



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:41 PM UTC

PDB ID : 3QRG / pdb_00003qrg
Title : Crystal structure of antiRSVF Fab B21m
Authors : Luo, J.; Tsui, P.; Lewandowski, F.; Spurlino, J.; Vecchio, F.D.
Deposited on : 2011-02-17
Resolution : 1.70 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

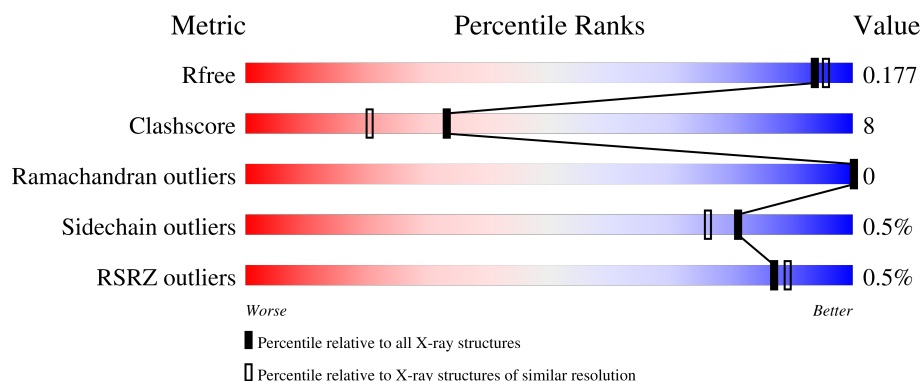
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	L	218	85% 12% .
2	H	227	88% 9% .

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
4	SO4	L	230	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4215 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.

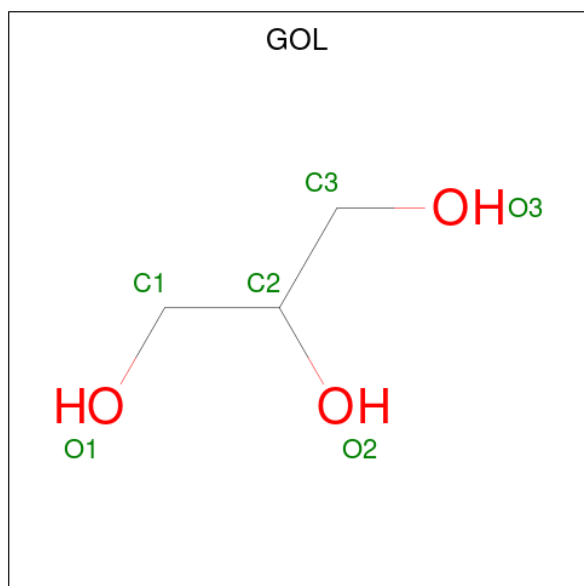
- Molecule 1 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	17	0
			1752	1108	286	352	6			

- Molecule 2 is a protein called Fab heavy chain Fd fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	17	0
			1726	1110	271	337	8			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



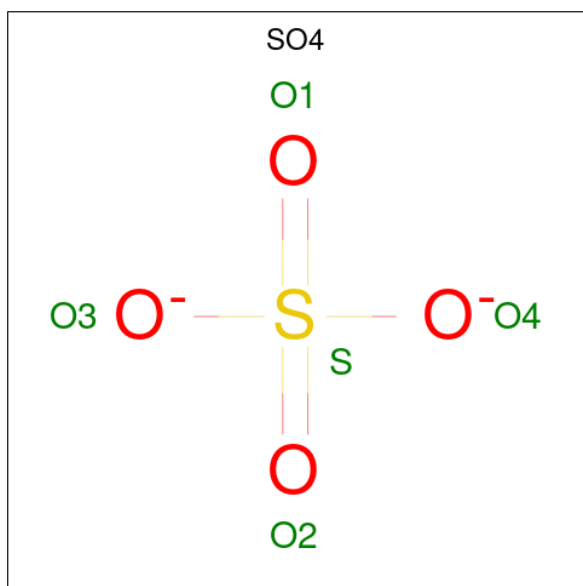
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



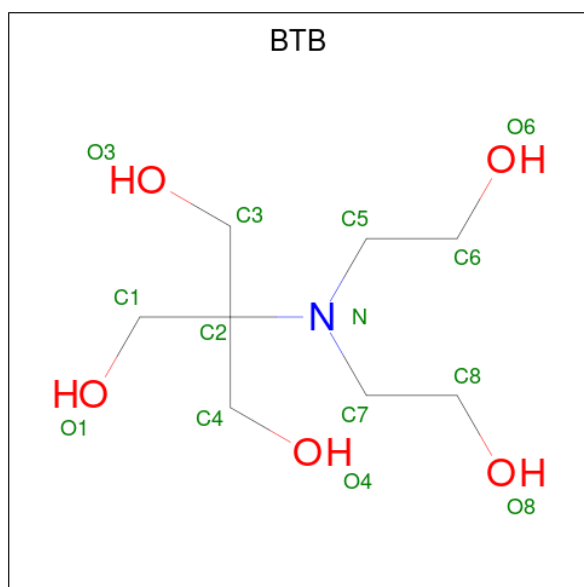
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	299	Total 299	O 299	0	0
6	H	300	Total 300	O 300	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	166.41Å 166.41Å 166.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.60 – 1.70 41.60 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.60-1.70) 99.1 (41.60-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650), CNX	Depositor
R, R_{free}	0.161 , 0.185 0.155 , 0.177	Depositor DCC
R_{free} test set	4167 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.012 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4215	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: PCA, SO4, BTB, GOL

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	L	1.35	5/1841 (0.3%)	1.32	2/2504 (0.1%)
2	H	1.32	0/1814	1.40	4/2481 (0.2%)
All	All	1.34	5/3655 (0.1%)	1.36	6/4985 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	207	SER	CA-C	5.89	1.58	1.52
1	L	54	ALA	CA-CB	5.61	1.62	1.53
1	L	42	GLN	CD-OE1	5.33	1.33	1.23
1	L	102	PHE	N-CA	5.26	1.52	1.45
1	L	119	VAL	CA-CB	-5.18	1.48	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	63	PRO	CB-CA-C	-5.26	104.43	112.11
2	H	167	THR	CA-C-O	5.23	124.57	118.77
2	H	62	ASN	CA-C-N	-5.06	113.83	119.19
2	H	62	ASN	C-N-CA	-5.06	113.83	119.19
1	L	12	ALA	CA-C-N	-5.02	116.20	123.03
1	L	12	ALA	C-N-CA	-5.02	116.20	123.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1752	0	1748	35	0
2	H	1726	0	1763	18	0
3	H	18	0	24	5	0
3	L	36	0	47	1	0
4	H	40	0	0	0	1
4	L	30	0	0	3	0
5	H	14	0	18	3	0
6	H	300	0	0	7	1
6	L	299	0	0	6	2
All	All	4215	0	3600	56	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (56) 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)
2:H:99:ARG:HH22	3:H:229:GOL:H32	1.13	1.11
1:L:12:ALA:N	4:L:230:SO4:O1	1.88	1.06
1:L:42:GLN:HE22	2:H:41:GLN:HE22	1.20	0.90
2:H:67[A]:SER:OG	6:H:563:HOH:O	1.88	0.89
1:L:87[B]:VAL:HG22	1:L:110[B]:ILE:HD13	1.53	0.87
1:L:87[B]:VAL:CG2	1:L:110[B]:ILE:HD13	2.06	0.84
2:H:99:ARG:NH2	3:H:229:GOL:H32	1.94	0.81
4:L:230:SO4:O4	6:L:403:HOH:O	2.03	0.75
1:L:110[B]:ILE:H	1:L:170:GLN:HE22	1.35	0.74
1:L:110[A]:ILE:H	1:L:170:GLN:HE22	1.36	0.73
1:L:44:PRO:O	6:L:360:HOH:O	2.07	0.71
1:L:44:PRO:HB3	1:L:169[B]:GLU:OE1	1.89	0.71
2:H:66:LYS:NZ	6:H:547:HOH:O	2.22	0.71
2:H:10[B]:THR:HG22	6:H:594:HOH:O	1.91	0.70
2:H:2:ILE:HD11	3:H:229:GOL:H11	1.74	0.70
3:H:228:GOL:H11	6:H:408:HOH:O	1.92	0.69
1:L:201[B]:THR:HG22	1:L:208:PRO:HG3	1.74	0.68
1:L:149:LYS:HB3	1:L:201[B]:THR:OG1	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180[B]:SER:OG	3:L:219:GOL:H12	1.96	0.65
2:H:168[B]:SER:OG	3:H:230:GOL:H31	1.96	0.65
1:L:38:HIS:CD2	1:L:54:ALA:H	2.15	0.64
1:L:211:LYS:HE2	6:H:459:HOH:O	1.95	0.64
1:L:159:GLN:HB3	1:L:162:ASN:HD21	1.63	0.64
4:L:229:SO4:O3	6:L:301:HOH:O	2.13	0.63
1:L:141:ASN:HD21	2:H:171:HIS:CD2	2.19	0.60
1:L:149:LYS:HB3	1:L:201[B]:THR:HG1	1.67	0.58
1:L:162:ASN:HD22	1:L:162:ASN:H	1.52	0.58
1:L:87[B]:VAL:HG23	1:L:110[B]:ILE:HD13	1.88	0.55
1:L:44:PRO:HB3	1:L:169[B]:GLU:CD	2.30	0.55
1:L:38:HIS:HD2	1:L:53:TYR:HA	1.73	0.54
1:L:156:ASN:O	1:L:156:ASN:ND2	2.42	0.52
1:L:169[A]:GLU:CD	6:L:393:HOH:O	2.52	0.52
1:L:98:ASP:HA	1:L:99:PRO:C	2.35	0.51
1:L:128:GLN:HE22	1:L:135:SER:HB2	1.76	0.50
1:L:128:GLN:HE22	1:L:135:SER:H	1.59	0.50
1:L:22[A]:ASN:OD1	6:L:435:HOH:O	2.20	0.48
2:H:10[B]:THR:HG21	6:H:455:HOH:O	2.13	0.48
2:H:8:GLY:HA3	2:H:20[B]:LEU:HD23	1.96	0.47
1:L:199:GLU:CD	6:L:541:HOH:O	2.58	0.47
1:L:128:GLN:NE2	1:L:135:SER:H	2.13	0.46
5:H:239:BTB:H41	5:H:239:BTB:H72	1.28	0.46
2:H:185:LEU:HD12	2:H:185:LEU:C	2.41	0.46
5:H:239:BTB:H82	5:H:239:BTB:H51	1.74	0.44
1:L:38:HIS:HD2	1:L:54:ALA:H	1.62	0.44
2:H:112[A]:GLN:NE2	6:H:323:HOH:O	2.40	0.44
1:L:162:ASN:HD22	1:L:162:ASN:N	2.14	0.43
5:H:239:BTB:H71	5:H:239:BTB:H32	1.68	0.43
1:L:4:MET:HE3	1:L:23:CYS:SG	2.59	0.43
2:H:84[B]:MET:SD	2:H:87:MET:SD	3.17	0.42
1:L:110[B]:ILE:H	1:L:170:GLN:NE2	2.09	0.42
1:L:141:ASN:HD21	2:H:171:HIS:HD2	1.62	0.42
1:L:11:LEU:C	1:L:11:LEU:HD12	2.45	0.41
1:L:110[A]:ILE:H	1:L:170:GLN:NE2	2.09	0.41
2:H:20[B]:LEU:HD23	2:H:20[B]:LEU:HA	1.90	0.41
2:H:69:LEU:HD21	2:H:84[B]:MET:HE2	2.03	0.41
2:H:33:GLY:H	2:H:55:TRP:CD1	2.40	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:477:HOH:O	6:H:592:HOH:O[17_553]	1.91	0.29
4:H:236:SO4:O3	6:L:389:HOH:O[3_655]	2.03	0.17

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	L	232/218 (106%)	224 (97%)	8 (3%)	0	100	100
2	H	235/227 (104%)	230 (98%)	5 (2%)	0	100	100
All	All	467/445 (105%)	454 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	L	207/191 (108%)	205 (99%)	2 (1%)	68	58
2	H	207/197 (105%)	207 (100%)	0	100	100
All	All	414/388 (107%)	412 (100%)	2 (0%)	81	76

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	156	ASN
1	L	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	32	ASN
1	L	38	HIS
1	L	41	GLN
1	L	42	GLN
1	L	93	GLN
1	L	128	GLN
1	L	141	ASN
1	L	151	GLN
1	L	159	GLN
1	L	162	ASN
1	L	170	GLN
1	L	214	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PCA	H	1	2	7,8,9	1.73	1 (14%)	9,10,12	2.60	5 (55%)

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	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	4.34	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-3.80	100.58	113.58
2	H	1	PCA	CG-CD-N	3.63	117.26	108.39
2	H	1	PCA	CB-CA-N	3.56	113.04	103.24
2	H	1	PCA	OE-CD-CG	-2.93	121.50	126.72
2	H	1	PCA	CB-CG-CD	-2.07	101.22	104.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	H	230	-	5,5,5	0.52	0	5,5,5	0.99	0
4	SO4	H	232	-	4,4,4	0.52	0	6,6,6	0.48	0
3	GOL	H	228	-	5,5,5	0.58	0	5,5,5	1.01	0
3	GOL	L	222	-	5,5,5	0.42	0	5,5,5	1.15	0
4	SO4	L	225	-	4,4,4	0.26	0	6,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	H	231	-	4,4,4	0.80	0	6,6,6	0.39	0
3	GOL	L	223	-	5,5,5	0.42	0	5,5,5	1.49	1 (20%)
4	SO4	H	234	-	4,4,4	0.48	0	6,6,6	0.68	0
4	SO4	H	235	-	4,4,4	0.30	0	6,6,6	0.74	0
5	BTB	H	239	-	13,13,13	0.98	1 (7%)	7,16,16	2.29	3 (42%)
4	SO4	L	226	-	4,4,4	0.40	0	6,6,6	0.55	0
4	SO4	L	230	-	4,4,4	0.37	0	6,6,6	0.60	0
4	SO4	H	233	-	4,4,4	0.17	0	6,6,6	0.30	0
3	GOL	L	224	-	5,5,5	1.39	1 (20%)	5,5,5	1.24	0
3	GOL	L	219	-	5,5,5	1.11	0	5,5,5	1.35	0
4	SO4	L	228	-	4,4,4	0.34	0	6,6,6	0.53	0
4	SO4	L	227	-	4,4,4	0.32	0	6,6,6	0.71	0
3	GOL	L	221	-	5,5,5	0.31	0	5,5,5	1.20	1 (20%)
4	SO4	H	237	-	4,4,4	0.37	0	6,6,6	0.58	0
3	GOL	H	229	-	5,5,5	0.46	0	5,5,5	1.53	0
4	SO4	H	236	-	4,4,4	0.69	0	6,6,6	1.46	1 (16%)
3	GOL	L	220	-	5,5,5	0.58	0	5,5,5	0.89	0
4	SO4	L	229	-	4,4,4	0.31	0	6,6,6	0.53	0
4	SO4	H	238	-	4,4,4	0.32	0	6,6,6	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	L	219	-	-	0/4/4/4	-
3	GOL	H	229	-	-	2/4/4/4	-
3	GOL	L	223	-	-	2/4/4/4	-
3	GOL	H	230	-	-	4/4/4/4	-
3	GOL	H	228	-	-	0/4/4/4	-
3	GOL	L	220	-	-	1/4/4/4	-
3	GOL	L	222	-	-	0/4/4/4	-
5	BTB	H	239	-	-	1/21/21/21	-
3	GOL	L	221	-	-	4/4/4/4	-
3	GOL	L	224	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	224	GOL	O2-C2	-2.68	1.35	1.43
5	H	239	BTB	O1-C1	-2.25	1.35	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	239	BTB	O4-C4-C2	3.71	120.12	111.40
5	H	239	BTB	O3-C3-C2	3.11	118.72	111.40
5	H	239	BTB	O1-C1-C2	-3.10	104.12	111.40
4	H	236	SO4	O3-S-O1	-2.58	96.08	109.56
3	L	221	GOL	O2-C2-C3	2.12	117.96	109.18
3	L	223	GOL	O3-C3-C2	2.08	119.72	110.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	221	GOL	O1-C1-C2-C3
3	L	221	GOL	C1-C2-C3-O3
3	L	223	GOL	O1-C1-C2-C3
3	H	229	GOL	O1-C1-C2-C3
3	H	230	GOL	O1-C1-C2-C3
3	H	230	GOL	C1-C2-C3-O3
3	L	221	GOL	O1-C1-C2-O2
3	L	223	GOL	O1-C1-C2-O2
3	H	229	GOL	O1-C1-C2-O2
3	H	230	GOL	O1-C1-C2-O2
3	L	221	GOL	O2-C2-C3-O3
3	L	224	GOL	C1-C2-C3-O3
3	H	230	GOL	O2-C2-C3-O3
3	L	220	GOL	O1-C1-C2-C3
5	H	239	BTB	C8-C7-N-C5

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	230	GOL	1	0
3	H	228	GOL	1	0
5	H	239	BTB	3	0
4	L	230	SO4	2	0
3	L	219	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	229	GOL	3	0
4	H	236	SO4	0	1
4	L	229	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	L	217/218 (99%)	-0.35	0 100 100	9, 19, 38, 56	17 (7%)
2	H	219/227 (96%)	-0.45	2 (0%) 81 83	7, 18, 33, 48	17 (7%)
All	All	436/445 (97%)	-0.40	2 (0%) 87 89	7, 18, 36, 56	34 (7%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	211	ASN	2.2
2	H	220	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	PCA	H	1	8/9	0.91	0.12	26,35,46,60	0

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(Å ²)	Q<0.9
3	GOL	H	230	6/6	0.82	0.19	46,58,64,68	0
4	SO4	H	233	5/5	0.83	0.16	52,57,63,80	5
3	GOL	L	224	6/6	0.85	0.18	22,42,50,60	0
3	GOL	L	222	6/6	0.86	0.17	25,48,59,63	0
3	GOL	H	229	6/6	0.86	0.14	25,36,54,62	0
3	GOL	L	223	6/6	0.87	0.15	27,40,55,67	0
4	SO4	H	238	5/5	0.87	0.14	48,52,53,66	5
4	SO4	H	236	5/5	0.88	0.13	22,24,29,34	5
3	GOL	L	221	6/6	0.89	0.13	29,38,46,46	0
3	GOL	L	219	6/6	0.90	0.12	19,26,38,39	0
4	SO4	H	235	5/5	0.91	0.13	30,34,40,42	5
4	SO4	L	230	5/5	0.91	0.21	21,31,40,47	5
3	GOL	H	228	6/6	0.91	0.14	28,47,50,53	0
5	BTB	H	239	14/14	0.91	0.16	15,26,41,59	14
4	SO4	L	228	5/5	0.92	0.12	23,33,38,42	5
4	SO4	L	229	5/5	0.92	0.23	19,28,32,43	5
4	SO4	H	232	5/5	0.93	0.11	29,34,45,52	5
4	SO4	H	237	5/5	0.93	0.10	34,42,46,47	5
3	GOL	L	220	6/6	0.95	0.10	17,35,37,49	0
4	SO4	L	226	5/5	0.95	0.10	35,39,44,48	5
4	SO4	H	234	5/5	0.96	0.08	29,37,40,51	5
4	SO4	L	227	5/5	0.96	0.09	20,30,37,46	5
4	SO4	L	225	5/5	0.98	0.05	29,32,39,41	5
4	SO4	H	231	5/5	0.99	0.04	17,19,21,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.