



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 08:01 PM EDT

PDB ID : 3VE2
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

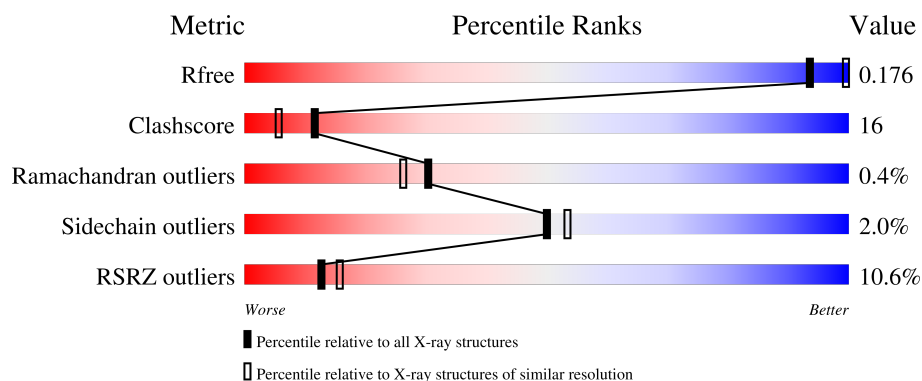
1 Overall quality at a glance

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}	164625	3336 (2.16-2.12)
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)
RSRZ outliers	164620	3337 (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	<div> <div>9%</div> <div>58%</div> <div>19%</div> <div>22%</div> </div>
1	B	658	<div> <div>8%</div> <div>59%</div> <div>18%</div> <div>21%</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
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.

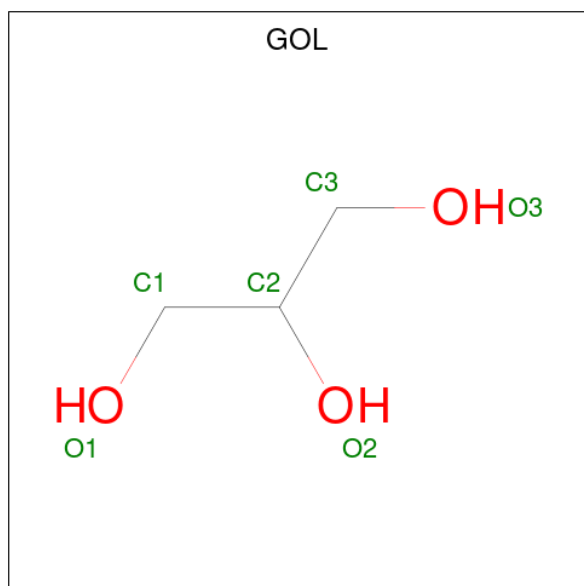
- Molecule 1 is a protein called Transferrin-binding protein 2.

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:

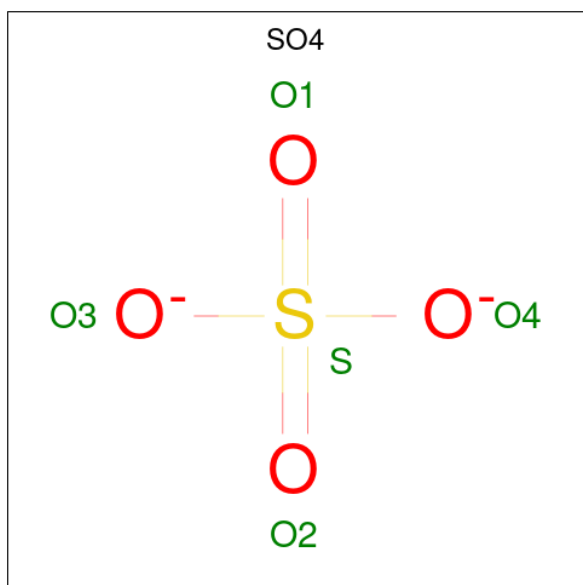
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q09057
A	35	SER	-	expression tag	UNP Q09057
B	34	GLY	-	expression tag	UNP Q09057
B	35	SER	-	expression tag	UNP Q09057

- Molecule 2 is GLYCEROL (three-letter code: 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 (three-letter code: SO4) (formula: O₄S).



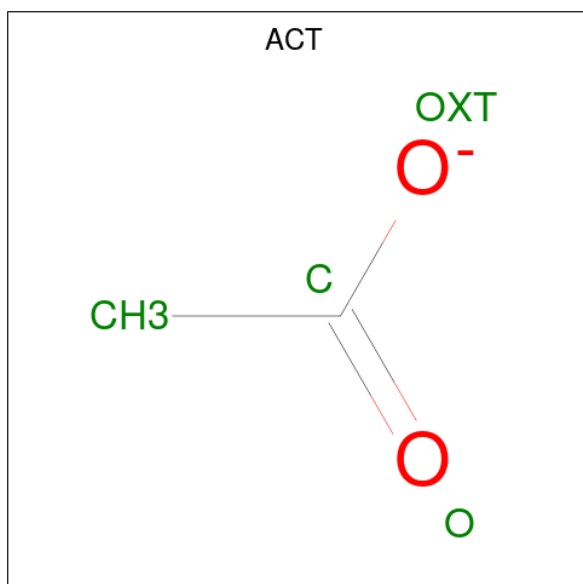
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

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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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



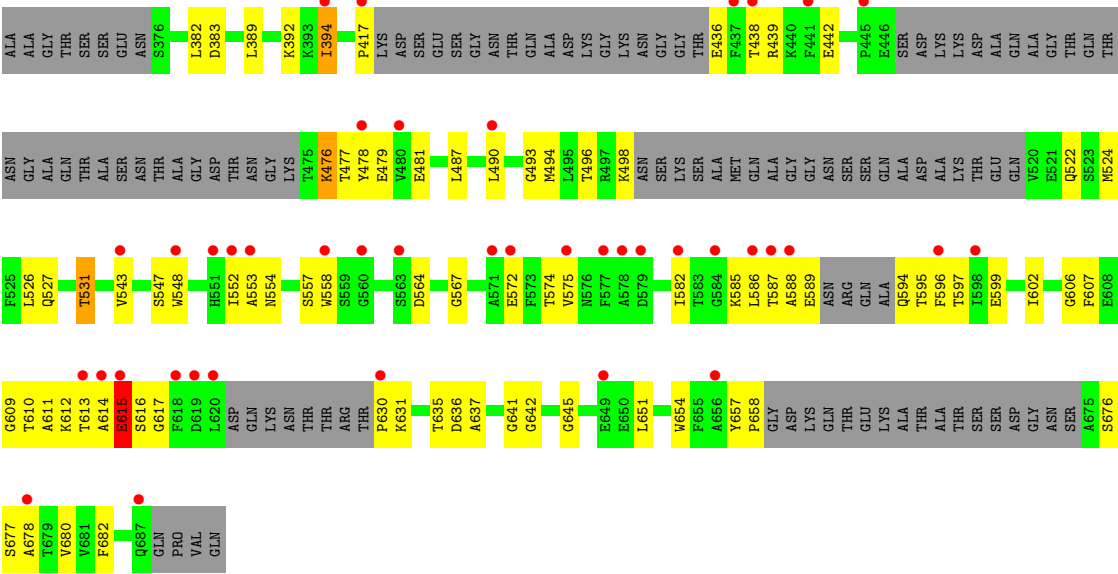
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (three-letter code: 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, GOL, ACT, NA

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	0.44	0/4147	0.63	3/5573 (0.1%)
1	B	0.45	0/4176	0.63	4/5611 (0.1%)
All	All	0.44	0/8323	0.63	7/11184 (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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	A	330	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	B	330	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	A	330	ARG	NE-CZ-NH2	10.03	125.31	120.30
1	B	330	ARG	CD-NE-CZ	5.61	131.45	123.60
1	A	330	ARG	CD-NE-CZ	5.57	131.40	123.60
1	B	105	LEU	CB-CG-CD1	5.25	119.92	111.00

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	126	0
1	B	4087	0	3927	127	0
2	A	36	0	48	17	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	15	0
All	All	8868	0	7920	254	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 (254) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:615:GLU:HA	1:B:616:SER:C	2.05	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: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:589:GLU:C	1:B:594:GLN:HG3	2.15	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
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:85:LYS:NZ	6:A:1011:HOH:O	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:46:ARG:HH22	2:A:704:GOL:C3	2.07	0.58
1:B:394:ILE:HG12	1:B:394:ILE:O	2.02	0.58
1:B:572:GLU:OE2	1:B:585:LYS:HB2	2.03	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:B:651:LEU:C	1:B:651:LEU:HD12	2.26	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: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:548:TRP:CE2	1:B:586:LEU:HB3	2.41	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:253:LEU:HD12	1:A:253:LEU:C	2.28	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:A:264:LEU:C	1:A:264:LEU:HD12	2.28	0.53
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: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:B:253:LEU:C	1:B:253:LEU:HD12	2.31	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: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:650:LEU:C	1:A:650:LEU:HD12	2.32	0.49
1:A:383:ASP:O	1:A:527:GLN:HA	2.12	0.49
1:B:56:ALA:C	6:B:914:HOH:O	2.51	0.49
1:A:646:LYS:N	6:A:1029:HOH:O	2.38	0.49
1:B:383:ASP:O	1:B:527:GLN:HA	2.11	0.49
1:B:607:PHE:CZ	1:B:641:GLY:HA3	2.47	0.49
1:B:288:ARG:NH2	6:B:845:HOH:O	2.46	0.48
1:B:302:GLU:HB3	1:B:303:THR:C	2.33	0.48
1:B:337[A]:LYS:CE	2:B:703:GOL:H11	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:SER:HB3	1:A:632:TYR:HE1	1.77	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: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: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: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:B:85:LYS:NZ	1:B:109:ASN:HB3	2.31	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
1:B:57:GLU:N	6:B:914:HOH:O	2.49	0.45
1:B:193:LYS:HZ2	2:B:703:GOL:H12	1.80	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: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: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:490:LEU:C	1:A:490:LEU:HD13	2.37	0.45
1:A:547:SER:OG	1:A:548:TRP:N	2.49	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:382:LEU:C	1:A:382:LEU:HD12	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:382:LEU:HD12	1:B:382:LEU:C	2.38	0.44
1:A:615:GLU:HA	1:A:616:SER:HA	1.76	0.44
1:A:477:THR:HG22	1:A:478:TYR:N	2.33	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:B:108:SER:O	1:B:109:ASN:C	2.56	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: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:617:GLY:HA2	1:A:631:ALA:C	2.39	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:494:MET:SD	1:A:524:MET:HG2	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:LEU:C	1:B:526:LEU:HD23	2.40	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:327:LEU:C	1:A:327:LEU:HD12	2.41	0.41
1:A:656:TYR:CG	1:A:657:PRO:HA	2.56	0.41
1:B:490:LEU:HD13	1:B:490:LEU:C	2.41	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: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
1:B:630:PRO:C	1:B:631:LYS:HG3	2.41	0.40
1:B:149:ASP:OD1	1:B:149:ASP:C	2.59	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:597:THR:O	1:B:611:ALA:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 ⓘ

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%)	424 (98%)	10 (2%)	45	47
1	B	437/533 (82%)	429 (98%)	8 (2%)	54	57
All	All	871/1066 (82%)	853 (98%)	18 (2%)	50	51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	127	THR
1	A	166	HIS
1	A	221	GLU
1	A	233[A]	ASP
1	A	233[B]	ASP
1	A	301	ASN
1	A	394	ILE

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Mol	Chain	Res	Type
1	A	582	ILE
1	A	635	ASP
1	B	105	LEU
1	B	127	THR
1	B	166	HIS
1	B	221	GLU
1	B	288	ARG
1	B	394	ILE
1	B	531	THR
1	B	615	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	590	ASN
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	$\# Z > 2$
2	GOL	B	702	-	5,5,5	0.34	0	5,5,5	0.29	0
3	SO4	B	706	-	4,4,4	0.27	0	6,6,6	0.16	0
3	SO4	B	709	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	B	711	-	4,4,4	0.29	0	6,6,6	0.10	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
3	SO4	A	707	-	4,4,4	0.25	0	6,6,6	0.06	0
2	GOL	B	704	-	5,5,5	0.33	0	5,5,5	0.26	0
2	GOL	A	702	-	5,5,5	0.45	0	5,5,5	0.18	0
2	GOL	A	706	-	5,5,5	0.38	0	5,5,5	0.25	0
2	GOL	A	704	-	5,5,5	0.33	0	5,5,5	0.43	0
2	GOL	A	705	-	5,5,5	0.34	0	5,5,5	0.34	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	B	701	-	5,5,5	0.48	0	5,5,5	0.46	0
3	SO4	B	707	-	4,4,4	0.29	0	6,6,6	0.17	0
2	GOL	B	703	-	5,5,5	0.36	0	5,5,5	0.36	0
3	SO4	B	708	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SO4	B	710	-	4,4,4	0.24	0	6,6,6	0.12	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	A	706	-	-	2/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	B	705	-	-	2/4/4/4	-
2	GOL	A	703	-	-	2/4/4/4	-
2	GOL	A	701	-	-	2/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-
2	GOL	B	704	-	-	2/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-
2	GOL	A	705	-	-	2/4/4/4	-
2	GOL	B	703	-	-	2/4/4/4	-
2	GOL	A	702	-	-	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
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 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	GOL	7	0
3	B	706	SO4	1	0
4	A	708	ACT	5	0
2	B	704	GOL	2	0
2	A	702	GOL	2	0
2	A	706	GOL	2	0
2	A	704	GOL	6	0
2	A	705	GOL	4	0
2	A	703	GOL	2	0
2	A	701	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	GOL	6	0
2	B	703	GOL	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.29	57 (11%)	12 14	13, 51, 132, 194	2 (0%)
1	B	519/658 (78%)	0.23	53 (10%)	13 17	13, 47, 129, 179	2 (0%)
All	All	1033/1316 (78%)	0.26	110 (10%)	13 16	13, 49, 131, 194	4 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	LEU	5.7
1	B	552	ILE	4.9
1	A	558	TRP	4.6
1	B	119	VAL	4.6
1	B	630	PRO	4.2
1	A	107	PRO	4.1
1	B	619	ASP	4.1
1	B	618	PHE	4.0
1	B	115	ALA	3.9
1	B	118	GLY	3.9
1	A	618	PHE	3.8
1	B	578	ALA	3.8
1	B	588	ALA	3.8
1	B	107	PRO	3.6
1	B	678	ALA	3.5
1	A	441	PHE	3.5
1	A	303	THR	3.4
1	A	571	ALA	3.4
1	A	438	THR	3.3
1	A	584	GLY	3.3
1	B	264	LEU	3.3
1	B	445	PRO	3.3
1	B	558	TRP	3.2
1	B	303	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	485	SER	3.2
1	A	629	PRO	3.1
1	B	560	GLY	3.1
1	A	299	LYS	3.1
1	A	679	THR	3.1
1	B	438	THR	3.1
1	A	552	ILE	3.0
1	A	587	THR	3.0
1	B	117	ASN	3.0
1	B	300	GLU	3.0
1	B	586	LEU	2.9
1	A	596	PHE	2.9
1	B	598	ILE	2.9
1	B	687	GLN	2.9
1	B	584	GLY	2.9
1	A	482	VAL	2.8
1	A	638	VAL	2.8
1	A	631	ALA	2.8
1	B	614	ALA	2.8
1	A	387	LEU	2.8
1	B	441	PHE	2.8
1	B	394	ILE	2.7
1	B	572	GLU	2.7
1	A	548	TRP	2.7
1	A	543	VAL	2.7
1	A	683	GLY	2.6
1	A	583	THR	2.6
1	B	656	ALA	2.6
1	B	649	GLU	2.6
1	B	121	GLN	2.6
1	B	615	GLU	2.6
1	A	595	THR	2.6
1	B	490	LEU	2.6
1	A	480	VAL	2.5
1	A	680	VAL	2.5
1	A	490	LEU	2.5
1	A	553	ALA	2.5
1	B	553	ALA	2.5
1	B	120	ASN	2.5
1	A	614	ALA	2.5
1	A	394	ILE	2.4
1	B	571	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	569	ASN	2.4
1	A	620	LEU	2.4
1	B	551	HIS	2.4
1	A	681	VAL	2.4
1	A	633	ILE	2.4
1	B	620	LEU	2.3
1	A	585	LYS	2.3
1	B	575	VAL	2.3
1	A	233[A]	ASP	2.3
1	A	606	GLY	2.3
1	B	563	SER	2.3
1	B	579	ASP	2.3
1	A	389	LEU	2.3
1	A	586	LEU	2.3
1	A	636	ALA	2.3
1	A	121	GLN	2.3
1	A	621	ASP	2.2
1	A	617	GLY	2.2
1	B	299	LYS	2.2
1	A	570	ARG	2.2
1	B	548	TRP	2.2
1	A	525	PHE	2.2
1	B	437	PHE	2.2
1	B	582	ILE	2.2
1	A	560	GLY	2.2
1	B	587	THR	2.2
1	A	494	MET	2.2
1	B	596	PHE	2.1
1	B	613	THR	2.1
1	A	302	GLU	2.1
1	A	689	PRO	2.1
1	B	57	GLU	2.1
1	A	678	ALA	2.1
1	B	417	PRO	2.1
1	B	543	VAL	2.1
1	A	416	LEU	2.1
1	A	301	ASN	2.0
1	A	566	GLU	2.0
1	B	478	TYR	2.0
1	B	480	VAL	2.0
1	A	551	HIS	2.0
1	B	577	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	589	GLU	2.0
1	A	562	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	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
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.