



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:54 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

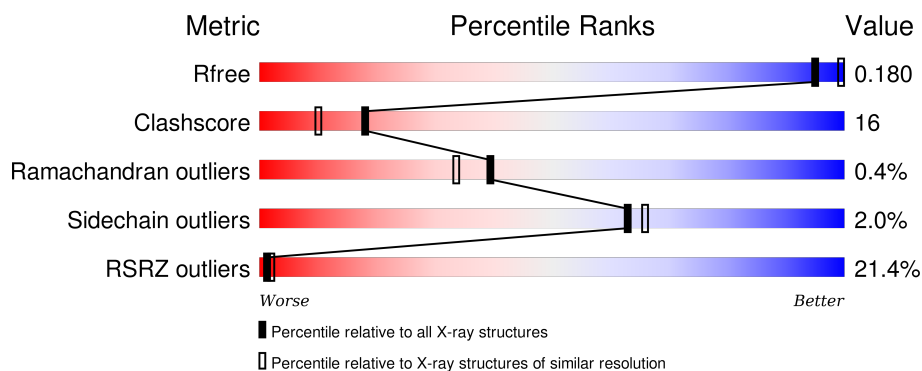
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	658	<div> <div>17%</div> <div>58%</div> <div>19%</div> <div>•</div> <div>22%</div> </div>
1	B	658	<div> <div>17%</div> <div>59%</div> <div>18%</div> <div>•</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	701	-	-	-	X
2	GOL	A	703	-	-	-	X
2	GOL	A	704	-	-	X	-
2	GOL	A	705	-	-	X	X
2	GOL	A	706	-	-	-	X
2	GOL	B	701	-	-	X	-
2	GOL	B	702	-	-	X	-
2	GOL	B	703	-	-	X	X
2	GOL	B	704	-	-	-	X
2	GOL	B	705	-	-	-	X
3	SO4	B	711	-	-	-	X
4	ACT	A	708	-	-	X	X
5	NA	B	712	-	-	-	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.

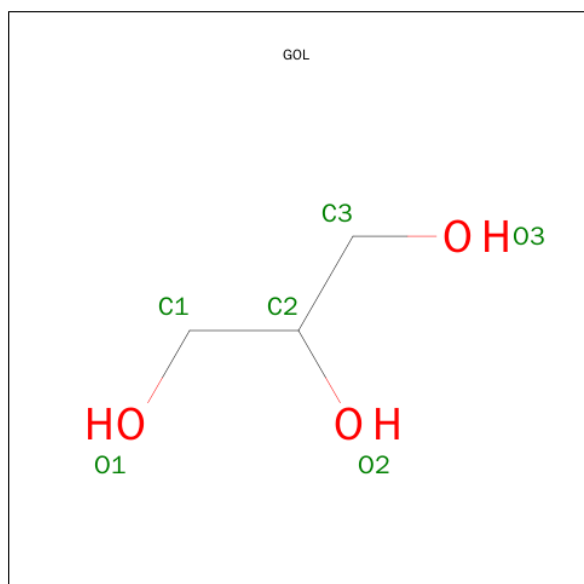
- Molecule 1 is a protein called Transferrin-binding protein 2.

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:

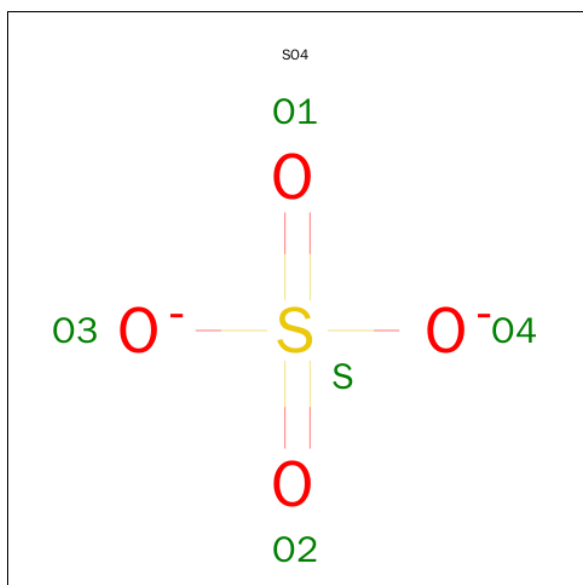
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	EXPRESSION TAG	UNP Q09057
A	35	SER	-	EXPRESSION TAG	UNP Q09057
B	34	GLY	-	EXPRESSION TAG	UNP Q09057
B	35	SER	-	EXPRESSION TAG	UNP Q09057

- 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: O<sub>4</sub>S).



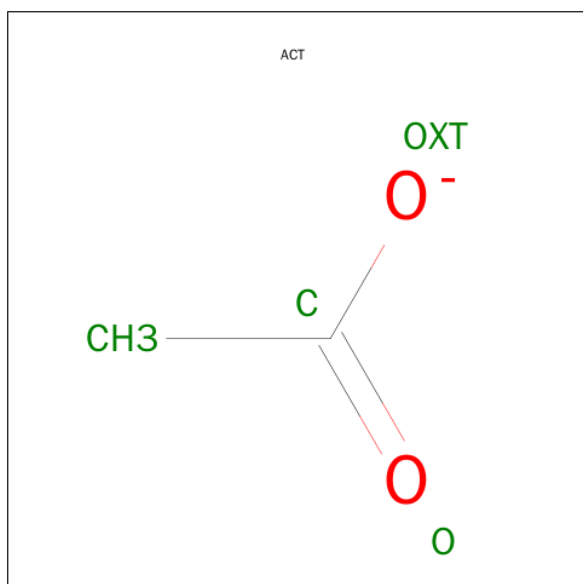
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

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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, $\alpha$ , $\beta$ , $\gamma$	46.60 Å 149.34 Å 199.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.38 – 2.14 46.60 – 2.14	Depositor EDS
% Data completeness (in resolution range)	93.4 (45.38-2.14) 93.4 (46.60-2.14)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.14 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.171 , 0.209 0.176 , 0.180	Depositor DCC
$R_{free}$ test set	3667 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 85.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72972 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ACT, SO4, 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:HG12	1:A:394:ILE:O	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
1:B:615:GLU:HA	1:B:617:GLY:N	2.06	0.69
4:A:708:ACT:H1	6:A:855:HOH:O	1.93	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:B:589:GLU:C	1:B:594:GLN:HG3	2.15	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
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:B:153:LYS:HE2	2:B:701:GOL:H2	1.83	0.60
1:A:147:GLU:HA	2:A:703:GOL:H31	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:HD12	1:B:651:LEU:C	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:582:ILE:HD13	1:A:583:THR:N	2.23	0.54
1:A:253:LEU:C	1:A:253:LEU:HD12	2.28	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:264:LEU:C	1:A:264:LEU:HD12	2.28	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:HD12	1:B:253:LEU:C	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:B:153:LYS:HE2	2:B:701:GOL:C2	2.41	0.50
1:A:206:LYS:NZ	6:B:973:HOH:O	2.45	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: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:288:ARG:NH2	6:B:845:HOH:O	2.46	0.48
1:B:654:TRP:HA	1:B:680:VAL:O	2.13	0.48
1:B:394:ILE:CG1	1:B:394:ILE:O	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:295:ALA:O	1:A:298:LYS:NZ	2.49	0.46
1:A:147:GLU:CA	2:A:703:GOL:H31	2.45	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:547:SER:OG	1:A:548:TRP:N	2.49	0.45
1:A:490:LEU:C	1:A:490:LEU:HD13	2.37	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

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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	0.44
1:B:382:LEU:HD12	1:B:382:LEU:C	2.38	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:477:THR:HG22	1:A:478:TYR:N	2.33	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:HD3	1:A:304:LYS:HA	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:N	1:B:436:GLU:OE1	2.51	0.43
1:B:108:SER:O	1:B:109:ASN:C	2.56	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:285:THR:HG23	6:A:1014:HOH:O	2.17	0.43
1:B:127:THR:HB	6:B:905:HOH:O	2.18	0.43
1:A:568:GLY:O	1:A:570:ARG:HG3	2.19	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:B:85:LYS:HE2	1:B:89:GLU:OE2	2.19	0.43
1:A:232:LYS:HG3	1:A:273:HIS:CD2	2.54	0.43
1:A:438:THR:CG2	1:A:439:ARG:N	2.74	0.43
1:A:122:PRO:CD	1:B:119:VAL:HA	2.46	0.43
1:A:617:GLY:HA2	1:A:631:ALA:C	2.39	0.43
1:B:127:THR:HG21	6:B:844:HOH:O	2.19	0.43
1:A:483:CYS:HA	1:A:484:CYS:HA	1.73	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:B:526:LEU:HD23	1:B:526:LEU:C	2.40	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:A:306:HIS:HB2	1:A:307:PRO:HD2	2.02	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:N	1:A:564:ASP:OD2	2.44	0.42
1:B:46:ARG:NH1	2:B:702:GOL:H12	2.18	0.42
1:B:304:LYS:HD3	1:B:304:LYS:HA	1.73	0.41
1:A:129:HIS:CG	1:A:183:LYS:HB2	2.55	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: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: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:575:VAL:HG13	1:B:602:ILE:HD11	2.02	0.41
1:A:315:LEU:HA	1:A:331:PHE:HB3	2.03	0.41
1:B:153:LYS:HZ2	2:B:701:GOL:H32	1.83	0.41
1:A:127:THR:HG22	1:A:237:GLY:HA2	2.02	0.41
1:A:252:LYS:HE2	1:A:252:LYS:HB3	1.81	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:43:PHE:HA	1:A:69:GLU:O	2.21	0.41
1:A:548:TRP:O	1:A:569:ASN:ND2	2.46	0.40
1:A:349:LYS:HG2	2:A:705:GOL:C3	2.41	0.40
1:B:630:PRO:C	1:B:631:LYS:HG3	2.41	0.40
1:B:188:PHE:CZ	1:B:201:ILE:HD12	2.56	0.40
1:B:149:ASP:C	1:B:149:ASP:OD1	2.59	0.40
1:A:298:LYS:O	1:A:304:LYS:HG3	2.22	0.40
1:A:38:GLN:O	1:A:38:GLN:HG2	2.21	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 [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%)	39	33
1	B	501/658 (76%)	467 (93%)	32 (6%)	2 (0%)	39	33
All	All	997/1316 (76%)	932 (94%)	61 (6%)	4 (0%)	39	33

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%)	58	60
1	B	437/533 (82%)	429 (98%)	8 (2%)	66	69
All	All	871/1066 (82%)	853 (98%)	18 (2%)	63	64

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

Some 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 carbohydrates 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	A	701	-	5,5,5	0.44	0	5,5,5	0.52	0
2	GOL	A	702	-	5,5,5	0.42	0	5,5,5	0.22	0
2	GOL	A	703	-	5,5,5	0.31	0	5,5,5	0.30	0
2	GOL	A	704	-	5,5,5	0.33	0	5,5,5	0.42	0
2	GOL	A	705	-	5,5,5	0.29	0	5,5,5	0.30	0
2	GOL	A	706	-	5,5,5	0.33	0	5,5,5	0.25	0
3	SO4	A	707	-	4,4,4	0.18	0	6,6,6	0.08	0
4	ACT	A	708	-	1,3,3	1.07	0	0,3,3	0.00	-
2	GOL	B	701	-	5,5,5	0.44	0	5,5,5	0.49	0
2	GOL	B	702	-	5,5,5	0.34	0	5,5,5	0.22	0
2	GOL	B	703	-	5,5,5	0.32	0	5,5,5	0.27	0
2	GOL	B	704	-	5,5,5	0.30	0	5,5,5	0.22	0
2	GOL	B	705	-	5,5,5	0.30	0	5,5,5	0.38	0
3	SO4	B	706	-	4,4,4	0.25	0	6,6,6	0.25	0
3	SO4	B	707	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	B	708	-	4,4,4	0.20	0	6,6,6	0.17	0
3	SO4	B	709	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	B	710	-	4,4,4	0.22	0	6,6,6	0.23	0
3	SO4	B	711	-	4,4,4	0.15	0	6,6,6	0.11	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	701	-	-	0/4/4/4	0/0/0/0
2	GOL	A	702	-	-	0/4/4/4	0/0/0/0
2	GOL	A	703	-	-	0/4/4/4	0/0/0/0
2	GOL	A	704	-	-	0/4/4/4	0/0/0/0
2	GOL	A	705	-	-	0/4/4/4	0/0/0/0
2	GOL	A	706	-	-	0/4/4/4	0/0/0/0
3	SO4	A	707	-	-	0/0/0/0	0/0/0/0
4	ACT	A	708	-	-	0/0/0/0	0/0/0/0
2	GOL	B	701	-	-	0/4/4/4	0/0/0/0
2	GOL	B	702	-	-	0/4/4/4	0/0/0/0
2	GOL	B	703	-	-	0/4/4/4	0/0/0/0
2	GOL	B	704	-	-	0/4/4/4	0/0/0/0
2	GOL	B	705	-	-	0/4/4/4	0/0/0/0
3	SO4	B	706	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	707	-	-	0/0/0/0	0/0/0/0
3	SO4	B	708	-	-	0/0/0/0	0/0/0/0
3	SO4	B	709	-	-	0/0/0/0	0/0/0/0
3	SO4	B	710	-	-	0/0/0/0	0/0/0/0
3	SO4	B	711	-	-	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.

12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GOL	1	0
2	A	702	GOL	2	0
2	A	703	GOL	2	0
2	A	704	GOL	6	0
2	A	705	GOL	4	0
2	A	706	GOL	2	0
4	A	708	ACT	5	0
2	B	701	GOL	6	0
2	B	702	GOL	7	0
2	B	703	GOL	4	0
2	B	704	GOL	2	0
3	B	706	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	514/658 (78%)	1.09	112 (21%)  	16, 51, 132, 194	0
1	B	519/658 (78%)	0.99	109 (21%)  	15, 47, 129, 179	0
All	All	1033/1316 (78%)	1.04	221 (21%)  	15, 49, 131, 194	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	PRO	20.7
1	B	614	ALA	12.5
1	A	618	PHE	9.7
1	A	264	LEU	9.5
1	B	615	GLU	9.3
1	A	617	GLY	9.2
1	A	558	TRP	9.1
1	B	618	PHE	8.1
1	A	565	LYS	7.9
1	A	436	GLU	7.8
1	A	441	PHE	7.6
1	A	299	LYS	7.5
1	A	614	ALA	7.5
1	B	119	VAL	7.5
1	B	565	LYS	7.2
1	B	578	ALA	7.1
1	A	569	ASN	7.1
1	B	445	PRO	6.8
1	A	418	LYS	6.3
1	A	632	TYR	6.3
1	A	498	LYS	6.2
1	B	476	LYS	6.2
1	B	118	GLY	6.1
1	A	630	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	416	LEU	6.0
1	A	438	THR	6.0
1	B	552	ILE	6.0
1	B	477	THR	5.9
1	B	567	GLY	5.9
1	A	616	SER	5.9
1	A	480	VAL	5.8
1	B	577	PHE	5.8
1	A	571	ALA	5.8
1	B	441	PHE	5.7
1	A	437	PHE	5.7
1	B	575	VAL	5.6
1	A	478	TYR	5.5
1	A	675	ALA	5.4
1	A	477	THR	5.3
1	B	540	GLN	5.3
1	A	620	LEU	5.3
1	A	631	ALA	5.2
1	A	392	LYS	5.2
1	B	558	TRP	5.2
1	B	579	ASP	5.2
1	B	443	HIS	5.2
1	A	677	SER	5.1
1	B	117	ASN	5.0
1	A	446	GLU	4.8
1	B	566	GLU	4.8
1	A	485	SER	4.8
1	A	520	VAL	4.7
1	B	589	GLU	4.7
1	B	115	ALA	4.7
1	B	120	ASN	4.6
1	A	476	LYS	4.6
1	B	560	GLY	4.6
1	B	444	THR	4.6
1	B	611	ALA	4.6
1	B	300	GLU	4.6
1	A	272	LYS	4.6
1	A	439	ARG	4.5
1	A	548	TRP	4.5
1	A	615	GLU	4.5
1	A	629	PRO	4.5
1	B	475	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	588	ALA	4.4
1	A	609	GLY	4.4
1	B	633	TYR	4.4
1	A	557	SER	4.4
1	B	548	TRP	4.4
1	B	520	VAL	4.4
1	B	636	ASP	4.4
1	B	598	ILE	4.3
1	A	585	LYS	4.3
1	B	601	MET	4.3
1	B	619	ASP	4.3
1	B	498	LYS	4.2
1	A	481	GLU	4.2
1	B	553	ALA	4.2
1	B	417	PRO	4.2
1	B	586	LEU	4.2
1	A	492	TYR	4.2
1	A	687	GLN	4.1
1	A	440	LYS	4.1
1	B	446	GLU	4.1
1	A	562	ALA	4.1
1	A	587	THR	4.1
1	A	612	LYS	3.9
1	B	568	GLY	3.9
1	A	688	GLN	3.9
1	B	536	ILE	3.8
1	B	613	THR	3.8
1	A	566	GLU	3.8
1	B	438	THR	3.8
1	B	635	THR	3.8
1	B	631	LYS	3.8
1	B	299	LYS	3.7
1	B	634	ILE	3.7
1	B	542	VAL	3.7
1	B	630	PRO	3.7
1	A	619	ASP	3.7
1	A	570	ARG	3.7
1	A	576	ASN	3.6
1	A	444	THR	3.6
1	A	636	ALA	3.6
1	B	392	LYS	3.6
1	B	582	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	633	ILE	3.5
1	B	440	LYS	3.5
1	B	442	GLU	3.5
1	B	437	PHE	3.5
1	B	436	GLU	3.5
1	B	534	LYS	3.5
1	A	443	HIS	3.5
1	B	270	ASN	3.5
1	A	676	SER	3.4
1	B	563	SER	3.4
1	B	678	ALA	3.4
1	A	596	PHE	3.4
1	A	482	VAL	3.4
1	A	586	LEU	3.4
1	B	620	LEU	3.4
1	B	557	SER	3.4
1	A	554	ASN	3.4
1	A	563	SER	3.3
1	B	535	GLU	3.3
1	B	349	LYS	3.3
1	A	271	ASP	3.3
1	B	612	LYS	3.2
1	B	551	HIS	3.2
1	B	637	ALA	3.2
1	B	479	GLU	3.2
1	B	677	SER	3.2
1	A	560	GLY	3.2
1	B	617	GLY	3.2
1	A	479	GLU	3.2
1	B	376	SER	3.2
1	B	616	SER	3.2
1	A	417	PRO	3.2
1	A	564	ASP	3.1
1	B	570	ARG	3.1
1	B	109	ASN	3.1
1	B	537	PRO	3.1
1	B	271	ASP	3.1
1	A	483	CYS	3.1
1	A	590	ASN	3.0
1	A	546	GLY	2.9
1	B	478	TYR	2.9
1	A	579	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	536	ILE	2.9
1	B	632	ALA	2.8
1	A	635	ASP	2.8
1	A	445	PRO	2.8
1	A	568	GLY	2.8
1	B	522	GLN	2.8
1	A	233[A]	ASP	2.7
1	A	634	THR	2.7
1	B	687	GLN	2.7
1	A	611	ALA	2.7
1	B	497	ARG	2.7
1	A	581	LYS	2.6
1	A	657	PRO	2.6
1	A	487	LEU	2.6
1	A	553	ALA	2.6
1	A	684	ALA	2.6
1	B	603	GLN	2.6
1	B	264	LEU	2.6
1	A	302	GLU	2.6
1	A	540	GLN	2.6
1	B	580	LYS	2.5
1	A	559	SER	2.5
1	B	597	THR	2.5
1	B	480	VAL	2.5
1	A	486	ASN	2.4
1	B	439	ARG	2.4
1	B	303	THR	2.4
1	A	601	MET	2.4
1	B	596	PHE	2.4
1	A	177	SER	2.4
1	A	686	ARG	2.4
1	B	585	LYS	2.4
1	A	599	GLU	2.4
1	A	349	LYS	2.4
1	A	303	THR	2.4
1	A	597	THR	2.4
1	A	613	THR	2.4
1	A	442	GLU	2.3
1	B	608	GLU	2.3
1	A	301	ASN	2.3
1	A	484	CYS	2.3
1	B	389	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	656	TYR	2.3
1	A	552	ILE	2.3
1	A	606	GLY	2.3
1	A	545	ARG	2.3
1	B	576	ASN	2.3
1	B	302	GLU	2.3
1	A	547	SER	2.3
1	A	475	THR	2.3
1	B	556	THR	2.2
1	B	538	THR	2.2
1	B	602	ILE	2.2
1	B	599	GLU	2.2
1	A	390	ASN	2.2
1	A	589	GLU	2.1
1	B	583	THR	2.1
1	A	607	PHE	2.1
1	A	544	TYR	2.1
1	A	555	GLY	2.1
1	B	416	LEU	2.1
1	B	390	ASN	2.1
1	B	562	ALA	2.1
1	A	37	ASP	2.1
1	B	492	TYR	2.1
1	A	181	ILE	2.1
1	B	272	LYS	2.1
1	B	581	LYS	2.0
1	B	571	ALA	2.0
1	B	569	ASN	2.0
1	A	524	MET	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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	701	6/6	0.98	0.25	5.23	22,64,76,77	0
3	SO4	B	711	5/5	0.92	0.17	4.72	59,122,134,139	0
2	GOL	B	705	6/6	0.76	0.20	4.45	63,76,81,84	0
5	NA	B	712	1/1	0.99	0.19	3.77	27,27,27,27	0
4	ACT	A	708	4/4	0.94	0.21	2.82	36,37,50,82	0
2	GOL	B	703	6/6	0.83	0.25	2.66	64,81,87,87	0
2	GOL	A	703	6/6	0.88	0.18	2.57	47,76,85,87	0
2	GOL	B	704	6/6	0.85	0.39	2.40	58,78,96,105	0
2	GOL	A	706	6/6	0.68	0.25	2.39	68,82,91,92	0
2	GOL	A	705	6/6	0.75	0.30	2.00	56,69,75,88	0
2	GOL	B	701	6/6	0.84	0.20	1.91	44,67,72,82	0
3	SO4	B	707	5/5	0.98	0.15	-0.33	47,49,79,91	0
3	SO4	B	710	5/5	0.98	0.17	-0.59	51,65,98,98	0
3	SO4	B	706	5/5	0.97	0.15	-0.76	47,59,90,125	0
2	GOL	A	702	6/6	0.61	0.21	-	40,62,65,74	0
3	SO4	B	708	5/5	0.94	0.15	-	52,85,109,122	0
3	SO4	B	709	5/5	0.85	0.12	-	91,113,118,124	0
2	GOL	B	702	6/6	0.91	0.17	-	31,46,72,80	0
3	SO4	A	707	5/5	0.96	0.17	-	56,96,119,121	0
2	GOL	A	704	6/6	0.94	0.16	-	35,52,59,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.