



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:06 AM UTC

PDB ID : 3VE2 / pdb_00003ve2
Title : The 2.1 angstrom crystal structure of Transferrin binding protein B (TbpB) from serogroup B M982 *Neisseria meningitidis*
Authors : Calmettes, C.; Moraes, T.F.
Deposited on : 2012-01-06
Resolution : 2.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

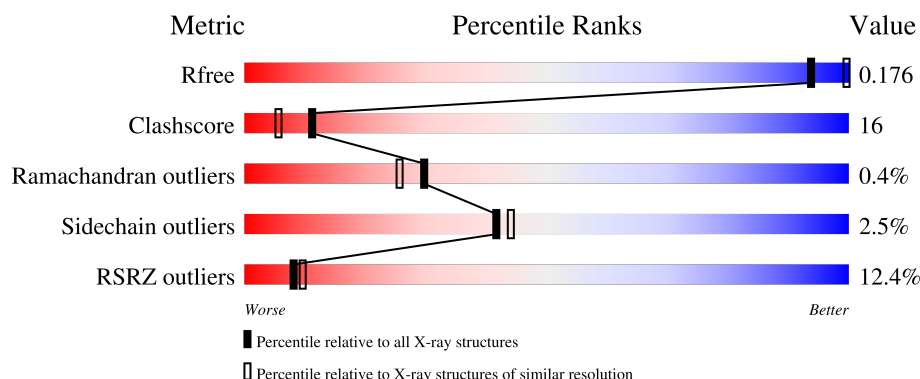
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	658	10% 58% 19% • 22%
1	B	658	9% 58% 19% • 21%

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	GOL	A	704	-	-	X	-
2	GOL	A	705	-	-	X	-
2	GOL	B	701	-	-	X	-
2	GOL	B	702	-	-	X	-
2	GOL	B	703	-	-	X	-
4	ACT	A	708	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8868 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.

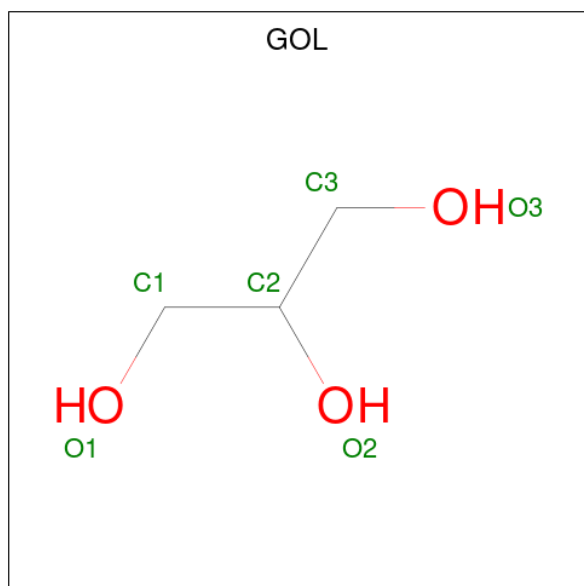
- Molecule 1 is a protein called Transferrin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	2	0
			4057	2557	687	806	7			
1	B	519	Total	C	N	O	S	0	2	0
			4087	2571	695	814	7			

There are 4 discrepancies between the modelled and reference sequences:

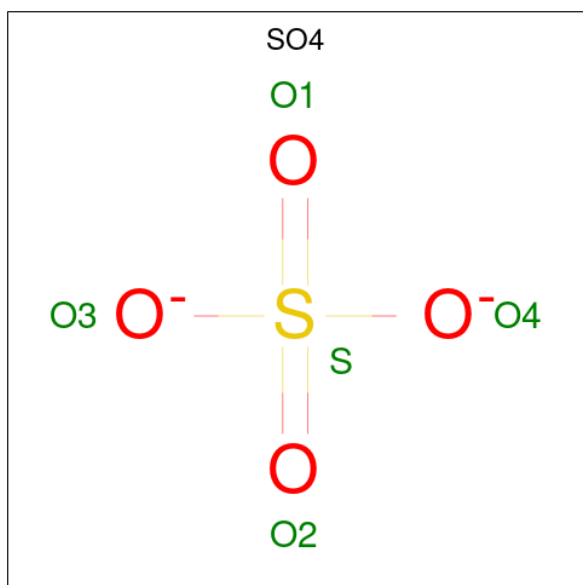
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q09057
A	35	SER	-	expression tag	UNP Q09057
B	34	GLY	-	expression tag	UNP Q09057
B	35	SER	-	expression tag	UNP Q09057

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



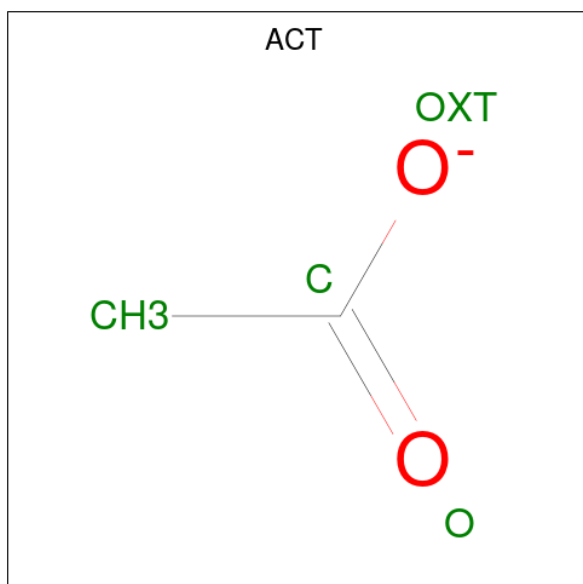
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	299	Total 299	O 299	0	0
6	B	319	Total 319	O 319	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	46.60Å 149.34Å 199.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.38 – 2.14 45.38 – 2.14	Depositor EDS
% Data completeness (in resolution range)	93.4 (45.38-2.14) 93.4 (45.38-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.171 , 0.209 0.171 , 0.176	Depositor DCC
R_{free} test set	3667 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8868	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.49	0/4147	0.83	4/5573 (0.1%)
1	B	0.52	1/4176 (0.0%)	0.82	4/5611 (0.1%)
All	All	0.50	1/8323 (0.0%)	0.82	8/11184 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	HIS	C-N	5.26	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	NE-CZ-NH1	-7.38	114.12	121.50
1	A	330	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	B	321	GLY	CA-C-N	6.51	126.01	119.24
1	B	321	GLY	C-N-CA	6.51	126.01	119.24
1	A	321	GLY	CA-C-N	6.31	125.80	119.24
1	A	321	GLY	C-N-CA	6.31	125.80	119.24
1	B	330	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	B	330	ARG	CD-NE-CZ	5.04	131.45	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ASN	Peptide

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	4057	0	3902	131	0
1	B	4087	0	3927	132	0
2	A	36	0	48	19	0
2	B	30	0	40	19	0
3	A	5	0	0	0	0
3	B	30	0	0	1	0
4	A	4	0	3	5	0
5	B	1	0	0	0	0
6	A	299	0	0	14	0
6	B	319	0	0	16	0
All	All	8868	0	7920	264	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 16.

All (264) 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:46:ARG:HH22	2:B:702:GOL:H32	1.14	1.09
1:B:302:GLU:HB3	1:B:303:THR:CA	1.82	1.07
1:A:46:ARG:HH22	2:A:704:GOL:H32	1.19	1.05
1:B:302:GLU:CB	1:B:303:THR:HA	1.87	1.04
1:B:615:GLU:O	1:B:615:GLU:HG2	1.57	1.02
1:B:302:GLU:HB3	1:B:303:THR:HA	1.03	1.01
1:B:438:THR:HG22	1:B:439:ARG:H	1.29	0.97
1:A:438:THR:HG22	1:A:439:ARG:H	1.29	0.96
1:A:595:THR:N	1:A:618:PHE:HE2	1.62	0.96
1:A:46:ARG:HH12	2:A:704:GOL:H12	1.35	0.91
2:A:701:GOL:H12	6:B:888:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201[B]:ILE:HG22	1:A:202:ILE:HG13	1.52	0.90
1:B:46:ARG:HH12	2:B:702:GOL:H12	1.37	0.89
1:A:299:LYS:HA	1:A:304:LYS:HE2	1.54	0.88
2:B:702:GOL:H31	6:B:847:HOH:O	1.75	0.86
1:B:73:LEU:HD12	1:B:74:PRO:HD2	1.59	0.83
1:A:554:ASN:H	1:A:620:LEU:HD21	1.44	0.82
1:B:615:GLU:HA	1:B:616:SER:C	2.05	0.82
1:B:612:LYS:HE2	1:B:636:ASP:H	1.44	0.82
1:A:349:LYS:HG2	2:A:705:GOL:H31	1.60	0.81
1:B:117:ASN:OD1	1:B:120:ASN:HB3	1.81	0.80
1:A:46:ARG:NH2	2:A:704:GOL:H32	1.97	0.80
1:A:487:LEU:HD13	1:A:490:LEU:HD12	1.63	0.80
1:B:487:LEU:HD13	1:B:490:LEU:HD12	1.65	0.79
1:A:595:THR:N	1:A:618:PHE:CE2	2.49	0.78
1:B:554:ASN:HB2	1:B:676:SER:HB3	1.63	0.78
1:A:554:ASN:HB2	1:A:676:SER:HB3	1.64	0.78
1:B:102:SER:HB2	1:B:105:LEU:HD22	1.64	0.77
1:A:648:GLU:OE2	1:A:648:GLU:N	2.15	0.77
1:A:41:TYR:CE1	1:A:73:LEU:HD13	2.20	0.76
1:B:46:ARG:NH2	2:B:702:GOL:H32	1.98	0.75
1:A:553:ALA:HB2	1:A:557:SER:HA	1.68	0.75
1:B:553:ALA:HB2	1:B:557:SER:HA	1.69	0.75
1:B:349:LYS:H	2:B:704:GOL:H2	1.52	0.74
1:A:211:ARG:HH21	4:A:708:ACT:C	2.00	0.74
1:B:153:LYS:NZ	2:B:701:GOL:H32	2.02	0.73
1:A:394:ILE:O	1:A:394:ILE:HG12	1.88	0.73
1:B:612:LYS:HE2	1:B:636:ASP:N	2.03	0.73
1:B:589:GLU:C	1:B:594:GLN:HG3	2.15	0.71
1:A:613:THR:HG23	1:A:633:ILE:HB	1.71	0.71
1:A:129:HIS:NE2	2:A:706:GOL:H32	2.06	0.70
1:A:648:GLU:HG2	1:A:649:GLU:HG3	1.72	0.70
1:A:122:PRO:HD3	1:B:119:VAL:HA	1.74	0.70
4:A:708:ACT:H1	6:A:855:HOH:O	1.93	0.69
1:B:615:GLU:HA	1:B:617:GLY:N	2.06	0.69
1:B:285:THR:HG23	6:B:955:HOH:O	1.94	0.69
1:B:37:ASP:N	6:B:1119:HOH:O	2.27	0.67
1:A:617:GLY:HA3	1:A:630:LYS:HB3	1.76	0.67
1:A:201[A]:ILE:HG13	1:A:202:ILE:HG13	1.74	0.67
1:A:173:GLN:NE2	6:A:926:HOH:O	2.26	0.67
1:B:438:THR:HG22	1:B:439:ARG:N	2.07	0.66
1:A:46:ARG:HH12	2:A:704:GOL:C1	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:VAL:HG22	1:A:582:ILE:HG12	1.79	0.65
1:B:106:THR:HG22	1:B:108:SER:HB2	1.76	0.65
1:A:46:ARG:NH1	2:A:704:GOL:H12	2.10	0.64
1:A:479:GLU:HB3	1:A:496:THR:OG1	1.97	0.64
1:B:301:ASN:OD1	1:B:301:ASN:N	2.30	0.64
1:B:337[A]:LYS:HE3	2:B:703:GOL:H11	1.79	0.64
1:B:479:GLU:HB3	1:B:496:THR:OG1	1.98	0.63
1:A:302:GLU:HB2	1:A:304:LYS:NZ	2.13	0.63
2:A:702:GOL:H2	4:A:708:ACT:H3	1.80	0.63
1:A:305:LEU:HA	6:A:1023:HOH:O	2.00	0.62
1:B:417:PRO:HD3	1:B:439:ARG:CZ	2.30	0.62
1:A:417:PRO:HD3	1:A:439:ARG:CZ	2.29	0.62
1:A:438:THR:HG22	1:A:439:ARG:N	2.07	0.62
1:A:552:ILE:HG13	1:A:677:SER:O	2.00	0.62
1:B:615:GLU:O	1:B:615:GLU:CG	2.39	0.61
1:B:651:LEU:C	1:B:651:LEU:HD12	2.26	0.61
1:B:288:ARG:NH1	1:B:317:GLY:O	2.34	0.61
1:B:442:GLU:HG2	1:B:479:GLU:HA	1.82	0.61
1:A:147:GLU:HA	2:A:703:GOL:H31	1.83	0.60
1:B:153:LYS:HE2	2:B:701:GOL:H2	1.83	0.60
1:B:588:ALA:O	1:B:589:GLU:HB3	2.01	0.60
1:B:552:ILE:HG13	1:B:677:SER:O	2.02	0.60
1:A:442:GLU:HG2	1:A:479:GLU:HA	1.84	0.59
1:B:657:TYR:N	1:B:678:ALA:O	2.35	0.59
1:B:606:GLY:HA2	1:B:642:GLY:HA2	1.83	0.59
1:A:253:LEU:HD12	1:A:253:LEU:C	2.28	0.58
1:A:46:ARG:HH22	2:A:704:GOL:C3	2.07	0.58
1:A:264:LEU:C	1:A:264:LEU:HD12	2.28	0.58
1:B:572:GLU:OE2	1:B:585:LYS:HB2	2.03	0.58
1:B:394:ILE:HG12	1:B:394:ILE:O	2.02	0.58
1:B:575:VAL:HG22	1:B:582:ILE:HG13	1.87	0.57
1:B:588:ALA:O	1:B:589:GLU:CB	2.53	0.57
1:B:349:LYS:H	2:B:704:GOL:C2	2.16	0.57
1:B:272:LYS:HG3	6:B:1082:HOH:O	2.04	0.56
1:A:687:GLN:O	1:A:688:GLN:HB3	2.05	0.56
1:B:567:GLY:O	1:B:589:GLU:HB3	2.05	0.56
1:A:85:LYS:NZ	6:A:1011:HOH:O	2.30	0.56
1:A:612:LYS:HD2	1:A:614:ALA:HA	1.88	0.56
1:A:638:VAL:HG22	1:A:654:PHE:HB3	1.88	0.56
1:B:253:LEU:C	1:B:253:LEU:HD12	2.31	0.56
1:B:548:TRP:CE2	1:B:586:LEU:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201[B]:ILE:HD11	1:A:277:TYR:OH	2.07	0.55
1:A:583:THR:HA	1:A:598:ILE:O	2.06	0.55
1:A:548:TRP:CE2	1:A:586:LEU:HB3	2.42	0.55
1:A:617:GLY:HA2	1:A:631:ALA:O	2.07	0.55
1:B:587:THR:HB	1:B:595:THR:HG22	1.87	0.55
1:B:586:LEU:O	1:B:596:PHE:N	2.32	0.55
1:A:302:GLU:HB2	1:A:304:LYS:HZ3	1.71	0.54
1:B:554:ASN:HA	1:B:676:SER:HA	1.88	0.54
1:A:389:LEU:O	1:A:392:LYS:HD3	2.07	0.54
1:B:56:ALA:C	6:B:914:HOH:O	2.51	0.54
1:B:389:LEU:O	1:B:392:LYS:HD3	2.08	0.54
1:A:305:LEU:HD23	6:A:1023:HOH:O	2.05	0.54
1:A:481:GLU:O	1:A:493:GLY:HA3	2.06	0.54
1:A:650:LEU:C	1:A:650:LEU:HD12	2.32	0.54
1:A:618:PHE:CD1	1:A:619:ASP:N	2.76	0.54
1:B:193:LYS:NZ	2:B:703:GOL:H12	2.22	0.54
1:A:582:ILE:HD13	1:A:583:THR:N	2.23	0.54
1:B:613:THR:HG22	1:B:614:ALA:N	2.23	0.54
1:B:612:LYS:NZ	1:B:635:THR:HG23	2.24	0.53
1:A:645:PRO:HA	6:A:1029:HOH:O	2.09	0.53
1:B:302:GLU:HB3	1:B:303:THR:C	2.33	0.53
1:B:106:THR:HA	6:B:1096:HOH:O	2.09	0.53
1:A:121:GLN:N	1:A:122:PRO:CD	2.71	0.53
1:A:349:LYS:CG	2:A:705:GOL:H31	2.37	0.53
1:A:122:PRO:HD2	1:B:119:VAL:HG13	1.90	0.52
1:A:612:LYS:HE2	1:A:614:ALA:HB2	1.90	0.52
1:B:153:LYS:CE	2:B:701:GOL:H32	2.39	0.52
1:A:554:ASN:HA	1:A:676:SER:HA	1.91	0.52
1:B:46:ARG:HH22	2:B:702:GOL:C3	2.04	0.52
1:B:481:GLU:O	1:B:493:GLY:HA3	2.10	0.51
1:A:236:GLU:OE1	6:A:993:HOH:O	2.20	0.51
1:B:188:PHE:CE2	1:B:216:SER:HB3	2.46	0.51
1:B:193:LYS:HZ3	2:B:703:GOL:H12	1.75	0.51
1:A:188:PHE:CE2	1:A:216:SER:HB3	2.45	0.51
1:A:617:GLY:HA3	1:A:630:LYS:CB	2.40	0.50
1:A:206:LYS:NZ	6:B:973:HOH:O	2.45	0.50
1:B:153:LYS:HE2	2:B:701:GOL:C2	2.41	0.50
1:B:615:GLU:N	1:B:616:SER:HB2	2.26	0.50
1:A:183:LYS:NZ	2:A:706:GOL:H31	2.27	0.49
1:A:383:ASP:O	1:A:527:GLN:HA	2.12	0.49
1:A:646:LYS:N	6:A:1029:HOH:O	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:C	1:A:382:LEU:HD12	2.37	0.49
1:B:383:ASP:O	1:B:527:GLN:HA	2.11	0.49
1:A:490:LEU:C	1:A:490:LEU:HD13	2.37	0.49
1:B:607:PHE:CZ	1:B:641:GLY:HA3	2.47	0.49
1:B:633:TYR:O	1:B:676:SER:OG	2.31	0.49
1:B:288:ARG:NH2	6:B:845:HOH:O	2.46	0.48
1:B:337[A]:LYS:CE	2:B:703:GOL:H11	2.43	0.48
1:B:382:LEU:HD12	1:B:382:LEU:C	2.38	0.48
1:B:654:TRP:HA	1:B:680:VAL:O	2.13	0.48
1:B:394:ILE:O	1:B:394:ILE:CG1	2.60	0.48
1:B:476:LYS:HG2	1:B:498:LYS:O	2.13	0.48
1:A:616:SER:HB3	1:A:632:TYR:HE1	1.77	0.48
1:B:108:SER:O	1:B:109:ASN:C	2.56	0.48
1:A:496:THR:HG22	1:A:522:GLN:HG2	1.95	0.48
1:A:531:THR:HB	1:A:644:GLY:O	2.14	0.48
1:A:347:LYS:O	1:A:349:LYS:HE3	2.13	0.48
1:A:479:GLU:HB3	1:A:496:THR:HG1	1.78	0.48
1:B:599:GLU:O	1:B:609:GLY:HA3	2.14	0.48
1:A:127:THR:HB	6:A:938:HOH:O	2.13	0.48
1:A:194:LYS:NZ	2:A:702:GOL:O2	2.33	0.48
1:B:57:GLU:OE2	3:B:706:SO4:O4	2.32	0.48
1:B:613:THR:HG22	1:B:614:ALA:H	1.79	0.47
1:B:564:ASP:OD2	1:B:564:ASP:N	2.41	0.47
1:A:476:LYS:HG2	1:A:498:LYS:O	2.15	0.47
1:A:617:GLY:HA2	1:A:631:ALA:C	2.39	0.47
1:B:554:ASN:CB	1:B:676:SER:HB3	2.40	0.47
1:B:287:ASN:OD1	1:B:288:ARG:HD3	2.14	0.47
1:B:526:LEU:C	1:B:526:LEU:HD23	2.40	0.47
1:A:677:SER:O	1:A:678:ALA:HB2	2.15	0.47
1:B:127:THR:CG2	6:B:844:HOH:O	2.63	0.46
1:A:554:ASN:CB	1:A:676:SER:HB3	2.42	0.46
1:B:496:THR:HG22	1:B:522:GLN:HG2	1.97	0.46
1:B:438:THR:O	1:B:439:ARG:HB2	2.16	0.46
1:B:552:ILE:HG22	1:B:558:TRP:HD1	1.81	0.46
1:A:327:LEU:C	1:A:327:LEU:HD12	2.41	0.46
1:B:85:LYS:NZ	1:B:109:ASN:HB3	2.31	0.46
1:B:490:LEU:HD13	1:B:490:LEU:C	2.41	0.46
1:B:586:LEU:O	1:B:595:THR:HB	2.16	0.46
1:A:147:GLU:CA	2:A:703:GOL:H31	2.45	0.46
1:A:295:ALA:O	1:A:298:LYS:NZ	2.49	0.46
1:B:677:SER:O	1:B:678:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLU:N	6:B:914:HOH:O	2.49	0.45
1:A:188:PHE:CZ	1:A:201[A]:ILE:HD12	2.52	0.45
1:B:179:LYS:HE3	6:B:1047:HOH:O	2.16	0.45
1:A:598:ILE:HA	1:A:610:THR:O	2.17	0.45
1:B:610:THR:HA	1:B:637:ALA:O	2.16	0.45
1:B:630:PRO:C	1:B:631:LYS:HG3	2.41	0.45
1:A:304:LYS:O	6:A:1023:HOH:O	2.21	0.45
1:B:73:LEU:HD12	1:B:74:PRO:CD	2.40	0.45
1:B:149:ASP:OD1	1:B:149:ASP:C	2.59	0.45
1:B:46:ARG:HH12	2:B:702:GOL:C1	2.19	0.45
1:B:99:ILE:H	1:B:115:ALA:N	2.15	0.45
1:A:543:VAL:HG22	1:A:574:THR:HG22	1.99	0.45
1:A:547:SER:OG	1:A:548:TRP:N	2.49	0.45
1:B:78:LYS:NZ	6:B:1026:HOH:O	2.50	0.45
1:A:436:GLU:N	1:A:436:GLU:OE1	2.50	0.45
1:B:494:MET:SD	1:B:524:MET:HG2	2.57	0.44
1:B:37:ASP:N	1:B:290:ASN:HD21	2.14	0.44
1:A:438:THR:O	1:A:439:ARG:HB2	2.17	0.44
6:A:952:HOH:O	1:B:206:LYS:HE3	2.18	0.44
1:A:615:GLU:HA	1:A:616:SER:HA	1.76	0.44
1:A:552:ILE:HG22	1:A:558:TRP:HD1	1.83	0.44
1:A:575:VAL:HG22	1:A:582:ILE:CG1	2.47	0.44
1:A:687:GLN:HB3	1:A:688:GLN:H	1.60	0.44
1:B:100:TYR:O	1:B:140:PHE:HA	2.17	0.44
1:B:477:THR:HG22	1:B:478:TYR:N	2.32	0.44
1:B:547:SER:OG	1:B:548:TRP:N	2.48	0.44
1:B:64:ASN:HB3	6:B:959:HOH:O	2.16	0.44
1:B:299:LYS:HB3	1:B:300:GLU:H	1.63	0.44
1:A:304:LYS:HA	1:A:304:LYS:HD3	1.73	0.44
1:A:348:ASP:HA	2:A:705:GOL:H2	2.00	0.44
1:B:657:TYR:HA	1:B:658:PRO:HA	1.61	0.44
1:B:436:GLU:OE1	1:B:436:GLU:N	2.51	0.43
1:A:477:THR:HG22	1:A:478:TYR:N	2.33	0.43
1:A:285:THR:HG23	6:A:1014:HOH:O	2.17	0.43
1:A:616:SER:HB3	1:A:632:TYR:CE1	2.53	0.43
1:B:127:THR:HG22	1:B:237:GLY:HA2	2.00	0.43
1:A:568:GLY:O	1:A:570:ARG:HG3	2.19	0.43
1:B:127:THR:HB	6:B:905:HOH:O	2.18	0.43
1:B:153:LYS:HZ3	2:B:701:GOL:H32	1.81	0.43
1:A:303:THR:HA	6:A:1045:HOH:O	2.17	0.43
1:A:92:GLU:CD	2:A:703:GOL:H12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HG3	1:A:273:HIS:CD2	2.54	0.43
1:B:85:LYS:HE2	1:B:89:GLU:OE2	2.19	0.43
1:A:122:PRO:CD	1:B:119:VAL:HA	2.46	0.43
1:A:438:THR:CG2	1:A:439:ARG:N	2.74	0.43
1:A:483:CYS:HA	1:A:484:CYS:HA	1.73	0.43
1:B:127:THR:HG21	6:B:844:HOH:O	2.19	0.43
1:B:302:GLU:HG2	1:B:304:LYS:HG2	2.01	0.42
1:A:645:PRO:O	1:A:648:GLU:OE2	2.37	0.42
1:B:548:TRP:HB3	1:B:682:PHE:HB3	2.01	0.42
1:A:586:LEU:O	1:A:595:THR:HA	2.20	0.42
1:A:620:LEU:N	1:A:620:LEU:HD12	2.35	0.42
1:B:543:VAL:HG22	1:B:574:THR:HG22	2.00	0.42
1:A:127:THR:CG2	6:A:954:HOH:O	2.67	0.42
1:A:306:HIS:HB2	1:A:307:PRO:HD2	2.02	0.42
1:A:411:ILE:HD12	1:A:411:ILE:C	2.45	0.42
1:A:494:MET:SD	1:A:524:MET:HG2	2.58	0.42
1:A:183:LYS:HZ1	2:A:706:GOL:H31	1.84	0.42
1:A:211:ARG:HH21	4:A:708:ACT:CH3	2.33	0.42
1:A:211:ARG:NH2	4:A:708:ACT:O	2.53	0.42
1:A:536:ILE:HD11	1:A:605:ASN:HA	2.02	0.42
1:A:564:ASP:OD2	1:A:564:ASP:N	2.44	0.42
1:B:46:ARG:NH1	2:B:702:GOL:H12	2.18	0.42
1:A:129:HIS:CG	1:A:183:LYS:HB2	2.55	0.41
1:B:304:LYS:HD3	1:B:304:LYS:HA	1.73	0.41
1:A:548:TRP:HB3	1:A:682:PHE:HB3	2.02	0.41
1:B:438:THR:CG2	1:B:439:ARG:N	2.75	0.41
1:B:531:THR:HB	1:B:645:GLY:O	2.21	0.41
1:A:656:TYR:CG	1:A:657:PRO:HA	2.56	0.41
1:B:587:THR:HA	1:B:595:THR:HA	2.03	0.41
1:A:315:LEU:HA	1:A:331:PHE:HB3	2.03	0.41
1:B:575:VAL:HG13	1:B:602:ILE:HD11	2.02	0.41
1:A:127:THR:HG22	1:A:237:GLY:HA2	2.02	0.41
1:A:252:LYS:HB3	1:A:252:LYS:HE2	1.81	0.41
1:B:153:LYS:HZ2	2:B:701:GOL:H32	1.83	0.41
1:A:43:PHE:HA	1:A:69:GLU:O	2.21	0.41
1:A:654:PHE:CZ	1:A:680:VAL:HB	2.55	0.41
1:B:38:GLN:O	1:B:38:GLN:HG2	2.20	0.41
1:B:289:PHE:C	1:B:290:ASN:OD1	2.63	0.41
1:B:327:LEU:HD12	1:B:327:LEU:C	2.46	0.41
1:A:349:LYS:HG2	2:A:705:GOL:C3	2.41	0.40
1:A:548:TRP:O	1:A:569:ASN:ND2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ILE:HD13	1:A:582:ILE:C	2.46	0.40
1:B:188:PHE:CZ	1:B:201:ILE:HD12	2.56	0.40
1:A:38:GLN:O	1:A:38:GLN:HG2	2.21	0.40
1:A:298:LYS:O	1:A:304:LYS:HG3	2.22	0.40
1:A:544:TYR:CE2	1:A:686:ARG:HB2	2.56	0.40
1:B:614:ALA:C	1:B:616:SER:HB2	2.46	0.40
1:B:597:THR:O	1:B:611:ALA:HA	2.20	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	496/658 (75%)	465 (94%)	29 (6%)	2 (0%)	30	26
1	B	501/658 (76%)	467 (93%)	32 (6%)	2 (0%)	30	26
All	All	997/1316 (76%)	932 (94%)	61 (6%)	4 (0%)	30	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	LYS
1	B	476	LYS
1	B	615	GLU
1	A	678	ALA

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	434/533 (81%)	423 (98%)	11 (2%)	42	44
1	B	437/533 (82%)	425 (97%)	12 (3%)	39	41
All	All	871/1066 (82%)	848 (97%)	23 (3%)	42	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	THR
1	A	233[A]	ASP
1	A	233[B]	ASP
1	A	300	GLU
1	A	301	ASN
1	A	394	ILE
1	A	582	ILE
1	A	635	ASP
1	A	639	LYS
1	A	650	LEU
1	A	687	GLN
1	B	105	LEU
1	B	127	THR
1	B	288	ARG
1	B	299	LYS
1	B	301	ASN
1	B	330	ARG
1	B	394	ILE
1	B	531	THR
1	B	615	GLU
1	B	619	ASP
1	B	651	LEU
1	B	687	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	590	ASN
1	B	64	ASN
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	125	GLN
1	B	173	GLN
1	B	187	HIS
1	B	594	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	SO4	B	707	-	4,4,4	0.29	0	6,6,6	0.17	0
2	GOL	A	705	-	5,5,5	0.34	0	5,5,5	0.34	0
2	GOL	B	704	-	5,5,5	0.33	0	5,5,5	0.26	0
2	GOL	B	705	-	5,5,5	0.34	0	5,5,5	0.43	0
4	ACT	A	708	-	3,3,3	0.76	0	3,3,3	1.34	0
2	GOL	A	704	-	5,5,5	0.33	0	5,5,5	0.43	0
3	SO4	A	707	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	B	708	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SO4	B	706	-	4,4,4	0.27	0	6,6,6	0.16	0
3	SO4	B	710	-	4,4,4	0.24	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	702	-	5,5,5	0.34	0	5,5,5	0.29	0
2	GOL	A	702	-	5,5,5	0.45	0	5,5,5	0.18	0
2	GOL	B	701	-	5,5,5	0.48	0	5,5,5	0.46	0
3	SO4	B	711	-	4,4,4	0.29	0	6,6,6	0.10	0
2	GOL	B	703	-	5,5,5	0.36	0	5,5,5	0.36	0
3	SO4	B	709	-	4,4,4	0.22	0	6,6,6	0.12	0
2	GOL	A	703	-	5,5,5	0.36	0	5,5,5	0.36	0
2	GOL	A	701	-	5,5,5	0.44	0	5,5,5	0.62	0
2	GOL	A	706	-	5,5,5	0.38	0	5,5,5	0.25	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
2	GOL	B	701	-	-	2/4/4/4	-
2	GOL	B	703	-	-	2/4/4/4	-
2	GOL	A	703	-	-	2/4/4/4	-
2	GOL	A	701	-	-	2/4/4/4	-
2	GOL	A	706	-	-	2/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	A	705	-	-	2/4/4/4	-
2	GOL	B	704	-	-	2/4/4/4	-
2	GOL	B	705	-	-	2/4/4/4	-
2	GOL	A	702	-	-	2/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-C3
2	A	702	GOL	O1-C1-C2-C3
2	A	703	GOL	O1-C1-C2-C3
2	A	704	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	705	GOL	O1-C1-C2-O2
2	A	705	GOL	O1-C1-C2-C3
2	A	706	GOL	O2-C2-C3-O3
2	B	701	GOL	O1-C1-C2-C3
2	B	702	GOL	O1-C1-C2-C3
2	B	703	GOL	O1-C1-C2-O2
2	A	701	GOL	O1-C1-C2-O2
2	A	703	GOL	O1-C1-C2-O2
2	A	706	GOL	C1-C2-C3-O3
2	B	703	GOL	O1-C1-C2-C3
2	B	704	GOL	O1-C1-C2-C3
2	B	705	GOL	O1-C1-C2-C3
2	A	702	GOL	O1-C1-C2-O2
2	A	704	GOL	O1-C1-C2-O2
2	B	705	GOL	O1-C1-C2-O2
2	B	701	GOL	O1-C1-C2-O2
2	B	702	GOL	O1-C1-C2-O2
2	B	704	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	705	GOL	4	0
2	B	704	GOL	2	0
4	A	708	ACT	5	0
2	A	704	GOL	6	0
3	B	706	SO4	1	0
2	B	702	GOL	7	0
2	A	702	GOL	2	0
2	B	701	GOL	6	0
2	B	703	GOL	4	0
2	A	703	GOL	3	0
2	A	701	GOL	1	0
2	A	706	GOL	3	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	514/658 (78%)	0.40	67 (13%) 7 9	13, 51, 132, 194	2 (0%)
1	B	519/658 (78%)	0.34	61 (11%) 9 11	13, 47, 129, 179	2 (0%)
All	All	1033/1316 (78%)	0.37	128 (12%) 8 9	13, 49, 131, 194	4 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	LEU	5.9
1	B	552	ILE	5.1
1	A	558	TRP	4.9
1	B	119	VAL	4.8
1	B	630	PRO	4.3
1	A	107	PRO	4.3
1	B	618	PHE	4.2
1	B	619	ASP	4.1
1	B	115	ALA	4.1
1	B	118	GLY	4.1
1	A	618	PHE	4.0
1	B	578	ALA	3.9
1	B	588	ALA	3.9
1	B	107	PRO	3.7
1	B	678	ALA	3.7
1	A	441	PHE	3.7
1	A	303	THR	3.6
1	A	571	ALA	3.6
1	A	584	GLY	3.5
1	A	438	THR	3.5
1	B	264	LEU	3.5
1	B	445	PRO	3.4
1	B	558	TRP	3.4
1	B	303	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	485	SER	3.3
1	B	560	GLY	3.2
1	A	629	PRO	3.2
1	A	679	THR	3.2
1	B	438	THR	3.2
1	A	552	ILE	3.1
1	A	587	THR	3.1
1	A	299	LYS	3.1
1	A	596	PHE	3.1
1	B	117	ASN	3.1
1	B	586	LEU	3.1
1	B	300	GLU	3.0
1	B	598	ILE	3.0
1	B	584	GLY	3.0
1	A	482	VAL	3.0
1	A	631	ALA	3.0
1	B	614	ALA	3.0
1	A	638	VAL	3.0
1	B	441	PHE	3.0
1	B	687	GLN	2.9
1	A	387	LEU	2.9
1	A	548	TRP	2.9
1	B	394	ILE	2.9
1	A	543	VAL	2.8
1	A	683	GLY	2.8
1	B	572	GLU	2.8
1	B	656	ALA	2.8
1	A	583	THR	2.8
1	A	595	THR	2.7
1	B	490	LEU	2.7
1	A	480	VAL	2.7
1	A	680	VAL	2.7
1	B	121	GLN	2.7
1	A	490	LEU	2.7
1	B	649	GLU	2.7
1	A	553	ALA	2.6
1	B	553	ALA	2.6
1	B	615	GLU	2.6
1	A	614	ALA	2.6
1	B	120	ASN	2.6
1	B	571	ALA	2.6
1	A	394	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	620	LEU	2.6
1	A	569	ASN	2.5
1	A	681	VAL	2.5
1	B	620	LEU	2.5
1	A	606	GLY	2.5
1	B	551	HIS	2.5
1	A	633	ILE	2.5
1	B	575	VAL	2.5
1	A	636	ALA	2.4
1	A	389	LEU	2.4
1	A	586	LEU	2.4
1	A	233[A]	ASP	2.4
1	B	548	TRP	2.4
1	B	563	SER	2.4
1	A	585	LYS	2.4
1	A	617	GLY	2.4
1	B	579	ASP	2.4
1	A	121	GLN	2.4
1	A	525	PHE	2.4
1	B	437	PHE	2.4
1	A	560	GLY	2.3
1	A	621	ASP	2.3
1	B	582	ILE	2.3
1	A	570	ARG	2.3
1	B	299	LYS	2.3
1	B	596	PHE	2.3
1	B	587	THR	2.3
1	B	613	THR	2.3
1	A	494	MET	2.3
1	A	689	PRO	2.2
1	A	678	ALA	2.2
1	B	417	PRO	2.2
1	B	543	VAL	2.2
1	A	302	GLU	2.2
1	A	416	LEU	2.2
1	B	478	TYR	2.2
1	B	577	PHE	2.2
1	B	480	VAL	2.2
1	B	57	GLU	2.2
1	A	562	ALA	2.2
1	A	301	ASN	2.2
1	A	551	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	566	GLU	2.1
1	A	520	VAL	2.1
1	B	567	GLY	2.1
1	A	589	GLU	2.1
1	A	522	GLN	2.1
1	A	531	THR	2.1
1	A	658	GLY	2.1
1	A	437	PHE	2.1
1	A	677	SER	2.1
1	B	585	LYS	2.1
1	B	680	VAL	2.1
1	B	675	ALA	2.1
1	B	677	SER	2.1
1	B	489	TYR	2.0
1	B	482	VAL	2.0
1	A	271	ASP	2.0
1	A	619	ASP	2.0
1	A	565	LYS	2.0
1	B	583	THR	2.0
1	A	644	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	702	6/6	0.75	0.15	40,62,65,74	0
2	GOL	B	701	6/6	0.83	0.16	44,67,72,82	0
2	GOL	B	704	6/6	0.83	0.18	58,78,96,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	705	6/6	0.83	0.17	63,76,81,84	0
3	SO4	B	709	5/5	0.87	0.11	91,113,118,124	0
3	SO4	B	711	5/5	0.87	0.10	59,122,134,139	0
4	ACT	A	708	4/4	0.87	0.19	36,37,50,82	0
3	SO4	A	707	5/5	0.88	0.10	56,96,119,121	0
2	GOL	A	706	6/6	0.88	0.16	68,82,91,92	0
2	GOL	B	702	6/6	0.89	0.11	31,46,72,80	0
2	GOL	A	705	6/6	0.90	0.12	56,69,75,88	0
3	SO4	B	710	5/5	0.91	0.11	51,65,98,98	0
3	SO4	B	708	5/5	0.91	0.09	52,85,109,122	0
2	GOL	B	703	6/6	0.91	0.11	64,81,87,87	0
2	GOL	A	704	6/6	0.92	0.10	35,52,59,68	0
2	GOL	A	703	6/6	0.94	0.15	47,76,85,87	0
2	GOL	A	701	6/6	0.95	0.14	22,64,76,77	0
3	SO4	B	707	5/5	0.96	0.07	47,49,79,91	0
3	SO4	B	706	5/5	0.96	0.09	47,59,90,125	0
5	NA	B	712	1/1	1.00	0.06	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.