



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:14 PM BST

PDB ID : 5BK2
Title : Crystal structure of maltose binding protein in complex with a peristeric synthetic antibody
Authors : Mukherjee, S.; Kossiakoff, A.A.
Deposited on : 2017-09-12
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

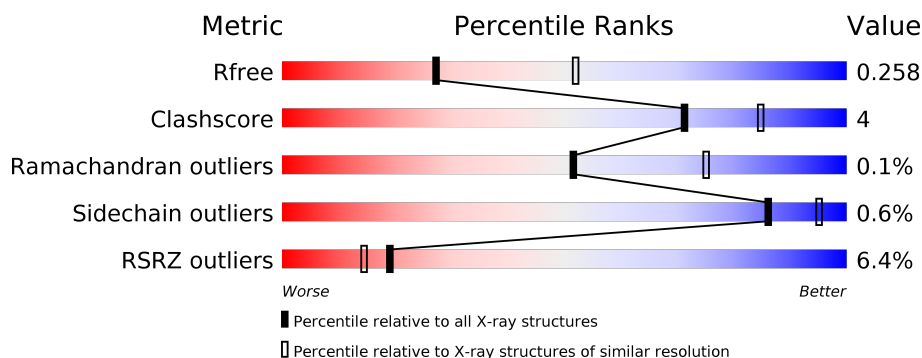
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



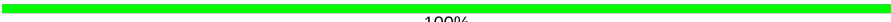
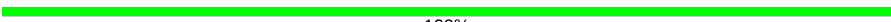
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	398	<div> <div>7%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	B	398	<div> <div>7%</div> <div>81%</div> <div>11%</div> <div>8%</div> </div>
2	C	237	<div> <div>5%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
2	H	237	<div> <div>8%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
3	D	216	<div> <div>3%</div> <div>94%</div> <div>6%</div> </div>
3	L	216	<div> <div>7%</div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 100%

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
6	GOL	C	307	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12849 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	367	Total	C	N	O	S	0	3	0
			2856	1843	465	542	6			
1	A	367	Total	C	N	O	S	0	1	0
			2842	1832	462	542	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	initiating methionine	UNP P0AEX9
B	-29	LYS	-	expression tag	UNP P0AEX9
B	-28	HIS	-	expression tag	UNP P0AEX9
B	-27	HIS	-	expression tag	UNP P0AEX9
B	-26	HIS	-	expression tag	UNP P0AEX9
B	-25	HIS	-	expression tag	UNP P0AEX9
B	-24	HIS	-	expression tag	UNP P0AEX9
B	-23	HIS	-	expression tag	UNP P0AEX9
B	-22	HIS	-	expression tag	UNP P0AEX9
B	-21	HIS	-	expression tag	UNP P0AEX9
B	-20	HIS	-	expression tag	UNP P0AEX9
B	-19	HIS	-	expression tag	UNP P0AEX9
B	-18	SER	-	expression tag	UNP P0AEX9
B	-17	SER	-	expression tag	UNP P0AEX9
B	-16	ASP	-	expression tag	UNP P0AEX9
B	-15	TYR	-	expression tag	UNP P0AEX9
B	-14	LYS	-	expression tag	UNP P0AEX9
B	-13	ASP	-	expression tag	UNP P0AEX9
B	-12	ASP	-	expression tag	UNP P0AEX9
B	-11	ASP	-	expression tag	UNP P0AEX9
B	-10	ASP	-	expression tag	UNP P0AEX9
B	-9	LYS	-	expression tag	UNP P0AEX9
B	-8	GLY	-	expression tag	UNP P0AEX9
B	-7	GLU	-	expression tag	UNP P0AEX9
B	-6	ASN	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP P0AEX9
B	-4	TYR	-	expression tag	UNP P0AEX9
B	-3	PHE	-	expression tag	UNP P0AEX9
B	-2	GLN	-	expression tag	UNP P0AEX9
B	-1	GLY	-	expression tag	UNP P0AEX9
B	0	SER	-	expression tag	UNP P0AEX9
B	367	ASN	-	expression tag	UNP P0AEX9
A	-30	MET	-	initiating methionine	UNP P0AEX9
A	-29	LYS	-	expression tag	UNP P0AEX9
A	-28	HIS	-	expression tag	UNP P0AEX9
A	-27	HIS	-	expression tag	UNP P0AEX9
A	-26	HIS	-	expression tag	UNP P0AEX9
A	-25	HIS	-	expression tag	UNP P0AEX9
A	-24	HIS	-	expression tag	UNP P0AEX9
A	-23	HIS	-	expression tag	UNP P0AEX9
A	-22	HIS	-	expression tag	UNP P0AEX9
A	-21	HIS	-	expression tag	UNP P0AEX9
A	-20	HIS	-	expression tag	UNP P0AEX9
A	-19	HIS	-	expression tag	UNP P0AEX9
A	-18	SER	-	expression tag	UNP P0AEX9
A	-17	SER	-	expression tag	UNP P0AEX9
A	-16	ASP	-	expression tag	UNP P0AEX9
A	-15	TYR	-	expression tag	UNP P0AEX9
A	-14	LYS	-	expression tag	UNP P0AEX9
A	-13	ASP	-	expression tag	UNP P0AEX9
A	-12	ASP	-	expression tag	UNP P0AEX9
A	-11	ASP	-	expression tag	UNP P0AEX9
A	-10	ASP	-	expression tag	UNP P0AEX9
A	-9	LYS	-	expression tag	UNP P0AEX9
A	-8	GLY	-	expression tag	UNP P0AEX9
A	-7	GLU	-	expression tag	UNP P0AEX9
A	-6	ASN	-	expression tag	UNP P0AEX9
A	-5	LEU	-	expression tag	UNP P0AEX9
A	-4	TYR	-	expression tag	UNP P0AEX9
A	-3	PHE	-	expression tag	UNP P0AEX9
A	-2	GLN	-	expression tag	UNP P0AEX9
A	-1	GLY	-	expression tag	UNP P0AEX9
A	0	SER	-	expression tag	UNP P0AEX9
A	367	ASN	-	expression tag	UNP P0AEX9

- Molecule 2 is a protein called sAB Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	228	Total	C	N	O	S	0	5	0
			1739	1108	282	341	8			
2	H	220	Total	C	N	O	S	0	7	0
			1697	1085	273	331	8			

- Molecule 3 is a protein called sAB Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	216	Total	C	N	O	S	0	5	0
			1673	1049	276	341	7			
3	L	216	Total	C	N	O	S	0	7	0
			1682	1055	276	344	7			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	2	Total	C	O	0	0	0
			23	12	11			
4	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

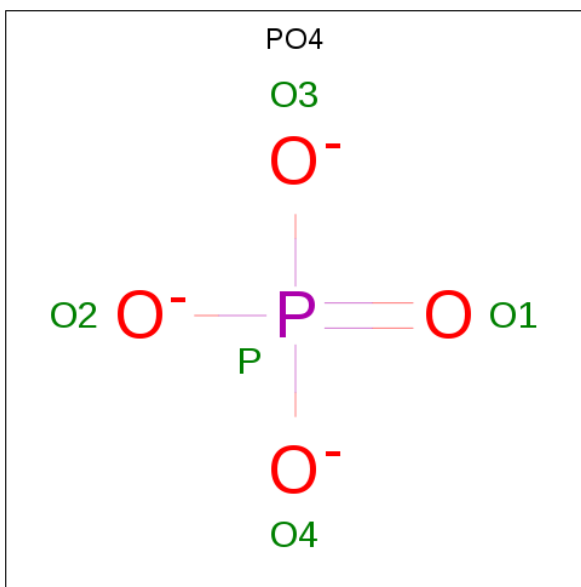
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	3	Total	Cl	0	0
			3	3		
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		
7	H	1	Total	O	P	0	0
			5	4	1		
7	H	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		

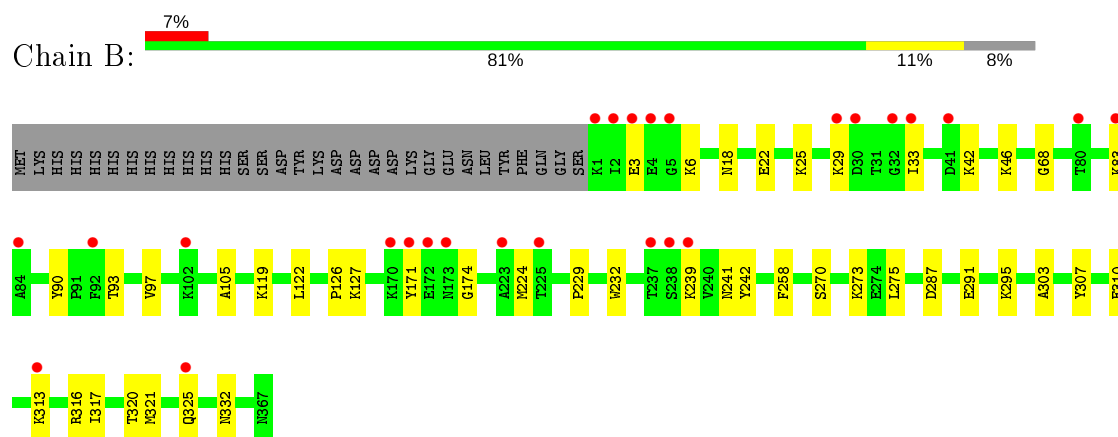
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	38	Total	O	0	0
			38	38		
8	A	23	Total	O	0	0
			23	23		
8	C	57	Total	O	0	0
			57	57		
8	H	29	Total	O	0	0
			29	29		
8	D	49	Total	O	0	0
			49	49		
8	L	25	Total	O	0	0
			25	25		

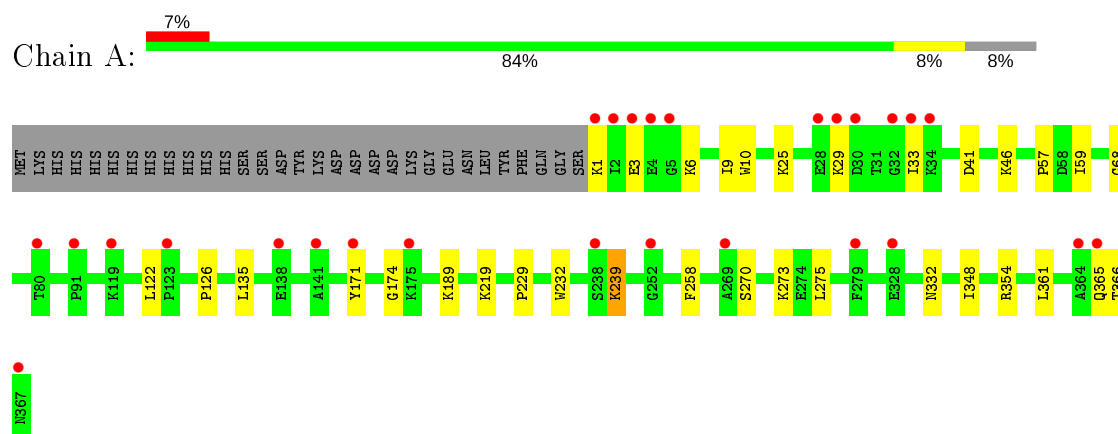
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

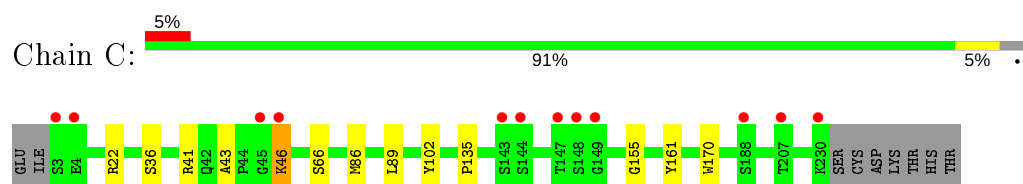
- Molecule 1: Maltose-binding periplasmic protein



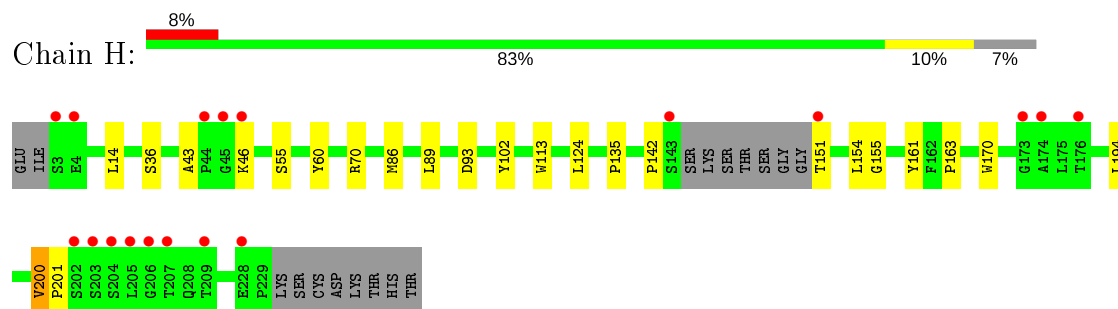
- Molecule 1: Maltose-binding periplasmic protein



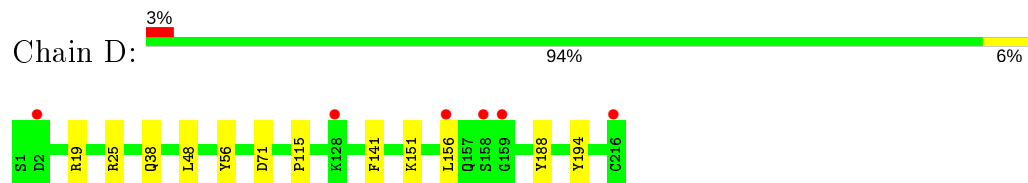
- Molecule 2: sAB Heavy Chain



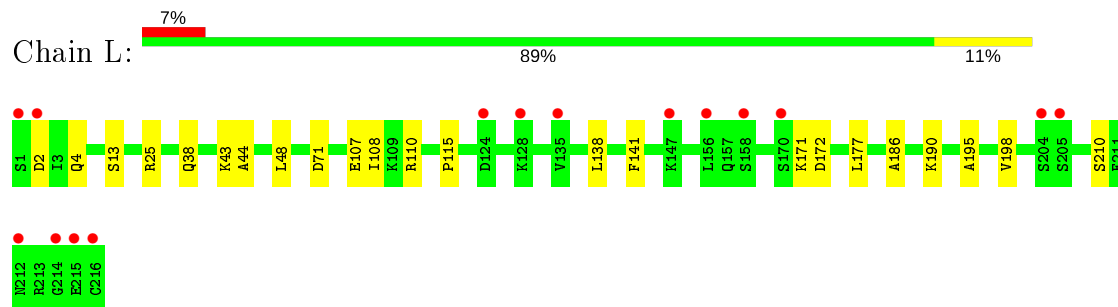
- Molecule 2: sAB Heavy Chain



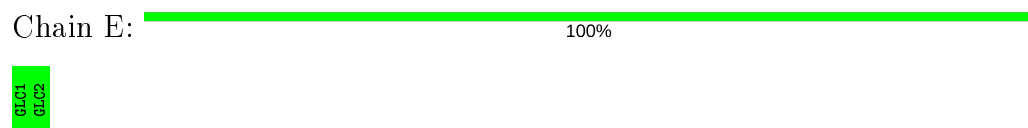
- Molecule 3: sAB Light Chain



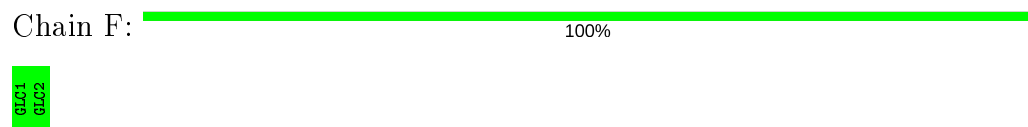
- Molecule 3: sAB Light Chain



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.17Å 42.38Å 200.66Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	19.94 – 2.60 19.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.94-2.60) 99.5 (19.94-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.59Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.259 0.212 , 0.258	Depositor DCC
R_{free} test set	2864 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12849	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, GLC, 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	A	0.25	0/2914	0.41	0/3958
1	B	0.25	0/2934	0.41	0/3982
2	C	0.26	0/1805	0.49	0/2465
2	H	0.25	0/1768	0.48	0/2415
3	D	0.26	0/1726	0.49	0/2344
3	L	0.25	0/1741	0.47	0/2364
All	All	0.25	0/12888	0.45	0/17528

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	A	2842	0	2808	19	0
1	B	2856	0	2841	25	0
2	C	1739	0	1673	8	0
2	H	1697	0	1637	15	0
3	D	1673	0	1631	9	0
3	L	1682	0	1642	12	0
4	E	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	23	0	21	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	H	3	0	0	0	0
6	C	42	0	56	3	0
6	H	18	0	24	2	0
6	L	6	0	8	0	0
7	C	5	0	0	0	0
7	D	5	0	0	1	0
7	H	10	0	0	0	0
8	A	23	0	0	2	0
8	B	38	0	0	1	0
8	C	57	0	0	1	0
8	D	49	0	0	2	0
8	H	29	0	0	1	0
8	L	25	0	0	0	0
All	All	12849	0	12362	88	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 4.

All (88) 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:C:41:ARG:HH22	6:C:304:GOL:H12	1.46	0.80
2:C:43:ALA:HB3	2:C:46:LYS:HG2	1.68	0.74
3:L:110:ARG:NH2	3:L:172:ASP:O	2.21	0.73
2:H:142:PRO:HG3	2:H:154:LEU:HB3	1.71	0.71
2:C:36:SER:HB2	2:C:102:TYR:HB3	1.73	0.69
1:A:41:ASP:O	1:A:46:LYS:NZ	2.28	0.66
2:H:194:LEU:HD12	6:H:303:GOL:H32	1.78	0.66
1:A:3:GLU:HB3	1:A:6:LYS:HE2	1.78	0.64
3:D:19:ARG:NH1	8:D:403:HOH:O	2.32	0.62
2:H:36:SER:HB2	2:H:102:TYR:HB3	1.84	0.59
2:H:70:ARG:NH2	2:H:93:ASP:OD2	2.34	0.59
1:A:1:LYS:N	8:A:501:HOH:O	2.34	0.58
3:L:115:PRO:HB3	3:L:141:PHE:HB3	1.85	0.58
1:B:3:GLU:HB3	1:B:6:LYS:HE2	1.84	0.58
3:L:25:ARG:NE	3:L:71:ASP:OD1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:SER:O	6:C:304:GOL:O1	2.21	0.57
1:B:270:SER:O	1:B:273:LYS:NZ	2.37	0.56
1:B:291:GLU:HG3	1:B:295:LYS:HD3	1.86	0.56
1:B:320:THR:HG22	8:B:519:HOH:O	2.05	0.56
3:L:138:LEU:HD21	3:L:198:VAL:HG21	1.87	0.56
1:B:119:LYS:NZ	1:B:242:TYR:O	2.37	0.55
1:B:90:TYR:O	1:B:93:THR:HG22	2.06	0.55
1:A:270:SER:O	1:A:273:LYS:NZ	2.39	0.55
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.88	0.54
2:C:22:ARG:NH2	8:C:408:HOH:O	2.40	0.54
2:H:200:VAL:HG22	2:H:201:PRO:HD2	1.89	0.54
1:A:348:ILE:HG22	1:A:354:ARG:NH1	2.22	0.54
2:H:151:THR:N	8:H:403:HOH:O	2.40	0.54
2:H:155:GLY:HA2	2:H:170:TRP:CH2	2.44	0.53
1:B:25:LYS:O	1:B:29:LYS:HG2	2.09	0.53
2:C:135:PRO:HB3	2:C:161:TYR:HB3	1.89	0.53
3:D:151:LYS:HG2	3:D:156:LEU:HD23	1.91	0.53
1:B:93:THR:HG21	1:B:303:ALA:HB1	1.90	0.52
3:D:38:GLN:HB2	3:D:48:LEU:HD11	1.90	0.52
1:B:33:ILE:HD13	1:B:275:LEU:HD13	1.91	0.52
3:D:71:ASP:OD2	8:D:402:HOH:O	2.18	0.51
1:A:348:ILE:HG22	1:A:354:ARG:HH12	1.75	0.51
1:A:219:LYS:NZ	8:A:502:HOH:O	2.43	0.51
3:L:186:ALA:O	3:L:190:LYS:HG3	2.11	0.50
1:A:25:LYS:O	1:A:29:LYS:HG2	2.10	0.50
1:B:119:LYS:NZ	1:B:241:ASN:OD1	2.45	0.49
3:L:107:GLU:HG2	3:L:108:ILE:N	2.27	0.49
2:H:14:LEU:HD22	2:H:163:PRO:HG3	1.95	0.49
2:C:86:MET:HB3	2:C:89:LEU:HD21	1.94	0.48
1:A:9:ILE:HG12	1:A:59:ILE:HB	1.96	0.48
2:H:135:PRO:HB3	2:H:161:TYR:HB3	1.96	0.47
3:L:138:LEU:HB2	3:L:177:LEU:HB3	1.96	0.47
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.49	0.47
1:B:239:LYS:HA	1:B:239:LYS:HD3	1.56	0.47
1:B:316:ARG:O	1:B:320:THR:HG23	2.15	0.47
3:D:115:PRO:HB3	3:D:141:PHE:HB3	1.97	0.47
1:B:18:ASN:O	1:B:22:GLU:HG2	2.15	0.47
1:B:310:GLU:HA	1:B:313:LYS:HE2	1.97	0.46
1:B:126:PRO:HD2	1:B:224:MET:HE3	1.97	0.46
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.51	0.46
1:B:295:LYS:HD2	1:B:295:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:HA3	1:B:332:ASN:O	2.15	0.46
1:A:122:LEU:HD21	1:A:126:PRO:HD3	1.96	0.46
3:L:43:LYS:HG2	3:L:44:ALA:N	2.31	0.46
1:B:321:MET:O	1:B:325:GLN:HG2	2.15	0.45
1:A:122:LEU:HD11	1:A:135:LEU:HD11	1.98	0.45
1:A:365:GLN:HA	1:A:366:THR:HA	1.56	0.45
2:H:86:MET:HE2	2:H:89:LEU:HD21	1.99	0.45
3:D:188:TYR:O	3:D:194:TYR:OH	2.33	0.45
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.16	0.45
2:H:124:LEU:HD23	6:H:302:GOL:H2	1.98	0.45
2:H:102:TYR:OH	2:H:113:TRP:HB2	2.17	0.45
1:A:68:GLY:HA3	1:A:332:ASN:O	2.18	0.44
2:H:86:MET:HB3	2:H:89:LEU:HD21	2.00	0.44
2:H:43:ALA:HB3	2:H:46:LYS:HD3	1.98	0.43
1:A:10:TRP:CG	1:A:57:PRO:HG3	2.53	0.43
1:B:122:LEU:HD21	1:B:126:PRO:HD3	2.00	0.43
3:D:38:GLN:NE2	7:D:302:PO4:O1	2.45	0.43
1:B:42[B]:LYS:HD2	1:B:46:LYS:NZ	2.34	0.43
1:A:33:ILE:HD13	1:A:275:LEU:HD13	2.01	0.43
2:H:55:SER:HB3	2:H:60:TYR:HB3	2.00	0.43
1:A:239:LYS:O	1:A:239:LYS:HD2	2.19	0.42
3:L:171:LYS:HA	3:L:171:LYS:HD3	1.92	0.42
3:D:25:ARG:NE	3:D:71:ASP:OD1	2.50	0.42
1:B:171:TYR:OH	1:B:174:GLY:HA2	2.20	0.42
1:A:189:LYS:HG2	1:A:361:LEU:HD12	2.02	0.42
6:C:305:GOL:H12	3:D:56:TYR:HE1	1.85	0.41
1:B:317:ILE:O	1:B:320:THR:OG1	2.31	0.41
1:B:127:LYS:HD3	1:B:127:LYS:HA	1.79	0.41
3:L:2:ASP:OD1	3:L:4:GLN:NE2	2.54	0.41
1:B:97:VAL:HG11	1:B:105:ALA:HB3	2.02	0.41
3:L:195:ALA:HB2	3:L:210:SER:HB3	2.02	0.40
2:C:155:GLY:HA2	2:C:170:TRP:CH2	2.56	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	366/398 (92%)	360 (98%)	6 (2%)	0	100	100
1	B	368/398 (92%)	358 (97%)	9 (2%)	1 (0%)	41	64
2	C	231/237 (98%)	223 (96%)	8 (4%)	0	100	100
2	H	223/237 (94%)	216 (97%)	7 (3%)	0	100	100
3	D	219/216 (101%)	210 (96%)	9 (4%)	0	100	100
3	L	221/216 (102%)	212 (96%)	9 (4%)	0	100	100
All	All	1628/1702 (96%)	1579 (97%)	48 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	TYR

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	291/323 (90%)	289 (99%)	2 (1%)	84	94
1	B	294/323 (91%)	291 (99%)	3 (1%)	76	90
2	C	194/199 (98%)	193 (100%)	1 (0%)	88	96
2	H	191/199 (96%)	190 (100%)	1 (0%)	88	96
3	D	195/190 (103%)	195 (100%)	0	100	100
3	L	197/190 (104%)	195 (99%)	2 (1%)	76	90
All	All	1362/1424 (96%)	1353 (99%)	9 (1%)	86	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	LYS
1	B	258	PHE
1	B	287	ASP
1	A	239	LYS
1	A	258	PHE
2	C	46	LYS
2	H	200	VAL
3	L	13[A]	SER
3	L	13[B]	SER

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](#)

4 monosaccharides 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	$\# Z > 2$
4	GLC	E	1	4	12,12,12	0.50	0	17,17,17	0.51	0
4	GLC	E	2	4	11,11,12	0.55	0	15,15,17	0.95	0
4	GLC	F	1	4	12,12,12	0.49	0	17,17,17	0.44	0
4	GLC	F	2	4	11,11,12	0.62	0	15,15,17	0.56	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
4	GLC	E	1	4	-	0/2/22/22	0/1/1/1
4	GLC	E	2	4	-	0/2/19/22	0/1/1/1
4	GLC	F	1	4	-	0/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1

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.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	$\# Z > 2$
7	PO4	C	309	-	4,4,4	0.91	0	6,6,6	0.48	0
6	GOL	H	301	-	5,5,5	1.05	0	5,5,5	0.89	0
6	GOL	H	302	-	5,5,5	0.89	0	5,5,5	0.98	0
6	GOL	C	301	-	5,5,5	0.90	0	5,5,5	1.00	0
6	GOL	C	306	-	5,5,5	0.86	0	5,5,5	1.04	0
6	GOL	C	305	-	5,5,5	0.90	0	5,5,5	0.98	0
6	GOL	L	301	-	5,5,5	0.89	0	5,5,5	0.98	0
7	PO4	H	308	-	4,4,4	0.93	0	6,6,6	0.39	0
6	GOL	H	303	-	5,5,5	0.94	0	5,5,5	0.94	0
7	PO4	H	307	-	4,4,4	0.91	0	6,6,6	0.42	0
6	GOL	C	302	-	5,5,5	0.96	0	5,5,5	0.96	0
7	PO4	D	302	-	4,4,4	0.92	0	6,6,6	0.45	0
6	GOL	C	303	-	5,5,5	0.90	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	C	307	-	5,5,5	0.94	0	5,5,5	0.95	0
6	GOL	C	304	-	5,5,5	0.82	0	5,5,5	1.24	1 (20%)

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
6	GOL	H	301	-	-	2/4/4/4	-
6	GOL	H	302	-	-	0/4/4/4	-
6	GOL	C	301	-	-	3/4/4/4	-
6	GOL	L	301	-	-	2/4/4/4	-
6	GOL	C	305	-	-	2/4/4/4	-
6	GOL	C	306	-	-	2/4/4/4	-
6	GOL	H	303	-	-	0/4/4/4	-
6	GOL	C	302	-	-	0/4/4/4	-
6	GOL	C	304	-	-	3/4/4/4	-
6	GOL	C	303	-	-	1/4/4/4	-
6	GOL	C	307	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	304	GOL	C3-C2-C1	-2.25	102.97	111.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	306	GOL	O1-C1-C2-O2
6	C	306	GOL	O1-C1-C2-C3
6	H	301	GOL	O1-C1-C2-C3
6	L	301	GOL	O1-C1-C2-O2
6	L	301	GOL	O1-C1-C2-C3
6	C	304	GOL	O1-C1-C2-C3
6	H	301	GOL	O1-C1-C2-O2
6	C	304	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	C	301	GOL	O1-C1-C2-C3
6	C	305	GOL	C1-C2-C3-O3
6	C	305	GOL	O2-C2-C3-O3
6	C	301	GOL	O1-C1-C2-O2
6	C	301	GOL	C1-C2-C3-O3
6	C	304	GOL	C1-C2-C3-O3
6	C	303	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	302	GOL	1	0
6	C	305	GOL	1	0
6	H	303	GOL	1	0
7	D	302	PO4	1	0
6	C	304	GOL	2	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	367/398 (92%)	0.38	27 (7%)	14 10	36, 59, 94, 143	0
1	B	367/398 (92%)	0.28	26 (7%)	16 11	29, 52, 94, 141	0
2	C	228/237 (96%)	-0.00	12 (5%)	26 20	24, 36, 76, 105	0
2	H	220/237 (92%)	0.16	18 (8%)	11 8	28, 43, 104, 122	0
3	D	216/216 (100%)	-0.01	6 (2%)	53 46	24, 41, 66, 149	1 (0%)
3	L	216/216 (100%)	0.43	15 (6%)	16 12	35, 61, 92, 152	1 (0%)
All	All	1614/1702 (94%)	0.23	104 (6%)	19 14	24, 50, 92, 152	2 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	216	CYS	10.6
3	D	216	CYS	7.7
1	B	2	ILE	5.9
1	B	80	THR	5.3
2	H	3	SER	4.8
1	B	83	LYS	4.7
3	D	2	ASP	4.7
1	A	34	LYS	4.6
1	A	238	SER	4.3
1	B	3	GLU	4.2
2	H	174	ALA	4.2
3	L	1	SER	4.1
3	L	214	GLY	4.1
1	A	32	GLY	4.0
3	L	215	GLU	4.0
1	A	141	ALA	3.9
2	H	205	LEU	3.7
1	A	2	ILE	3.6
3	L	204	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	3	SER	3.5
1	B	84	ALA	3.5
1	A	4	GLU	3.5
2	H	143	SER	3.4
1	B	1	LYS	3.4
1	A	3	GLU	3.4
1	B	239	LYS	3.3
2	C	143	SER	3.3
1	B	29	LYS	3.2
3	L	124	ASP	3.1
2	C	45	GLY	3.1
3	L	212	ASN	3.1
2	H	203	SER	3.1
1	A	80	THR	3.1
1	A	5	GLY	3.0
3	L	128	LYS	3.0
1	A	269	ALA	3.0
2	H	4	GLU	3.0
2	H	44	PRO	3.0
3	L	2	ASP	2.9
2	H	176	THR	2.9
1	B	33	ILE	2.9
3	L	205[A]	SER	2.9
1	B	172	GLU	2.9
2	H	45	GLY	2.9
2	H	207	THR	2.9
1	B	5	GLY	2.8
2	H	206	GLY	2.7
2	C	148	SER	2.7
1	B	237	THR	2.7
2	C	147	THR	2.6
1	B	173	ASN	2.6
2	C	4	GLU	2.6
1	A	364	ALA	2.6
1	A	365	GLN	2.6
3	D	158[A]	SER	2.6
2	C	230	LYS	2.6
2	H	202	SER	2.6
3	L	158[A]	SER	2.6
2	H	228	GLU	2.6
1	B	4	GLU	2.5
1	B	41	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	46	LYS	2.5
2	H	151	THR	2.5
1	A	279	PHE	2.5
1	A	91	PRO	2.5
1	A	138	GLU	2.4
3	D	156	LEU	2.4
1	B	32	GLY	2.4
2	C	149	GLY	2.4
1	B	102	LYS	2.4
1	B	313	LYS	2.4
1	B	30	ASP	2.4
3	L	170	SER	2.4
2	H	46	LYS	2.4
2	C	207	THR	2.3
2	H	204	SER	2.3
1	A	28	GLU	2.3
1	B	92	PHE	2.2
1	B	238	SER	2.2
3	L	156	LEU	2.2
1	A	29	LYS	2.2
2	H	173	GLY	2.2
1	B	171	TYR	2.2
3	L	135	VAL	2.2
3	D	128	LYS	2.2
1	A	171	TYR	2.1
3	D	159	GLY	2.1
1	A	175	LYS	2.1
2	C	144	SER	2.1
1	A	30	ASP	2.1
1	A	367	ASN	2.1
1	A	33	ILE	2.1
1	A	119	LYS	2.1
1	A	1	LYS	2.1
2	H	209	THR	2.1
1	A	252	GLY	2.1
1	B	170[A]	LYS	2.1
1	B	223	ALA	2.1
1	B	225	THR	2.1
3	L	147	LYS	2.0
2	C	188	SER	2.0
1	A	123	PRO	2.0
1	A	328	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	325	GLN	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](#)

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
4	GLC	F	1	12/12	0.94	0.12	37,44,48,50	0
4	GLC	E	1	12/12	0.96	0.10	30,34,39,39	0
4	GLC	F	2	11/12	0.97	0.12	35,38,40,42	0
4	GLC	E	2	11/12	0.98	0.11	25,31,34,35	0

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
6	GOL	C	307	6/6	0.68	0.43	68,74,78,80	0
6	GOL	H	301	6/6	0.81	0.24	58,68,70,71	0
6	GOL	C	306	6/6	0.81	0.28	58,62,65,68	0
5	CL	A	402	1/1	0.83	0.19	63,63,63,63	0
6	GOL	H	302	6/6	0.83	0.26	75,78,78,81	0
7	PO4	C	309	5/5	0.85	0.20	91,94,96,97	0
5	CL	H	305	1/1	0.88	0.10	73,73,73,73	0
5	CL	B	402	1/1	0.89	0.09	69,69,69,69	0
5	CL	D	301	1/1	0.89	0.23	82,82,82,82	0
6	GOL	C	301	6/6	0.89	0.18	42,48,51,56	0
7	PO4	H	308	5/5	0.89	0.24	97,98,101,102	0
7	PO4	H	307	5/5	0.89	0.43	101,102,102,104	0
5	CL	C	308	1/1	0.90	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	C	304	6/6	0.90	0.21	31,38,44,52	0
6	GOL	C	302	6/6	0.91	0.27	41,45,48,49	0
7	PO4	D	302	5/5	0.91	0.28	87,90,94,96	0
6	GOL	H	303	6/6	0.91	0.20	51,52,53,55	0
5	CL	H	304	1/1	0.92	0.10	71,71,71,71	0
6	GOL	C	303	6/6	0.93	0.20	43,47,53,57	0
5	CL	H	306	1/1	0.94	0.14	79,79,79,79	0
6	GOL	L	301	6/6	0.95	0.22	48,49,51,53	0
6	GOL	C	305	6/6	0.96	0.15	38,42,43,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.