



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 11:09 AM BST

PDB ID : 5OKE
Title : Conservatively refined structure of Gan1D-E170Q, a catalytic mutant of a putative 6-phospho-beta-galactosidase from *Geobacillus stearothermophilus*, in complex with cellobiose-6-phosphate
Authors : Lansky, S.; Zehavi, A.; Shoham, Y.; Shoham, G.
Deposited on : 2017-07-25
Resolution : 1.31 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
buster-report : 1.1.7 (2018)
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

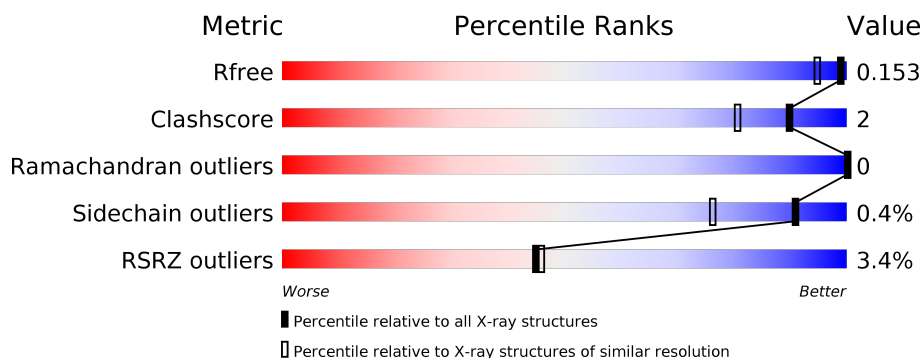
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.31 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	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

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 ≥ 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	485	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	B	485	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	C	485	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	D	485	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18080 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 Putative 6-phospho-beta-galactobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	26	0
			3949	2550	681	704	14			
1	B	462	Total	C	N	O	S	0	23	0
			3947	2545	675	713	14			
1	C	462	Total	C	N	O	S	0	23	0
			3933	2537	672	711	13			
1	D	461	Total	C	N	O	S	0	18	0
			3882	2504	656	708	14			

There are 36 discrepancies between the modelled and reference sequences:

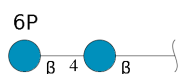
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	UNP W8QF82
A	1	HIS	-	expression tag	UNP W8QF82
A	170	GLN	GLU	engineered mutation	UNP W8QF82
B	-6	MET	-	initiating methionine	UNP W8QF82
B	-5	ILE	-	expression tag	UNP W8QF82
B	-4	HIS	-	expression tag	UNP W8QF82
B	-3	HIS	-	expression tag	UNP W8QF82
B	-2	HIS	-	expression tag	UNP W8QF82
B	-1	HIS	-	expression tag	UNP W8QF82
B	0	HIS	-	expression tag	UNP W8QF82
B	1	HIS	-	expression tag	UNP W8QF82
B	170	GLN	GLU	engineered mutation	UNP W8QF82
C	-6	MET	-	initiating methionine	UNP W8QF82
C	-5	ILE	-	expression tag	UNP W8QF82
C	-4	HIS	-	expression tag	UNP W8QF82

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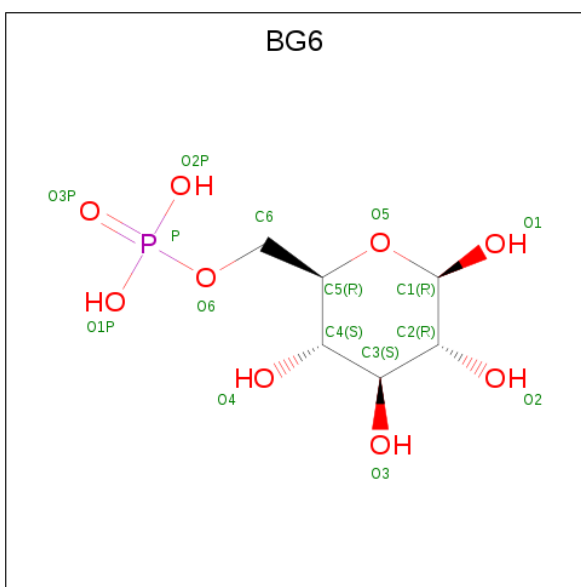
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP W8QF82
C	-2	HIS	-	expression tag	UNP W8QF82
C	-1	HIS	-	expression tag	UNP W8QF82
C	0	HIS	-	expression tag	UNP W8QF82
C	1	HIS	-	expression tag	UNP W8QF82
C	170	GLN	GLU	engineered mutation	UNP W8QF82
D	-6	MET	-	initiating methionine	UNP W8QF82
D	-5	ILE	-	expression tag	UNP W8QF82
D	-4	HIS	-	expression tag	UNP W8QF82
D	-3	HIS	-	expression tag	UNP W8QF82
D	-2	HIS	-	expression tag	UNP W8QF82
D	-1	HIS	-	expression tag	UNP W8QF82
D	0	HIS	-	expression tag	UNP W8QF82
D	1	HIS	-	expression tag	UNP W8QF82
D	170	GLN	GLU	engineered mutation	UNP W8QF82

- Molecule 2 is an oligosaccharide called 6-O-phosphono-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	F	2	Total	C	O	P	0	0	0
			27	12	14	1			

- Molecule 3 is 6-O-phosphono-beta-D-glucopyranose (three-letter code: BG6) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



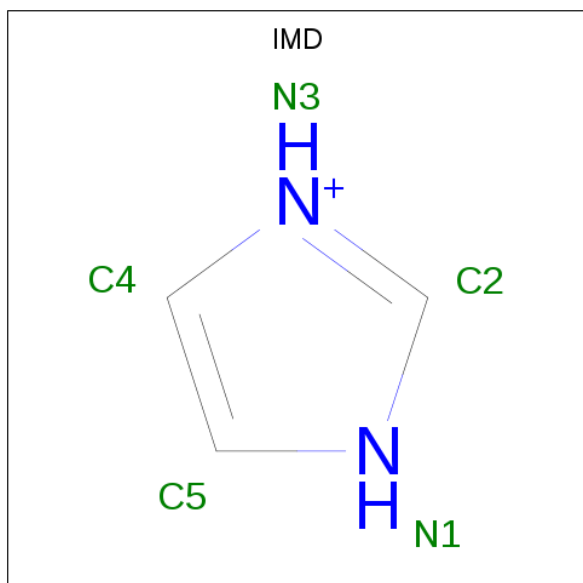
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

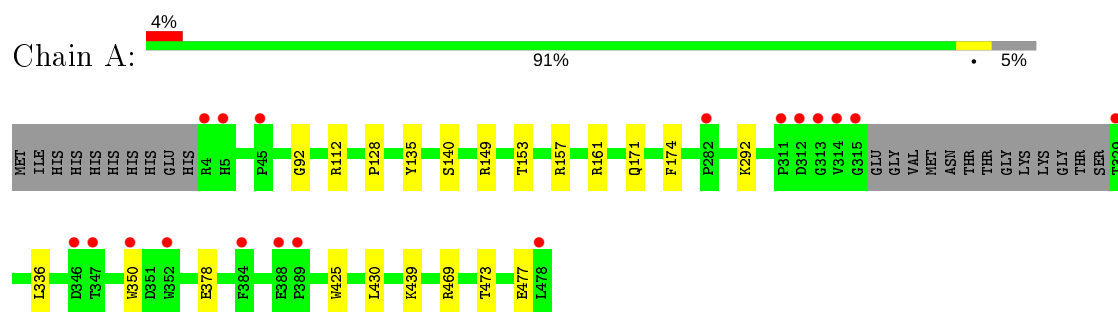
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	542	Total	O	0	0
			542	542		
6	B	560	Total	O	0	0
			560	560		
6	C	574	Total	O	0	0
			574	574		
6	D	520	Total	O	0	0
			520	520		

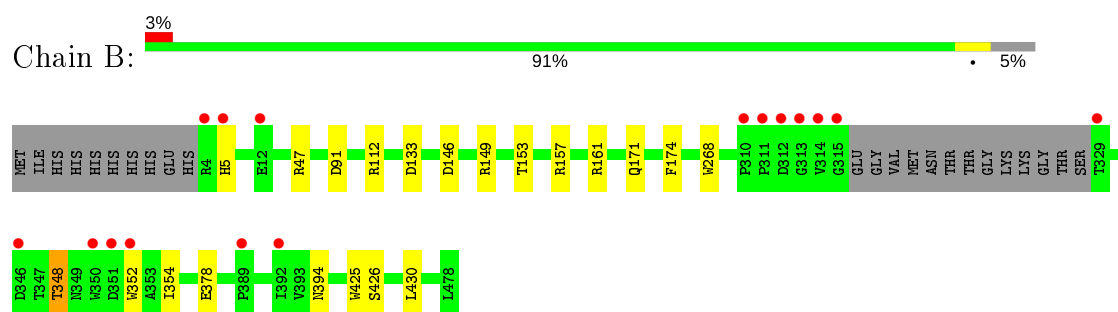
3 Residue-property plots [i](#)

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.

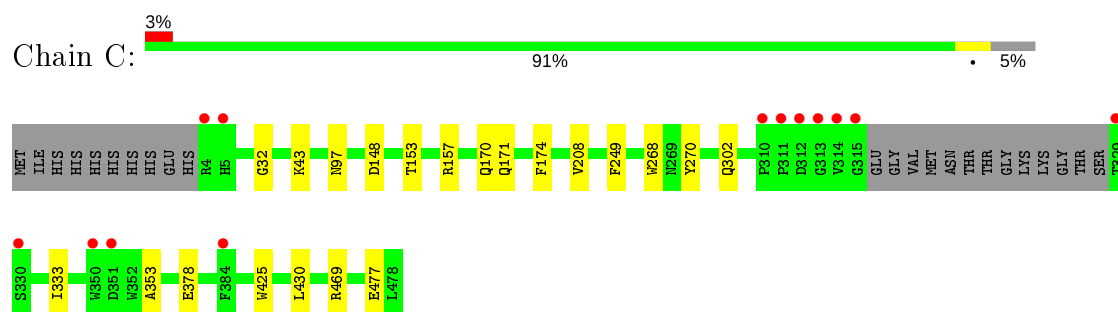
- Molecule 1: Putative 6-phospho-beta-galactobiosidase



- Molecule 1: Putative 6-phospho-beta-galactobiosidase

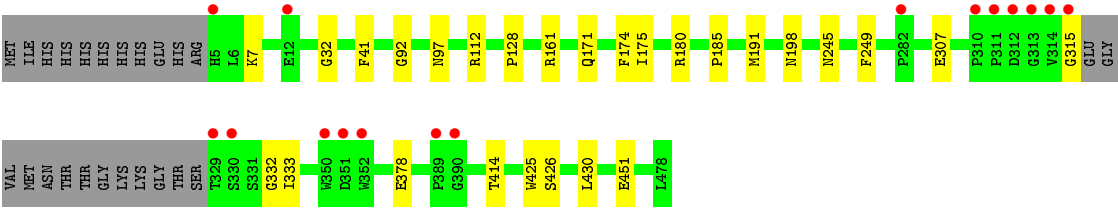


- Molecule 1: Putative 6-phospho-beta-galactobiosidase



- Molecule 1: Putative 6-phospho-beta-galactobiosidase





- Molecule 2: 6-O-phosphono-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:

50%

50%



- Molecule 2: 6-O-phosphono-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:

50%

50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.60Å 97.48Å 105.27Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	34.78 – 1.31 36.14 – 1.31	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.78-1.31) 98.4 (36.14-1.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.31Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.133 , 0.155 0.133 , 0.153	Depositor DCC
R_{free} test set	4697 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	9.8	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	18080	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4937e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, BGC, IMD, BG6

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	0.34	0/4149	0.58	0/5636
1	B	0.33	0/4131	0.58	0/5618
1	C	0.36	0/4128	0.59	0/5610
1	D	0.37	2/4060 (0.0%)	0.57	0/5522
All	All	0.35	2/16468 (0.0%)	0.58	0/22386

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	307	GLU	CD-OE1	-6.44	1.18	1.25
1	D	307	GLU	CD-OE2	-5.06	1.20	1.25

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	3949	0	3831	13	0
1	B	3947	0	3790	15	0
1	C	3933	0	3783	12	0
1	D	3882	0	3717	15	0
2	E	27	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	27	0	20	0	0
3	A	16	0	11	0	0
3	B	16	0	10	0	0
4	A	30	0	40	1	0
4	B	12	0	16	1	0
4	C	24	0	32	1	0
4	D	6	0	8	0	0
5	A	5	0	5	0	0
5	C	5	0	5	0	0
5	D	5	0	5	1	0
6	A	542	0	0	2	0
6	B	560	0	0	5	0
6	C	574	0	0	1	0
6	D	520	0	0	3	0
All	All	18080	0	15291	56	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 (56) 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:D:97[A]:ASN:ND2	6:D:601:HOH:O	2.23	0.72
1:B:91[A]:ASP:OD1	6:B:601:HOH:O	2.14	0.65
1:B:348[A]:THR:OG1	6:B:602:HOH:O	2.16	0.60
1:D:112[B]:ARG:HD2	1:D:161:ARG:HB3	1.84	0.58
1:D:112[A]:ARG:HD2	1:D:161:ARG:HB3	1.89	0.55
1:A:112[A]:ARG:HD2	1:A:161:ARG:HB3	1.89	0.54
1:B:348[A]:THR:HG23	1:B:352[A]:TRP:HB2	1.91	0.52
1:A:473:THR:HG21	1:A:477[A]:GLU:HG3	1.91	0.52
1:C:32:GLY:HA3	1:C:97[B]:ASN:HD21	1.76	0.50
1:C:153:THR:O	1:C:157[B]:ARG:HG2	2.11	0.50
1:B:149[A]:ARG:NH2	6:B:611:HOH:O	2.44	0.50
1:B:394:ASN:ND2	6:B:612:HOH:O	2.44	0.49
1:B:146:ASP:OD1	1:B:149[B]:ARG:NH1	2.47	0.48
1:A:336:LEU:CD2	4:A:506:GOL:H2	2.45	0.47
1:C:249[A]:PHE:CE2	1:C:333:ILE:HD11	2.49	0.47
1:B:378:GLU:HG3	1:B:425:TRP:HB2	1.97	0.47
1:B:133:ASP:OD2	6:B:603:HOH:O	2.21	0.46
1:A:469[A]:ARG:NE	1:A:477[A]:GLU:OE1	2.48	0.46
1:D:249:PHE:CE2	1:D:333:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180[A]:ARG:HD3	1:D:191[A]:MET:HG2	1.98	0.45
1:B:47:ARG:HA	1:B:47:ARG:HD3	1.84	0.45
1:D:92:GLY:HA2	1:D:128:PRO:HG2	1.99	0.45
1:A:378:GLU:HG3	1:A:425:TRP:HB2	1.98	0.44
1:D:315:GLY:HA2	1:D:332:GLY:O	2.17	0.44
1:D:32:GLY:HA3	1:D:97[B]:ASN:HD21	1.82	0.44
1:C:378:GLU:HG3	1:C:425:TRP:HB2	1.98	0.44
1:D:425:TRP:HA	1:D:426:SER:HA	1.85	0.44
1:A:292[B]:LYS:NZ	6:A:618:HOH:O	2.49	0.44
1:C:43:LYS:HE3	6:C:809:HOH:O	2.17	0.44
1:B:268:TRP:CE2	4:B:503:GOL:H32	2.52	0.43
1:C:302:GLN:HB2	1:C:353:ALA:HB3	1.99	0.43
1:D:378:GLU:HG3	1:D:425:TRP:HB2	2.00	0.43
1:A:149[A]:ARG:NH2	6:A:620:HOH:O	2.51	0.43
1:B:348[A]:THR:HB	1:B:354:ILE:HD11	2.01	0.43
1:A:112[B]:ARG:HD2	1:A:161:ARG:HB3	2.01	0.43
1:C:268:TRP:CE2	4:C:504:GOL:H32	2.54	0.43
1:C:469:ARG:HE	1:C:477:GLU:CD	2.23	0.42
1:A:350[A]:TRP:CE2	1:A:439:LYS:HD2	2.54	0.42
1:B:425:TRP:HA	1:B:426:SER:HA	1.83	0.42
1:C:171:GLN:HA	1:C:174:PHE:CE2	2.54	0.42
1:C:249[B]:PHE:HZ	1:C:270:TYR:HD2	1.68	0.42
5:D:503:IMD:H5	6:D:632:HOH:O	2.18	0.42
1:D:41:PHE:CD2	1:D:185:PRO:HD3	2.54	0.42
1:B:153:THR:O	1:B:157[B]:ARG:HG2	2.20	0.42
1:B:171:GLN:HA	1:B:174:PHE:CE2	2.55	0.42
1:C:148:ASP:HA	1:C:208[A]:VAL:HG12	2.02	0.42
1:C:170:GLN:OE1	2:E:1:BGC:O6	2.38	0.42
1:A:153:THR:O	1:A:157[A]:ARG:HG2	2.20	0.42
1:D:171:GLN:HA	1:D:174:PHE:CE2	2.55	0.41
1:A:171:GLN:HA	1:A:174:PHE:CE2	2.56	0.41
1:D:7:LYS:HG3	1:D:414:THR:HA	2.01	0.41
1:A:135:TYR:CD1	1:A:140:SER:HB3	2.55	0.41
1:D:175:ILE:HG21	1:D:198:ASN:HB2	2.03	0.40
1:D:245:ASN:ND2	6:D:628:HOH:O	2.53	0.40
1:B:112:ARG:HD2	1:B:161:ARG:HB3	2.03	0.40
1:A:92:GLY:HA2	1:A:128:PRO:HG2	2.03	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	484/485 (100%)	469 (97%)	15 (3%)	0	100	100
1	B	482/485 (99%)	470 (98%)	12 (2%)	0	100	100
1	C	482/485 (99%)	467 (97%)	15 (3%)	0	100	100
1	D	476/485 (98%)	461 (97%)	15 (3%)	0	100	100
All	All	1924/1940 (99%)	1867 (97%)	57 (3%)	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	417/412 (101%)	416 (100%)	1 (0%)	93	79
1	B	416/412 (101%)	412 (99%)	4 (1%)	76	47
1	C	416/412 (101%)	415 (100%)	1 (0%)	93	79
1	D	410/412 (100%)	408 (100%)	2 (0%)	88	69
All	All	1659/1648 (101%)	1651 (100%)	8 (0%)	91	69

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	LEU
1	B	5	HIS

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Mol	Chain	Res	Type
1	B	348[A]	THR
1	B	348[B]	THR
1	B	430	LEU
1	C	430	LEU
1	D	430	LEU
1	D	451	GLU

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	$\# Z > 2$
2	BGC	E	1	2	12,12,12	0.92	0	17,17,17	2.87	8 (47%)
2	BG6	E	2	2	15,15,16	2.14	6 (40%)	22,22,24	3.16	11 (50%)
2	BGC	F	1	2	12,12,12	0.45	0	17,17,17	0.70	0
2	BG6	F	2	2	15,15,16	0.56	0	22,22,24	1.73	4 (18%)

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	E	1	2	-	1/2/22/22	0/1/1/1
2	BG6	E	2	2	-	0/6/23/26	0/1/1/1
2	BGC	F	1	2	-	1/2/22/22	0/1/1/1
2	BG6	F	2	2	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	BG6	O2-C2	-4.34	1.34	1.43
2	E	2	BG6	P-O1P	-4.11	1.39	1.54
2	E	2	BG6	O3-C3	2.76	1.49	1.43
2	E	2	BG6	C4-C3	2.41	1.58	1.52
2	E	2	BG6	O5-C1	-2.21	1.40	1.43
2	E	2	BG6	P-O2P	-2.07	1.46	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	BG6	C1-C2-C3	9.32	121.12	109.67
2	E	2	BG6	O3-C3-C4	6.07	124.38	110.35
2	E	1	BGC	O5-C1-C2	-5.92	99.72	110.28
2	F	2	BG6	C1-C2-C3	5.39	116.29	109.67
2	E	1	BGC	O5-C5-C6	-5.07	93.84	106.44
2	E	2	BG6	O2P-P-O3P	4.61	128.75	110.68
2	E	1	BGC	O1-C1-C2	4.61	122.02	109.03
2	E	1	BGC	C6-C5-C4	3.89	122.12	113.00
2	E	1	BGC	O2-C2-C1	3.74	117.84	109.16
2	E	2	BG6	O3-C3-C2	-3.47	103.35	109.99
2	E	2	BG6	O2-C2-C3	-3.44	103.26	110.14
2	F	2	BG6	O2-C2-C3	-3.28	103.57	110.14
2	E	1	BGC	C1-C2-C3	-3.11	103.85	110.31
2	E	2	BG6	O2-C2-C1	-2.94	103.13	109.15
2	E	1	BGC	O5-C5-C4	-2.78	104.65	109.69
2	E	2	BG6	O1P-P-O6	2.69	113.90	106.73
2	E	2	BG6	O4-C4-C3	2.61	116.37	110.35
2	F	2	BG6	O3-C3-C4	2.57	116.28	110.35
2	E	2	BG6	O1P-P-O3P	-2.50	100.90	110.68
2	E	1	BGC	O4-C4-C5	-2.43	103.27	109.30
2	F	2	BG6	O3-C3-C2	-2.42	105.35	109.99
2	E	2	BG6	O4-C4-C5	-2.21	103.81	109.30
2	E	2	BG6	C1-O5-C5	-2.04	109.43	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

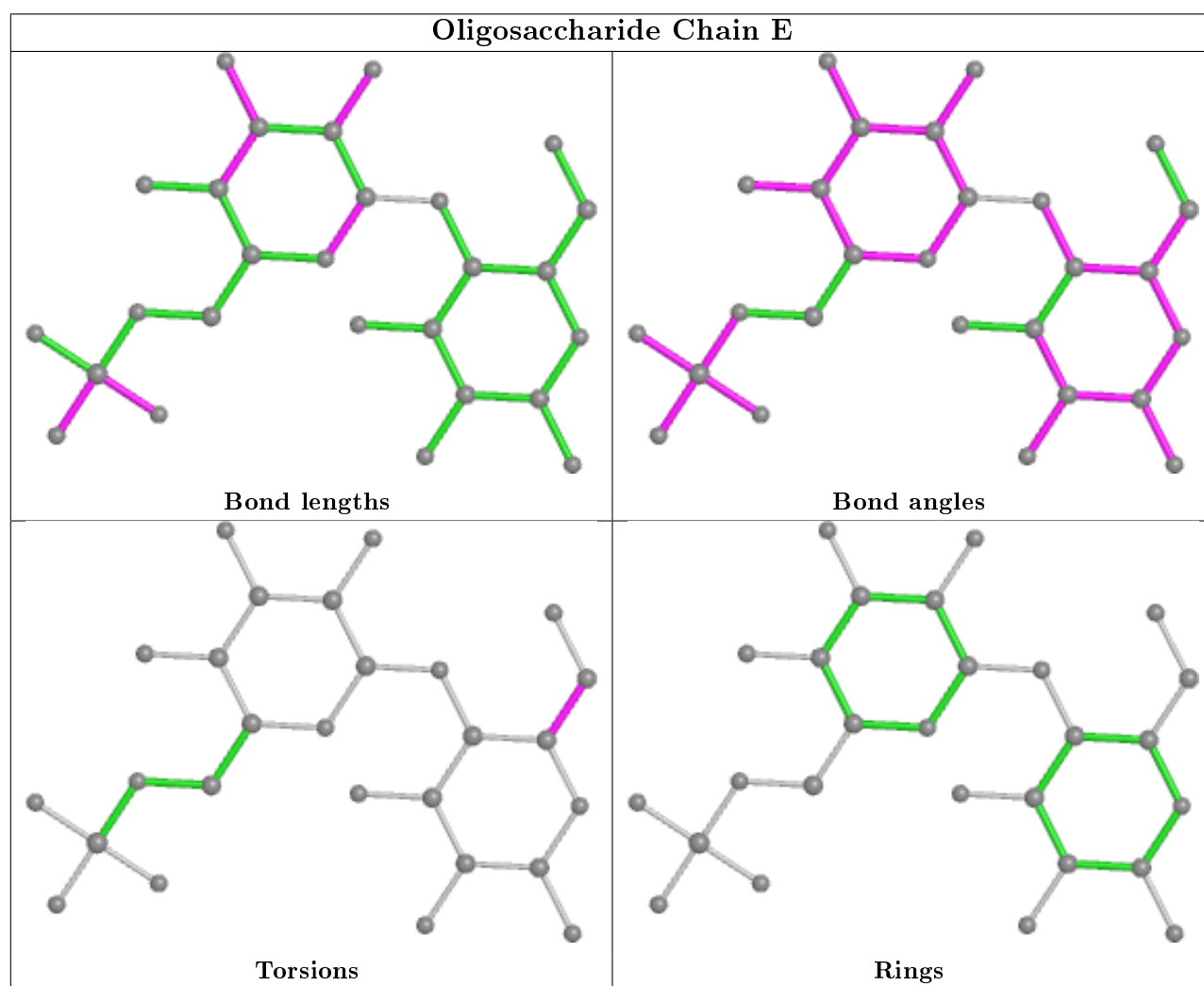
Mol	Chain	Res	Type	Atoms
2	F	1	BGC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6

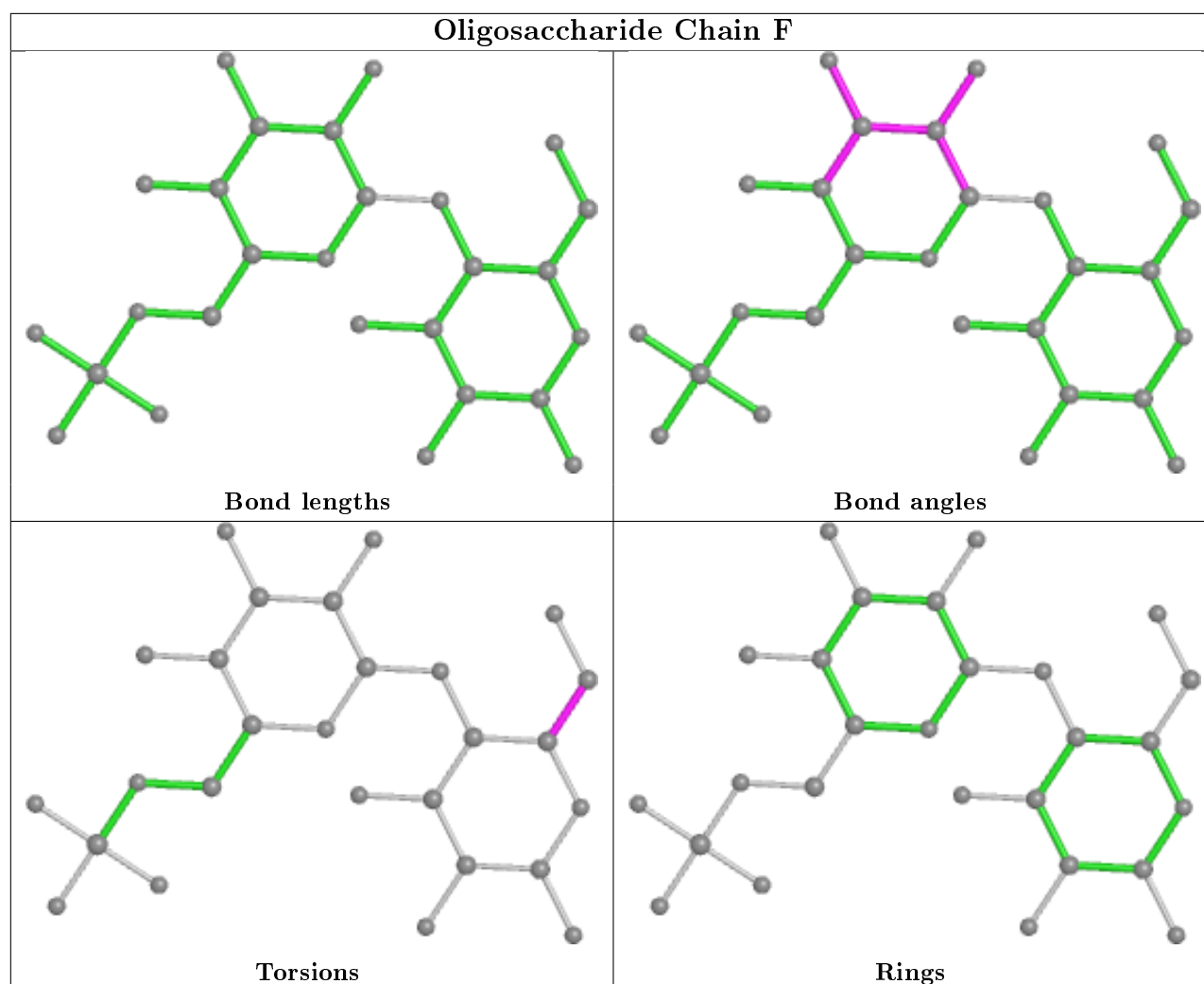
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

17 ligands 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	GOL	A	505	-	5,5,5	0.37	0	5,5,5	0.31	0
5	IMD	C	506	-	3,5,5	0.42	0	4,5,5	0.56	0
4	GOL	D	502	-	5,5,5	0.37	0	5,5,5	0.29	0
3	BG6	A	501	-	16,16,16	0.59	0	24,24,24	1.22	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	504	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.42	0
4	GOL	B	502	-	5,5,5	0.38	0	5,5,5	0.18	0
5	IMD	A	507	-	3,5,5	0.41	0	4,5,5	0.59	0
4	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.40	0
4	GOL	C	503	-	5,5,5	0.35	0	5,5,5	0.46	0
5	IMD	D	503	-	3,5,5	0.43	0	4,5,5	0.49	0
3	BG6	B	501	-	16,16,16	2.15	5 (31%)	24,24,24	3.05	13 (54%)
4	GOL	B	503	-	5,5,5	0.36	0	5,5,5	0.30	0
4	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.34	0
4	GOL	A	502	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	C	505	-	5,5,5	0.38	0	5,5,5	0.21	0
4	GOL	C	502	-	5,5,5	0.35	0	5,5,5	0.44	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
4	GOL	A	505	-	-	4/4/4/4	-
5	IMD	C	506	-	-	-	0/1/1/1
4	GOL	D	502	-	-	2/4/4/4	-
3	BG6	A	501	-	-	0/6/26/26	0/1/1/1
4	GOL	C	504	-	-	2/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	502	-	-	2/4/4/4	-
5	IMD	A	507	-	-	-	0/1/1/1
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	C	503	-	-	0/4/4/4	-
5	IMD	D	503	-	-	-	0/1/1/1
3	BG6	B	501	-	-	1/6/26/26	0/1/1/1
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	C	505	-	-	0/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	BG6	O2-C2	-5.41	1.30	1.43
3	B	501	BG6	O3-C3	3.65	1.51	1.43
3	B	501	BG6	C4-C3	3.12	1.60	1.52
3	B	501	BG6	O4-C4	2.36	1.48	1.43
3	B	501	BG6	P-O2P	-2.26	1.46	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	BG6	O3-C3-C4	6.76	125.97	110.35
3	B	501	BG6	C1-C2-C3	6.49	123.77	110.31
3	B	501	BG6	O4-C4-C3	4.33	120.35	110.35
3	B	501	BG6	O1P-P-O6	-4.24	95.46	106.73
3	B	501	BG6	O2-C2-C3	-4.03	101.03	110.35
3	B	501	BG6	O2P-P-O6	3.96	117.27	106.73
3	B	501	BG6	O3-C3-C2	-3.50	102.25	110.35
3	B	501	BG6	O4-C4-C5	-3.40	100.84	109.30
3	B	501	BG6	O1P-P-O3P	2.66	121.08	110.68
3	B	501	BG6	O2-C2-C1	-2.32	103.78	109.16
3	A	501	BG6	C1-C2-C3	2.29	115.06	110.31
3	A	501	BG6	O2-C2-C3	-2.25	105.15	110.35
3	B	501	BG6	O5-C5-C6	2.23	111.17	106.67
3	B	501	BG6	O5-C1-C2	-2.11	106.52	110.28
3	B	501	BG6	C1-O5-C5	-2.10	109.71	113.66
3	A	501	BG6	O3-C3-C4	2.04	115.07	110.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	502	GOL	O1-C1-C2-C3
4	C	504	GOL	O1-C1-C2-C3
4	B	502	GOL	O1-C1-C2-O2
4	B	502	GOL	O1-C1-C2-C3
4	B	503	GOL	O1-C1-C2-C3
4	A	505	GOL	O1-C1-C2-C3
4	A	505	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-C3
4	A	502	GOL	O1-C1-C2-C3
4	A	506	GOL	O1-C1-C2-O2
4	C	504	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	501	BG6	C4-C5-C6-O6
4	D	502	GOL	O1-C1-C2-O2
4	A	505	GOL	O1-C1-C2-O2
4	A	502	GOL	O1-C1-C2-O2
4	A	505	GOL	O2-C2-C3-O3

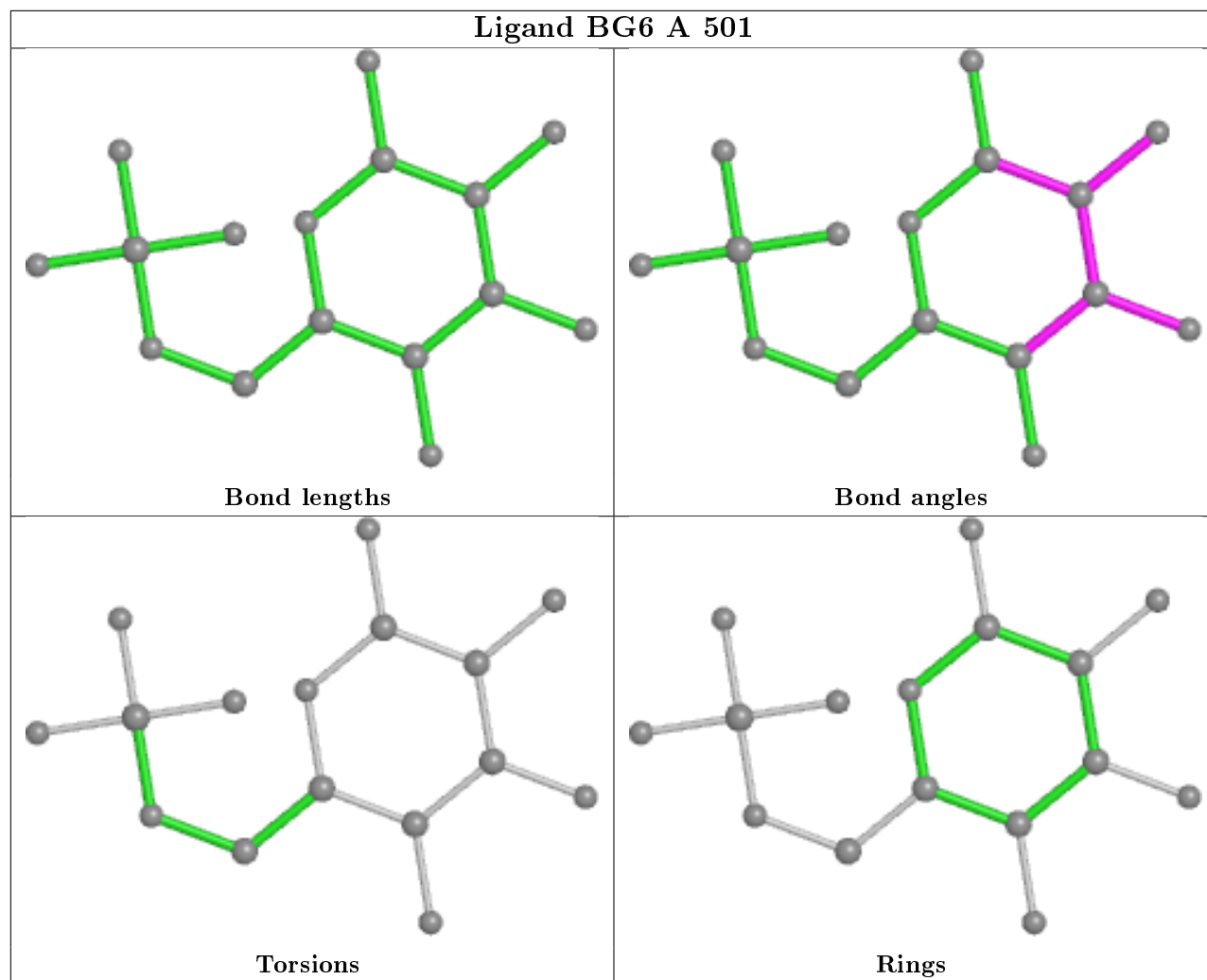
There are no ring outliers.

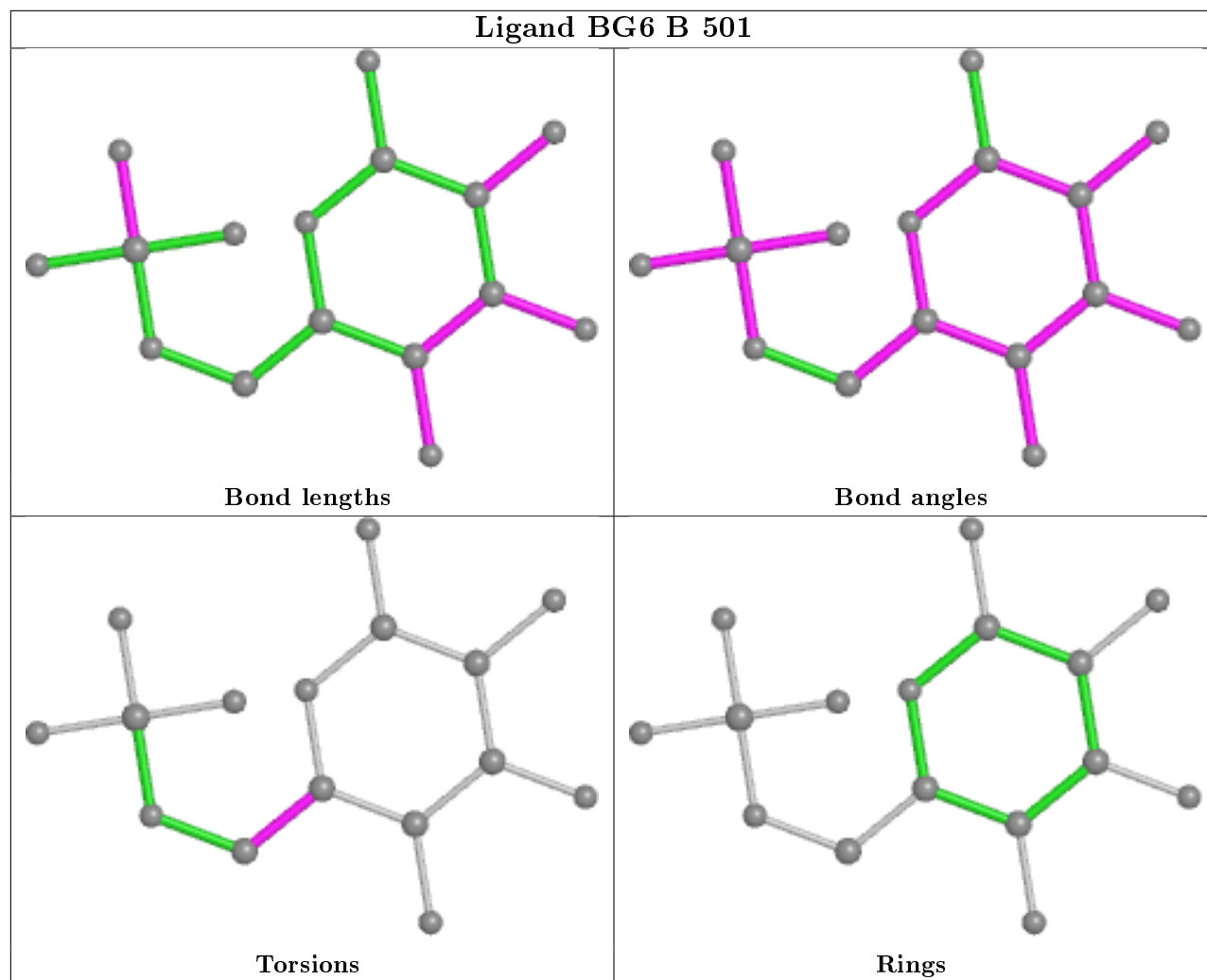
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	GOL	1	0
5	D	503	IMD	1	0
4	B	503	GOL	1	0
4	A	506	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BG6 A 501





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	462/485 (95%)	-0.04	18 (3%) 39 40	7, 13, 28, 51	0
1	B	462/485 (95%)	-0.06	16 (3%) 44 44	7, 12, 26, 52	0
1	C	462/485 (95%)	-0.09	13 (2%) 53 53	7, 11, 23, 59	0
1	D	461/485 (95%)	-0.08	16 (3%) 44 44	7, 13, 27, 59	0
All	All	1847/1940 (95%)	-0.07	63 (3%) 45 46	7, 12, 27, 59	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	THR	9.5
1	A	350[A]	TRP	8.7
1	B	329	THR	8.1
1	D	329	THR	8.1
1	D	312	ASP	7.9
1	D	315	GLY	7.6
1	D	311	PRO	7.4
1	C	329	THR	7.2
1	C	312	ASP	6.9
1	C	4	ARG	6.4
1	C	5	HIS	5.9
1	D	310	PRO	5.9
1	D	313	GLY	5.7
1	A	312	ASP	5.5
1	B	312	ASP	5.5
1	B	315	GLY	5.4
1	B	352[A]	TRP	5.4
1	B	350[A]	TRP	5.2
1	C	311	PRO	5.2
1	C	314	VAL	5.2
1	D	5	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	310	PRO	5.1
1	C	313	GLY	5.0
1	A	315	GLY	4.7
1	D	314	VAL	4.6
1	B	5	HIS	4.5
1	A	313	GLY	4.5
1	D	350	TRP	4.4
1	C	315	GLY	4.3
1	A	311	PRO	3.8
1	A	389	PRO	3.5
1	B	12	GLU	3.4
1	B	311	PRO	3.4
1	B	314	VAL	3.3
1	B	313	GLY	3.3
1	A	4	ARG	3.3
1	D	352	TRP	3.0
1	B	4	ARG	3.0
1	C	384	PHE	3.0
1	D	330	SER	3.0
1	A	5	HIS	2.9
1	B	392	ILE	2.9
1	C	350	TRP	2.8
1	A	314	VAL	2.6
1	B	389	PRO	2.6
1	D	12	GLU	2.5
1	A	282	PRO	2.4
1	B	346	ASP	2.4
1	A	45	PRO	2.4
1	A	346	ASP	2.3
1	B	351[A]	ASP	2.3
1	D	282	PRO	2.3
1	A	478	LEU	2.3
1	D	390	GLY	2.3
1	B	310	PRO	2.2
1	A	384	PHE	2.2
1	D	351	ASP	2.2
1	A	352	TRP	2.2
1	C	351	ASP	2.1
1	A	347	THR	2.1
1	D	389	PRO	2.1
1	A	388	GLU	2.1
1	C	330	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

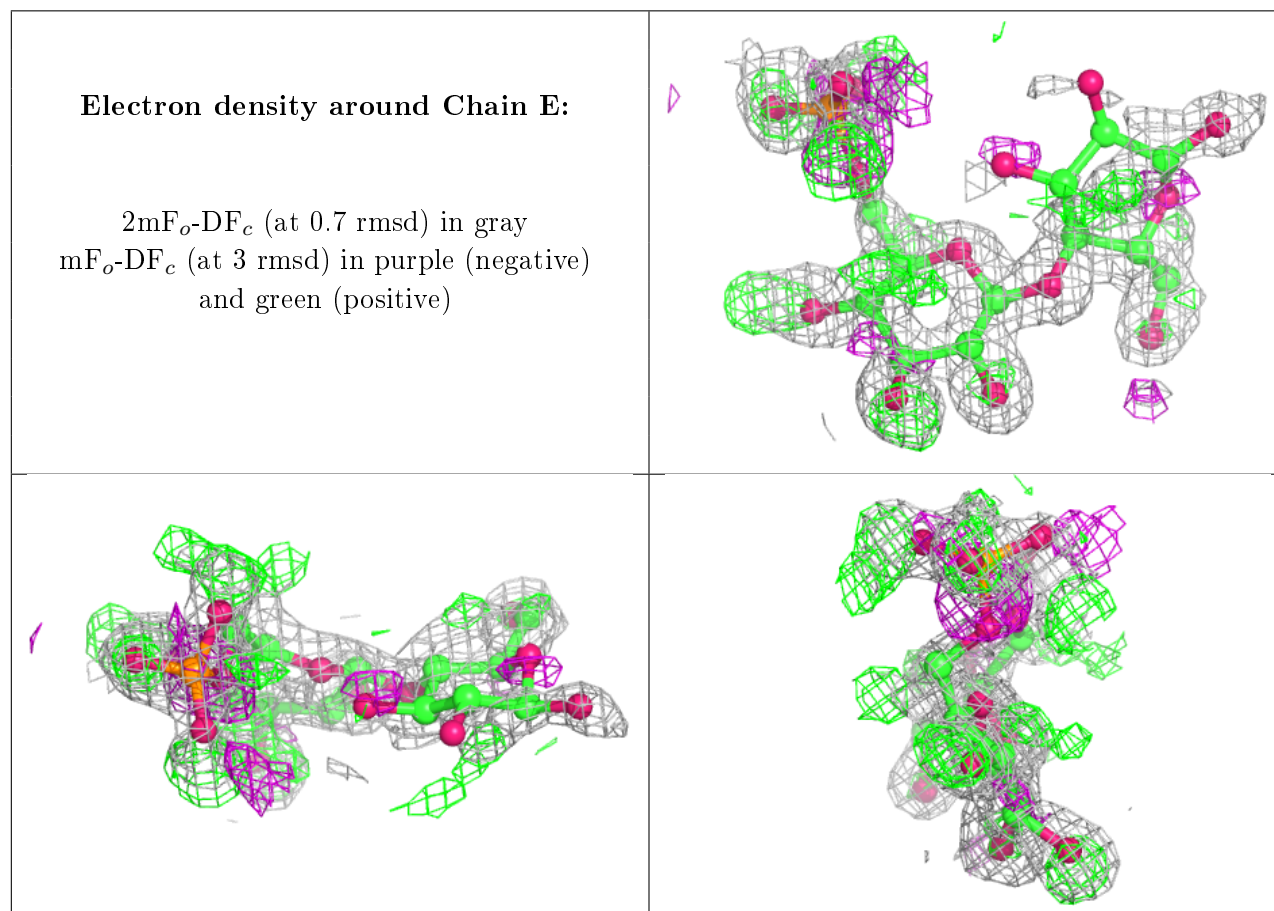
There are no non-standard protein/DNA/RNA residues in this entry.

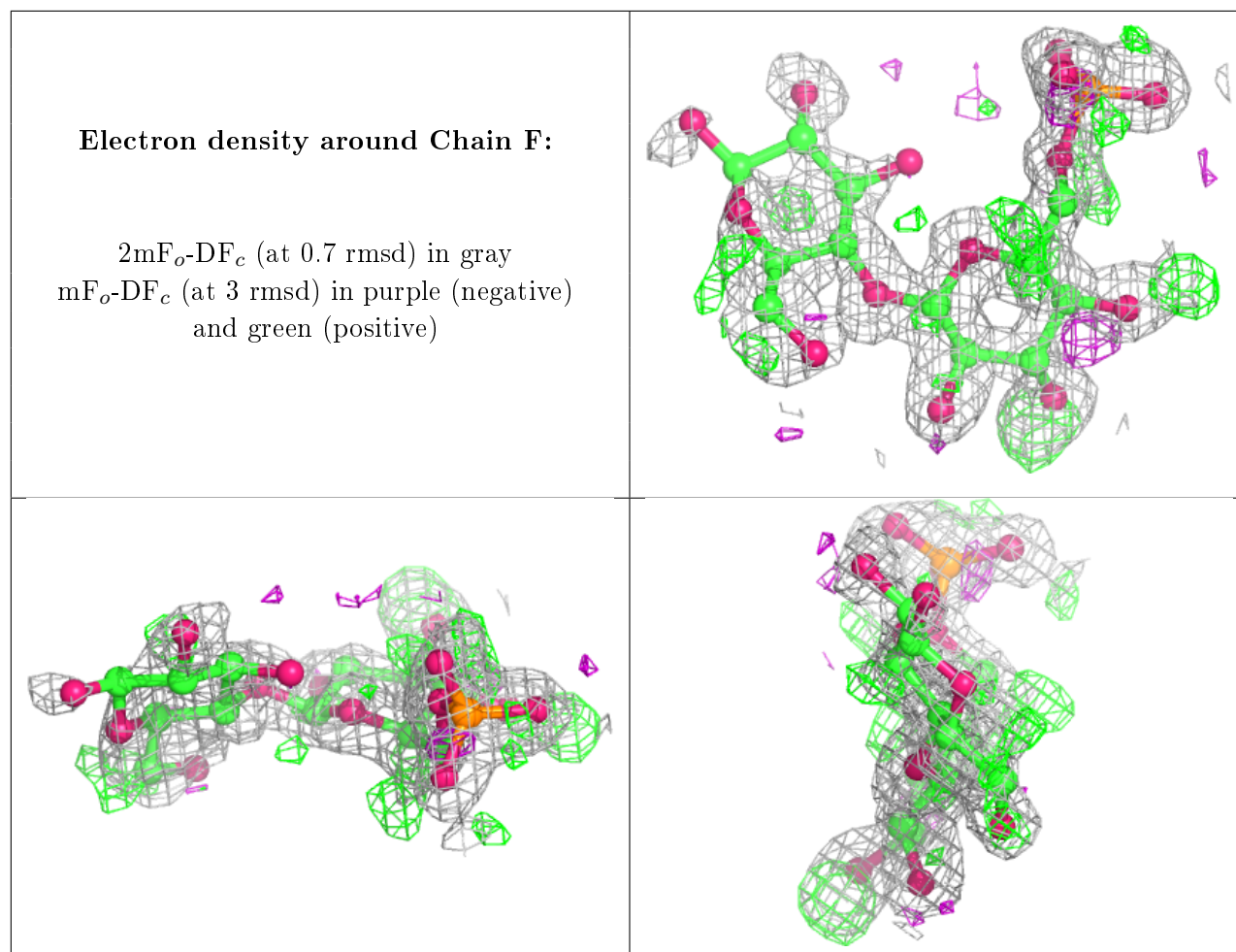
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	BGC	E	1	12/12	0.47	0.30	33,42,43,44	12
2	BGC	F	1	12/12	0.63	0.24	24,34,36,36	12
2	BG6	E	2	15/16	0.67	0.23	19,30,42,43	15
2	BG6	F	2	15/16	0.83	0.16	15,19,25,27	15

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





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(\AA^2)	Q<0.9
4	GOL	A	505	6/6	0.44	0.27	53,54,55,55	0
4	GOL	C	505	6/6	0.53	0.24	57,57,58,58	0
3	BG6	A	501	16/16	0.65	0.25	23,33,42,43	16
3	BG6	B	501	16/16	0.66	0.25	20,31,41,41	16
4	GOL	B	502	6/6	0.67	0.21	43,45,46,47	0
5	IMD	A	507	5/5	0.73	0.13	41,41,42,42	0
5	IMD	D	503	5/5	0.76	0.17	44,45,45,45	0
4	GOL	C	504	6/6	0.80	0.14	46,47,48,49	0
4	GOL	D	502	6/6	0.80	0.15	51,51,51,51	0
4	GOL	A	502	6/6	0.82	0.11	44,44,44,45	0
5	IMD	C	506	5/5	0.82	0.17	51,52,52,52	0

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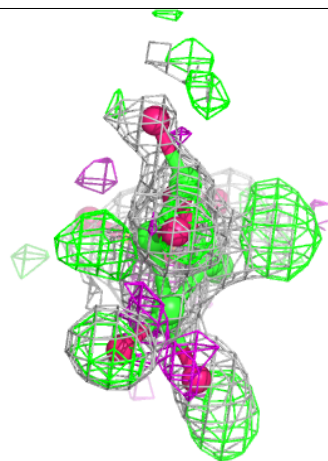
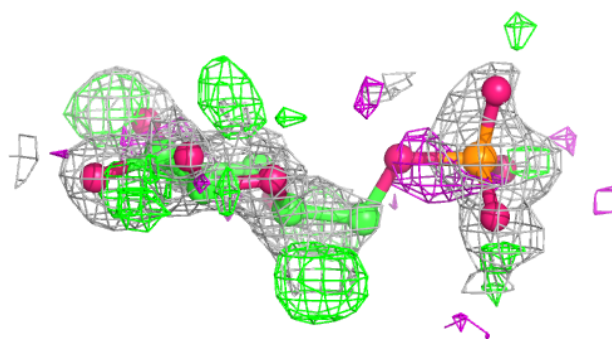
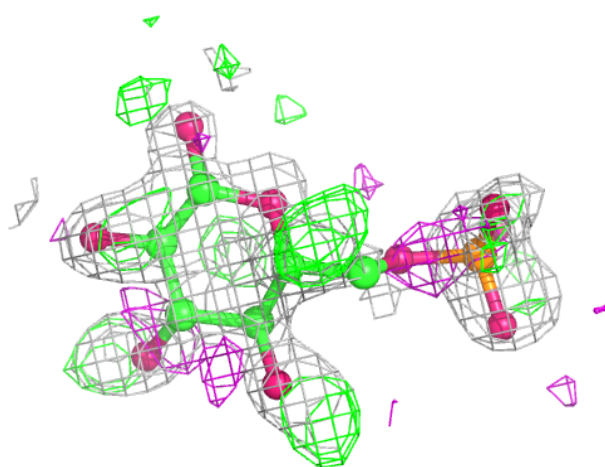
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	506	6/6	0.85	0.19	47,47,48,48	0
4	GOL	B	503	6/6	0.88	0.16	48,49,49,50	0
4	GOL	C	503	6/6	0.90	0.11	16,21,23,25	0
4	GOL	A	504	6/6	0.92	0.11	16,22,24,25	0
4	GOL	C	502	6/6	0.92	0.12	15,22,24,25	0
4	GOL	A	503	6/6	0.95	0.12	17,22,24,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

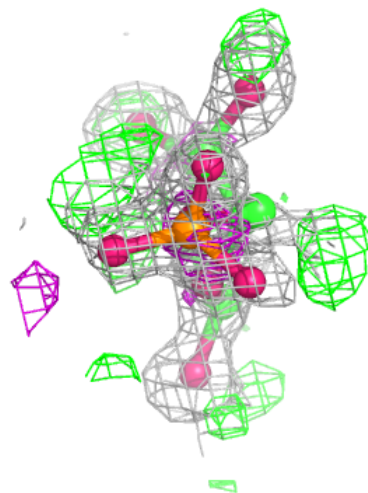
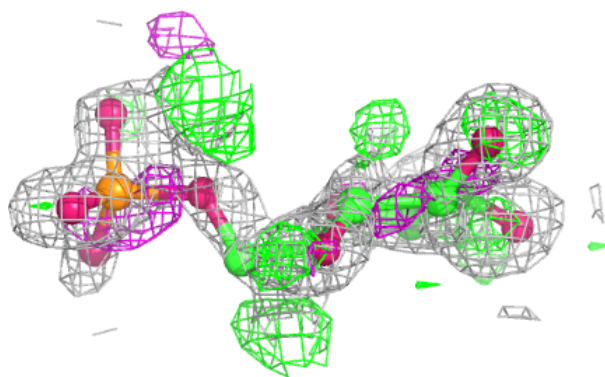
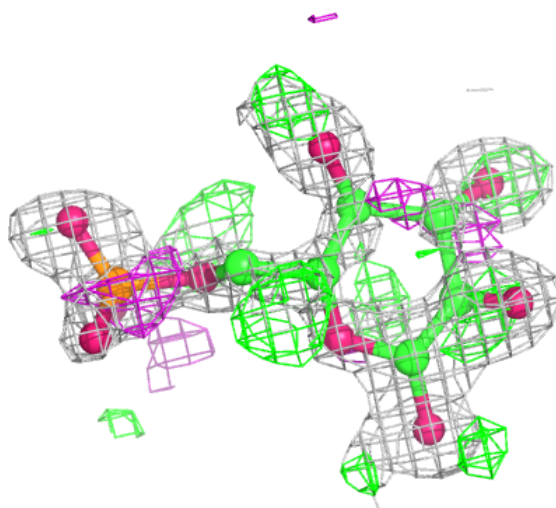
Electron density around BG6 A 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BG6 B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.