Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:35 PM GMT

PDB ID	:	4IUG
Title	:	Crystal structure of beta-galactosidase from Aspergillus oryzae in complex with galactose
Authors	:	Maksimainen, M.; Rouvinen, J.
Deposited on	:	2013-01-21
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

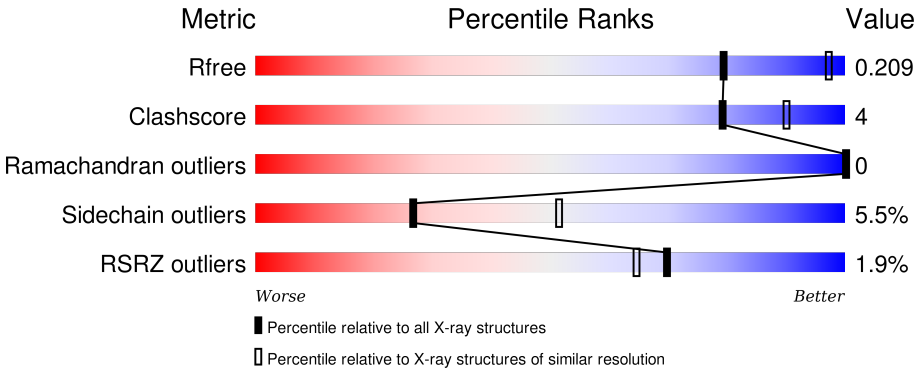
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1005	2% 84% 10% • 5%

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
10	M6D	A	1163	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GAL	A	1130	-	-	-	X
5	NAG	A	1136	-	-	-	X
8	MAN	A	1156	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8208 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.

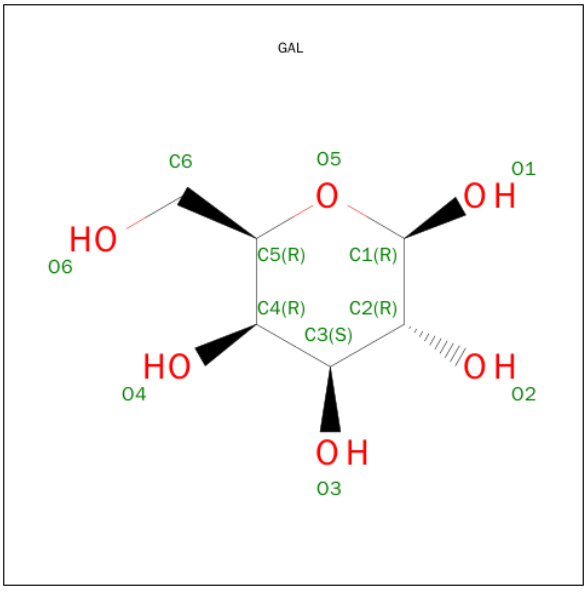
- Molecule 1 is a protein called Beta-galactosidase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	957	Total	C	N	O	P	S	0	0	0
			7441	4752	1227	1452	1	9			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	Cd	0	0
			29	29		

- Molecule 3 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).

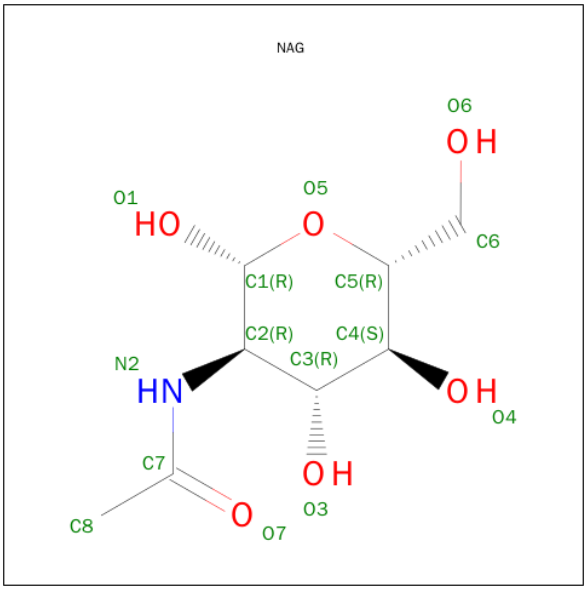


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	2	Total	C	N	O	0	0
			28	16	2	10		
7	A	2	Total	C	N	O	0	0
			28	16	2	10		

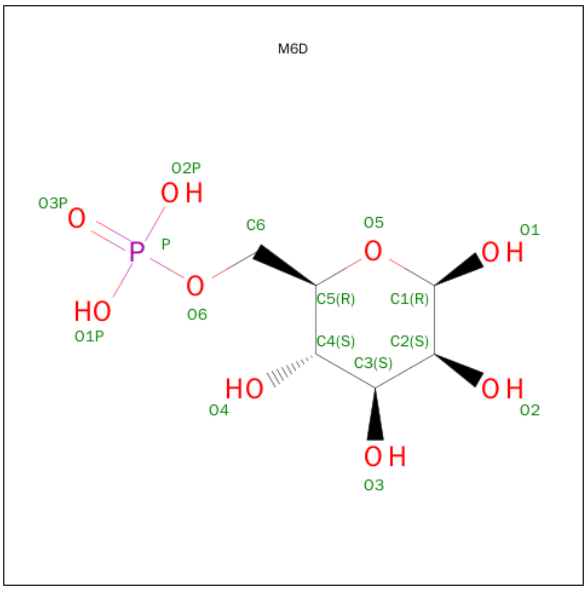
- Molecule 8 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	5	Total	C	N	O	0	0
			62	34	2	26		

- Molecule 10 is 6-O-PHOSPHONO-BETA-D-MANNOPYRANOSE (three-letter code: M6D) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is water.

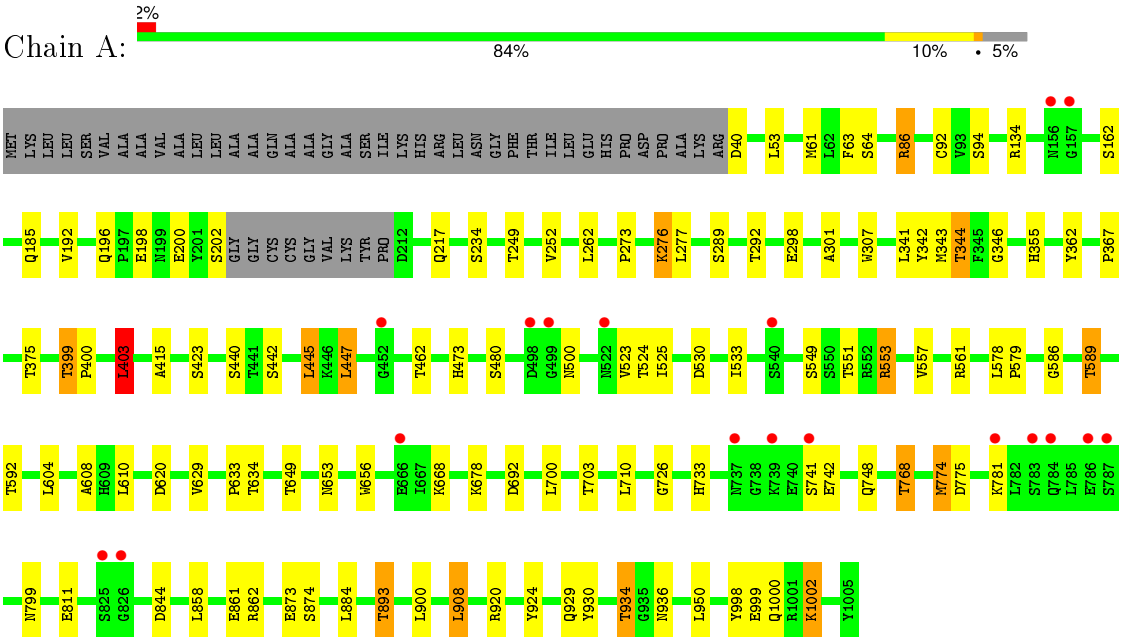
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	280	Total	O	0	0
			280	280		

3 Residue-property plots (i)

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: Beta-galactosidase A

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.38Å 146.38Å 136.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.91 – 2.60 47.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.91-2.60) 99.9 (47.91-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.180 , 0.214 0.177 , 0.209	Depositor DCC
R_{free} test set	2608 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 34.7	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 52147 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8208	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, SEP, CD, GAL, M6D, MAN

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	0.44	0/7640	0.59	1/10408 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	403	LEU	CA-CB-CG	6.28	129.75	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7441	0	7109	52	0
2	A	29	0	0	0	0
3	A	12	0	12	2	0
4	A	61	0	52	1	0
5	A	14	0	13	0	0
6	A	83	0	70	1	0
7	A	56	0	50	0	0
8	A	116	0	97	0	0
9	A	62	0	52	0	0
10	A	15	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	39	0	33	1	0
12	A	280	0	0	1	0
All	All	8208	0	7496	54	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 (54) 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)
1:A:134:ARG:NH2	1:A:298:GLU:OE2	2.20	0.70
1:A:589:THR:HG22	1:A:592:THR:H	1.61	0.67
1:A:861:GLU:OE2	1:A:924:TYR:OH	2.14	0.65
1:A:298:GLU:OE1	3:A:1130:GAL:H1	1.95	0.65
1:A:134:ARG:HG2	1:A:196:GLN:HB3	1.85	0.58
1:A:200:GLU:OE2	3:A:1130:GAL:O1	2.24	0.54
1:A:742:GLU:HG2	1:A:781:LYS:HD2	1.90	0.53
1:A:579:PRO:HD2	1:A:608:ALA:O	2.08	0.53
1:A:86:ARG:NH2	1:A:586:GLY:O	2.42	0.52
1:A:774:MET:H	1:A:774:MET:CE	2.23	0.52
1:A:94:SER:OG	1:A:134:ARG:HD2	2.10	0.51
1:A:64:SER:HB2	1:A:92:CYS:HB3	1.93	0.51
1:A:604:LEU:HB3	1:A:620:ASP:HB2	1.94	0.49
1:A:341:LEU:HB2	1:A:344:THR:HG22	1.94	0.49
1:A:273:PRO:HB2	1:A:276:LYS:HD3	1.95	0.49
1:A:445:LEU:HD21	1:A:473:HIS:CD2	2.47	0.48
1:A:442:SER:HB3	1:A:462:THR:HG21	1.96	0.48
1:A:403:LEU:HD13	1:A:415:ALA:HB1	1.96	0.47
1:A:768:THR:HG23	1:A:936:ASN:ND2	2.29	0.47
1:A:445:LEU:HG	1:A:447:LEU:HD13	1.97	0.46
1:A:523:VAL:HG22	1:A:557:VAL:HG22	1.98	0.46
1:A:858:LEU:O	1:A:862:ARG:HG3	2.15	0.45
1:A:301:ALA:HB2	1:A:341:LEU:HB3	1.97	0.45
6:A:1139:BMA:H61	6:A:1140:MAN:H2	1.72	0.45
1:A:307:TRP:CZ3	1:A:934:THR:HG23	2.52	0.45
1:A:610:LEU:HD22	1:A:633:PRO:HG2	1.99	0.45
1:A:998:TYR:O	1:A:999:GLU:HG3	2.16	0.44
1:A:185:GLN:HA	1:A:192:VAL:HB	1.99	0.44
1:A:344:THR:HA	1:A:367:PRO:HD2	2.00	0.44
1:A:86:ARG:HD2	12:A:3223:HOH:O	2.17	0.44
1:A:726:GLY:O	1:A:799:ASN:HB3	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LYS:HB2	1:A:893:THR:HG22	1.99	0.43
1:A:342:TYR:HA	1:A:343:MET:HA	1.90	0.43
1:A:692:ASP:OD2	1:A:733:HIS:NE2	2.47	0.43
1:A:561:ARG:NH1	1:A:653:ASN:HB3	2.34	0.43
1:A:629:VAL:HB	1:A:656:TRP:HB2	2.01	0.43
1:A:748:GLN:OE1	1:A:775:ASP:HB3	2.18	0.43
1:A:289:SER:HG	1:A:292:THR:HG1	1.67	0.43
1:A:920:ARG:HG2	1:A:934:THR:HB	2.00	0.43
1:A:549:SER:HB3	1:A:553:ARG:NH2	2.34	0.42
1:A:399:THR:HA	1:A:400:PRO:HD3	1.76	0.42
1:A:217:GLN:HB2	1:A:249:THR:HG23	2.01	0.42
10:A:1163:M6D:H6A	11:A:1164:NAG:C1	2.50	0.42
1:A:908:LEU:HD23	1:A:950:LEU:HD13	2.01	0.42
1:A:1002:LYS:HB3	1:A:1002:LYS:HE3	1.78	0.42
1:A:375:THR:HG21	4:A:1131:NAG:H82	2.00	0.41
1:A:500:ASN:OD1	1:A:500:ASN:N	2.53	0.41
1:A:774:MET:H	1:A:774:MET:HE3	1.86	0.41
1:A:533:ILE:HD11	1:A:553:ARG:HG2	2.02	0.41
1:A:703:THR:HB	1:A:710:LEU:HD21	2.03	0.41
1:A:346:GLY:HA3	1:A:362:TYR:O	2.22	0.40
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.83	0.40
1:A:525:ILE:HD12	1:A:530:ASP:HB3	2.02	0.40
1:A:234:SER:HB3	1:A:252:VAL:HG21	2.03	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	952/1005 (95%)	907 (95%)	45 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	794/828 (96%)	750 (94%)	44 (6%)	27 51

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	53	LEU
1	A	61	MET
1	A	63	PHE
1	A	86	ARG
1	A	162	SER
1	A	198	GLU
1	A	202	SER
1	A	276	LYS
1	A	277	LEU
1	A	344	THR
1	A	355	HIS
1	A	399	THR
1	A	403	LEU
1	A	423	SER
1	A	440	SER
1	A	445	LEU
1	A	447	LEU
1	A	480	SER
1	A	524	THR
1	A	551	THR
1	A	553	ARG
1	A	578	LEU
1	A	589	THR
1	A	634	THR
1	A	649	THR
1	A	668	LYS
1	A	700	LEU
1	A	741	SER
1	A	768	THR

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Mol	Chain	Res	Type
1	A	774	MET
1	A	811	GLU
1	A	844	ASP
1	A	873	GLU
1	A	874	SER
1	A	884	LEU
1	A	893	THR
1	A	900	LEU
1	A	908	LEU
1	A	929	GLN
1	A	930	TYR
1	A	934	THR
1	A	1000	GLN
1	A	1002	LYS

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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	SEP	A	569	1	8,9,10	1.83	3 (37%)	8,12,14	2.38	1 (12%)

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
1	SEP	A	569	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	SEP	P-OG	2.24	1.67	1.60
1	A	569	SEP	P-O3P	2.29	1.62	1.54
1	A	569	SEP	P-O1P	3.17	1.61	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	569	SEP	OG-CB-CA	5.97	113.36	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

34 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	$\#\|Z\| > 2$
4	NAG	A	1131	1,4	14,14,15	0.69	0	15,19,21	1.51	1 (6%)
4	NAG	A	1132	4	14,14,15	0.77	0	15,19,21	1.86	1 (6%)
4	BMA	A	1133	4	11,11,12	2.19	4 (36%)	14,15,17	1.74	3 (21%)
4	MAN	A	1134	4	11,11,12	0.70	0	14,15,17	1.32	2 (14%)
4	MAN	A	1135	4	11,11,12	0.72	0	14,15,17	1.51	3 (21%)
6	NAG	A	1137	1,6	14,14,15	0.56	0	15,19,21	1.06	2 (13%)
6	NAG	A	1138	6	14,14,15	0.56	0	15,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	A	1139	6	11,11,12	2.15	2 (18%)	14,15,17	2.62	7 (50%)
6	MAN	A	1140	6	11,11,12	0.63	0	14,15,17	1.14	2 (14%)
6	MAN	A	1141	6	11,11,12	0.59	0	14,15,17	0.93	1 (7%)
6	MAN	A	1142	6	11,11,12	0.73	0	14,15,17	0.99	0
6	MAN	A	1143	6	11,11,12	0.54	0	14,15,17	1.65	2 (14%)
7	NAG	A	1144	1,7	14,14,15	0.53	0	15,19,21	1.15	1 (6%)
7	NAG	A	1145	7	14,14,15	0.50	0	15,19,21	1.65	2 (13%)
7	NAG	A	1146	1,7	14,14,15	0.45	0	15,19,21	1.02	2 (13%)
7	NAG	A	1147	7	14,14,15	0.54	0	15,19,21	0.91	1 (6%)
8	NAG	A	1148	1,8	14,14,15	0.71	0	15,19,21	0.92	0
8	NAG	A	1149	8	14,14,15	0.68	0	15,19,21	0.83	0
8	BMA	A	1150	8	11,11,12	2.28	4 (36%)	14,15,17	1.13	1 (7%)
8	MAN	A	1151	8	11,11,12	0.62	0	14,15,17	2.54	3 (21%)
8	MAN	A	1152	8	11,11,12	0.56	0	14,15,17	1.36	2 (14%)
8	MAN	A	1153	8	11,11,12	0.81	1 (9%)	14,15,17	1.09	1 (7%)
8	MAN	A	1154	8	11,11,12	0.52	0	14,15,17	1.03	1 (7%)
8	MAN	A	1155	8	11,11,12	0.67	0	14,15,17	1.15	2 (14%)
8	MAN	A	1156	8	11,11,12	0.40	0	14,15,17	1.55	2 (14%)
8	MAN	A	1157	8	11,11,12	1.03	1 (9%)	14,15,17	1.94	4 (28%)
9	NAG	A	1158	9	14,14,15	0.67	0	15,19,21	1.40	2 (13%)
9	BMA	A	1159	9	11,11,12	0.99	1 (9%)	14,15,17	2.27	2 (14%)
9	BMA	A	1160	9,2	11,11,12	1.13	2 (18%)	14,15,17	2.10	3 (21%)
9	NAG	A	1161	9,10	14,14,15	0.65	0	15,19,21	0.96	1 (6%)
9	BMA	A	1162	9	12,12,12	1.52	2 (16%)	17,17,17	1.76	5 (29%)
11	NAG	A	1164	11,10	14,14,15	0.58	0	15,19,21	1.77	2 (13%)
11	BMA	A	1165	11,2	11,11,12	1.33	2 (18%)	14,15,17	2.19	4 (28%)
11	NAG	A	1166	11	14,14,15	0.81	0	15,19,21	1.38	3 (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
4	NAG	A	1131	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1132	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1133	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	1134	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1135	4	-	0/2/19/22	0/1/1/1
6	NAG	A	1137	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1138	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1139	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1140	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1141	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1142	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1143	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1144	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1145	7	-	0/6/23/26	0/1/1/1
7	NAG	A	1146	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1147	7	-	0/6/23/26	0/1/1/1
8	NAG	A	1148	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1149	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1150	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1151	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1152	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1153	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1154	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1155	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1156	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1157	8	-	0/2/19/22	0/1/1/1
9	NAG	A	1158	9	-	0/6/23/26	0/1/1/1
9	BMA	A	1159	9	-	0/2/19/22	0/1/1/1
9	BMA	A	1160	9,2	-	0/2/19/22	0/1/1/1
9	NAG	A	1161	9,10	-	0/6/23/26	0/1/1/1
9	BMA	A	1162	9	-	0/2/22/22	0/1/1/1
11	NAG	A	1164	11,10	-	0/6/23/26	0/1/1/1
11	BMA	A	1165	11,2	-	0/2/19/22	0/1/1/1
11	NAG	A	1166	11	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1150	BMA	C2-C3	-4.44	1.46	1.52
6	A	1139	BMA	C4-C3	-4.41	1.40	1.52
4	A	1133	BMA	C2-C3	-4.24	1.46	1.52
8	A	1150	BMA	C4-C3	-4.15	1.41	1.52
6	A	1139	BMA	C2-C3	-3.99	1.47	1.52
4	A	1133	BMA	C4-C3	-3.78	1.42	1.52
9	A	1162	BMA	C4-C3	-3.72	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1133	BMA	O5-C1	-3.27	1.38	1.43
8	A	1150	BMA	O5-C1	-2.97	1.38	1.43
11	A	1165	BMA	O5-C1	-2.36	1.39	1.43
8	A	1150	BMA	O2-C2	-2.33	1.38	1.43
4	A	1133	BMA	O2-C2	-2.23	1.38	1.43
9	A	1160	BMA	O5-C1	-2.18	1.40	1.43
8	A	1153	MAN	O5-C1	-2.14	1.40	1.43
9	A	1162	BMA	O2-C2	-2.02	1.38	1.43
9	A	1160	BMA	C2-C3	2.09	1.55	1.52
9	A	1159	BMA	C2-C3	2.29	1.55	1.52
11	A	1165	BMA	C2-C3	2.87	1.56	1.52
8	A	1157	MAN	C2-C3	3.14	1.56	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1132	NAG	C2-N2-C7	-6.38	114.85	123.04
6	A	1139	BMA	C6-C5-C4	-5.62	99.16	113.02
11	A	1164	NAG	C2-N2-C7	-5.33	116.20	123.04
7	A	1145	NAG	C2-N2-C7	-4.68	117.02	123.04
6	A	1143	MAN	C1-O5-C5	-4.66	106.33	112.25
4	A	1135	MAN	O5-C1-C2	-3.94	104.47	110.86
8	A	1151	MAN	C6-C5-C4	-3.78	103.69	113.02
8	A	1156	MAN	C2-C3-C4	-3.47	105.15	111.04
6	A	1139	BMA	O3-C3-C4	-3.22	103.08	110.34
11	A	1165	BMA	C1-O5-C5	-3.21	108.17	112.25
8	A	1156	MAN	C1-C2-C3	-3.13	105.84	109.54
4	A	1133	BMA	O3-C3-C2	-3.10	104.40	110.00
6	A	1139	BMA	O3-C3-C2	-2.96	104.65	110.00
9	A	1161	NAG	C2-N2-C7	-2.84	119.39	123.04
11	A	1166	NAG	C3-C4-C5	-2.74	105.42	110.20
8	A	1152	MAN	O5-C1-C2	-2.67	106.52	110.86
9	A	1158	NAG	C2-N2-C7	-2.65	119.63	123.04
7	A	1146	NAG	C2-N2-C7	-2.51	119.82	123.04
4	A	1133	BMA	O4-C4-C5	-2.50	102.61	109.24
8	A	1157	MAN	O5-C1-C2	-2.47	106.86	110.86
11	A	1166	NAG	C1-O5-C5	-2.44	109.14	112.25
11	A	1165	BMA	O6-C6-C5	-2.38	103.46	111.33
8	A	1154	MAN	O5-C1-C2	-2.35	107.04	110.86
6	A	1137	NAG	C6-C5-C4	-2.35	107.22	113.02
7	A	1147	NAG	C2-N2-C7	-2.35	120.03	123.04
9	A	1162	BMA	C1-O5-C5	-2.21	109.38	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1160	BMA	O6-C6-C5	-2.11	104.35	111.33
8	A	1155	MAN	O5-C1-C2	-2.09	107.47	110.86
8	A	1153	MAN	O5-C1-C2	-2.08	107.49	110.86
6	A	1140	MAN	O5-C1-C2	-2.07	107.50	110.86
9	A	1162	BMA	O3-C3-C2	-2.05	105.73	110.34
6	A	1143	MAN	O3-C3-C2	-2.04	106.31	110.00
8	A	1152	MAN	O2-C2-C3	-2.03	106.04	110.12
4	A	1135	MAN	O2-C2-C1	-2.01	105.17	109.21
7	A	1146	NAG	C1-O5-C5	2.01	114.80	112.25
6	A	1137	NAG	O5-C5-C6	2.07	111.84	107.35
8	A	1155	MAN	O3-C3-C2	2.08	113.76	110.00
8	A	1157	MAN	O4-C4-C5	2.10	114.80	109.24
6	A	1141	MAN	C1-C2-C3	2.17	112.11	109.54
4	A	1135	MAN	O3-C3-C2	2.22	114.01	110.00
11	A	1166	NAG	O3-C3-C2	2.31	113.69	109.11
4	A	1134	MAN	O2-C2-C1	2.42	114.05	109.21
6	A	1139	BMA	C1-C2-C3	2.45	112.44	109.54
8	A	1150	BMA	C1-C2-C3	2.52	112.52	109.54
9	A	1162	BMA	O5-C5-C6	2.63	112.99	106.36
4	A	1134	MAN	C1-O5-C5	2.68	115.65	112.25
6	A	1139	BMA	O6-C6-C5	2.69	120.21	111.33
6	A	1139	BMA	O5-C1-C2	2.75	115.32	110.86
7	A	1144	NAG	C1-O5-C5	2.77	115.77	112.25
6	A	1140	MAN	C1-C2-C3	2.81	112.87	109.54
9	A	1162	BMA	O5-C1-C2	3.18	114.86	109.80
4	A	1133	BMA	C1-C2-C3	3.26	113.40	109.54
11	A	1165	BMA	C2-C3-C4	3.39	116.80	111.04
8	A	1151	MAN	C3-C4-C5	3.45	116.21	110.20
9	A	1158	NAG	O3-C3-C2	3.47	115.98	109.11
8	A	1157	MAN	O2-C2-C3	3.51	117.17	110.12
11	A	1164	NAG	C1-O5-C5	3.57	116.78	112.25
6	A	1139	BMA	C3-C4-C5	3.65	116.56	110.20
9	A	1162	BMA	C1-C2-C3	3.67	115.89	110.43
9	A	1159	BMA	C2-C3-C4	3.71	117.34	111.04
9	A	1160	BMA	C2-C3-C4	3.78	117.45	111.04
7	A	1145	NAG	C1-O5-C5	3.89	117.18	112.25
8	A	1157	MAN	O3-C3-C2	4.01	117.25	110.00
4	A	1131	NAG	C1-O5-C5	5.03	118.63	112.25
11	A	1165	BMA	C1-C2-C3	5.90	116.52	109.54
9	A	1160	BMA	C1-C2-C3	5.92	116.55	109.54
9	A	1159	BMA	C1-C2-C3	6.74	117.52	109.54
8	A	1151	MAN	C1-O5-C5	7.22	121.41	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1131	NAG	1	0
6	A	1139	BMA	1	0
6	A	1140	MAN	1	0
11	A	1164	NAG	1	0

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 29 are monoatomic - leaving 3 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	GAL	A	1130	-	12,12,12	0.88	1 (8%)	17,17,17	1.13	1 (5%)
5	NAG	A	1136	1	14,14,15	0.48	0	15,19,21	1.36	3 (20%)
10	M6D	A	1163	9,11	15,15,16	1.10	3 (20%)	20,22,24	1.03	1 (5%)

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	GAL	A	1130	-	-	0/2/22/22	0/1/1/1
5	NAG	A	1136	1	-	0/6/23/26	0/1/1/1
10	M6D	A	1163	9,11	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1163	M6D	O4-C4	-2.54	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1163	M6D	C4-C5	-2.23	1.48	1.53
3	A	1130	GAL	O2-C2	-2.12	1.37	1.43
10	A	1163	M6D	C4-C3	-2.00	1.47	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1136	NAG	C2-N2-C7	-3.53	118.50	123.04
10	A	1163	M6D	C1-O5-C5	-3.51	107.79	112.25
3	A	1130	GAL	O5-C5-C4	-2.11	105.72	109.68
5	A	1136	NAG	C3-C4-C5	-2.06	106.61	110.20
5	A	1136	NAG	C1-O5-C5	2.25	115.10	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1130	GAL	2	0
10	A	1163	M6D	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, 95^{th} 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	956/1005 (95%)	-0.37	18 (1%) 70 64	24, 32, 47, 64	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	ASP	4.9
1	A	499	GLY	3.4
1	A	739	LYS	3.4
1	A	781	LYS	3.0
1	A	787	SER	2.9
1	A	741	SER	2.6
1	A	737	ASN	2.5
1	A	786	GLU	2.5
1	A	826	GLY	2.5
1	A	666	GLU	2.3
1	A	784	GLN	2.3
1	A	783	SER	2.2
1	A	522	ASN	2.1
1	A	157	GLY	2.1
1	A	825	SER	2.1
1	A	452	GLY	2.0
1	A	540	SER	2.0
1	A	156	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	A	569	10/11	0.93	0.13	-	32,34,39,41	0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MAN	A	1156	11/12	0.87	0.23	2.82	38,41,46,49	0
6	MAN	A	1140	11/12	0.95	0.14	1.13	30,32,34,34	0
7	NAG	A	1146	14/15	0.95	0.14	1.09	36,43,50,52	0
11	NAG	A	1166	14/15	0.92	0.14	0.86	45,50,51,52	0
11	NAG	A	1164	14/15	0.90	0.14	0.58	51,52,54,55	0
9	BMA	A	1159	11/12	0.93	0.11	-0.30	35,37,39,42	0
7	NAG	A	1144	14/15	0.95	0.12	-0.48	42,46,51,52	0
9	NAG	A	1158	14/15	0.96	0.11	-0.53	36,39,41,42	0
8	BMA	A	1150	11/12	0.98	0.11	-0.58	30,31,33,37	0
8	NAG	A	1149	14/15	0.96	0.13	-0.62	28,31,35,35	0
8	MAN	A	1153	11/12	0.96	0.11	-0.70	32,33,34,38	0
8	MAN	A	1154	11/12	0.97	0.12	-0.73	31,33,34,35	0
4	NAG	A	1131	14/15	0.98	0.12	-0.80	25,28,31,33	0
6	NAG	A	1137	14/15	0.96	0.10	-0.95	26,29,30,30	0
4	NAG	A	1132	14/15	0.96	0.12	-0.96	30,32,34,37	0
8	NAG	A	1148	14/15	0.97	0.10	-1.22	27,30,35,37	0
6	MAN	A	1141	11/12	0.97	0.09	-1.27	31,32,35,38	0
9	NAG	A	1161	14/15	0.98	0.10	-1.32	36,40,42,43	0
6	NAG	A	1138	14/15	0.97	0.09	-1.84	27,29,30,30	0
11	BMA	A	1165	11/12	0.95	0.11	-1.90	51,53,53,54	0
8	MAN	A	1152	11/12	0.98	0.08	-2.03	31,32,33,34	0
7	NAG	A	1145	14/15	0.82	0.23	-	50,58,62,62	0
6	MAN	A	1142	11/12	0.98	0.10	-	35,36,41,45	0
8	MAN	A	1151	11/12	0.95	0.12	-	37,41,43,44	0
4	MAN	A	1134	11/12	0.96	0.12	-	38,41,44,47	0
8	MAN	A	1157	11/12	0.74	0.21	-	48,50,51,52	0
7	NAG	A	1147	14/15	0.92	0.26	-	55,58,61,63	0
6	MAN	A	1143	11/12	0.85	0.22	-	49,54,57,57	0
9	BMA	A	1160	11/12	0.94	0.16	-	42,44,47,48	0
4	BMA	A	1133	11/12	0.96	0.09	-	35,38,39,39	0
6	BMA	A	1139	11/12	0.95	0.11	-	29,32,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	BMA	A	1162	12/12	0.87	0.24	-	50,55,60,65	0
4	MAN	A	1135	11/12	0.87	0.31	-	50,53,56,56	0
8	MAN	A	1155	11/12	0.95	0.13	-	31,32,34,35	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	1136	14/15	0.85	0.34	7.57	42,47,50,50	0
10	M6D	A	1163	15/16	0.83	0.20	4.77	47,52,59,60	0
3	GAL	A	1130	12/12	0.87	0.20	2.02	27,30,34,35	0
2	CD	A	1105	1/1	1.00	0.11	0.05	42,42,42,42	0
2	CD	A	1104	1/1	1.00	0.10	-0.52	42,42,42,42	0
2	CD	A	1117	1/1	0.87	0.17	-	119,119,119,119	0
2	CD	A	1124	1/1	0.98	0.12	-	91,91,91,91	0
2	CD	A	1101	1/1	0.92	0.17	-	104,104,104,104	0
2	CD	A	1110	1/1	0.98	0.05	-	91,91,91,91	0
2	CD	A	1129	1/1	0.91	0.06	-	108,108,108,108	0
2	CD	A	1127	1/1	0.88	0.19	-	113,113,113,113	0
2	CD	A	1115	1/1	0.98	0.03	-	78,78,78,78	0
2	CD	A	1109	1/1	0.96	0.14	-	95,95,95,95	0
2	CD	A	1118	1/1	0.88	0.08	-	110,110,110,110	0
2	CD	A	1106	1/1	0.98	0.03	-	85,85,85,85	0
2	CD	A	1108	1/1	0.99	0.06	-	70,70,70,70	0
2	CD	A	1103	1/1	0.99	0.06	-	47,47,47,47	0
2	CD	A	1107	1/1	0.97	0.05	-	97,97,97,97	0
2	CD	A	1120	1/1	0.98	0.07	-	98,98,98,98	0
2	CD	A	1125	1/1	0.98	0.03	-	89,89,89,89	0
2	CD	A	1123	1/1	0.96	0.16	-	105,105,105,105	0
2	CD	A	1122	1/1	0.97	0.08	-	95,95,95,95	0
2	CD	A	1113	1/1	0.95	0.09	-	94,94,94,94	0
2	CD	A	1121	1/1	0.91	0.13	-	104,104,104,104	0
2	CD	A	1128	1/1	0.99	0.06	-	73,73,73,73	0
2	CD	A	1116	1/1	0.89	0.17	-	113,113,113,113	0
2	CD	A	1126	1/1	0.96	0.15	-	110,110,110,110	0
2	CD	A	1112	1/1	0.95	0.09	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CD	A	1119	1/1	0.93	0.06	-	88,88,88,88	0
2	CD	A	1102	1/1	0.99	0.08	-	49,49,49,49	0
2	CD	A	1111	1/1	0.79	0.26	-	108,108,108,108	0
2	CD	A	1114	1/1	0.95	0.09	-	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.