



Full wwPDB X-ray Structure Validation 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 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

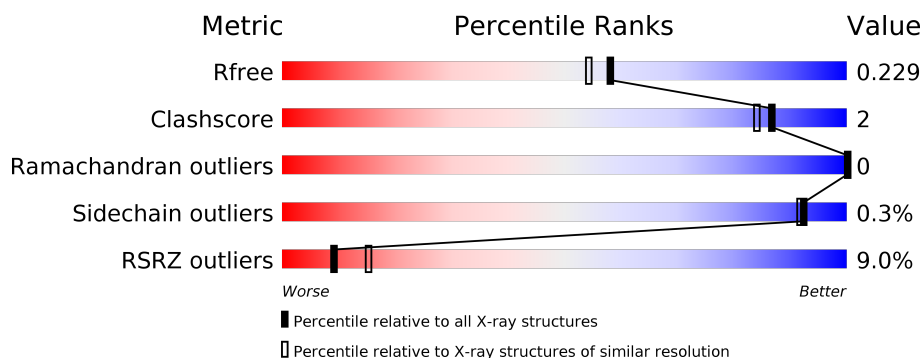
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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%</div> <div>8%</div> </div>
1	B	398	<div> <div>%</div> <div>87%</div> <div>8%</div> </div>
2	C	238	<div> <div>5%</div> <div>91%</div> <div>5%</div> </div>
2	D	238	<div> <div>22%</div> <div>92%</div> <div>5%</div> </div>
3	H	216	<div> <div>23%</div> <div>89%</div> <div>9%</div> </div>
3	L	216	<div> <div>5%</div> <div>92%</div> <div>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.

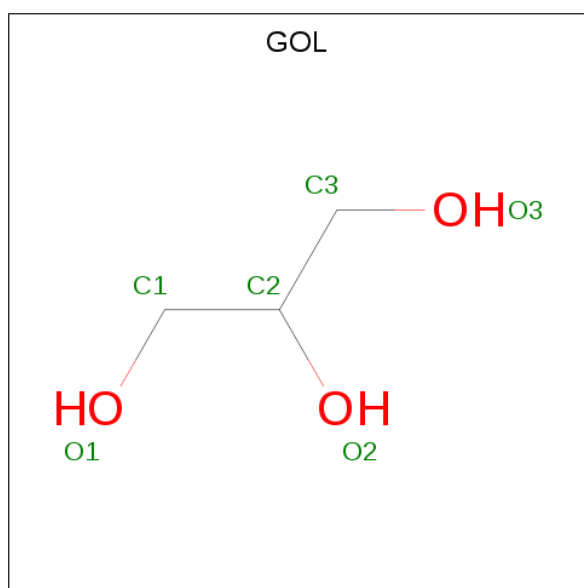
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	11	0
			1662	1037	279	339	7			
3	H	213	Total	C	N	O	S	0	9	0
			1643	1026	272	336	9			

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



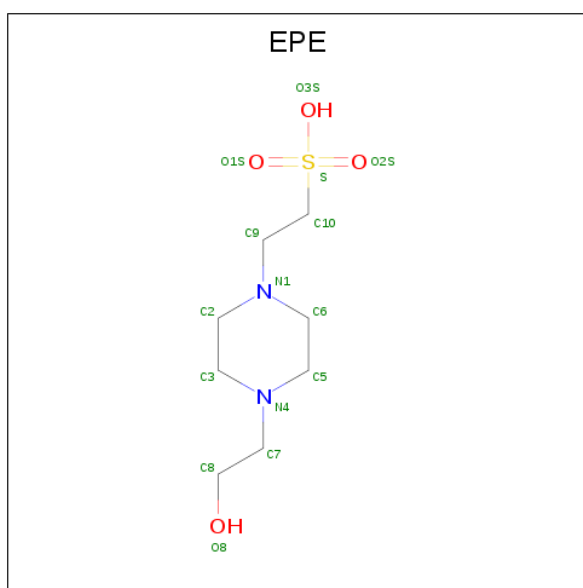
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	2	Total	C	O	0	0	0
			23	12	11			
4	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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: C₈H₁₈N₂O₄S).



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

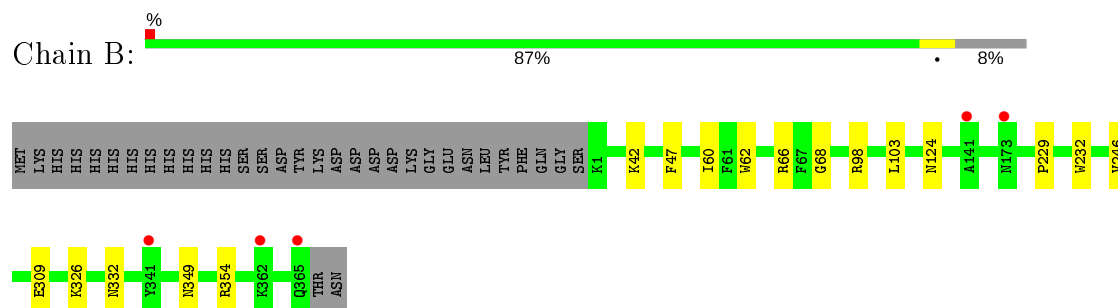
- Molecule 8 is water.

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

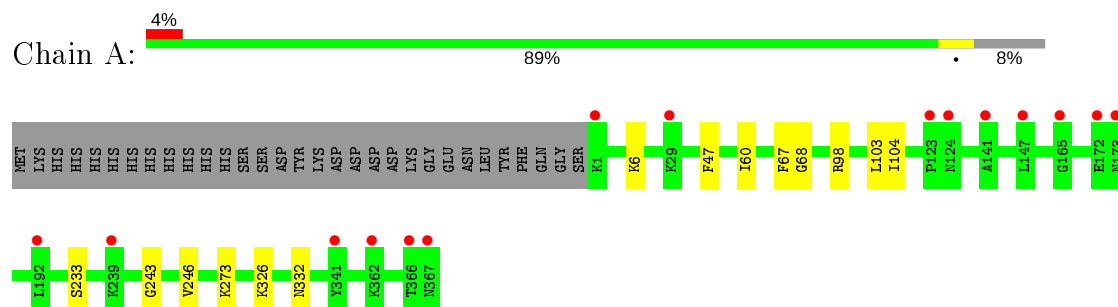
3 Residue-property plots [i](#)

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.

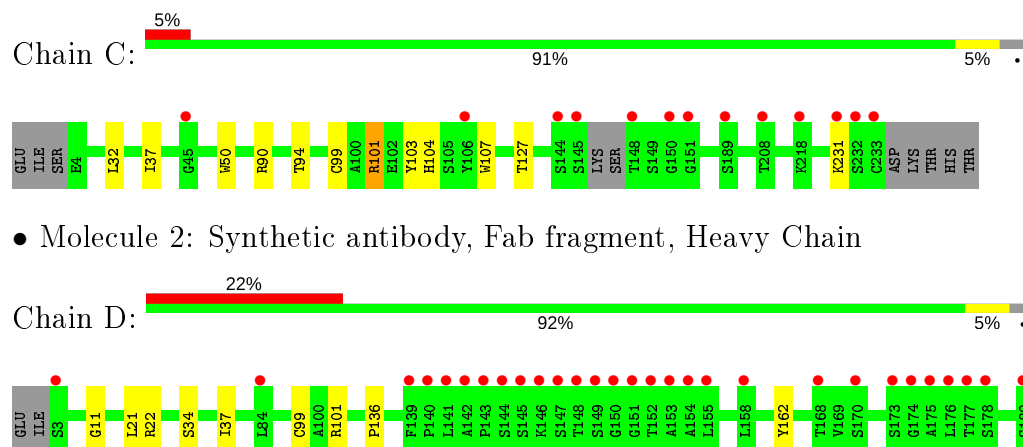
- Molecule 1: Maltose-binding periplasmic protein



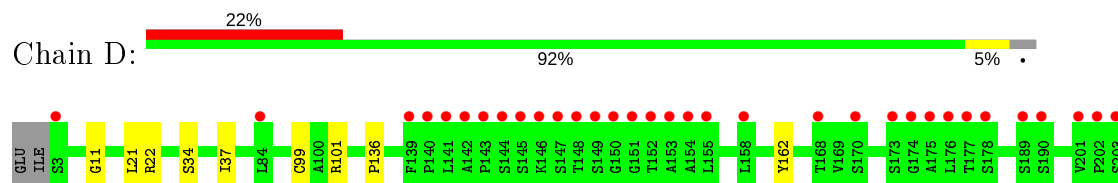
- Molecule 1: Maltose-binding periplasmic protein

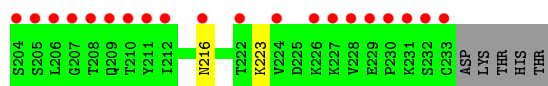


- Molecule 2: Synthetic antibody, Fab fragment, Heavy Chain



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

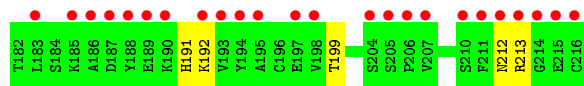
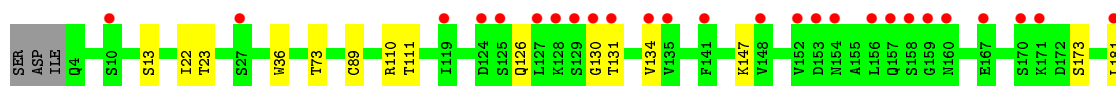
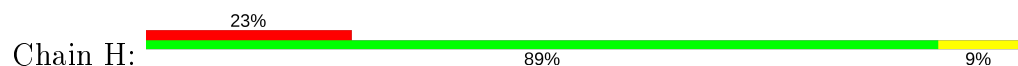




- Molecule 3: Synthetic antibody, Fab fragment, Light Chain



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	31.3	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: 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.

All (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
1:B:349:ASN:OD1	1:B:354:ARG:NH1	2.34	0.60
1:A:243:GLY:HA2	5:A:402:GOL:H32	1.82	0.60
2:C:90:ARG:NH1	8:C:307:HOH:O	2.36	0.58
1:B:42[A]:LYS:NZ	8:B:507:HOH:O	2.37	0.58
2:C:101:ARG:NH1	2:C:103:TYR:HB3	2.20	0.57
2:D:11:GLY:O	2:D:21:LEU:HD21	2.06	0.56
3:L:110[A]:ARG:HH12	3:L:113:ALA:HB2	1.72	0.54
2:C:37:ILE:HD11	2:C:99[B]:CYS:SG	2.48	0.54
1:B:68:GLY:HA3	1:B:332:ASN:O	2.07	0.53
3:H:110:ARG:HD2	3:H:173:SER:HB2	1.91	0.53
3:L:110[A]:ARG:HD2	3:L:173:SER:HB2	1.92	0.52
1:B:309:GLU:OE2	8:B:501:HOH:O	2.19	0.51
2:C:32:LEU:HD11	2:C:37:ILE:HD13	1.93	0.50
3:H:134:VAL:HB	3:H:181:LEU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:THR:HG23	2:C:127:THR:HA	1.94	0.49
3:L:149:GLN:OE1	8:L:401:HOH:O	2.19	0.49
1:A:68:GLY:HA3	1:A:332:ASN:O	2.12	0.49
2:D:37:ILE:HD11	2:D:99[B]:CYS:SG	2.54	0.48
3:H:130:GLY:N	8:H:401:HOH:O	2.46	0.48
2:D:34:SER:OG	8:D:401:HOH:O	2.09	0.48
3:H:131:THR:N	8:H:401:HOH:O	2.21	0.48
3:H:147:LYS:HB3	3:H:199:THR:HB	1.96	0.48
1:B:124:ASN:ND2	8:C:303:HOH:O	2.31	0.47
2:C:104:HIS:HB3	2:C:107:TRP:CD1	2.50	0.47
1:B:62:TRP:CD1	1:B:66:ARG:HG3	2.50	0.47
3:L:191:HIS:O	3:L:213:ARG:NH1	2.47	0.47
1:A:98:ARG:HG2	1:A:103:LEU:HD23	1.97	0.46
3:H:192:LYS:HE3	3:H:212:ASN:HB3	1.96	0.46
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.98	0.46
1:A:47:PHE:CG	1:A:60:ILE:HD12	2.51	0.46
1:B:246:VAL:HG11	1:B:326:LYS:HE3	1.98	0.45
2:D:216[B]:ASN:HD22	2:D:223:LYS:HG2	1.83	0.43
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.52	0.43
3:H:110:ARG:NH1	3:H:111:THR:O	2.51	0.43
3:L:168:GLN:HG3	3:L:175:TYR:CZ	2.54	0.42
1:B:47:PHE:CG	1:B:60:ILE:HD12	2.55	0.42
2:D:136:PRO:HB3	2:D:162:TYR:HB3	2.00	0.42
3:H:36:TRP:CZ3	3:H:89[A]:CYS:HB3	2.54	0.42
3:H:23:THR:HG22	3:H:73:THR:OG1	2.19	0.41
2:D:21:LEU:HD23	2:D:22:ARG:N	2.35	0.41
2:C:50:TRP:CG	3:L:98:LEU:HB2	2.55	0.41
3:L:107:GLU:OE2	3:L:144:ARG:NH2	2.54	0.41
3:H:22:ILE:O	3:H:73:THR:HA	2.21	0.41
1:A:6:LYS:NZ	8:A:508:HOH:O	2.42	0.40
1:B:98:ARG:HG2	1:B:103:LEU:HD23	2.03	0.40
1:A:67:PHE:HB3	1:A:104[A]:ILE:HD13	2.04	0.40
2:C:231:LYS:NZ	8:C:306:HOH:O	2.33	0.40
1:A:246:VAL:HG21	1:A:326:LYS:NZ	2.37	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	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

All (6) residues with a non-rotameric sidechain are listed below:

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

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
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 [i](#)

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(°)	Ideal(°)
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.

All (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
5	H	301	GOL	O2-C2-C3-O3
5	H	301	GOL	O1-C1-C2-C3
5	B	402	GOL	C1-C2-C3-O3
5	A	403	GOL	C1-C2-C3-O3
5	D	301	GOL	O1-C1-C2-O2
5	A	403	GOL	O2-C2-C3-O3
6	B	403	EPE	N4-C7-C8-O8
5	A	402	GOL	O2-C2-C3-O3
5	A	402	GOL	C1-C2-C3-O3
6	B	403	EPE	C8-C7-N4-C3
6	B	403	EPE	C9-C10-S-O2S
6	B	403	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
5	H	301	GOL	O1-C1-C2-O2

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 ⓘ

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%)	0.33	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%)

All (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
2	D	209	GLN	10.0
3	L	216	CYS	9.6
2	D	232	SER	9.5
2	D	175	ALA	9.4
1	A	367	ASN	8.9
2	D	149	SER	8.9
3	H	194	TYR	8.9
2	D	145	SER	8.6
2	D	207	GLY	8.0
3	H	156	LEU	7.5
2	D	142	ALA	7.5
3	H	124	ASP	6.9
2	D	146	LYS	6.8
3	H	186	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
3	H	192	LYS	6.4
2	D	210	THR	6.2
3	H	214	GLY	6.2
3	H	171	LYS	6.1
3	L	214	GLY	6.1
3	H	128	LYS	6.0
2	D	208	THR	5.9
2	D	144	SER	5.8
2	D	155	LEU	5.8
3	H	211	PHE	5.7
2	C	232	SER	5.6
3	H	185	LYS	5.5
3	H	212	ASN	5.5
3	H	129	SER	5.4
2	D	3	SER	5.1
2	D	173	SER	5.1
2	D	143	PRO	5.1
2	D	177	THR	5.0
3	H	213	ARG	5.0
2	D	148	THR	4.9
1	A	366	THR	4.8
3	H	215	GLU	4.8
2	D	231	LYS	4.8
3	H	154	ASN	4.7
1	A	141	ALA	4.6
3	H	170	SER	4.6
3	H	193	VAL	4.5
3	H	153	ASP	4.4
3	H	189	GLU	4.4
3	H	127	LEU	4.3
2	D	211	TYR	4.2
3	H	158[A]	SER	4.1
2	D	227	LYS	4.1
3	H	204	SER	4.1
2	D	176	LEU	4.0
3	H	188	TYR	4.0
3	H	131	THR	4.0
2	D	151	GLY	4.0
3	H	152	VAL	4.0
3	H	183	LEU	3.9
1	B	173	ASN	3.9
3	H	205[A]	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	204	SER	3.9
2	C	148	THR	3.8
3	H	159	GLY	3.8
2	D	139	PHE	3.8
2	D	203	SER	3.7
3	H	210	SER	3.7
3	H	160	ASN	3.7
2	C	144	SER	3.6
2	D	206	LEU	3.6
2	C	150	GLY	3.6
2	D	205	SER	3.5
2	C	145	SER	3.5
1	B	141	ALA	3.5
2	D	170[A]	SER	3.2
2	D	229	GLU	3.2
2	C	189	SER	3.2
2	D	174	GLY	3.2
3	H	167[A]	GLU	3.2
2	D	224	VAL	3.1
1	A	124	ASN	3.1
2	D	216[A]	ASN	3.1
3	H	130	GLY	3.0
3	L	205[A]	SER	3.0
2	D	201	VAL	3.0
2	C	231	LYS	3.0
2	D	230	PRO	2.9
3	H	207	VAL	2.9
3	H	206	PRO	2.9
1	A	165	GLY	2.9
1	B	341	TYR	2.8
3	H	134	VAL	2.8
2	D	158	LEU	2.8
1	A	341	TYR	2.8
3	H	119	ILE	2.8
2	C	151	GLY	2.8
3	H	125	SER	2.8
2	C	208	THR	2.8
3	H	148	VAL	2.8
2	D	152	THR	2.7
2	D	154	ALA	2.7
3	H	190	LYS	2.7
3	L	27	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	212	ILE	2.6
2	D	202	PRO	2.6
1	A	1	LYS	2.5
1	A	173	ASN	2.5
1	A	239	LYS	2.5
1	B	362	LYS	2.5
2	D	168	THR	2.4
3	L	204	SER	2.4
2	D	141	LEU	2.4
2	D	226	LYS	2.4
2	C	106	TYR	2.4
3	H	187	ASP	2.3
3	H	10	SER	2.3
2	D	140	PRO	2.3
2	D	84	LEU	2.3
1	B	365	GLN	2.3
1	A	172	GLU	2.3
3	H	181	LEU	2.3
1	A	123	PRO	2.2
2	D	153	ALA	2.2
2	D	190	SER	2.2
3	L	74	LEU	2.2
1	A	147	LEU	2.2
3	H	195	ALA	2.2
3	H	198	VAL	2.2
3	H	197	GLU	2.2
2	C	45	GLY	2.2
3	L	25	ARG	2.1
3	L	4	GLN	2.1
3	H	141	PHE	2.1
2	D	189	SER	2.1
1	A	29	LYS	2.1
2	C	218	LYS	2.1
2	D	178	SER	2.1
2	D	222	THR	2.1
1	A	192	LEU	2.1
3	L	170[A]	SER	2.1
2	D	228	VAL	2.1
3	H	157	GLN	2.1
3	L	24	CYS	2.0
3	H	135	VAL	2.0
1	A	362	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	H	27	SER	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	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, 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
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.