



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:10 PM GMT

PDB ID : 4BQ5  
Title : Structural analysis of an exo-beta-agarase  
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Deposited on : 2013-05-29  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

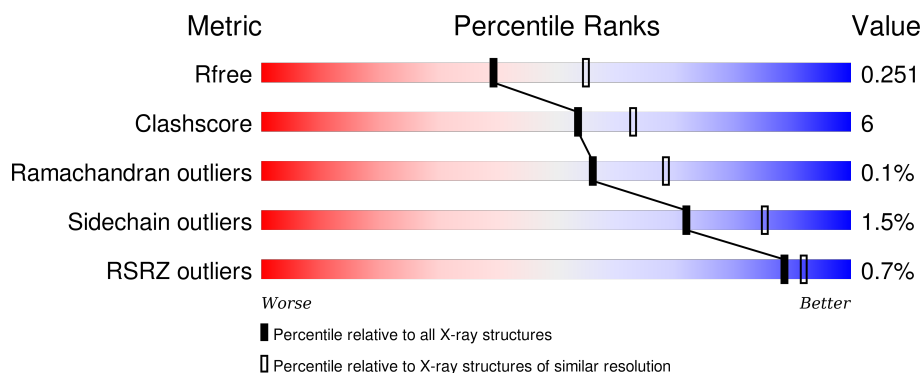
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	750	<div> <div></div> <div>86%</div> <div>13%</div> </div>
1	B	750	<div> <div></div> <div>84%</div> <div>16%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GAL	A	1796	-	-	X	-
5	GOL	A	1801	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12994 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 B-AGARASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	3	3	0
			5920	3776	991	1130	23			
1	B	749	Total	C	N	O	S	14	2	0
			5912	3770	997	1122	23			

There are 8 discrepancies between the modelled and reference sequences:

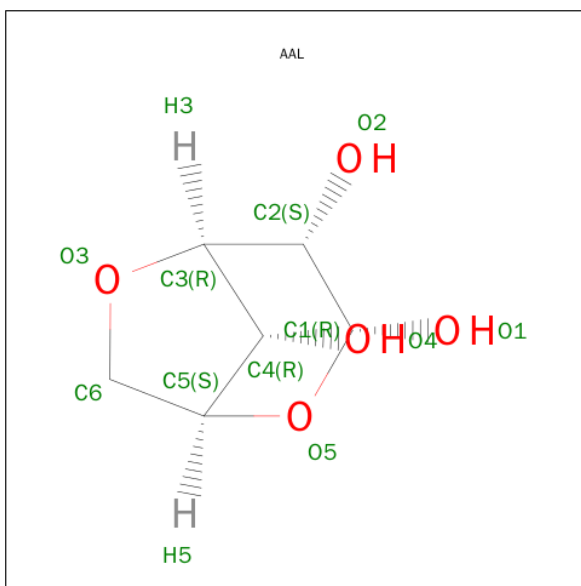
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	EXPRESSION TAG	UNP Q21HC5
A	45	SER	-	EXPRESSION TAG	UNP Q21HC5
A	46	HIS	-	EXPRESSION TAG	UNP Q21HC5
A	534	GLN	GLU	ENGINEERED MUTATION	UNP Q21HC5
B	44	GLY	-	EXPRESSION TAG	UNP Q21HC5
B	45	SER	-	EXPRESSION TAG	UNP Q21HC5
B	46	HIS	-	EXPRESSION TAG	UNP Q21HC5
B	534	GLN	GLU	ENGINEERED MUTATION	UNP Q21HC5

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			21	12	9		
2	A	2	Total	C	O	0	0
			21	12	9		
2	A	2	Total	C	O	0	0
			22	12	10		
2	B	2	Total	C	O	0	0
			21	12	9		
2	B	2	Total	C	O	0	0
			22	12	10		

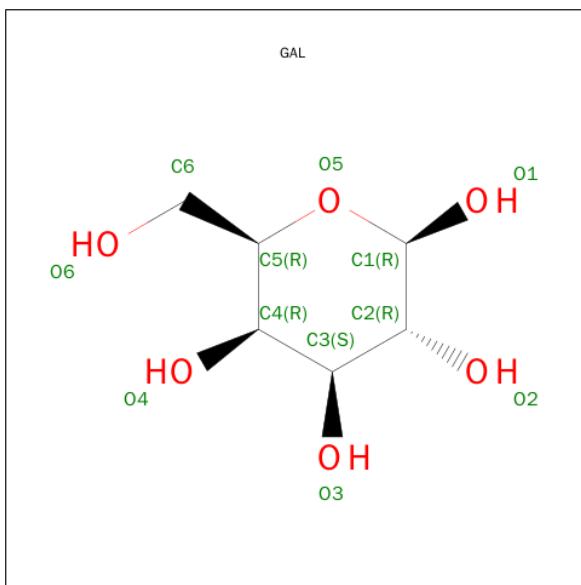
- Molecule 3 is SUGAR (3,6-ANHYDRO-L-GALACTOSE) (three-letter code: AAL) (formula:

C<sub>6</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- 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	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Ca	0	0
			3	3		
6	A	3	Total	Ca	0	0
			3	3		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	4	Total	C	O	0	0
			42	24	18		

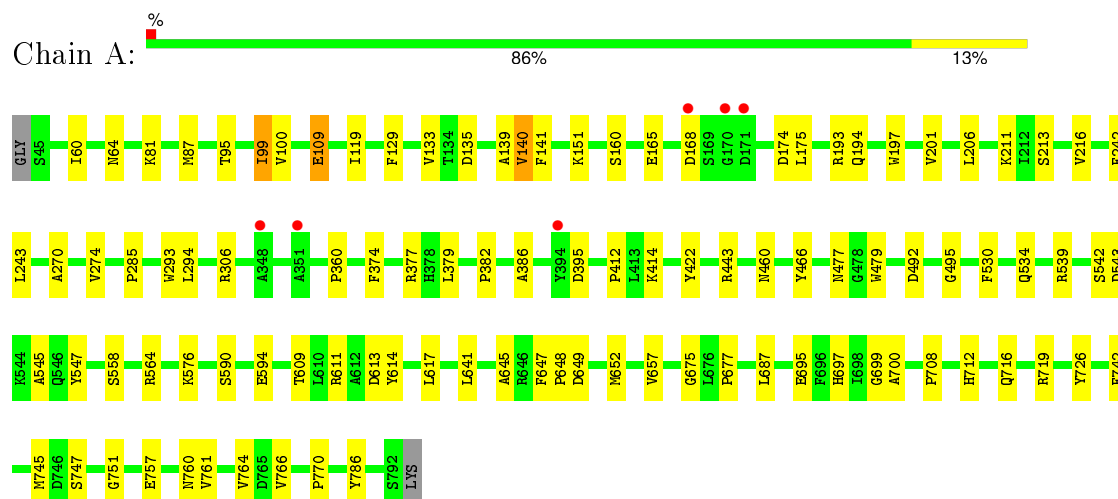
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	512	Total 512	O 512	0	0
8	B	450	Total 450	O 450	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 errors 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: B-AGARASE



#### • Molecule 1: B-AGARASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.03Å 116.17Å 207.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 2.30 39.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.1 (39.19-2.30) 94.1 (39.16-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.189 , 0.251 0.189 , 0.251	Depositor DCC
$R_{free}$ test set	3787 reflections (5.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 70781 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12994	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.67	1/6094 (0.0%)	0.76	3/8293 (0.0%)
1	B	0.68	4/6085 (0.1%)	0.74	4/8277 (0.0%)
All	All	0.67	5/12179 (0.0%)	0.75	7/16570 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	GLU	CG-CD	-20.29	1.21	1.51
1	B	84	LYS	CE-NZ	-15.21	1.11	1.49
1	B	259	LYS	CG-CD	-15.01	1.01	1.52
1	B	414	LYS	CD-CE	-12.48	1.20	1.51
1	B	588	LYS	CG-CD	7.52	1.78	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	LYS	CB-CG-CD	11.21	140.74	111.60
1	B	588	LYS	CB-CG-CD	-7.41	92.32	111.60
1	B	581	LEU	CA-CB-CG	6.19	129.53	115.30
1	A	539	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	193	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	165	GLU	CB-CG-CD	5.24	128.34	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	LYS	CD-CE-NZ	5.10	123.42	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	PRO	Peptide

## 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	5920	0	5586	60	0
1	B	5912	0	5576	67	0
2	A	64	0	53	10	0
2	B	43	0	36	7	0
3	A	10	0	8	5	0
4	A	11	0	10	6	0
5	A	6	0	8	0	0
5	B	18	0	24	1	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	B	42	0	33	6	0
8	A	512	0	0	11	0
8	B	450	0	0	5	0
All	All	12994	0	11334	145	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 6.

All (145) 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)
7:B:1797:GAL:C1	2:B:1798:AAL:HO4	1.47	1.18
4:A:1796:GAL:C1	2:A:1797:AAL:HO4	1.67	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HD21	8:B:2095:HOH:O	1.67	0.93
1:A:700:ALA:H	1:A:760:ASN:HD22	1.13	0.93
2:A:1794:GAL:C1	3:A:1795:AAL:HO4	1.79	0.92
1:A:109:GLU:HG2	8:A:2049:HOH:O	1.71	0.91
7:B:1797:GAL:C1	2:B:1798:AAL:C4	2.50	0.89
3:A:1795:AAL:C1	4:A:1796:GAL:HO3	1.78	0.88
4:A:1796:GAL:C1	2:A:1797:AAL:C4	2.54	0.84
1:A:649:ASP:HB3	8:A:2452:HOH:O	1.81	0.81
3:A:1795:AAL:C1	4:A:1796:GAL:C3	2.60	0.80
1:A:700:ALA:H	1:A:760:ASN:ND2	1.82	0.76
1:B:764:VAL:HG12	1:B:770:PRO:HA	1.67	0.76
4:A:1796:GAL:C2	2:A:1797:AAL:O4	2.34	0.75
1:B:742:PHE:CZ	7:B:1795:GAL:H4	2.23	0.74
1:B:700:ALA:H	1:B:760:ASN:HD22	1.37	0.73
1:A:716:GLN:HE22	1:A:719:ARG:HH11	1.36	0.72
1:B:716:GLN:HE22	1:B:719:ARG:HH11	1.35	0.71
2:A:1798:GAL:C1	2:A:1799:AAL:C4	2.70	0.70
2:B:1799:GAL:H2	2:B:1800:AAL:O4	1.92	0.69
1:B:162:HIS:HA	1:B:238:GLN:OE1	1.93	0.67
1:A:151:LYS:O	8:A:2095:HOH:O	2.13	0.66
1:A:87:MET:SD	1:A:216:VAL:HG23	2.35	0.65
2:A:1794:GAL:C2	3:A:1795:AAL:O4	2.43	0.65
1:B:492:ASP:HB3	1:B:495:GLY:O	1.96	0.65
2:B:1799:GAL:C2	2:B:1800:AAL:O4	2.47	0.63
1:B:703:HIS:O	5:B:1802:GOL:H12	1.99	0.63
1:A:492:ASP:HB3	1:A:495:GLY:O	1.99	0.61
1:B:48:LEU:HD11	1:B:232:ILE:CD1	2.31	0.61
1:B:141:PHE:HB3	1:B:201:VAL:O	2.01	0.60
1:A:422:TYR:CE1	1:A:745:MET:HG2	2.38	0.59
1:A:141:PHE:HB3	1:A:201:VAL:O	2.02	0.59
1:B:176:ASN:HD22	1:B:182:ARG:HA	1.65	0.58
1:A:697:HIS:CE1	1:A:761:VAL:HG11	2.38	0.58
1:B:176:ASN:ND2	1:B:182:ARG:HE	2.03	0.57
1:A:708:PRO:HG2	1:A:712:HIS:CD2	2.41	0.56
1:B:294:LEU:HD23	1:B:322:TYR:CE1	2.41	0.56
1:A:194:GLN:HB3	8:A:2140:HOH:O	2.05	0.56
1:B:764:VAL:HG12	1:B:770:PRO:CA	2.36	0.55
1:A:87:MET:SD	1:A:216:VAL:CG2	2.95	0.54
1:B:85:LEU:HD22	1:B:97:LEU:HD23	1.89	0.54
1:A:422:TYR:CZ	1:A:745:MET:HG2	2.42	0.54
7:B:1797:GAL:C1	2:B:1798:AAL:H4	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:GLN:HA	1:A:648:PRO:HD3	1.90	0.53
1:A:64:ASN:HB2	1:A:95:THR:HG22	1.90	0.53
1:A:645:ALA:HB2	8:A:2370:HOH:O	2.09	0.53
1:B:742:PHE:CE1	7:B:1795:GAL:H4	2.44	0.52
1:A:386:ALA:HB3	8:A:2174:HOH:O	2.08	0.52
1:B:654:MET:HG3	1:B:658:LYS:HD2	1.90	0.52
1:B:680:LYS:HG3	8:B:2120:HOH:O	2.10	0.52
1:A:675:GLY:O	1:A:677:PRO:HD3	2.09	0.51
1:B:661:ALA:O	1:B:689:LYS:HE2	2.11	0.51
1:B:247:VAL:HG22	1:B:749:LEU:HD23	1.92	0.51
1:A:766:VAL:HB	8:A:2493:HOH:O	2.11	0.51
1:B:270:ALA:O	1:B:274:VAL:HG23	2.11	0.51
1:B:697:HIS:O	1:B:698:ILE:HG13	2.10	0.51
4:A:1796:GAL:C1	2:A:1797:AAL:H4	2.40	0.50
1:B:61:HIS:O	1:B:97:LEU:HA	2.11	0.50
1:B:500:VAL:HG12	1:B:505:PHE:CE2	2.46	0.50
1:B:528:GLY:HA3	1:B:643:LEU:HD11	1.93	0.50
1:A:306:ARG:HA	1:A:641:LEU:HD21	1.93	0.50
1:A:700:ALA:N	1:A:760:ASN:HD22	1.96	0.50
1:B:48:LEU:HD11	1:B:232:ILE:HD12	1.93	0.50
1:B:409:HIS:HE1	1:B:493:PHE:O	1.95	0.50
1:B:488:SER:HB2	8:B:2301:HOH:O	2.12	0.50
1:B:727:MET:O	1:B:731:ILE:HG13	2.11	0.49
1:A:60:ILE:HG12	1:A:99:ILE:HG23	1.94	0.49
1:B:121:SER:O	1:B:149:VAL:HA	2.12	0.49
1:A:168:ASP:HB2	1:A:174:ASP:OD2	2.13	0.49
1:B:44:GLY:HA2	1:B:46:HIS:N	2.27	0.49
1:B:119:ILE:HG22	1:B:147:ILE:HG21	1.95	0.49
1:A:443:ARG:HG2	1:A:466:TYR:CZ	2.47	0.49
1:A:590:SER:OG	1:A:594:GLU:OE1	2.28	0.49
1:B:623:ASP:O	1:B:627:LYS:HB2	2.12	0.49
1:A:716:GLN:NE2	1:A:719:ARG:HH11	2.09	0.49
1:B:374:PHE:CD2	1:B:394:TYR:HB2	2.48	0.48
1:B:647:PHE:HB3	1:B:652:MET:HB3	1.95	0.48
1:B:449:ARG:HD3	1:B:453:TRP:CZ2	2.49	0.48
1:A:100:VAL:HG22	1:A:211:LYS:HG3	1.96	0.48
1:B:285:PRO:O	1:B:286:SER:HB2	2.13	0.48
1:A:460:ASN:OD1	1:A:477:ASN:HB3	2.14	0.47
1:A:675:GLY:HA2	1:A:726:TYR:CD2	2.49	0.47
1:A:764:VAL:HG12	1:A:770:PRO:HA	1.96	0.47
1:A:379:LEU:HD21	1:A:382:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:PHE:O	1:B:144:SER:HA	2.15	0.47
1:A:558:SER:HA	1:A:564:ARG:HG3	1.97	0.47
1:B:115:LEU:HD21	1:B:212:ILE:HD13	1.97	0.46
1:B:669:TYR:O	1:B:693:ILE:HA	2.15	0.46
1:B:44:GLY:HA2	1:B:45:SER:C	2.36	0.46
1:B:396:HIS:CG	1:B:397:PRO:HD2	2.50	0.46
1:B:697:HIS:HB3	1:B:742:PHE:O	2.16	0.46
1:B:118:ASP:HB3	1:B:152:MET:SD	2.56	0.46
1:A:613:ASP:O	1:A:617:LEU:HG	2.15	0.46
1:B:709:GLY:HA2	1:B:759:TYR:CG	2.51	0.45
1:B:218:SER:HB2	1:B:673:LYS:HD2	1.99	0.45
1:A:293:TRP:CD2	1:A:786:TYR:HB3	2.51	0.45
1:B:781:VAL:HG22	8:B:2425:HOH:O	2.16	0.45
1:B:515:VAL:O	1:B:519:GLU:HG3	2.17	0.45
1:A:360:PRO:HD2	1:A:479:TRP:CD1	2.51	0.45
2:A:1798:GAL:C2	2:A:1799:AAL:O4	2.61	0.45
1:B:697:HIS:CE1	1:B:761:VAL:HG11	2.52	0.45
1:A:160:SER:HB3	1:A:206:LEU:HD11	1.99	0.45
1:A:270:ALA:O	1:A:274:VAL:HG23	2.17	0.45
1:A:374:PHE:O	1:A:377:ARG:HB2	2.16	0.44
1:A:751:GLY:HA2	1:A:757:GLU:O	2.17	0.44
2:A:1794:GAL:H2	3:A:1795:AAL:O4	2.14	0.44
1:B:174:ASP:OD1	1:B:410:SER:HB2	2.17	0.44
1:A:695:GLU:HG2	1:A:742:PHE:HB2	2.00	0.44
7:B:1797:GAL:C2	2:B:1798:AAL:O4	2.54	0.44
1:A:657:VAL:CG1	1:A:687:LEU:HD11	2.48	0.44
1:B:539:ARG:HD3	8:B:2335:HOH:O	2.16	0.44
1:A:412:PRO:HD2	8:A:2050:HOH:O	2.17	0.44
1:B:342:GLY:HA2	1:B:413:LEU:HD11	2.00	0.43
1:A:699:GLY:HA3	1:A:708:PRO:O	2.18	0.43
1:B:755:ASP:OD1	1:B:757:GLU:HG3	2.18	0.43
1:A:133:VAL:O	1:A:140:VAL:HA	2.18	0.43
1:A:543:ASP:CG	1:A:611:ARG:HH12	2.22	0.43
2:B:1799:GAL:C1	2:B:1800:AAL:C4	2.96	0.43
1:A:657:VAL:HG12	1:A:687:LEU:HD11	2.00	0.43
1:A:175:LEU:O	1:A:197:TRP:NE1	2.52	0.43
1:A:294:LEU:HA	1:A:294:LEU:HD23	1.76	0.42
1:B:708:PRO:HG2	1:B:712:HIS:CD2	2.54	0.42
1:B:542:SER:H	1:B:545:ALA:HB3	1.85	0.42
1:B:218:SER:CB	1:B:673:LYS:HD2	2.49	0.42
1:B:318:ASP:C	1:B:318:ASP:OD1	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:HB1	1:B:83:LEU:HD11	2.01	0.42
1:B:667:VAL:O	1:B:691:SER:HA	2.19	0.42
1:A:547:TYR:CD1	1:A:614:TYR:HB3	2.54	0.42
1:A:647:PHE:HB3	1:A:652:MET:HB3	2.01	0.42
1:A:609:THR:HG23	8:A:2398:HOH:O	2.19	0.42
1:B:484:PHE:CE1	1:B:498:PRO:HB3	2.55	0.42
1:A:695:GLU:OE1	2:A:1794:GAL:C1	2.67	0.42
1:B:49:PHE:HB2	1:B:230:ILE:HD12	2.01	0.42
1:A:81:LYS:NZ	8:A:2004:HOH:O	2.52	0.41
1:A:477:ASN:HA	1:A:530:PHE:O	2.20	0.41
1:B:123:GLY:O	1:B:149:VAL:HG11	2.20	0.41
1:B:297:PRO:HD2	1:B:323:PRO:HG2	2.03	0.41
1:B:97:LEU:O	1:B:97:LEU:HD12	2.21	0.40
1:B:143:ARG:HG2	1:B:197:TRP:HA	2.03	0.40
1:A:135:ASP:OD2	1:A:139:ALA:HB3	2.21	0.40
1:A:242:PHE:CE2	1:A:243:LEU:HG	2.57	0.40
1:B:242:PHE:CZ	1:B:243:LEU:HG	2.56	0.40
1:A:109:GLU:CG	8:A:2049:HOH:O	2.47	0.40
1:B:460:ASN:OD1	1:B:477:ASN:HB3	2.22	0.40
1:A:542:SER:H	1:A:545:ALA:HB3	1.86	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	A	749/750 (100%)	722 (96%)	26 (4%)	1 (0%)	56	68
1	B	747/750 (100%)	721 (96%)	26 (4%)	0	100	100
All	All	1496/1500 (100%)	1443 (96%)	52 (4%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	576	LYS

### 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	622/630 (99%)	613 (99%)	9 (1%)	74	86
1	B	617/630 (98%)	608 (98%)	9 (2%)	72	85
All	All	1239/1260 (98%)	1221 (98%)	18 (2%)	72	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ILE
1	A	109	GLU
1	A	119	ILE
1	A	129	PHE
1	A	140	VAL
1	A	213	SER
1	A	395	ASP
1	A	414	LYS
1	A	747	SER
1	B	63	LEU
1	B	175	LEU
1	B	190	SER
1	B	309	LYS
1	B	356	ASP
1	B	488	SER
1	B	599	VAL
1	B	745	MET
1	B	792	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	194	GLN
1	A	409	HIS
1	A	716	GLN
1	A	760	ASN
1	B	176	ASN
1	B	194	GLN
1	B	409	HIS
1	B	546	GLN
1	B	716	GLN
1	B	760	ASN

### 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 ⓘ

14 carbohydrates 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$
2	AAL	A	1793	2	11,11,12	1.64	2 (18%)	14,16,18	1.25	1 (7%)
2	GAL	A	1794	3,2	11,11,12	0.84	1 (9%)	14,15,17	2.55	5 (35%)
2	AAL	A	1797	2,4	11,11,12	0.46	0	14,16,18	0.61	0
2	GAL	A	1798	2	11,11,12	0.99	0	14,15,17	2.54	3 (21%)
2	AAL	A	1799	2	11,11,12	1.63	1 (9%)	14,16,18	1.98	2 (14%)
2	GAL	A	1800	2	12,12,12	0.62	0	17,17,17	1.14	2 (11%)
7	AAL	B	1794	7	11,11,12	1.36	2 (18%)	14,16,18	1.81	4 (28%)
7	GAL	B	1795	7	11,11,12	1.85	3 (27%)	14,15,17	3.34	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	AAL	B	1796	7	11,11,12	1.09	1 (9%)	14,16,18	1.84	3 (21%)
7	GAL	B	1797	2,7	11,11,12	1.02	1 (9%)	14,15,17	2.24	3 (21%)
2	AAL	B	1798	2,7	11,11,12	1.19	2 (18%)	14,16,18	1.16	2 (14%)
2	GAL	B	1799	2	11,11,12	0.87	0	14,15,17	3.01	3 (21%)
2	AAL	B	1800	2	11,11,12	1.54	1 (9%)	14,16,18	1.60	3 (21%)
2	GAL	B	1801	2	12,12,12	0.55	0	17,17,17	2.07	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AAL	A	1793	2	-	0/0/22/25	0/0/2/2
2	GAL	A	1794	3,2	-	0/2/19/22	0/1/1/1
2	AAL	A	1797	2,4	-	0/0/22/25	0/0/2/2
2	GAL	A	1798	2	-	0/2/19/22	0/1/1/1
2	AAL	A	1799	2	-	0/0/22/25	0/0/2/2
2	GAL	A	1800	2	-	0/2/22/22	0/1/1/1
7	AAL	B	1794	7	-	0/0/22/25	0/0/2/2
7	GAL	B	1795	7	-	0/2/19/22	0/1/1/1
7	AAL	B	1796	7	-	0/0/22/25	0/0/2/2
7	GAL	B	1797	2,7	-	0/2/19/22	0/1/1/1
2	AAL	B	1798	2,7	-	0/0/22/25	0/0/2/2
2	GAL	B	1799	2	-	0/2/19/22	0/1/1/1
2	AAL	B	1800	2	-	0/0/22/25	0/0/2/2
2	GAL	B	1801	2	-	0/2/22/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1795	GAL	O5-C5	2.02	1.47	1.43
2	A	1794	GAL	C2-C3	2.04	1.55	1.52
2	A	1793	AAL	O3-C3	2.11	1.49	1.43
2	B	1798	AAL	O5-C5	2.13	1.48	1.43
7	B	1797	GAL	O5-C1	2.19	1.47	1.43
2	B	1798	AAL	O5-C1	2.29	1.47	1.43
7	B	1796	AAL	O5-C5	2.45	1.48	1.43
7	B	1794	AAL	O5-C1	2.46	1.47	1.43
7	B	1794	AAL	O5-C5	2.50	1.48	1.43
7	B	1795	GAL	O5-C1	3.44	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1800	AAL	O5-C1	3.46	1.49	1.43
7	B	1795	GAL	C2-C3	3.62	1.57	1.52
2	A	1793	AAL	O5-C1	3.62	1.49	1.43
2	A	1799	AAL	O5-C1	4.69	1.51	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1799	GAL	O5-C1-C2	-10.00	94.63	110.86
2	A	1798	GAL	C1-O5-C5	-7.52	102.70	112.25
7	B	1797	GAL	O3-C3-C2	-5.59	99.89	110.00
7	B	1795	GAL	O3-C3-C4	-5.51	97.93	110.34
2	A	1799	AAL	C2-C3-C4	-5.27	100.63	112.89
7	B	1797	GAL	C1-C2-C3	-4.88	103.77	109.54
7	B	1796	AAL	C1-C2-C3	-4.51	103.71	109.24
2	B	1799	GAL	C1-O5-C5	-3.51	107.79	112.25
2	A	1798	GAL	O3-C3-C2	-3.45	103.77	110.00
7	B	1794	AAL	O4-C4-C5	-3.18	101.53	111.05
2	A	1794	GAL	O3-C3-C4	-3.13	103.30	110.34
7	B	1796	AAL	O5-C5-C6	-2.94	108.60	113.33
2	A	1794	GAL	O2-C2-C1	-2.79	103.62	109.21
2	A	1800	GAL	C1-O5-C5	-2.74	108.40	113.47
2	A	1798	GAL	C6-C5-C4	-2.72	106.30	113.02
7	B	1794	AAL	C6-C5-C4	-2.63	97.42	102.18
2	B	1799	GAL	O3-C3-C2	-2.53	105.42	110.00
7	B	1795	GAL	O2-C2-C1	-2.28	104.64	109.21
7	B	1797	GAL	C2-C3-C4	-2.16	107.36	111.04
7	B	1796	AAL	C1-O5-C5	-2.14	109.54	112.25
2	B	1798	AAL	C6-C5-C4	-2.11	98.38	102.18
2	B	1800	AAL	C2-C3-C4	-2.01	108.22	112.89
2	B	1798	AAL	O5-C5-C6	2.16	116.81	113.33
2	A	1794	GAL	C1-C2-C3	2.31	112.28	109.54
2	A	1800	GAL	O5-C5-C6	2.34	112.27	106.36
2	A	1793	AAL	C1-O5-C5	2.35	115.23	112.25
2	B	1801	GAL	C1-O5-C5	2.38	117.87	113.47
7	B	1795	GAL	C3-C4-C5	2.63	114.78	110.20
2	B	1801	GAL	C4-C3-C2	2.87	116.15	110.79
2	B	1800	AAL	O5-C1-C2	2.90	115.56	110.86
7	B	1794	AAL	O5-C1-C2	3.58	116.67	110.86
7	B	1794	AAL	O5-C5-C6	3.67	119.23	113.33
2	B	1800	AAL	C1-O5-C5	4.06	117.40	112.25
2	B	1801	GAL	O5-C1-C2	4.25	116.58	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1799	AAL	O5-C1-C2	4.60	118.32	110.86
7	B	1795	GAL	C2-C3-C4	4.79	119.18	111.04
2	B	1801	GAL	C1-C2-C3	5.25	118.23	110.43
2	A	1794	GAL	O5-C1-C2	5.36	119.55	110.86
2	A	1794	GAL	C1-O5-C5	5.42	119.12	112.25
7	B	1795	GAL	C1-O5-C5	6.16	120.06	112.25
7	B	1795	GAL	O5-C1-C2	6.36	121.18	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1794	GAL	4	0
2	A	1797	AAL	4	0
2	A	1798	GAL	2	0
2	A	1799	AAL	2	0
7	B	1795	GAL	2	0
7	B	1797	GAL	4	0
2	B	1798	AAL	4	0
2	B	1799	GAL	3	0
2	B	1800	AAL	3	0

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 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
3	AAL	A	1795	2,4	11,11,12	2.11	3 (27%)	14,16,18	1.56	2 (14%)
4	GAL	A	1796	3,2	11,11,12	0.97	1 (9%)	14,15,17	2.96	4 (28%)
5	GOL	A	1801	-	5,5,5	0.53	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	1802	-	5,5,5	0.43	0	5,5,5	0.38	0
5	GOL	B	1803	-	5,5,5	0.28	0	5,5,5	0.19	0
5	GOL	B	1804	-	5,5,5	0.26	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AAL	A	1795	2,4	-	0/0/22/25	0/0/2/2
4	GAL	A	1796	3,2	-	0/2/19/22	0/1/1/1
5	GOL	A	1801	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1802	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1803	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1804	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1796	GAL	O3-C3	-2.00	1.38	1.43
3	A	1795	AAL	O3-C6	3.37	1.51	1.43
3	A	1795	AAL	O5-C5	3.51	1.51	1.43
3	A	1795	AAL	O5-C1	4.40	1.51	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1796	GAL	O3-C3-C2	-7.90	95.72	110.00
4	A	1796	GAL	O5-C1-C2	-5.29	102.27	110.86
3	A	1795	AAL	C1-C2-C3	-3.75	104.64	109.24
4	A	1796	GAL	C1-O5-C5	-3.59	107.70	112.25
4	A	1796	GAL	C1-C2-C3	-2.63	106.43	109.54
3	A	1795	AAL	O5-C1-C2	3.01	115.74	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1795	AAL	5	0
4	A	1796	GAL	6	0
5	B	1802	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	748/750 (99%)	-0.05	6 (0%) 87 90	6, 15, 33, 60	1 (0%)
1	B	749/750 (99%)	0.00	5 (0%) 89 92	7, 18, 35, 69	6 (0%)
All	All	1497/1500 (99%)	-0.03	11 (0%) 89 92	6, 16, 35, 69	7 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	ASP	3.6
1	A	394	TYR	2.9
1	B	166	VAL	2.9
1	B	172	VAL	2.9
1	B	394	TYR	2.9
1	A	348	ALA	2.4
1	A	171	ASP	2.3
1	A	170	GLY	2.3
1	A	168	ASP	2.3
1	A	351	ALA	2.2
1	B	169	SER	2.1

### 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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	AAL	B	1796	10/11	0.96	0.16	0.73	8,8,9,9	0
2	AAL	A	1793	10/11	0.95	0.15	0.16	8,8,8,9	0
2	GAL	A	1794	11/12	0.97	0.16	0.14	7,8,8,8	0
2	GAL	A	1798	11/12	0.95	0.12	0.12	14,15,16,17	0
7	GAL	B	1795	11/12	0.95	0.16	-0.04	7,8,8,9	0
7	AAL	B	1794	10/11	0.96	0.15	-0.10	7,7,8,8	0
7	GAL	B	1797	11/12	0.96	0.14	-0.36	13,14,15,17	0
2	GAL	B	1801	12/12	0.84	0.20	-	53,63,70,77	0
2	AAL	A	1797	10/11	0.95	0.14	-	14,15,16,16	0
2	AAL	B	1798	10/11	0.92	0.14	-	21,24,25,26	0
2	GAL	A	1800	12/12	0.81	0.23	-	44,52,56,57	0
2	AAL	A	1799	10/11	0.94	0.11	-	26,28,30,32	0
2	GAL	B	1799	11/12	0.89	0.14	-	24,27,28,29	0
2	AAL	B	1800	10/11	0.80	0.15	-	40,45,46,47	0

## 6.4 Ligands ⓘ

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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	1801	6/6	0.90	0.16	2.45	22,23,26,27	0
5	GOL	B	1803	6/6	0.93	0.16	1.63	32,36,39,47	0
3	AAL	A	1795	10/11	0.96	0.17	0.55	7,7,7,7	0
5	GOL	B	1802	6/6	0.93	0.13	0.10	16,19,19,19	0
4	GAL	A	1796	11/12	0.98	0.14	-1.02	11,11,12,12	0
6	CA	A	1802	1/1	1.00	0.07	-2.00	17,17,17,17	0
6	CA	A	1804	1/1	0.97	0.07	-2.87	35,35,35,35	0
6	CA	A	1803	1/1	0.99	0.07	-3.43	16,16,16,16	0
6	CA	B	1805	1/1	0.99	0.02	-3.90	19,19,19,19	0
6	CA	B	1806	1/1	0.98	0.02	-4.31	26,26,26,26	0
6	CA	B	1807	1/1	0.99	0.03	-5.04	21,21,21,21	0
5	GOL	B	1804	6/6	0.84	0.26	-	52,57,58,58	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.