WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2018 – 10:44 AM EST

PDB ID	:	5BK1
Title	:	Crystal structure of maltose binding protein in complex with an endosteric synthetic antibody
Authors	:	Mukherjee, S.; Kossiakoff, A.A.
Deposited on	:	2017-09-12
Resolution	:	2.15 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.
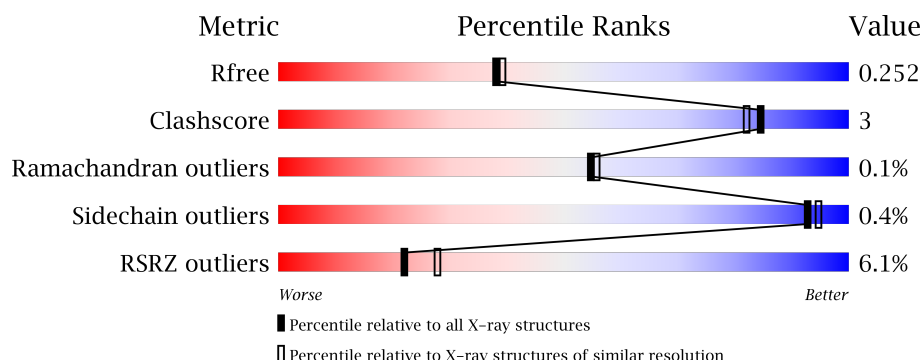
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	236	5% / 87% / 8% ·
1	H	236	4% / 89% / 8% ·
2	D	216	8% / 92% / 5% ·
2	L	216	6% / 89% / 7% ·
3	A	398	4% / 88% / · / 8%

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Mol	Chain	Length	Quality of chain
3	B	398	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13253 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 Synthetic antibody, Fab fragment, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	227	Total	C	N	O	S	0	2	0
			1713	1086	280	340	7			
1	C	226	Total	C	N	O	S	0	0	0
			1698	1078	278	335	7			

- Molecule 2 is a protein called Synthetic antibody, Fab fragment, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	1	0
			1584	984	263	332	5			
2	D	209	Total	C	N	O	S	0	3	0
			1584	985	264	329	6			

- Molecule 3 is a protein called Maltose binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	366	Total	C	N	O	S	0	1	0
			2840	1829	460	545	6			
3	B	366	Total	C	N	O	S	0	1	0
			2837	1828	459	544	6			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	167	Total 167	O 167	0	0
6	L	130	Total 130	O 130	0	0
6	C	142	Total 142	O 142	0	0
6	D	148	Total 148	O 148	0	0
6	A	240	Total 240	O 240	0	0
6	B	157	Total 157	O 157	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
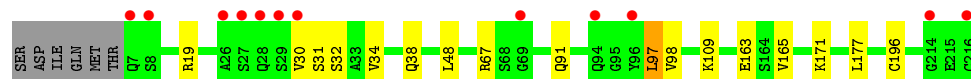
- Molecule 1: Synthetic antibody, Fab fragment, Heavy Chain
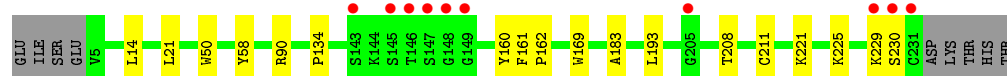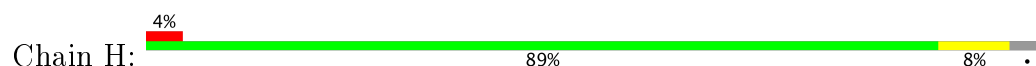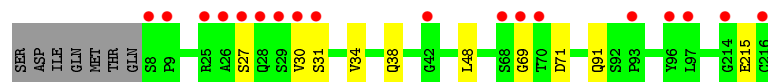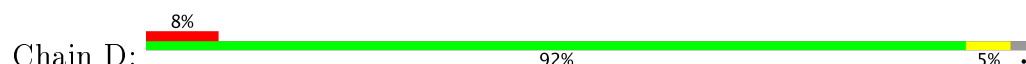
Chain H:

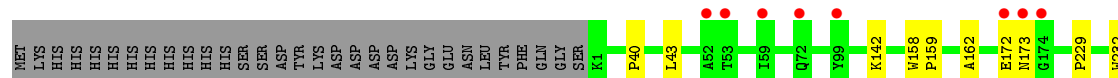- Molecule 1: Synthetic antibody, Fab fragment, Heavy Chain

Chain C:

- Molecule 2: Synthetic antibody, Fab fragment, Light Chain
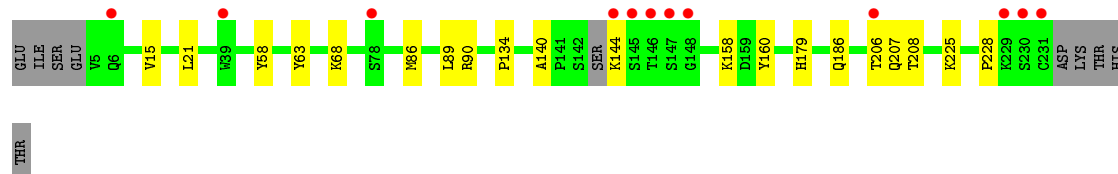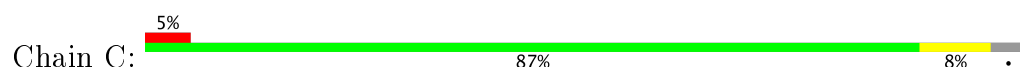
Chain L:

- Molecule 2: Synthetic antibody, Fab fragment, Light Chain

Chain D:

- Molecule 3: Maltose binding protein

Chain A:
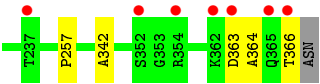
• Molecule 3: Maltose binding protein
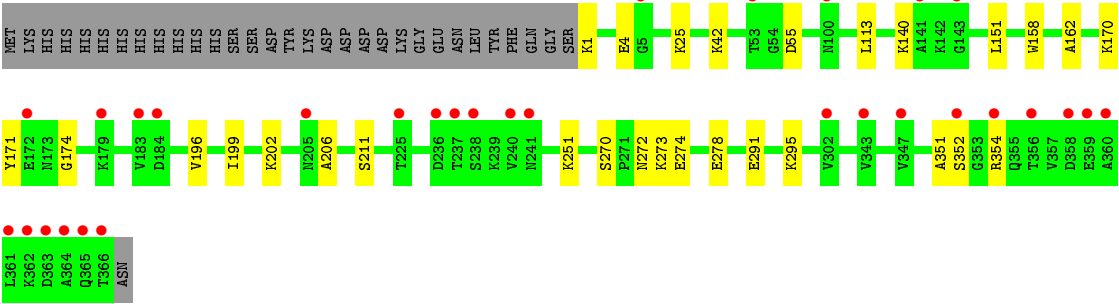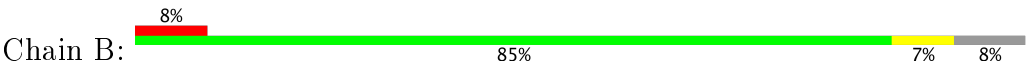
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.83Å 120.81Å 193.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.15 19.81 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.81-2.15) 99.2 (19.81-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.87 (at 2.15Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.253 0.203 , 0.252	Depositor DCC
R_{free} test set	4854 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.2	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13253	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	C	0.27	0/1743	0.50	0/2378
1	H	0.27	0/1762	0.49	0/2405
2	D	0.28	0/1624	0.49	0/2209
2	L	0.27	0/1618	0.49	0/2202
3	A	0.26	0/2912	0.43	0/3957
3	B	0.26	0/2909	0.42	0/3952
All	All	0.27	0/12568	0.47	0/17103

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	C	1698	0	1640	13	0
1	H	1713	0	1655	11	0
2	D	1584	0	1518	6	0
2	L	1584	0	1508	12	0
3	A	2840	0	2801	9	0
3	B	2837	0	2797	18	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	0	0
5	C	6	0	8	1	0
6	A	240	0	0	2	0
6	B	157	0	0	4	0
6	C	142	0	0	1	0
6	D	148	0	0	0	0
6	H	167	0	0	2	0
6	L	130	0	0	4	0
All	All	13253	0	11935	66	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 3.

All (66) 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:L:196:CYS:SG	6:L:301:HOH:O	2.49	0.71
3:B:4:GLU:O	3:B:272:ASN:ND2	2.24	0.71
2:L:196:CYS:O	6:L:301:HOH:O	2.14	0.66
2:L:31:SER:OG	2:L:67:ARG:NH2	2.30	0.64
3:A:342:ALA:HA	3:A:364:ALA:HB1	1.81	0.63
2:D:34:VAL:HG22	2:D:91[B]:GLN:HG2	1.80	0.63
2:L:19:ARG:NH2	6:L:304:HOH:O	2.30	0.63
2:L:30:VAL:HG13	2:L:32:SER:H	1.66	0.61
1:C:208:THR:HG23	1:C:225:LYS:HE3	1.85	0.59
2:L:30:VAL:HG22	2:L:31:SER:H	1.66	0.59
3:B:270:SER:O	3:B:273:LYS:NZ	2.37	0.57
1:H:90:ARG:NH2	6:H:304:HOH:O	2.30	0.57
3:A:142:LYS:NZ	6:A:405:HOH:O	2.39	0.55
2:L:109:LYS:NZ	6:L:310:HOH:O	2.38	0.55
1:H:14:LEU:HD21	1:H:162:PRO:HG3	1.91	0.52
3:B:140:LYS:NZ	3:B:202:LYS:O	2.40	0.52
1:C:206:THR:OG1	1:C:207:GLN:N	2.42	0.52
1:H:221:LYS:NZ	6:H:314:HOH:O	2.43	0.51
1:C:144:LYS:NZ	2:D:215:GLU:OE2	2.44	0.50
1:C:179:HIS:ND1	5:C:302:GOL:H32	2.27	0.50
1:C:134:PRO:HB3	1:C:160:TYR:HB3	1.94	0.49
2:L:34:VAL:HG22	2:L:91:GLN:HG3	1.95	0.49
3:B:158:TRP:CE2	3:B:162:ALA:HB2	2.48	0.49
1:C:86:MET:HB3	1:C:89:LEU:HD21	1.95	0.48
1:H:208:THR:HG23	1:H:225:LYS:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:LYS:HG2	1:H:230:SER:H	1.78	0.48
1:C:86:MET:HE2	1:C:89:LEU:HD21	1.95	0.47
2:L:38:GLN:HB2	2:L:48:LEU:HD11	1.95	0.47
2:D:38:GLN:HB2	2:D:48:LEU:HD11	1.96	0.47
3:A:142:LYS:NZ	6:A:408:HOH:O	2.39	0.47
1:H:134:PRO:HB3	1:H:160:TYR:HB3	1.96	0.47
1:C:90:ARG:NH2	6:C:415:HOH:O	2.48	0.46
1:C:15:VAL:HG11	1:C:89:LEU:HD13	1.98	0.45
3:B:1:LYS:HB2	3:B:55:ASP:OD1	2.17	0.45
3:B:199:ILE:HG21	3:B:206:ALA:HB2	1.98	0.45
3:A:158:TRP:CE2	3:A:162:ALA:HB2	2.52	0.45
3:A:363:ASP:HA	3:A:366:THR:HG22	1.99	0.44
3:A:229:PRO:HA	3:A:232:TRP:CE2	2.53	0.44
1:C:158:LYS:NZ	1:C:186:GLN:OE1	2.50	0.44
3:B:251:LYS:NZ	6:B:504:HOH:O	2.36	0.44
3:B:352:SER:OG	3:B:354:ARG:HG2	2.18	0.44
3:B:151:LEU:HD13	3:B:199:ILE:HD11	2.00	0.44
3:B:196:VAL:HG13	3:B:351:ALA:HA	1.99	0.43
3:B:42:LYS:NZ	6:B:512:HOH:O	2.47	0.43
2:D:31:SER:HB2	3:B:211:SER:CB	2.48	0.43
1:H:50:TRP:CG	2:L:98:VAL:HB	2.53	0.43
1:H:169:TRP:CH2	1:H:211:CYS:HB3	2.54	0.43
2:L:97:LEU:HA	2:L:97:LEU:HD12	1.91	0.43
3:B:171:TYR:OH	3:B:174:GLY:HA2	2.19	0.43
1:H:183:ALA:HA	1:H:193:LEU:HB3	2.01	0.43
1:H:21:LEU:HD23	1:H:21:LEU:HA	1.91	0.43
3:B:113:LEU:HG	6:B:547:HOH:O	2.19	0.43
2:D:30:VAL:HG11	2:D:91[A]:GLN:NE2	2.34	0.43
3:B:274:GLU:O	3:B:278:GLU:HG3	2.19	0.42
3:B:291:GLU:OE2	3:B:295:LYS:HE2	2.19	0.42
1:C:63:TYR:HB2	1:C:68:LYS:HE2	2.01	0.42
3:B:25:LYS:NZ	6:B:517:HOH:O	2.53	0.42
3:A:159:PRO:HG3	3:A:257:PRO:HA	2.01	0.41
3:A:172:GLU:HB3	3:A:173:ASN:H	1.64	0.41
3:A:40:PRO:HG2	3:A:43:LEU:HB3	2.01	0.41
1:H:161:PHE:HA	1:H:162:PRO:HA	1.85	0.41
1:C:21:LEU:HA	1:C:21:LEU:HD23	1.86	0.41
2:L:165:VAL:HG22	2:L:177:LEU:HD12	2.03	0.40
1:C:140:ALA:HB1	1:C:228:PRO:HA	2.02	0.40
3:B:170:LYS:HD3	3:B:170:LYS:HA	1.95	0.40
2:D:69:GLY:C	2:D:71:ASP:H	2.25	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	C	222/236 (94%)	217 (98%)	5 (2%)	0	100	100
1	H	227/236 (96%)	219 (96%)	8 (4%)	0	100	100
2	D	209/216 (97%)	197 (94%)	11 (5%)	1 (0%)	32	25
2	L	209/216 (97%)	201 (96%)	8 (4%)	0	100	100
3	A	365/398 (92%)	354 (97%)	11 (3%)	0	100	100
3	B	365/398 (92%)	357 (98%)	8 (2%)	0	100	100
All	All	1597/1700 (94%)	1545 (97%)	51 (3%)	1 (0%)	55	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	27	SER

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	C	189/199 (95%)	188 (100%)	1 (0%)	91	94
1	H	192/199 (96%)	191 (100%)	1 (0%)	91	94
2	D	184/190 (97%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	183/190 (96%)	180 (98%)	3 (2%)	68	73
3	A	292/323 (90%)	292 (100%)	0	100	100
3	B	291/323 (90%)	291 (100%)	0	100	100
All	All	1331/1424 (94%)	1326 (100%)	5 (0%)	93	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	58	TYR
2	L	97	LEU
2	L	163	GLU
2	L	171	LYS
1	C	58	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	#$|Z| > 2$
5	GOL	B	401	-	5,5,5	0.81	0	5,5,5	0.97	0
5	GOL	C	302	-	5,5,5	0.86	0	5,5,5	1.06	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
5	GOL	B	401	-	-	0/4/4/4	0/0/0/0
5	GOL	C	302	-	-	0/4/4/4	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	302	GOL	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	C	226/236 (95%)	0.39	12 (5%)	27	34	22, 32, 59, 173	0
1	H	227/236 (96%)	0.27	10 (4%)	35	43	22, 31, 66, 153	0
2	D	209/216 (96%)	0.38	18 (8%)	11	15	22, 31, 84, 175	0
2	L	210/216 (97%)	0.30	12 (5%)	24	32	21, 31, 74, 168	0
3	A	366/398 (91%)	0.22	15 (4%)	38	45	22, 34, 62, 150	0
3	B	366/398 (91%)	0.54	31 (8%)	11	15	25, 40, 77, 156	0
All	All	1604/1700 (94%)	0.36	98 (6%)	22	28	21, 34, 73, 175	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	SER	15.5
3	A	366	THR	13.7
1	H	231	CYS	13.6
3	B	366	THR	10.4
2	L	216	CYS	10.3
1	C	148	GLY	9.9
1	C	145	SER	9.9
2	D	27	SER	9.0
2	D	29	SER	7.9
2	D	216	CYS	7.1
3	B	364	ALA	6.9
1	H	230	SER	6.8
2	D	28	GLN	6.6
2	L	29	SER	6.5
2	D	96	TYR	6.5
1	C	231	CYS	6.3
2	L	96	TYR	5.9
3	B	365	GLN	5.8
2	D	26	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
3	A	173	ASN	5.1
1	C	230	SER	4.8
3	B	362	LYS	4.6
3	B	363	ASP	4.6
1	H	229	LYS	4.1
3	B	354	ARG	4.1
3	B	356	THR	4.0
3	B	143	GLY	3.9
1	H	146	THR	3.9
2	L	28	GLN	3.8
3	B	359	GLU	3.8
3	A	354	ARG	3.7
3	A	352	SER	3.6
3	B	240	VAL	3.6
3	A	52	ALA	3.6
1	C	144	LYS	3.6
2	L	214	GLY	3.6
3	A	53	THR	3.6
2	L	8	SER	3.6
1	C	39	TRP	3.5
2	D	70	THR	3.5
1	H	148	GLY	3.4
3	B	237	THR	3.3
1	H	147	SER	3.3
2	L	7	GLN	3.3
3	B	361	LEU	3.2
3	A	365	GLN	3.2
3	A	99	TYR	3.1
2	L	27	SER	3.1
3	B	236	ASP	3.1
2	D	25	ARG	3.1
2	D	69	GLY	3.0
1	H	143	SER	3.0
3	A	237	THR	3.0
2	D	8	SER	2.9
3	B	343	VAL	2.9
3	A	172	GLU	2.9
1	H	205	GLY	2.9
1	C	229	LYS	2.9
3	A	363	ASP	2.8
1	H	145	SER	2.8
3	A	174	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	31	SER	2.7
2	L	30	VAL	2.7
2	D	97	LEU	2.6
3	B	183	VAL	2.6
2	D	9	PRO	2.5
3	B	360	ALA	2.5
2	L	94	GLN	2.5
1	C	78	SER	2.5
3	B	172	GLU	2.5
2	D	93	PRO	2.4
3	A	59	ILE	2.4
3	B	347	VAL	2.3
1	C	146	THR	2.3
1	H	149	GLY	2.3
3	B	225	THR	2.3
3	B	241	ASN	2.3
3	B	141	ALA	2.3
2	D	30	VAL	2.3
3	B	53	THR	2.3
3	B	238	SER	2.3
3	B	184	ASP	2.3
2	D	42	GLY	2.3
3	B	352	SER	2.3
3	B	302	VAL	2.2
2	D	214	GLY	2.2
3	B	358	ASP	2.2
2	L	26	ALA	2.2
3	B	100	ASN	2.1
1	C	6	GLN	2.1
1	C	206	THR	2.1
3	A	362	LYS	2.1
3	A	72	GLN	2.1
3	B	5	GLY	2.1
2	D	68	SER	2.1
3	B	179	LYS	2.0
2	L	69	GLY	2.0
3	B	205	ASN	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 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, 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	LLDF	B-factors($Å^2$)	Q<0.9
5	GOL	C	302	6/6	0.72	0.27	1.89	43,48,50,55	0
5	GOL	B	401	6/6	0.74	0.21	-	58,60,62,66	0
4	CL	C	301	1/1	0.96	0.30	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.