



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 03:04 AM BST

PDB ID : 5BJZ  
Title : Crystal structure of maltose binding protein in complex with an allosteric synthetic antibody  
Authors : Mukherjee, S.; Kossiakoff, A.A.  
Deposited on : 2017-09-12  
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (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

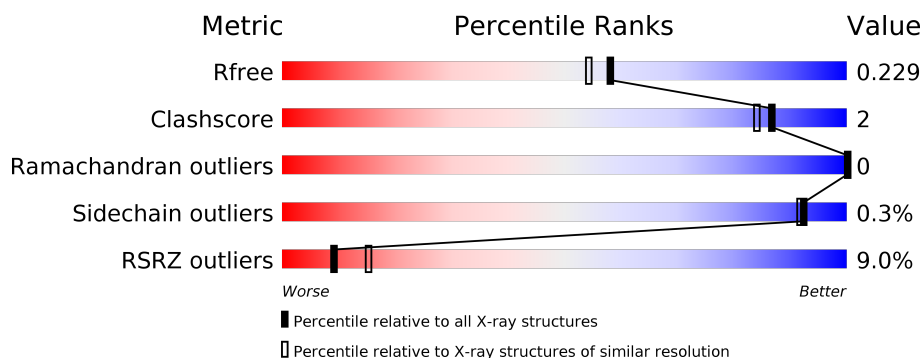
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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>4%</div> <div>89% 8%</div> </div>
1	B	398	<div> <div>%</div> <div>87% 8%</div> </div>
2	C	238	<div> <div>5%</div> <div>91% 5%</div> </div>
2	D	238	<div> <div>22%</div> <div>92% 5%</div> </div>
3	H	216	<div> <div>23%</div> <div>89% 9%</div> </div>
3	L	216	<div> <div>5%</div> <div>92% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	2	 50%50%
4	F	2	 50%50%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13778 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	365	Total	C	N	O	S	0	4	0
			2858	1847	463	542	6			
1	A	367	Total	C	N	O	S	0	4	0
			2871	1852	465	548	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	expression tag	UNP P0AEY0
B	-29	LYS	-	expression tag	UNP P0AEY0
B	-28	HIS	-	expression tag	UNP P0AEY0
B	-27	HIS	-	expression tag	UNP P0AEY0
B	-26	HIS	-	expression tag	UNP P0AEY0
B	-25	HIS	-	expression tag	UNP P0AEY0
B	-24	HIS	-	expression tag	UNP P0AEY0
B	-23	HIS	-	expression tag	UNP P0AEY0
B	-22	HIS	-	expression tag	UNP P0AEY0
B	-21	HIS	-	expression tag	UNP P0AEY0
B	-20	HIS	-	expression tag	UNP P0AEY0
B	-19	HIS	-	expression tag	UNP P0AEY0
B	-18	SER	-	expression tag	UNP P0AEY0
B	-17	SER	-	expression tag	UNP P0AEY0
B	-16	ASP	-	expression tag	UNP P0AEY0
B	-15	TYR	-	expression tag	UNP P0AEY0
B	-14	LYS	-	expression tag	UNP P0AEY0
B	-13	ASP	-	expression tag	UNP P0AEY0
B	-12	ASP	-	expression tag	UNP P0AEY0
B	-11	ASP	-	expression tag	UNP P0AEY0
B	-10	ASP	-	expression tag	UNP P0AEY0
B	-9	LYS	-	expression tag	UNP P0AEY0
B	-8	GLY	-	expression tag	UNP P0AEY0
B	-7	GLU	-	expression tag	UNP P0AEY0
B	-6	ASN	-	expression tag	UNP P0AEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP P0AEY0
B	-4	TYR	-	expression tag	UNP P0AEY0
B	-3	PHE	-	expression tag	UNP P0AEY0
B	-2	GLN	-	expression tag	UNP P0AEY0
B	-1	GLY	-	expression tag	UNP P0AEY0
B	0	SER	ALA	conflict	UNP P0AEY0
B	367	ASN	ARG	expression tag	UNP P0AEY0
A	-30	MET	-	expression tag	UNP P0AEY0
A	-29	LYS	-	expression tag	UNP P0AEY0
A	-28	HIS	-	expression tag	UNP P0AEY0
A	-27	HIS	-	expression tag	UNP P0AEY0
A	-26	HIS	-	expression tag	UNP P0AEY0
A	-25	HIS	-	expression tag	UNP P0AEY0
A	-24	HIS	-	expression tag	UNP P0AEY0
A	-23	HIS	-	expression tag	UNP P0AEY0
A	-22	HIS	-	expression tag	UNP P0AEY0
A	-21	HIS	-	expression tag	UNP P0AEY0
A	-20	HIS	-	expression tag	UNP P0AEY0
A	-19	HIS	-	expression tag	UNP P0AEY0
A	-18	SER	-	expression tag	UNP P0AEY0
A	-17	SER	-	expression tag	UNP P0AEY0
A	-16	ASP	-	expression tag	UNP P0AEY0
A	-15	TYR	-	expression tag	UNP P0AEY0
A	-14	LYS	-	expression tag	UNP P0AEY0
A	-13	ASP	-	expression tag	UNP P0AEY0
A	-12	ASP	-	expression tag	UNP P0AEY0
A	-11	ASP	-	expression tag	UNP P0AEY0
A	-10	ASP	-	expression tag	UNP P0AEY0
A	-9	LYS	-	expression tag	UNP P0AEY0
A	-8	GLY	-	expression tag	UNP P0AEY0
A	-7	GLU	-	expression tag	UNP P0AEY0
A	-6	ASN	-	expression tag	UNP P0AEY0
A	-5	LEU	-	expression tag	UNP P0AEY0
A	-4	TYR	-	expression tag	UNP P0AEY0
A	-3	PHE	-	expression tag	UNP P0AEY0
A	-2	GLN	-	expression tag	UNP P0AEY0
A	-1	GLY	-	expression tag	UNP P0AEY0
A	0	SER	ALA	conflict	UNP P0AEY0
A	367	ASN	ARG	expression tag	UNP P0AEY0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	228	Total	C	N	O	S	0	7	0
			1735	1100	286	341	8			
2	D	231	Total	C	N	O	S	0	7	0
			1756	1112	289	347	8			

- Molecule 3 is a protein called Synthetic antibody, Fab fragment, Light Chain.

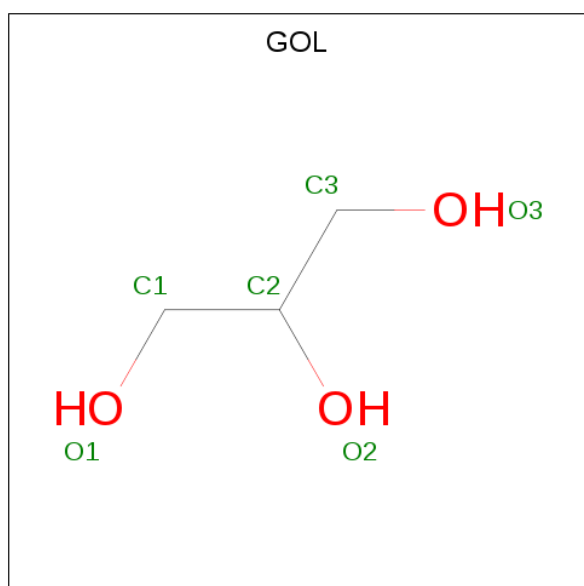
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	11	0
			1662	1037	279	339	7			
3	H	213	Total	C	N	O	S	0	9	0
			1643	1026	272	336	9			

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



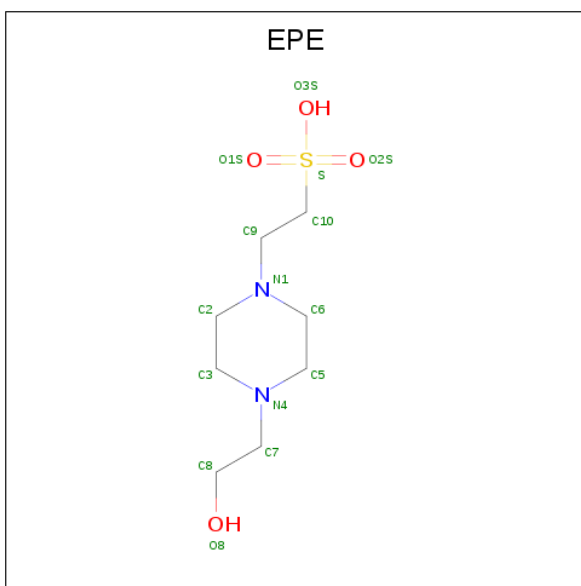
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	2	Total	C	O	0	0	0
			23	12	11			
4	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total Cl 1 1	0	0
7	L	1	Total Cl 1 1	0	0

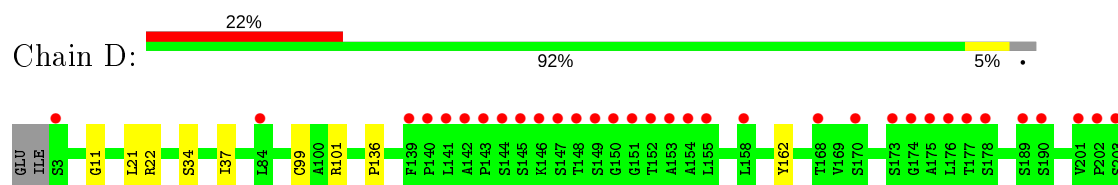
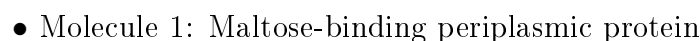
- Molecule 8 is water.

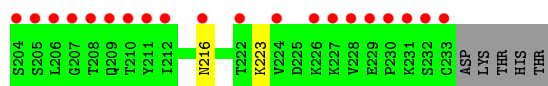
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	292	Total 292	O 292	0	0
8	C	200	Total 200	O 200	0	0
8	L	160	Total 160	O 160	0	0
8	A	252	Total 252	O 252	0	0
8	D	161	Total 161	O 161	0	0
8	H	95	Total 95	O 95	0	0





- Molecule 1: Maltose-binding periplasmic protein

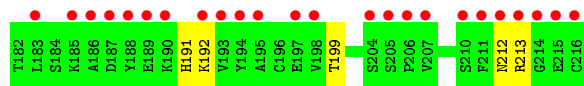
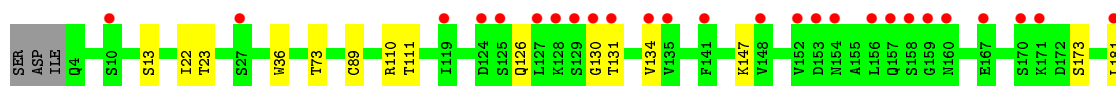
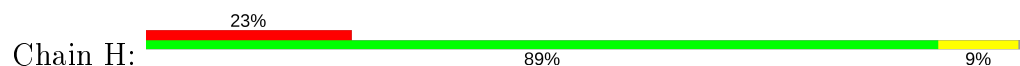




- Molecule 3: Synthetic antibody, Fab fragment, Light Chain



- Molecule 3: Synthetic antibody, Fab fragment, 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	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.39Å 87.59Å 114.65Å 90.00° 114.29° 90.00°	Depositor
Resolution (Å)	19.96 – 1.95 19.96 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.96-1.95) 97.6 (19.96-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 1.94Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.194 , 0.229 0.194 , 0.229	Depositor DCC
$R_{free}$ test set	6258 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, 0.333 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: GLC, GOL, EPE, 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	0.33	0/2952	0.50	0/4004
1	B	0.35	0/2939	0.51	0/3986
2	C	0.38	0/1804	0.57	0/2463
2	D	0.34	0/1826	0.55	0/2493
3	H	0.31	0/1703	0.49	0/2310
3	L	0.34	0/1725	0.54	0/2339
All	All	0.34	0/12949	0.52	0/17595

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	2871	0	2863	8	0
1	B	2858	0	2858	10	0
2	C	1735	0	1677	8	0
2	D	1756	0	1699	7	0
3	H	1643	0	1618	12	0
3	L	1662	0	1645	9	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	12	0	16	2	0
5	B	6	0	8	0	0
5	D	6	0	8	0	0
5	H	6	0	8	0	0
6	B	15	0	17	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	A	252	0	0	1	0
8	B	292	0	0	2	0
8	C	200	0	0	3	0
8	D	161	0	0	2	0
8	H	95	0	0	3	0
8	L	160	0	0	1	0
All	All	13778	0	12459	53	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 2.

The worst 5 of 53 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)
3:L:110[B]:ARG:NH1	3:L:172:ASP:O	2.06	0.88
3:H:126:GLN:O	8:H:401:HOH:O	2.11	0.69
2:D:216[B]:ASN:ND2	8:D:404:HOH:O	2.26	0.69
3:H:191:HIS:O	3:H:213:ARG:NH1	2.28	0.66
1:A:273:LYS:HB2	5:A:403:GOL:H2	1.81	0.62

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	369/398 (93%)	362 (98%)	7 (2%)	0	100	100
1	B	367/398 (92%)	362 (99%)	5 (1%)	0	100	100
2	C	231/238 (97%)	227 (98%)	4 (2%)	0	100	100
2	D	236/238 (99%)	230 (98%)	6 (2%)	0	100	100
3	H	220/216 (102%)	214 (97%)	6 (3%)	0	100	100
3	L	222/216 (103%)	219 (99%)	3 (1%)	0	100	100
All	All	1645/1704 (96%)	1614 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	298/323 (92%)	296 (99%)	2 (1%)	84	82
1	B	296/323 (92%)	296 (100%)	0	100	100
2	C	197/201 (98%)	196 (100%)	1 (0%)	88	88
2	D	200/201 (100%)	199 (100%)	1 (0%)	88	88
3	H	194/189 (103%)	192 (99%)	2 (1%)	76	74
3	L	196/189 (104%)	196 (100%)	0	100	100
All	All	1381/1426 (97%)	1375 (100%)	6 (0%)	92	90

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233[B]	SER
3	H	13[B]	SER
2	D	101	ARG
1	A	233[A]	SER
3	H	13[A]	SER

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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	0.59	0	17,17,17	0.84	0
4	GLC	E	2	4	11,11,12	0.76	0	15,15,17	1.01	1 (6%)
4	GLC	F	1	4	12,12,12	0.53	0	17,17,17	0.55	0
4	GLC	F	2	4	11,11,12	0.53	0	15,15,17	0.96	1 (6%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	GLC	C1-O5-C5	2.63	115.76	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	GLC	O5-C5-C6	2.16	110.58	107.20

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	A	402	-	5,5,5	0.96	0	5,5,5	1.05	0
5	GOL	H	301	-	5,5,5	0.86	0	5,5,5	1.03	0
6	EPE	B	403	-	15,15,15	0.58	0	18,20,20	1.60	5 (27%)
5	GOL	D	301	-	5,5,5	0.91	0	5,5,5	0.98	0
5	GOL	B	402	-	5,5,5	0.90	0	5,5,5	0.95	0
5	GOL	A	403	-	5,5,5	0.98	0	5,5,5	1.10	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	A	402	-	-	2/4/4/4	-
5	GOL	H	301	-	-	4/4/4/4	-
6	EPE	B	403	-	-	7/9/19/19	0/1/1/1
5	GOL	D	301	-	-	2/4/4/4	-
5	GOL	B	402	-	-	1/4/4/4	-
5	GOL	A	403	-	-	2/4/4/4	-



There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	B	403	EPE	C5-N4-C3	3.31	116.29	108.83
6	B	403	EPE	C7-N4-C3	2.85	118.52	111.23
6	B	403	EPE	C7-N4-C5	2.69	118.12	111.23
6	B	403	EPE	O1S-S-C10	2.43	109.84	106.92
6	B	403	EPE	O2S-S-C10	2.04	109.37	106.92

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	GOL	C1-C2-C3-O3
6	B	403	EPE	C10-C9-N1-C2
6	B	403	EPE	C9-C10-S-O1S
6	B	403	EPE	C9-C10-S-O3S
5	D	301	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	GOL	1	0
5	A	403	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, 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	367/398 (92%)	0.33	15 (4%) 37 46	20, 33, 53, 143	0
1	B	365/398 (91%)	0.10	5 (1%) 75 82	18, 29, 47, 62	0
2	C	228/238 (95%)	0.37	13 (5%) 23 32	20, 30, 55, 145	0
2	D	231/238 (97%)	1.37	53 (22%) 0 0	21, 36, 105, 159	0
3	H	213/216 (98%)	1.40	50 (23%) 0 0	21, 43, 100, 136	0
3	L	213/216 (98%)	0.34	10 (4%) 31 41	20, 32, 48, 128	1 (0%)
All	All	1617/1704 (94%)	0.58	146 (9%) 9 15	18, 33, 75, 159	1 (0%)

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	150	GLY	28.8
2	C	233	CYS	15.0
3	H	216	CYS	14.4
2	D	233	CYS	11.7
2	D	147	SER	10.6

### 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GLC	F	2	11/12	0.94	0.12	22,25,28,32	0
4	GLC	E	1	12/12	0.95	0.07	21,26,29,32	0
4	GLC	E	2	11/12	0.96	0.07	19,21,24,24	0
4	GLC	F	1	12/12	0.97	0.07	25,28,34,36	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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	402	6/6	0.57	0.37	78,82,82,84	0
5	GOL	D	301	6/6	0.78	0.20	57,58,59,59	0
5	GOL	A	403	6/6	0.83	0.27	41,43,51,55	0
5	GOL	H	301	6/6	0.84	0.18	42,47,50,52	0
5	GOL	A	402	6/6	0.85	0.15	42,42,45,48	0
6	EPE	B	403	15/15	0.87	0.19	60,61,66,67	0
7	CL	H	302	1/1	0.91	0.07	74,74,74,74	0
7	CL	L	301	1/1	0.97	0.09	68,68,68,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.