Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:35 PM GMT

PDB ID	:	1GA2
Title	:	THE CRYSTAL STRUCTURE OF ENDOGLUCANASE 9G FROM CLOSTRIDIUM CELLULOLYTICUM COMPLEXED WITH CELLOBIOSE
Authors	:	Mandelman, D.; Belaich, A.; Belaich, J.P.; Aghajari, N.; Driguez, H.; Haser, R.
Deposited on	:	2000-11-29
Resolution	:	1.70 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 (i)) were used in the production of this report:

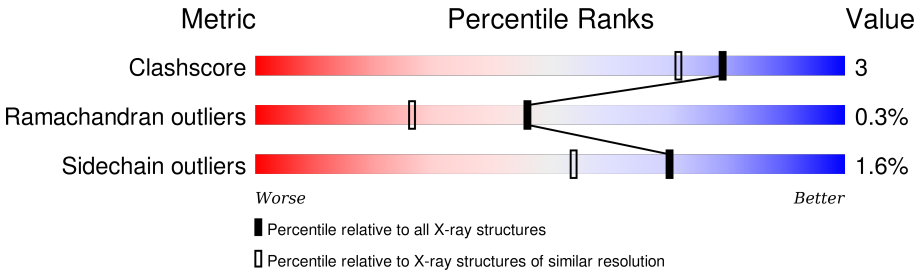
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.70 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))
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	614	92% 7%
1	B	614	91% 8%

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
7	ACY	A	790	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10474 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 ENDOGLUCANASE 9G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	5	0
			4795	3047	786	943	19			
1	B	613	Total	C	N	O	S	0	0	0
			4797	3050	787	941	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	574	THR	ARG	CONFLICT	UNP P37700
A	575	THR	ARG	CONFLICT	UNP P37700
B	574	THR	ARG	CONFLICT	UNP P37700
B	575	THR	ARG	CONFLICT	UNP P37700

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			34	18	16		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			23	12	11		
3	B	2	Total	C	O	0	0
			23	12	11		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

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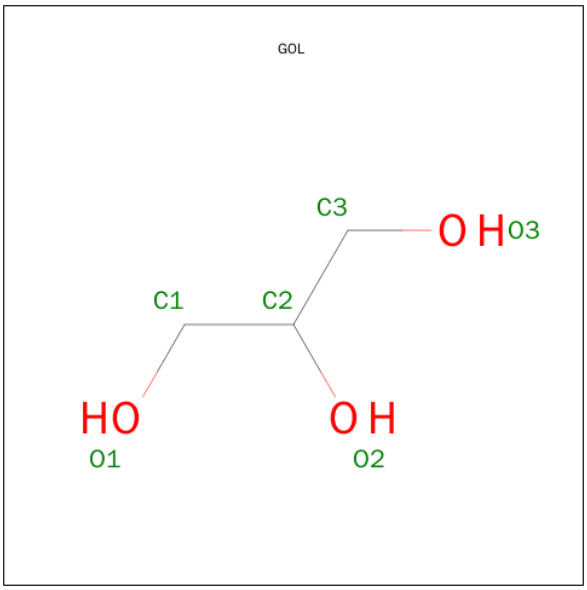
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

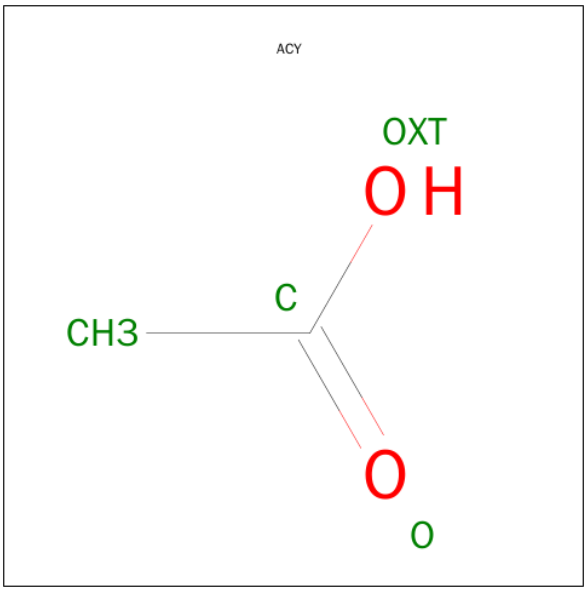
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Mg 3 3	0	0
5	A	4	Total Mg 4 4	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	401	Total O 401 401	0	0
8	B	356	Total O 356 356	0	0

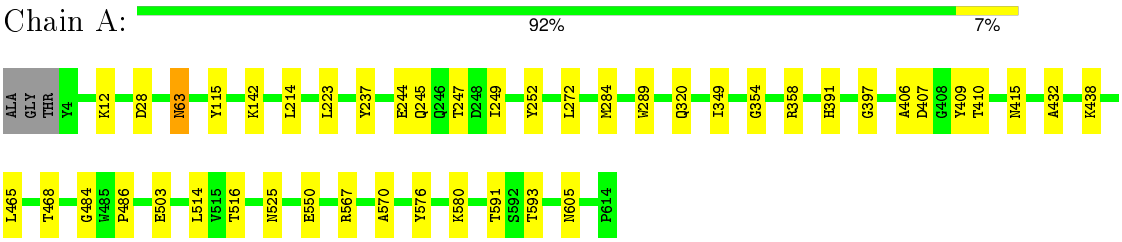
3 Residue-property plots (i)

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.

Note EDS was not executed.

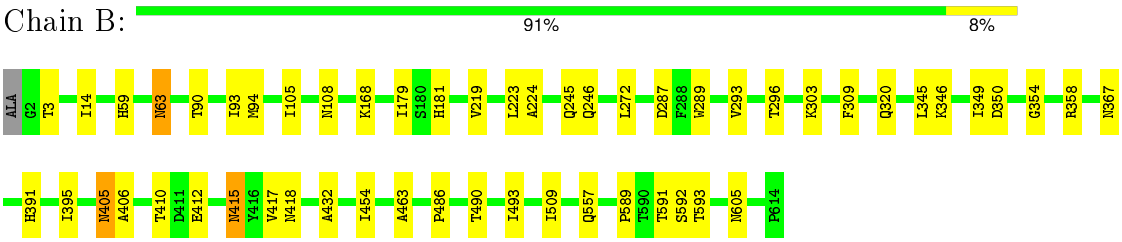
- Molecule 1: ENDOGLUCANASE 9G

Chain A:



- Molecule 1: ENDOGLUCANASE 9G

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.85Å 57.67Å 86.58Å 93.82° 100.86° 99.46°	Depositor
Resolution (Å)	43.54 – 1.70	Depositor
% Data completeness (in resolution range)	89.8 (43.54-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.170 , 0.197	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10474	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, GOL, MG, BGC, CA

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	0.39	0/4935	0.64	0/6727
1	B	0.40	0/4938	0.66	1/6729 (0.0%)
All	All	0.40	0/9873	0.65	1/13456 (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	1	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	B	415	ASN	N-CA-C	-5.87	95.14	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	454	ILE	CB

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	4795	0	4473	29	0
1	B	4797	0	4501	36	0
2	A	34	0	30	0	0
3	A	23	0	20	0	0
3	B	23	0	21	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
6	A	24	0	32	0	0
6	B	6	0	8	0	0
7	A	4	0	3	4	0
8	A	401	0	0	2	0
8	B	356	0	0	4	0
All	All	10474	0	9088	65	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 3.

All (65) 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:B:179:ILE:HD11	1:B:224:ALA:HB1	1.58	0.84
1:B:410:THR:HG22	1:B:412:GLU:HG3	1.67	0.76
1:B:345:LEU:O	1:B:349:ILE:HD13	1.85	0.76
1:B:591:THR:O	1:B:593:THR:N	2.17	0.76
1:A:247[A]:THR:HG21	1:A:249:ILE:HD12	1.69	0.75
1:B:287:ASP:HB3	1:B:293:VAL:HG13	1.68	0.73
1:A:410:THR:H	7:A:790:ACY:H1	1.55	0.70
1:B:223:LEU:HD11	1:B:272:LEU:HD11	1.75	0.66
1:B:349:ILE:HD11	1:B:432:ALA:HB1	1.77	0.66
1:A:247[A]:THR:HG22	1:A:249:ILE:HG13	1.79	0.64
1:A:591:THR:HG23	1:A:593:THR:H	1.61	0.64
1:B:14:ILE:HD12	1:B:93:ILE:HB	1.80	0.64
1:A:580:LYS:HE2	8:A:969:HOH:O	1.98	0.63
1:A:465:LEU:HD11	1:A:468:THR:HB	1.79	0.62
1:B:245:GLN:O	1:B:246:GLN:HB2	1.99	0.62
1:A:438:LYS:HD2	8:A:1112:HOH:O	2.00	0.61
1:B:219:VAL:O	1:B:223:LEU:HD13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:HD12	1:B:181:HIS:ND1	2.19	0.57
1:B:287:ASP:HB3	1:B:293:VAL:CG1	2.32	0.57
1:B:593:THR:O	1:B:593:THR:HG23	2.05	0.56
1:B:179:ILE:CD1	1:B:224:ALA:HB1	2.35	0.55
1:B:108:ASN:OD1	1:B:181:HIS:HD2	1.91	0.53
1:B:463:ALA:O	1:B:589:PRO:HG2	2.08	0.53
1:A:247[A]:THR:HG21	1:A:249:ILE:CD1	2.39	0.52
1:B:245:GLN:HE21	1:B:246:GLN:HG2	1.74	0.52
1:A:245:GLN:O	1:A:247[B]:THR:HG23	2.11	0.51
1:A:525:ASN:HB2	1:A:550:GLU:OE2	2.10	0.51
1:B:59:HIS:HD2	8:B:849:HOH:O	1.94	0.50
1:B:289:TRP:CE2	1:B:320:GLN:HG3	2.47	0.50
1:A:410:THR:H	7:A:790:ACY:CH3	2.24	0.50
1:A:349:ILE:HD11	1:A:432:ALA:HB3	1.94	0.49
1:B:405:ASN:HD22	1:B:406:ALA:N	2.11	0.49
1:A:252:TYR:CD2	1:A:284:MET:HG2	2.48	0.48
1:B:14:ILE:HD11	1:B:93:ILE:HD12	1.96	0.48
1:B:509:ILE:N	1:B:509:ILE:HD12	2.29	0.48
1:A:244:GLU:HG3	1:A:252:TYR:CE1	2.49	0.48
1:A:63:ASN:N	1:A:63:ASN:HD22	2.12	0.47
1:B:490:THR:OG1	1:B:493:ILE:HD11	2.15	0.47
1:A:516:THR:HA	1:A:567:ARG:O	2.15	0.46
1:B:415:ASN:CG	1:B:418:ASN:HB2	2.36	0.45
1:A:503:GLU:HG3	1:A:576:TYR:O	2.17	0.45
1:B:63:ASN:N	1:B:63:ASN:HD22	2.14	0.45
1:B:367:ASN:ND2	8:B:1049:HOH:O	2.47	0.44
1:A:223:LEU:HD21	1:A:272:LEU:HD21	1.98	0.44
1:B:490:THR:CB	1:B:493:ILE:HD11	2.47	0.44
1:A:252:TYR:CG	1:A:284:MET:HG2	2.52	0.44
1:B:395:ILE:O	1:B:395:ILE:HG23	2.18	0.43
1:A:289:TRP:CE2	1:A:320:GLN:HG3	2.54	0.43
1:B:90:THR:HG22	1:B:94:MET:CE	2.49	0.43
1:A:12:LYS:O	1:A:397:GLY:HA3	2.19	0.42
1:B:415:ASN:C	1:B:417:VAL:H	2.22	0.42
1:A:406:ALA:O	1:A:407:ASP:HB2	2.20	0.42
1:B:14:ILE:HD12	1:B:93:ILE:CB	2.47	0.42
1:B:346:LYS:NZ	1:B:350:ASP:OD2	2.52	0.42
1:B:454:ILE:HD12	1:B:454:ILE:N	2.35	0.42
1:A:247[A]:THR:CG2	1:A:249:ILE:HG13	2.47	0.42
1:A:410:THR:N	7:A:790:ACY:H1	2.27	0.41
1:B:168:LYS:CE	8:B:1018:HOH:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HD22	1:A:570:ALA:HA	2.02	0.41
1:B:303:LYS:HE3	8:B:1118:HOH:O	2.20	0.41
1:A:409:TYR:HA	7:A:790:ACY:H2	2.03	0.41
1:A:115:TYR:CD1	1:A:142:LYS:HB3	2.55	0.41
1:A:214:LEU:HB3	1:A:237:TYR:CE2	2.56	0.41
1:A:28:ASP:C	1:A:28:ASP:OD1	2.58	0.41
1:B:105:ILE:HG23	1:B:181:HIS:CE1	2.57	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	614/614 (100%)	595 (97%)	17 (3%)	2 (0%)	46 26
1	B	611/614 (100%)	590 (97%)	19 (3%)	2 (0%)	46 26
All	All	1225/1228 (100%)	1185 (97%)	36 (3%)	4 (0%)	46 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	592	SER
1	B	354	GLY
1	A	354	GLY
1	A	484	GLY

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	503/507 (99%)	497 (99%)	6 (1%)	78 65
1	B	506/507 (100%)	496 (98%)	10 (2%)	63 44
All	All	1009/1014 (100%)	993 (98%)	16 (2%)	70 54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	358	ARG
1	A	391	HIS
1	A	415	ASN
1	A	486	PRO
1	A	605	ASN
1	B	3	THR
1	B	63	ASN
1	B	296	THR
1	B	309	PHE
1	B	358	ARG
1	B	391	HIS
1	B	405	ASN
1	B	486	PRO
1	B	557	GLN
1	B	605	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	117	GLN
1	A	276	GLN
1	A	310	GLN
1	A	415	ASN
1	A	466	ASN
1	A	525	ASN
1	A	565	GLN
1	A	605	ASN
1	B	59	HIS
1	B	63	ASN

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Mol	Chain	Res	Type
1	B	89	GLN
1	B	117	GLN
1	B	181	HIS
1	B	245	GLN
1	B	276	GLN
1	B	294	ASN
1	B	367	ASN
1	B	405	ASN
1	B	466	ASN
1	B	519	ASN
1	B	544	ASN
1	B	557	GLN
1	B	572	GLN
1	B	605	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

7 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	BGC	A	775	2	11,11,12	0.41	0	14,15,17	0.37	0
2	BGC	A	776	2	11,11,12	0.54	0	14,15,17	0.50	0
2	BGC	A	777	2	12,12,12	0.57	0	17,17,17	0.77	0
3	BGC	A	778	3,5	11,11,12	0.53	0	14,15,17	0.48	0
3	BGC	A	779	3	12,12,12	0.40	0	17,17,17	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BGC	B	780	3	11,11,12	0.45	0	14,15,17	0.51	0
3	BGC	B	781	3	12,12,12	0.48	0	17,17,17	0.38	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
2	BGC	A	775	2	-	0/2/19/22	0/1/1/1
2	BGC	A	776	2	-	0/2/19/22	0/1/1/1
2	BGC	A	777	2	-	0/2/22/22	0/1/1/1
3	BGC	A	778	3,5	-	0/2/19/22	0/1/1/1
3	BGC	A	779	3	-	0/2/22/22	0/1/1/1
3	BGC	B	780	3	-	0/2/19/22	0/1/1/1
3	BGC	B	781	3	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 11 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	$\#\|Z\|>2$
6	GOL	A	786	-	5,5,5	0.76	0	5,5,5	0.58	0
6	GOL	A	787	-	5,5,5	1.10	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	788	-	5,5,5	1.01	0	5,5,5	0.89	0
6	GOL	A	789	-	5,5,5	0.72	0	5,5,5	2.26	2 (40%)
7	ACY	A	790	-	1,3,3	1.65	0	0,3,3	0.00	-
6	GOL	B	787	-	5,5,5	1.18	0	5,5,5	0.68	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
6	GOL	A	786	-	-	0/4/4/4	0/0/0/0
6	GOL	A	787	-	-	0/4/4/4	0/0/0/0
6	GOL	A	788	-	-	0/4/4/4	0/0/0/0
6	GOL	A	789	-	-	0/4/4/4	0/0/0/0
7	ACY	A	790	-	-	0/0/0/0	0/0/0/0
6	GOL	B	787	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	789	GOL	O3-C3-C2	3.37	126.51	110.18
6	A	789	GOL	O1-C1-C2	3.42	126.77	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	790	ACY	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.