



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:56 AM UTC

PDB ID : 5OKG / pdb_00005okg
Title : Non-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 : 1.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

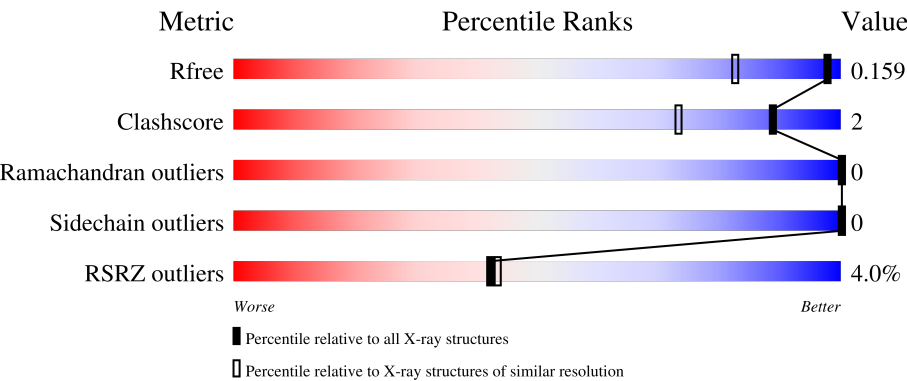
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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}	180053	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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 of 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	4% 91% 5%
1	B	485	3% 91% 5%
1	C	485	4% 90% 5% 5%
1	D	485	4% 91% 5% 5%

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18082 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	462	Total	C	N	O	S	0	18	0
			3893	2510	660	709	14			

There are 36 discrepancies between the modelled and reference sequences:

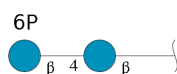
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	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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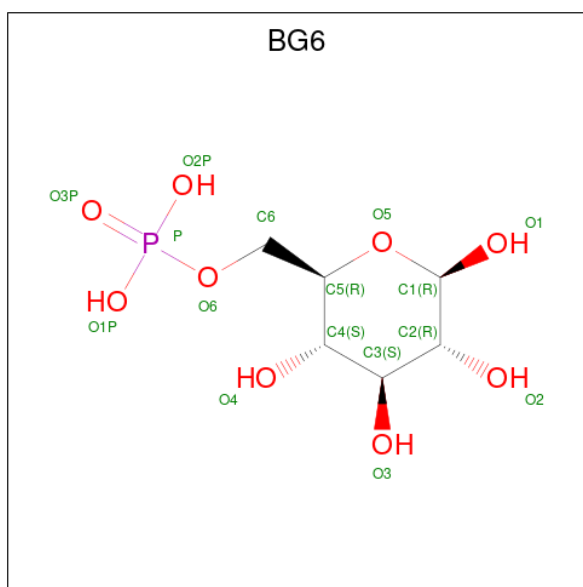
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP W8QF82
C	-2	HIS	-	expression tag	UNP W8QF82
C	-1	HIS	-	expression tag	UNP W8QF82
C	0	HIS	-	expression tag	UNP W8QF82
C	1	HIS	-	expression tag	UNP W8QF82
C	170	GLN	GLU	engineered mutation	UNP W8QF82
D	-6	MET	-	initiating methionine	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 (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



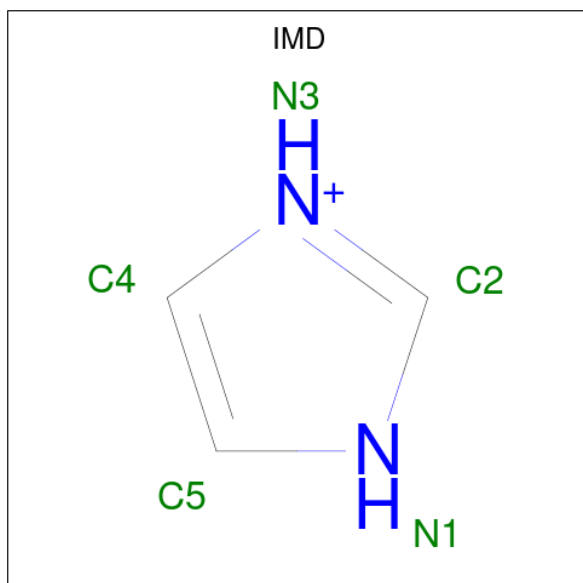
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: IMD) (formula: $C_3H_5N_2$).



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

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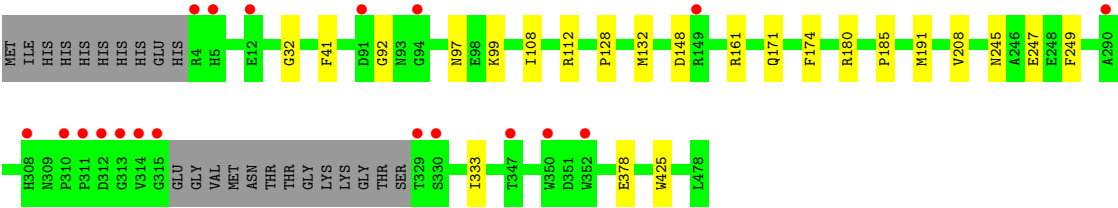
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	535	Total	O	0	0
			535	535		
6	B	564	Total	O	0	0
			564	564		
6	C	573	Total	O	0	0
			573	573		
6	D	515	Total	O	0	0
			515	515		

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





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

Chain E: 100%



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

Chain F: 100%



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)	36.14 – 1.25 36.14 – 1.25	Depositor EDS
% Data completeness (in resolution range)	96.2 (36.14-1.25) 96.3 (36.14-1.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.25Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.139 , 0.158 0.139 , 0.159	Depositor DCC
R_{free} test set	5417 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	9.6	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.1	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	18082	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 69.79 % 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 3.4860e-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: BG6, IMD, BGC, GOL

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	0.35	2/4149 (0.0%)	0.51	0/5636
1	B	0.33	0/4131	0.52	0/5618
1	C	0.31	0/4128	0.55	3/5610 (0.1%)
1	D	0.32	1/4071 (0.0%)	0.52	0/5536
All	All	0.33	3/16479 (0.0%)	0.52	3/22400 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	477[A]	GLU	CA-C	9.28	1.65	1.53
1	A	477[B]	GLU	CA-C	9.28	1.65	1.53
1	D	99	LYS	C-O	-5.17	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214[A]	HIS	CA-C-O	5.29	126.11	120.24
1	C	214[B]	HIS	CA-C-O	5.29	126.11	120.24
1	C	472	GLU	CB-CA-C	-5.21	100.99	110.63

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	14	0
1	B	3947	0	3790	14	0
1	C	3933	0	3783	17	0
1	D	3893	0	3730	14	0
2	E	27	0	18	0	0
2	F	27	0	19	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
4	A	30	0	40	1	0
4	B	12	0	16	1	0
4	C	24	0	32	0	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	535	0	0	2	1
6	B	564	0	0	4	0
6	C	573	0	0	5	0
6	D	515	0	0	4	1
All	All	18082	0	15304	60	1

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 (60) 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:469[A]:ARG:NE	1:A:477[A]:GLU:OE1	2.26	0.67
1:B:91[A]:ASP:OD1	6:B:602:HOH:O	2.15	0.64
1:B:146:ASP:OD1	1:B:149[B]:ARG:NH1	2.33	0.60
1:D:112[B]:ARG:HD2	1:D:161:ARG:HB3	1.83	0.60
1:B:97:ASN:ND2	6:B:609:HOH:O	2.35	0.59
1:C:469:ARG:HE	1:C:477:GLU:CD	2.14	0.56
1:A:473:THR:HG21	1:A:477[A]:GLU:HG3	1.90	0.53
1:A:112[A]:ARG:HD2	1:A:161:ARG:HB3	1.90	0.52
5:D:503:IMD:H5	6:D:634:HOH:O	2.09	0.52
1:B:149[A]:ARG:NH2	6:B:613:HOH:O	2.42	0.52
1:D:249:PHE:CE2	1:D:333:ILE:HD11	2.46	0.50
1:B:394:ASN:ND2	6:B:614:HOH:O	2.42	0.50
1:C:153:THR:O	1:C:157[B]:ARG:HG2	2.12	0.49
1:C:32:GLY:HA3	1:C:97[B]:ASN:HD21	1.78	0.49
1:A:336:LEU:CD2	4:A:506:GOL:H2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ASN:ND2	6:D:618:HOH:O	2.46	0.47
1:C:249[A]:PHE:CE2	1:C:333:ILE:HD11	2.50	0.47
1:C:43:LYS:HE3	6:C:804:HOH:O	2.14	0.47
1:B:378:GLU:HG3	1:B:425:TRP:HB2	1.97	0.46
1:D:112[A]:ARG:HD2	1:D:161:ARG:HB3	1.97	0.46
1:C:249[B]:PHE:HZ	1:C:270:TYR:HD2	1.64	0.46
1:C:302:GLN:HB2	1:C:353:ALA:HB3	1.97	0.46
1:B:171:GLN:HA	1:B:174:PHE:CE2	2.52	0.45
1:C:132[A]:MET:HE1	6:C:698:HOH:O	2.18	0.44
1:D:32:GLY:HA3	1:D:97[B]:ASN:HD21	1.82	0.44
1:D:92:GLY:HA2	1:D:128:PRO:HG2	2.00	0.44
1:B:47:ARG:HD3	1:B:47:ARG:HA	1.82	0.44
1:A:378:GLU:HG3	1:A:425:TRP:HB2	1.98	0.44
1:B:348[A]:THR:HB	1:B:354:ILE:HD11	2.00	0.44
1:B:268:TRP:CE2	4:B:503:GOL:H32	2.52	0.44
1:A:112[B]:ARG:HD2	1:A:161:ARG:HB3	2.00	0.44
1:C:249[B]:PHE:HZ	1:C:270:TYR:CD2	2.35	0.44
1:C:378:GLU:HG3	1:C:425:TRP:HB2	1.99	0.43
1:D:180[A]:ARG:HD3	1:D:191[A]:MET:HG2	2.00	0.43
1:C:148:ASP:HA	1:C:208[A]:VAL:HG12	2.00	0.43
1:B:425:TRP:HA	1:B:426:SER:HA	1.83	0.43
1:A:350[A]:TRP:CE2	1:A:439:LYS:HD2	2.54	0.42
1:D:378:GLU:HG3	1:D:425:TRP:HB2	2.01	0.42
1:D:148:ASP:HA	1:D:208[A]:VAL:HG12	2.01	0.42
1:D:108:ILE:O	1:D:112[B]:ARG:HG3	2.20	0.42
1:C:30[A]:GLU:HG3	6:C:620:HOH:O	2.20	0.42
1:C:171:GLN:HA	1:C:174:PHE:CE2	2.55	0.41
1:D:41:PHE:CD2	1:D:185:PRO:HD3	2.55	0.41
1:D:171:GLN:HA	1:D:174:PHE:CE2	2.55	0.41
1:A:153:THR:O	1:A:157[A]:ARG:HG2	2.20	0.41
1:C:192:LYS:HD2	6:C:743:HOH:O	2.21	0.41
1:D:247:GLU:OE2	6:D:601:HOH:O	2.22	0.41
1:A:149[A]:ARG:NH2	6:A:624:HOH:O	2.52	0.41
1:A:171:GLN:HA	1:A:174:PHE:CE2	2.56	0.41
1:A:30[A]:GLU:HG3	6:A:616:HOH:O	2.21	0.41
1:A:148:ASP:HA	1:A:208[A]:VAL:HG12	2.03	0.41
1:B:302:GLN:HB2	1:B:353:ALA:HB3	2.03	0.41
1:A:92:GLY:HA2	1:A:128:PRO:HG2	2.02	0.41
1:C:292[A]:LYS:HB3	6:C:715:HOH:O	2.21	0.41
1:B:112:ARG:HG2	1:B:112:ARG:HH11	1.86	0.40
1:C:180[B]:ARG:HB2	1:C:194[B]:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249[B]:PHE:CZ	1:C:270:TYR:CD2	3.09	0.40
1:A:135:TYR:CD1	1:A:140:SER:HB3	2.56	0.40
1:B:350[B]:TRP:HZ2	1:B:384:PHE:HZ	1.69	0.40
1:D:132[A]:MET:HE1	6:D:662:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:972:HOH:O	6:D:822:HOH:O[2_454]	2.17	0.03

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	484/485 (100%)	470 (97%)	14 (3%)	0	100	100
1	B	482/485 (99%)	468 (97%)	14 (3%)	0	100	100
1	C	482/485 (99%)	468 (97%)	14 (3%)	0	100	100
1	D	477/485 (98%)	462 (97%)	15 (3%)	0	100	100
All	All	1925/1940 (99%)	1868 (97%)	57 (3%)	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	417/412 (101%)	417 (100%)	0	100	100
1	B	416/412 (101%)	416 (100%)	0	100	100
1	C	416/412 (101%)	416 (100%)	0	100	100
1	D	411/412 (100%)	411 (100%)	0	100	100
All	All	1660/1648 (101%)	1660 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	344	HIS
1	A	379	ASN
1	B	214	HIS
1	B	379	ASN
1	B	394	ASN
1	B	468	GLN
1	C	379	ASN
1	D	274	GLN
1	D	379	ASN
1	D	410	GLN

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	0.91	0	17,17,17	2.87	8 (47%)
2	BG6	E	2	2	15,15,16	2.15	6 (40%)	21,22,24	2.98	11 (52%)
2	BGC	F	1	2	12,12,12	0.97	1 (8%)	17,17,17	2.62	9 (52%)
2	BG6	F	2	2	15,15,16	1.63	3 (20%)	21,22,24	2.42	7 (33%)

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	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	BG6	O2-C2	-4.38	1.34	1.43
2	E	2	BG6	P-O2P	-4.24	1.39	1.54
2	F	2	BG6	O2-C2	-3.45	1.36	1.43
2	F	2	BG6	O3-C3	3.33	1.51	1.43
2	E	2	BG6	O3-C3	2.64	1.49	1.43
2	E	2	BG6	C4-C3	2.36	1.58	1.52
2	F	2	BG6	P-O1P	-2.33	1.46	1.54
2	E	2	BG6	P-O1P	-2.16	1.46	1.54
2	E	2	BG6	O5-C1	-2.09	1.40	1.43
2	F	1	BGC	O1-C1	2.02	1.45	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	BG6	C1-C2-C3	7.88	121.12	109.64
2	F	2	BG6	C1-C2-C3	6.50	119.11	109.64
2	E	1	BGC	O5-C1-C2	-6.01	99.73	110.30
2	E	2	BG6	O3-C3-C4	5.94	124.38	110.38
2	F	1	BGC	O5-C5-C6	-5.24	93.44	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	BGC	O5-C5-C6	-5.09	93.82	106.44
2	F	2	BG6	O3-C3-C4	5.01	122.19	110.38
2	E	2	BG6	O1P-P-O3P	4.61	128.81	110.83
2	E	1	BGC	O1-C1-C2	4.49	122.01	108.98
2	F	1	BGC	C6-C5-C4	4.35	123.70	113.02
2	F	2	BG6	O2-C2-C3	-4.21	101.43	110.15
2	E	1	BGC	O2-C2-C1	3.73	117.86	109.25
2	E	1	BGC	C6-C5-C4	3.71	122.13	113.02
2	F	1	BGC	C4-C3-C2	3.53	117.02	110.83
2	E	2	BG6	O2-C2-C3	-3.33	103.26	110.15
2	F	1	BGC	O5-C5-C4	-3.30	103.75	109.70
2	E	2	BG6	O3-C3-C2	-3.28	103.35	110.05
2	F	1	BGC	O5-C1-C2	-3.22	104.64	110.30
2	E	1	BGC	C1-C2-C3	-3.18	103.86	110.36
2	F	1	BGC	O3-C3-C2	-2.87	103.61	110.38
2	E	1	BGC	O5-C5-C4	-2.83	104.60	109.70
2	F	1	BGC	O2-C2-C1	2.80	115.70	109.25
2	E	2	BG6	O2P-P-O6	2.76	113.85	106.67
2	F	2	BG6	O3-C3-C2	-2.72	104.51	110.05
2	E	2	BG6	O2-C2-C1	-2.66	103.13	109.22
2	F	2	BG6	O2-C2-C1	-2.65	103.16	109.22
2	F	2	BG6	O2P-P-O3P	2.63	121.07	110.83
2	E	2	BG6	O2P-P-O3P	-2.56	100.86	110.83
2	E	2	BG6	O4-C4-C3	2.54	116.37	110.38
2	E	1	BGC	O4-C4-C5	-2.47	103.23	109.32
2	F	1	BGC	O3-C3-C4	2.32	115.84	110.38
2	F	2	BG6	C1-O5-C5	-2.24	109.19	112.19
2	E	2	BG6	O4-C4-C5	-2.23	103.83	109.32
2	F	1	BGC	O4-C4-C5	-2.09	104.17	109.32
2	E	2	BG6	C1-O5-C5	-2.04	109.45	112.19

There are no chirality outliers.

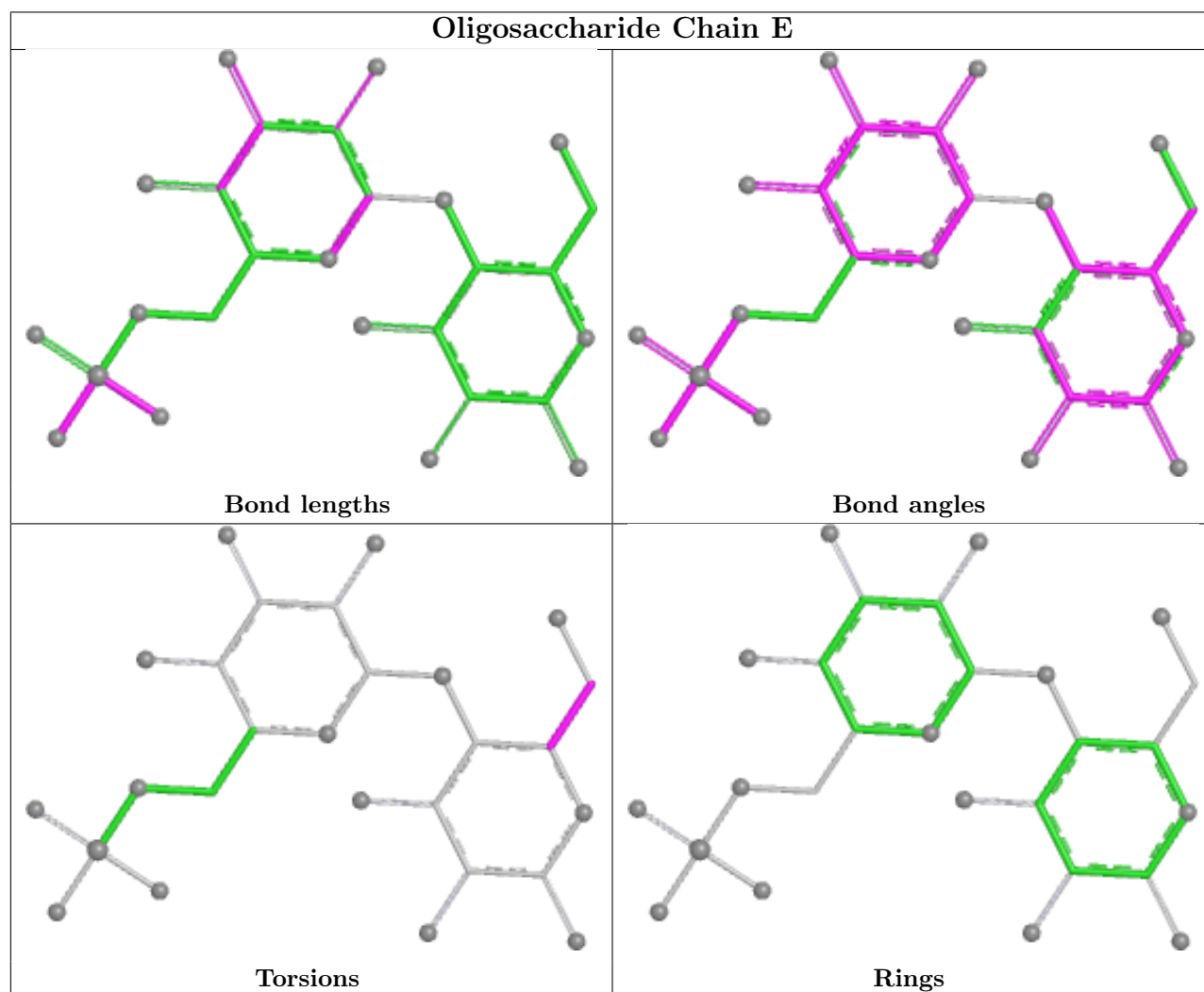
All (3) torsion outliers are listed below:

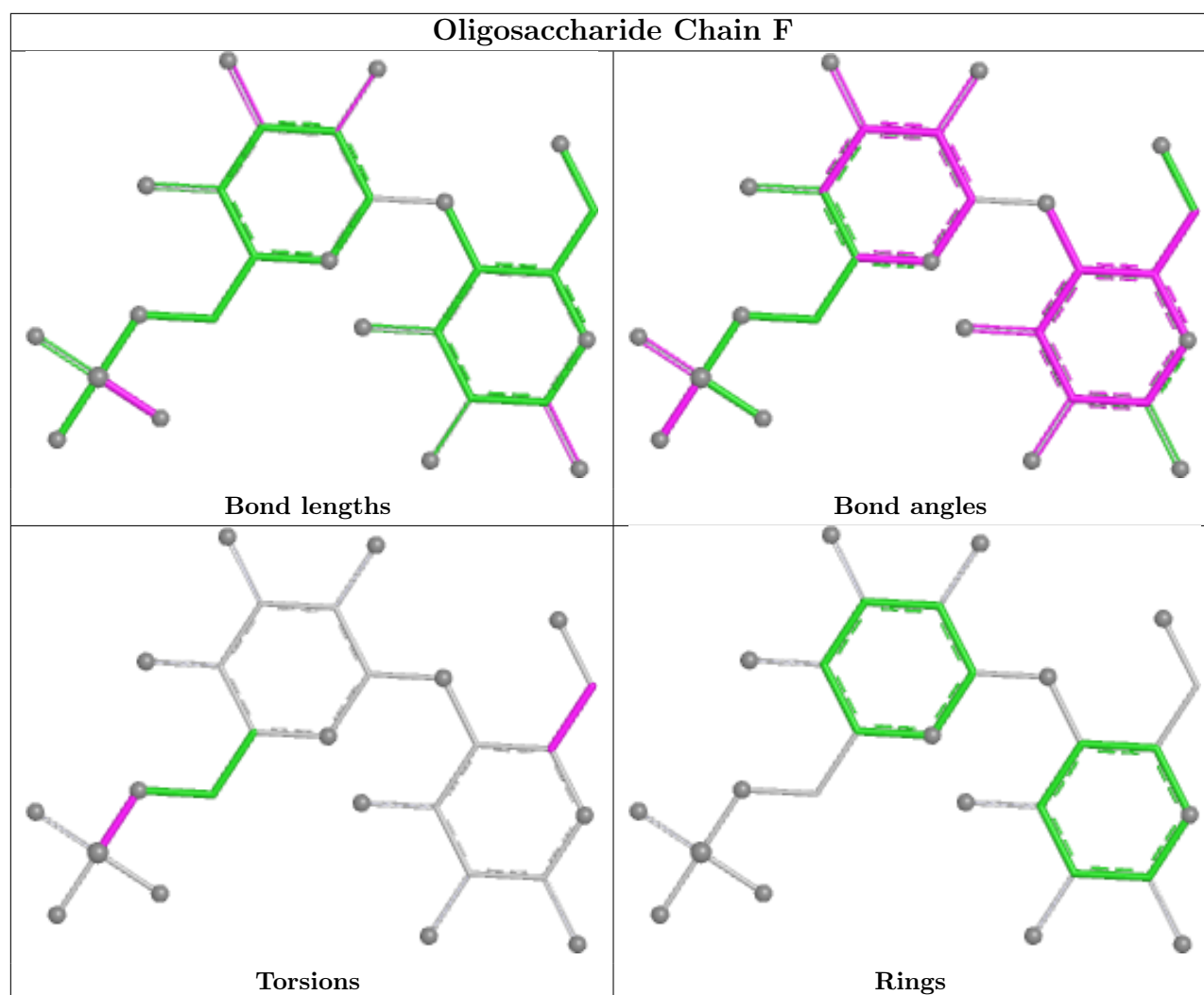
Mol	Chain	Res	Type	Atoms
2	F	1	BGC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	F	2	BG6	C6-O6-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
5	IMD	D	503	-	5,5,5	0.65	0	5,5,5	0.31	0
4	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.46	0
4	GOL	B	503	-	5,5,5	0.37	0	5,5,5	0.32	0
5	IMD	A	507	-	5,5,5	0.64	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	506	-	5,5,5	0.40	0	5,5,5	0.37	0
4	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.48	0
4	GOL	B	502	-	5,5,5	0.38	0	5,5,5	0.20	0
4	GOL	C	505	-	5,5,5	0.38	0	5,5,5	0.24	0
4	GOL	C	504	-	5,5,5	0.39	0	5,5,5	0.33	0
3	BG6	B	501	-	16,16,16	0.64	0	23,24,24	1.32	4 (17%)
4	GOL	A	502	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GOL	A	505	-	5,5,5	0.38	0	5,5,5	0.31	0
4	GOL	C	502	-	5,5,5	0.36	0	5,5,5	0.44	0
3	BG6	A	501	-	16,16,16	0.59	0	23,24,24	1.22	3 (13%)
5	IMD	C	506	-	5,5,5	0.64	0	5,5,5	0.42	0
4	GOL	D	502	-	5,5,5	0.37	0	5,5,5	0.33	0
4	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	D	503	-	-	-	0/1/1/1
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	503	-	-	2/4/4/4	-
5	IMD	A	507	-	-	-	0/1/1/1
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	B	502	-	-	2/4/4/4	-
4	GOL	C	505	-	-	0/4/4/4	-
4	GOL	C	504	-	-	2/4/4/4	-
3	BG6	B	501	-	-	0/6/26/26	0/1/1/1
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	A	505	-	-	3/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-
3	BG6	A	501	-	-	0/6/26/26	0/1/1/1
5	IMD	C	506	-	-	-	0/1/1/1
4	GOL	D	502	-	-	2/4/4/4	-
4	GOL	C	503	-	-	0/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	BG6	C1-C2-C3	2.58	115.61	110.36
3	B	501	BG6	O2-C2-C3	-2.54	104.39	110.38
3	A	501	BG6	C1-C2-C3	2.37	115.19	110.36
3	B	501	BG6	O5-C5-C6	2.17	110.99	106.69
3	A	501	BG6	O2-C2-C3	-2.11	105.41	110.38
3	A	501	BG6	O5-C5-C6	2.06	110.78	106.69
3	B	501	BG6	O3-C3-C4	2.02	115.14	110.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

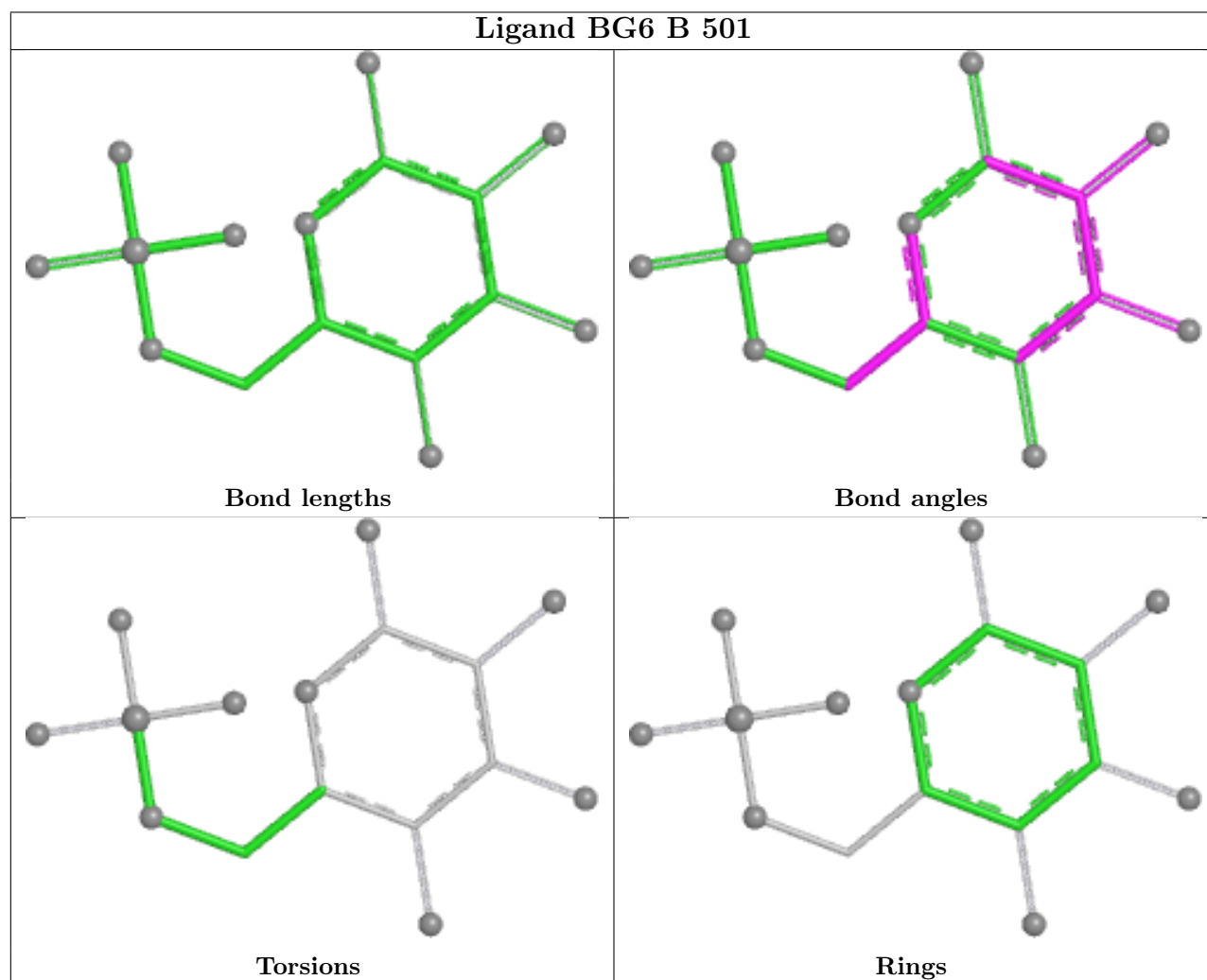
There are no ring outliers.

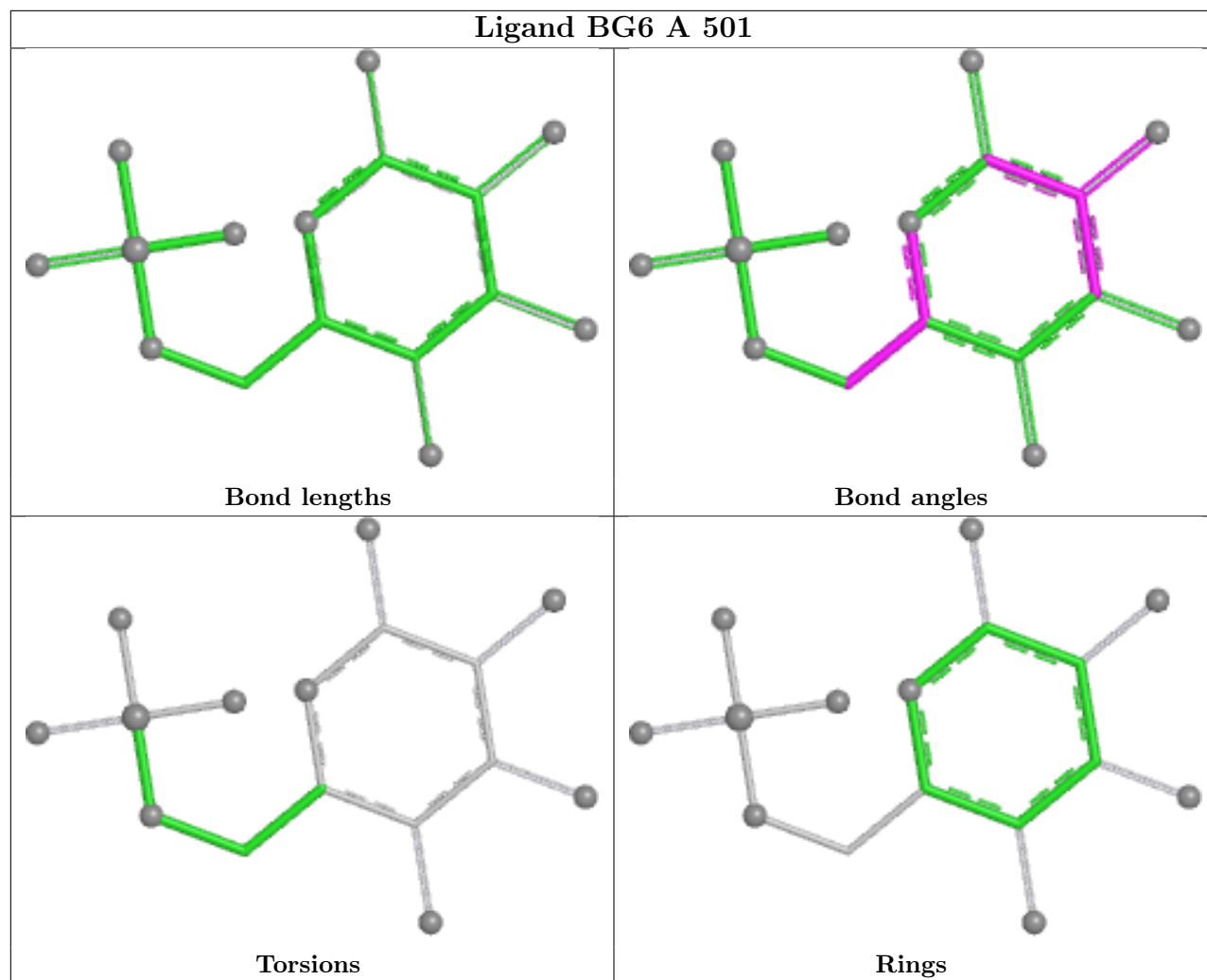
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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.





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, 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%)	-0.23	21 (4%) 38 39	6, 12, 28, 49	26 (5%)
1	B	462/485 (95%)	-0.24	16 (3%) 47 49	5, 12, 25, 51	23 (4%)
1	C	462/485 (95%)	-0.34	18 (3%) 43 45	5, 11, 23, 58	23 (4%)
1	D	462/485 (95%)	-0.22	19 (4%) 41 42	5, 13, 26, 59	18 (3%)
All	All	1848/1940 (95%)	-0.26	74 (4%) 42 43	5, 12, 26, 59	90 (4%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350[A]	TRP	9.4
1	A	350[A]	TRP	8.3
1	B	352[A]	TRP	6.9
1	A	329	THR	5.5
1	D	314	VAL	5.4
1	C	314	VAL	5.1
1	D	350	TRP	5.0
1	D	315	GLY	4.9
1	B	329	THR	4.7
1	D	5	HIS	4.3
1	B	351[A]	ASP	4.2
1	C	315	GLY	4.2
1	B	5	HIS	4.1
1	B	349[A]	ASN	4.1
1	B	290	ALA	4.0
1	D	310	PRO	4.0
1	D	329	THR	3.9
1	C	311	PRO	3.9
1	D	4	ARG	3.9
1	B	315	GLY	3.8
1	D	12	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	290	ALA	3.6
1	C	4	ARG	3.6
1	D	313	GLY	3.6
1	D	352	TRP	3.6
1	A	315	GLY	3.5
1	A	478	LEU	3.5
1	C	310	PRO	3.4
1	A	384	PHE	3.4
1	B	314	VAL	3.4
1	C	313	GLY	3.4
1	C	329	THR	3.4
1	A	352	TRP	3.3
1	A	351	ASP	3.3
1	D	312	ASP	3.3
1	C	312	ASP	3.3
1	C	384	PHE	3.1
1	D	311	PRO	3.1
1	B	348[A]	THR	3.0
1	C	352	TRP	3.0
1	A	313	GLY	2.9
1	A	4	ARG	2.8
1	B	311	PRO	2.8
1	C	5	HIS	2.8
1	C	214[A]	HIS	2.8
1	A	311	PRO	2.8
1	B	346	ASP	2.7
1	D	149	ARG	2.6
1	D	290	ALA	2.6
1	C	350	TRP	2.6
1	A	314	VAL	2.6
1	A	477[A]	GLU	2.6
1	A	6	LEU	2.6
1	B	312	ASP	2.6
1	C	290	ALA	2.4
1	C	12	GLU	2.4
1	C	472	GLU	2.4
1	A	5	HIS	2.4
1	B	12	GLU	2.4
1	D	308	HIS	2.3
1	D	91	ASP	2.3
1	A	349	ASN	2.3
1	B	4	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	476	ALA	2.2
1	B	478	LEU	2.2
1	A	347	THR	2.2
1	D	347	THR	2.2
1	A	346	ASP	2.2
1	D	330	SER	2.1
1	C	160	ASP	2.1
1	C	351	ASP	2.1
1	D	94	GLY	2.1
1	A	348	THR	2.1
1	A	312	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

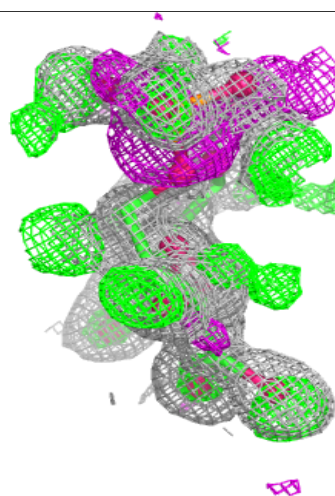
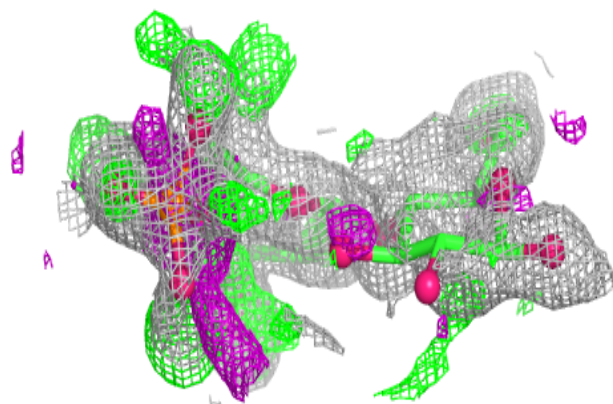
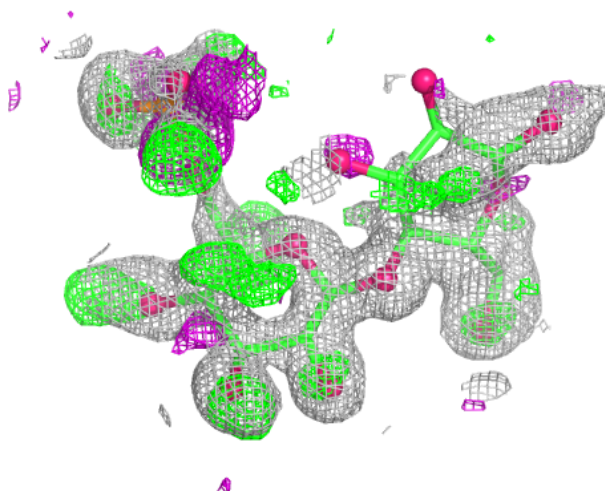
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

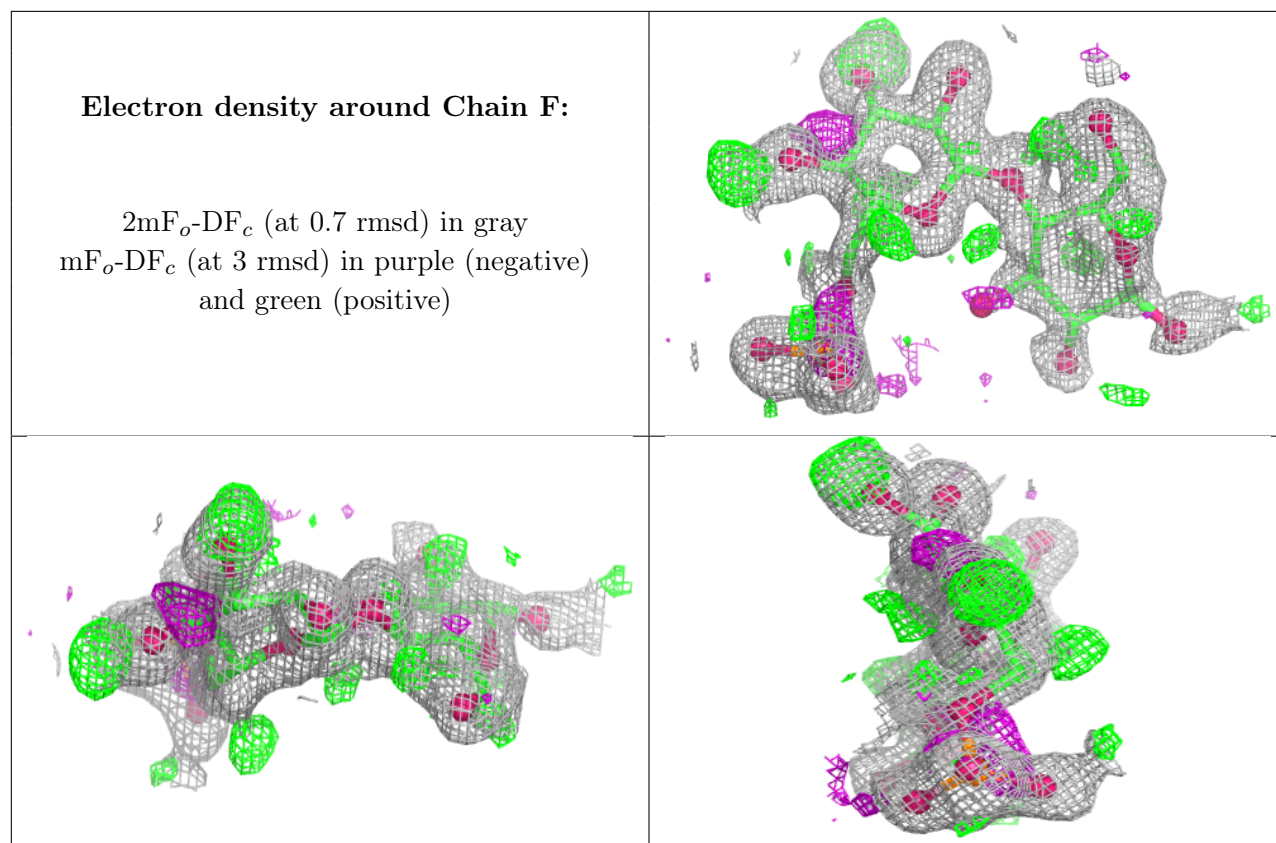
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	E	1	12/12	0.72	0.17	33,42,43,44	12
2	BG6	E	2	15/16	0.79	0.19	17,29,41,42	15
2	BGC	F	1	12/12	0.81	0.14	24,35,36,37	12
2	BG6	F	2	15/16	0.90	0.12	15,19,25,27	15

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.

Electron density around Chain E:

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BG6	B	501	16/16	0.75	0.19	20,31,42,42	16
3	BG6	A	501	16/16	0.76	0.17	22,34,43,44	16
4	GOL	A	505	6/6	0.76	0.20	52,53,54,54	0
4	GOL	C	505	6/6	0.76	0.19	56,56,56,56	0
4	GOL	D	502	6/6	0.81	0.16	50,50,50,50	0
4	GOL	A	502	6/6	0.82	0.19	44,44,45,45	0
4	GOL	B	502	6/6	0.83	0.16	44,46,46,47	0
4	GOL	C	504	6/6	0.83	0.16	46,46,47,48	0
4	GOL	A	506	6/6	0.85	0.17	47,48,48,48	0
5	IMD	A	507	5/5	0.85	0.12	41,41,42,42	0
4	GOL	B	503	6/6	0.86	0.17	48,49,49,49	0
5	IMD	D	503	5/5	0.87	0.16	40,40,40,40	5
5	IMD	C	506	5/5	0.88	0.17	48,48,49,49	0
4	GOL	A	504	6/6	0.93	0.09	16,21,23,25	0

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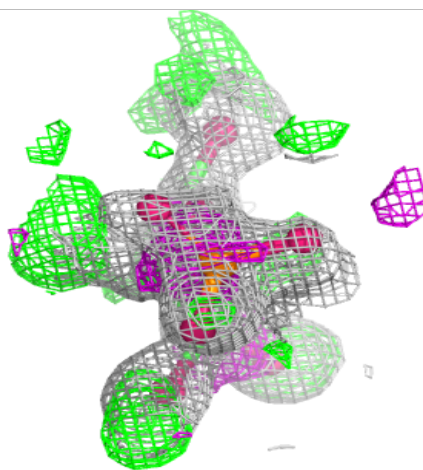
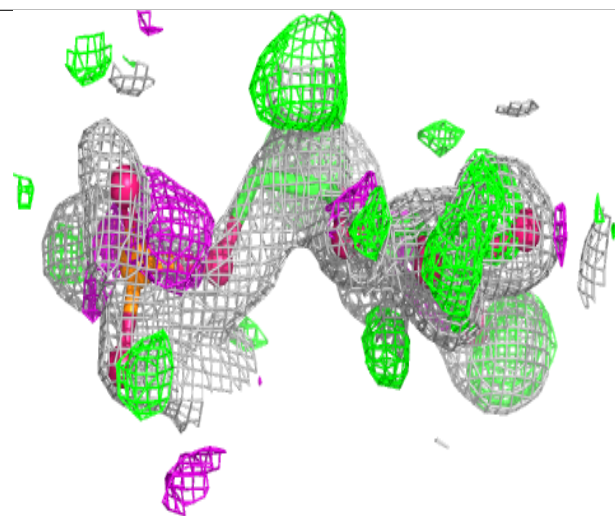
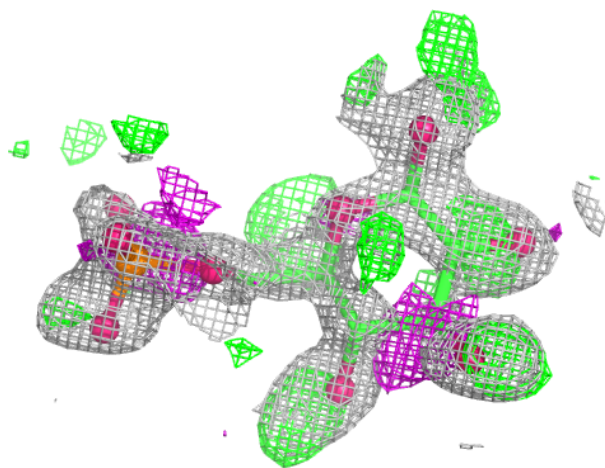
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	503	6/6	0.94	0.08	16,21,23,25	0
4	GOL	C	502	6/6	0.96	0.07	16,21,23,25	0
4	GOL	A	503	6/6	0.96	0.08	17,22,24,25	0

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.

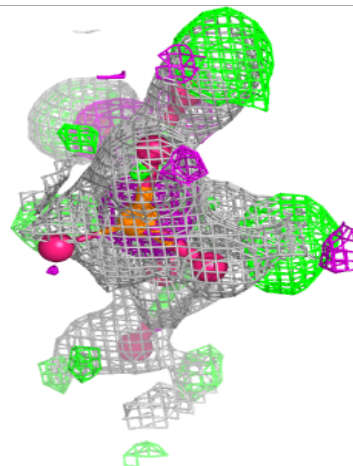
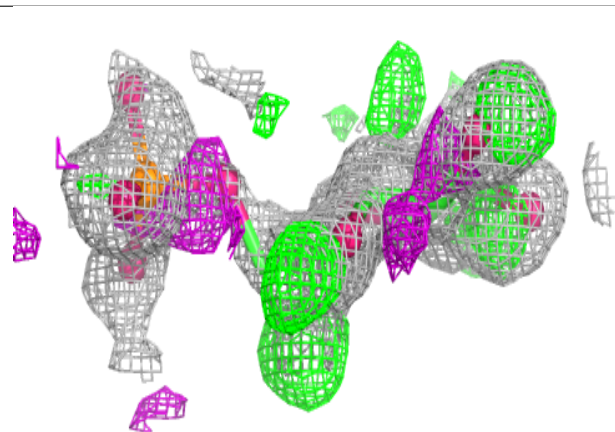
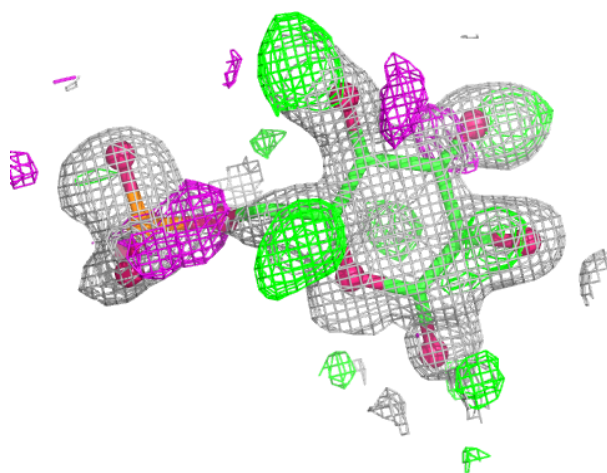
Electron density around BG6 B 501:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.