
1:B:493:LEU:HD11	1:B:512:LEU:HD12	1.93	0.46
1:A:690:THR:HG23	1:A:691:ARG:O	2.15	0.46
1:B:648:LEU:HD12	1:B:648:LEU:O	2.14	0.46
1:B:648:LEU:CA	1:B:649:THR:CG2	2.89	0.46
1:A:538:TYR:O	1:A:579:TYR:HA	2.16	0.46
1:A:60:HIS:CE1	1:A:639:ARG:NH2	2.71	0.46
1:B:651:ARG:HA	1:B:687:ARG:HB3	1.98	0.46
1:B:390:GLU:HG2	1:B:395:PRO:HG3	1.98	0.46
1:A:682:LEU:HD22	1:A:704:LEU:HD11	1.97	0.46
1:B:255:TRP:CZ3	1:B:256:GLN:NE2	2.84	0.46
1:B:690:THR:HG23	1:B:691:ARG:O	2.16	0.46
1:A:190:ASP:HB3	1:A:202:LEU:O	2.16	0.46
1:A:301:ARG:HA	1:A:302:PRO:HD3	1.83	0.46
1:B:667:LEU:HB2	1:B:671:GLU:HB2	1.96	0.46
1:A:74:ARG:HB3	1:A:538:TYR:CE2	2.51	0.46
1:A:639:ARG:HD2	1:A:659:TYR:CD1	2.50	0.46
1:B:222:LYS:HB2	1:B:317:TRP:CB	2.45	0.46
1:B:473:PRO:HA	1:B:474:GLN:HA	1.51	0.46
1:B:538:TYR:O	1:B:579:TYR:HA	2.16	0.46
1:A:651:ARG:HA	1:A:687:ARG:HB3	1.97	0.46
1:A:29:THR:OG1	1:A:119:VAL:HG13	2.16	0.45
1:A:686:TYR:HD1	1:A:687:ARG:N	2.14	0.45
1:B:218:TRP:O	1:B:219:VAL:HG23	2.15	0.45
1:B:697:TRP:HD1	1:B:730:VAL:HG13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:MET:SD	1:A:352:ASN:HB2	2.56	0.45
1:A:674:THR:HG22	1:A:675:PRO:O	2.16	0.45
1:B:486:ARG:HB3	1:B:515:GLU:HB2	1.97	0.45
1:A:473:PRO:HA	1:A:474:GLN:HA	1.52	0.45
1:B:53:LEU:HD22	1:B:114:ILE:HD11	1.99	0.45
1:B:178:VAL:O	1:B:216:LEU:HA	2.15	0.45
1:B:143:MET:HG2	1:B:219:VAL:CG1	2.45	0.45
1:A:418:PHE:CE1	4:A:806:C8E:H31	2.47	0.45
1:B:221:GLU:CB	1:B:222:LYS:HA	2.40	0.45
1:B:566:MET:HG3	1:B:566:MET:O	2.16	0.45
1:A:152:LEU:O	1:A:732:VAL:N	2.46	0.45
1:B:682:LEU:HD22	1:B:704:LEU:HD11	1.97	0.45
1:A:218:TRP:CE3	1:A:219:VAL:O	2.70	0.45
1:A:526:TYR:HB3	1:A:533:TYR:CE2	2.52	0.45
1:A:60:HIS:HE1	1:A:639:ARG:HH21	1.53	0.45
1:B:219:VAL:CG1	1:B:220:GLY:H	2.29	0.45
1:B:674:THR:HG22	1:B:675:PRO:O	2.17	0.45
1:A:221:GLU:OE1	1:A:318:LYS:HE2	2.17	0.44
1:B:347:GLU:HB3	1:B:500:VAL:HG11	1.99	0.44
1:B:35:LYS:HE3	1:B:584:GLU:OE2	2.18	0.44
1:B:74:ARG:HB3	1:B:538:TYR:CE2	2.52	0.44
1:A:74:ARG:HH11	1:A:116:ARG:HD3	1.82	0.44
1:B:74:ARG:HH11	1:B:116:ARG:CD	2.31	0.44
1:B:686:TYR:HD1	1:B:687:ARG:N	2.15	0.44
1:A:74:ARG:HH11	1:A:116:ARG:CD	2.31	0.44
1:A:694:GLU:O	1:A:732:VAL:HA	2.18	0.44
1:B:81:ILE:HG22	1:B:129:ALA:HB3	2.00	0.44
1:B:152:LEU:O	1:B:732:VAL:N	2.46	0.44
1:B:539:ARG:HD2	1:B:541:ARG:HH12	1.83	0.44
1:A:321:PHE:CD1	1:A:321:PHE:N	2.85	0.44
1:A:43:ARG:HD2	1:A:151:GLU:OE1	2.18	0.44
1:A:160:ASN:H	1:A:161:LEU:HA	1.83	0.44
1:A:84:LEU:HD11	1:A:123:TYR:CE1	2.53	0.44
1:A:346:VAL:HG11	1:A:349:PHE:CE1	2.53	0.44
1:A:493:LEU:HD11	1:A:512:LEU:HD12	1.95	0.44
1:B:43:ARG:HD2	1:B:151:GLU:OE1	2.17	0.44
1:B:694:GLU:O	1:B:732:VAL:HA	2.18	0.44
1:B:122:LEU:O	1:B:358:ARG:NH2	2.32	0.43
1:B:335:ASP:OD2	1:B:337:ARG:NH2	2.50	0.43
1:A:324:PHE:CE1	1:A:361:LEU:CD1	3.02	0.43
1:A:324:PHE:CE1	1:A:361:LEU:HD13	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ARG:HD2	1:B:307:ARG:HD3	2.00	0.43
1:A:222:LYS:HB2	1:A:317:TRP:CB	2.45	0.43
1:A:469:TRP:CB	4:A:806:C8E:H32	2.47	0.43
1:B:517:SER:OG	1:B:519:ASN:OD1	2.36	0.43
1:B:401:LYS:HB3	1:B:432:SER:HB2	2.00	0.43
1:B:84:LEU:HD11	1:B:123:TYR:CE1	2.52	0.43
1:B:221:GLU:OE1	1:B:318:LYS:HE2	2.19	0.43
1:B:324:PHE:CE1	1:B:361:LEU:HD13	2.54	0.43
1:B:690:THR:OG1	1:B:691:ARG:N	2.52	0.43
1:A:347:GLU:HB3	1:A:500:VAL:HG11	1.99	0.43
1:B:94:ALA:HA	1:B:100:HIS:HB2	2.00	0.43
1:B:539:ARG:HD3	1:B:539:ARG:HH11	1.63	0.43
1:A:210:GLN:O	1:A:232:ARG:HA	2.19	0.43
1:A:35:LYS:HE3	1:A:584:GLU:OE2	2.19	0.43
1:A:648:LEU:CA	1:A:649:THR:CG2	2.89	0.43
1:B:210:GLN:O	1:B:232:ARG:HA	2.19	0.43
1:B:321:PHE:N	1:B:321:PHE:CD1	2.86	0.43
1:A:213:SER:HA	1:A:229:TYR:O	2.19	0.43
1:A:220:GLY:N	1:A:223:GLY:O	2.52	0.43
1:A:552:ASN:ND2	1:A:552:ASN:O	2.52	0.43
1:A:492:GLU:HA	1:A:571:TYR:CD2	2.54	0.43
1:A:592:ARG:NH2	1:A:649:THR:CG2	2.77	0.43
1:B:700:LYS:HB3	1:B:727:THR:HB	2.01	0.43
1:A:126:GLY:O	1:A:128:VAL:HG13	2.19	0.42
1:A:254:ILE:HG21	1:A:393:LYS:HZ1	1.80	0.42
1:A:458:GLN:OE1	1:A:458:GLN:N	2.53	0.42
1:B:190:ASP:O	1:B:201:ARG:HD3	2.19	0.42
1:A:94:ALA:HA	1:A:100:HIS:HB2	2.02	0.42
1:A:700:LYS:HB3	1:A:727:THR:HB	2.02	0.42
1:B:37:ILE:HB	1:B:112:VAL:CG1	2.50	0.42
1:B:643:HIS:HE1	1:B:659:TYR:OH	2.02	0.42
1:A:512:LEU:HD13	1:A:546:ILE:HD13	2.02	0.42
1:B:160:ASN:H	1:B:161:LEU:HA	1.84	0.42
1:B:603:ARG:NH2	1:B:666:LYS:HE3	2.35	0.42
1:A:530:ARG:HA	1:A:530:ARG:HD2	1.95	0.42
1:B:346:VAL:HG11	1:B:349:PHE:CE1	2.55	0.42
1:B:526:TYR:HB3	1:B:533:TYR:CE2	2.54	0.42
1:A:212:GLY:O	1:A:230:SER:HA	2.20	0.42
1:B:212:GLY:O	1:B:230:SER:HA	2.20	0.42
1:A:140:PRO:C	1:A:142:LYS:H	2.23	0.42
1:A:218:TRP:HE3	1:A:219:VAL:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:O	1:A:524:LEU:HD12	2.20	0.42
1:B:274:GLU:HG2	1:B:277:ASP:HB3	2.02	0.42
1:B:306:LEU:HB2	1:B:338:HIS:HB3	2.01	0.42
1:B:593:TYR:HE1	1:B:646:ALA:CB	2.20	0.42
1:A:220:GLY:HA2	1:A:221:GLU:C	2.40	0.42
1:A:306:LEU:HB2	1:A:338:HIS:HB3	2.02	0.42
1:B:252:ASP:O	1:B:254:ILE:HG13	2.19	0.42
1:B:598:SER:O	1:B:641:GLY:N	2.36	0.42
1:A:138:LYS:HE2	1:A:213:SER:OG	2.19	0.42
1:A:60:HIS:HE1	1:A:639:ARG:NH2	2.16	0.42
1:A:274:GLU:HG2	1:A:277:ASP:HB3	2.02	0.41
1:A:27:LEU:HD22	1:A:371:GLY:HA2	2.02	0.41
1:A:37:ILE:HB	1:A:112:VAL:CG1	2.50	0.41
1:A:401:LYS:HB3	1:A:432:SER:HB2	2.01	0.41
1:A:539:ARG:HD2	1:A:541:ARG:HH12	1.84	0.41
1:A:169:ILE:N	1:A:181:THR:O	2.45	0.41
1:A:42:LEU:HD11	1:A:112:VAL:CG1	2.45	0.41
1:B:60:HIS:HE1	1:B:639:ARG:NH2	2.15	0.41
1:A:690:THR:OG1	1:A:691:ARG:N	2.53	0.41
1:B:136:ASP:CG	1:B:138:LYS:HD3	2.40	0.41
1:B:492:GLU:HA	1:B:571:TYR:CD2	2.55	0.41
1:A:552:ASN:ND2	1:A:552:ASN:N	2.69	0.41
1:B:324:PHE:CE1	1:B:361:LEU:CD1	3.03	0.41
1:B:400:ASN:HD22	1:B:402:VAL:HG23	1.85	0.41
1:B:532:GLN:O	1:B:586:TYR:N	2.44	0.41
1:A:259:LEU:HB2	1:A:272:THR:HA	2.03	0.41
1:B:27:LEU:HD22	1:B:371:GLY:HA2	2.02	0.41
1:A:458:GLN:HB3	1:A:487:LEU:HD21	2.03	0.41
1:A:530:ARG:O	1:A:587:PHE:HD1	2.03	0.41
1:B:190:ASP:HB3	1:B:202:LEU:O	2.21	0.41
1:A:651:ARG:NH1	1:A:688:ARG:HA	2.36	0.41
1:B:651:ARG:NH1	1:B:688:ARG:HA	2.36	0.41
1:A:401:LYS:HD3	1:A:432:SER:HB2	2.03	0.41
1:A:400:ASN:HD22	1:A:402:VAL:HG23	1.85	0.40
1:A:429:GLN:HE21	1:A:431:ALA:HB2	1.86	0.40
1:A:603:ARG:NH2	1:A:666:LYS:HE3	2.35	0.40
1:A:643:HIS:HE1	1:A:659:TYR:OH	2.03	0.40
1:A:667:LEU:HD12	1:A:668:ALA:O	2.22	0.40
1:A:724:ARG:HD3	1:A:726:PHE:CE1	2.56	0.40
1:B:140:PRO:C	1:B:142:LYS:H	2.25	0.40
1:B:356:ASN:ND2	6:B:901:HOH:O	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LEU:HD12	1:B:369:LEU:O	2.21	0.40
1:A:412:GLN:NE2	1:A:414:ASN:HD21	2.19	0.40
1:B:126:GLY:O	1:B:128:VAL:HG13	2.21	0.40
1:B:223:GLY:HA3	1:B:317:TRP:HA	2.02	0.40
1:B:486:ARG:HH21	1:B:515:GLU:CD	2.25	0.40
1:A:161:LEU:N	1:A:189:GLY:H	2.19	0.40
1:B:259:LEU:HB2	1:B:272:THR:HA	2.03	0.40
1:B:539:ARG:HD3	5:B:802:SO4:S	2.62	0.40
1:B:724:ARG:HD3	1:B:726:PHE:CE1	2.57	0.40
4:A:806:C8E:C1	4:A:806:C8E:H52	2.48	0.40
1:B:429:GLN:HE21	1:B:431:ALA:HB2	1.86	0.40
1:B:551:LEU:HA	1:B:551:LEU:HD23	1.79	0.40
1:B:213:SER:HA	1:B:229:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	622/748 (83%)	569 (92%)	51 (8%)	2 (0%)	43	79
1	B	621/748 (83%)	569 (92%)	50 (8%)	2 (0%)	43	79
All	All	1243/1496 (83%)	1138 (92%)	101 (8%)	4 (0%)	43	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ALA
1	B	251	ALA
1	A	636	PRO
1	B	636	PRO

5.3.2 Protein sidechains ⓘ

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	527/625 (84%)	500 (95%)	27 (5%)	26	64
1	B	526/625 (84%)	497 (94%)	29 (6%)	24	62
All	All	1053/1250 (84%)	997 (95%)	56 (5%)	25	62

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	152	LEU
1	A	177	PHE
1	A	197	ARG
1	A	218	TRP
1	A	250	HIS
1	A	255	TRP
1	A	306	LEU
1	A	321	PHE
1	A	369	LEU
1	A	463	PHE
1	A	496	HIS
1	A	509	ASN
1	A	511	HIS
1	A	514	LYS
1	A	522	LEU
1	A	544	ASN
1	A	552	ASN
1	A	564	SER
1	A	592	ARG
1	A	603	ARG
1	A	605	ARG
1	A	666	LYS
1	A	686	TYR
1	A	691	ARG
1	A	692	TYR
1	A	707	GLN

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Mol	Chain	Res	Type
1	B	43	ARG
1	B	152	LEU
1	B	177	PHE
1	B	216	LEU
1	B	218	TRP
1	B	250	HIS
1	B	254	ILE
1	B	255	TRP
1	B	306	LEU
1	B	321	PHE
1	B	369	LEU
1	B	457	ARG
1	B	458	GLN
1	B	463	PHE
1	B	487	LEU
1	B	496	HIS
1	B	509	ASN
1	B	511	HIS
1	B	514	LYS
1	B	544	ASN
1	B	552	ASN
1	B	592	ARG
1	B	603	ARG
1	B	605	ARG
1	B	666	LYS
1	B	686	TYR
1	B	691	ARG
1	B	692	TYR
1	B	707	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	355	GLN
1	A	400	ASN
1	A	403	GLN
1	A	412	GLN
1	A	429	GLN
1	A	549	GLN
1	A	552	ASN
1	A	630	GLN

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Mol	Chain	Res	Type
1	A	685	ASN
1	A	712	HIS
1	B	60	HIS
1	B	355	GLN
1	B	394	GLN
1	B	400	ASN
1	B	403	GLN
1	B	412	GLN
1	B	549	GLN
1	B	630	GLN
1	B	685	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	802	-	5,5,5	0.36	0	5,5,5	0.24	0
3	GOL	A	803	-	5,5,5	0.41	0	5,5,5	0.15	0
3	GOL	A	804	-	5,5,5	0.39	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	C8E	A	805	-	20,20,20	0.32	0	19,19,19	0.48	0
4	C8E	A	806	-	20,20,20	0.33	0	19,19,19	0.46	0
5	SO4	A	807	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	802	-	4,4,4	0.15	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	802	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	C8E	A	805	-	-	0/18/18/18	0/0/0/0
4	C8E	A	806	-	-	0/18/18/18	0/0/0/0
5	SO4	A	807	-	-	0/0/0/0	0/0/0/0
5	SO4	B	802	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	GOL	1	0
3	A	804	GOL	1	0
4	A	805	C8E	1	0
4	A	806	C8E	23	0
5	A	807	SO4	3	0
5	B	802	SO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	635/748 (84%)	0.16	35 (5%) 25 14	43, 87, 164, 259	0
1	B	635/748 (84%)	0.49	56 (8%) 10 5	94, 137, 213, 273	0
All	All	1270/1496 (84%)	0.33	91 (7%) 15 9	43, 119, 195, 273	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	647	SER	7.4
1	B	28	HIS	6.5
1	B	29	THR	6.4
1	A	591	PRO	6.0
1	B	646	ALA	5.5
1	B	593	TYR	5.0
1	B	591	PRO	4.9
1	B	429	GLN	4.8
1	B	25	GLY	4.7
1	B	26	LEU	4.6
1	A	29	THR	4.6
1	A	647	SER	4.4
1	A	241	HIS	4.3
1	A	27	LEU	4.3
1	A	250	HIS	4.3
1	B	590	THR	4.2
1	B	649	THR	4.0
1	B	457	ARG	3.9
1	B	287	PHE	3.8
1	B	652	ILE	3.8
1	A	254	ILE	3.7
1	B	648	LEU	3.7
1	A	649	THR	3.7
1	B	255	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	589	PRO	3.6
1	A	590	THR	3.5
1	B	254	ILE	3.5
1	B	327	LEU	3.5
1	B	27	LEU	3.5
1	A	646	ALA	3.4
1	A	287	PHE	3.4
1	B	300	GLY	3.3
1	B	587	PHE	3.3
1	A	394	GLN	3.3
1	A	277	ASP	3.3
1	B	653	ASP	3.3
1	B	592	ARG	3.3
1	B	24	SER	3.3
1	B	299	SER	3.2
1	A	650	ASP	3.0
1	A	251	ALA	3.0
1	B	250	HIS	3.0
1	A	652	ILE	3.0
1	A	327	LEU	3.0
1	A	300	GLY	2.9
1	A	398	LEU	2.9
1	B	277	ASP	2.9
1	B	21	ARG	2.8
1	B	682	LEU	2.8
1	B	644	LEU	2.7
1	B	185	TYR	2.7
1	B	30	SER	2.7
1	B	595	ILE	2.7
1	B	650	ASP	2.7
1	A	429	GLN	2.7
1	B	186	ARG	2.7
1	A	592	ARG	2.7
1	A	593	TYR	2.6
1	B	251	ALA	2.6
1	B	686	TYR	2.6
1	B	530	ARG	2.6
1	B	315	ALA	2.6
1	A	255	TRP	2.6
1	B	394	GLN	2.6
1	A	653	ASP	2.6
1	B	187	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	257	LYS	2.5
1	A	28	HIS	2.5
1	A	393	LYS	2.5
1	B	594	ARG	2.4
1	B	479	LEU	2.4
1	B	220	GLY	2.4
1	A	278	TYR	2.3
1	B	692	TYR	2.3
1	A	253	ILE	2.3
1	A	252	ASP	2.3
1	A	686	TYR	2.3
1	A	594	ARG	2.3
1	B	415	TRP	2.3
1	B	280	ASN	2.3
1	A	648	LEU	2.2
1	B	552	ASN	2.2
1	B	398	LEU	2.2
1	A	257	LYS	2.2
1	A	274	GLU	2.2
1	B	388	ILE	2.2
1	B	278	TYR	2.1
1	B	393	LYS	2.1
1	B	664	GLN	2.1
1	B	522	LEU	2.0
1	A	589	PRO	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, 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(\AA^2)	Q<0.9
5	SO4	B	802	5/5	0.61	0.23	173,176,176,177	0
3	GOL	A	803	6/6	0.62	0.74	92,113,117,123	0
3	GOL	A	802	6/6	0.67	0.66	118,132,135,137	0
3	GOL	A	804	6/6	0.70	0.82	97,104,112,113	0
5	SO4	A	807	5/5	0.74	0.26	157,158,162,169	0
4	C8E	A	806	21/21	0.86	0.52	80,98,130,132	0
4	C8E	A	805	21/21	0.89	0.32	39,92,137,142	0
2	ZN	A	801	1/1	0.93	0.34	127,127,127,127	0
2	ZN	B	801	1/1	0.95	0.20	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.