



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 11:48 AM BST

PDB ID : 4ZFM
Title : Structure of Gan1D-E170Q in complex with cellobiose-6-phosphate
Authors : Lansky, S.; Zehavi, A.; Dvir, H.; Shoham, Y.; Shoham, G.
Deposited on : 2015-04-21
Resolution : 1.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

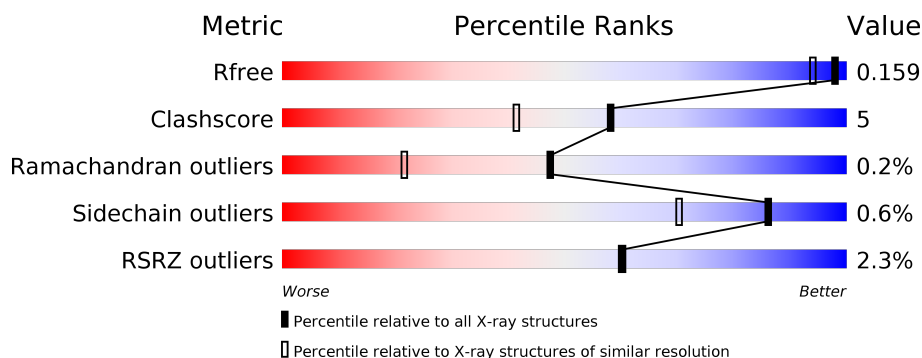
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	B	485	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	C	485	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	D	485	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• 5%</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18396 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	461	Total	C	N	O	S	0	27	0
			3945	2545	680	706	14			
1	B	461	Total	C	N	O	S	0	20	0
			3911	2521	667	709	14			
1	C	461	Total	C	N	O	S	0	22	0
			3914	2525	664	710	15			
1	D	461	Total	C	N	O	S	0	17	0
			3875	2500	653	708	14			

There are 36 discrepancies between the modelled and reference sequences:

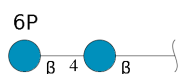
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag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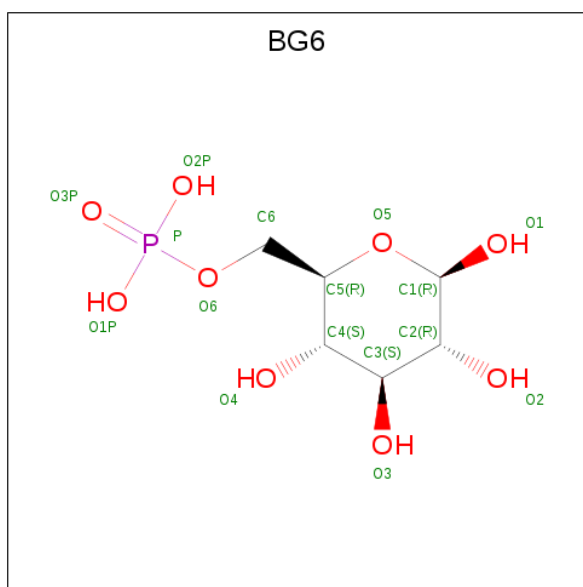
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP W8QF82
C	-2	HIS	-	expression tag	UNP W8QF82
C	-1	HIS	-	expression tag	UNP W8QF82
C	0	HIS	-	expression tag	UNP W8QF82
C	1	HIS	-	expression tag	UNP W8QF82
C	170	GLN	GLU	engineered mutation	UNP W8QF82
D	-6	MET	-	initiating methionine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

- 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: $C_3H_8O_3$).



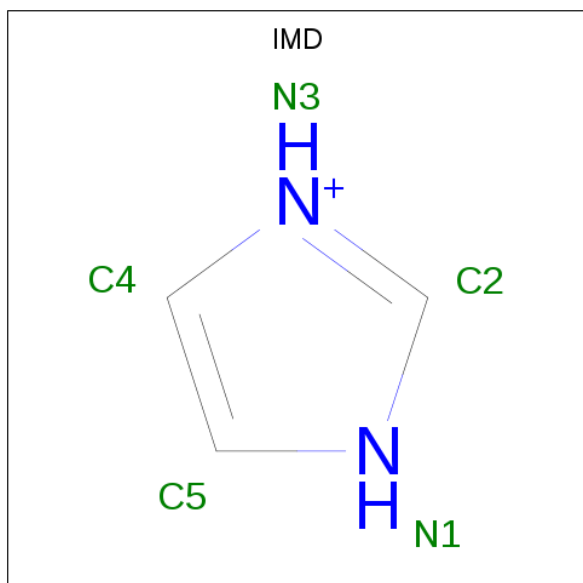
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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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	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



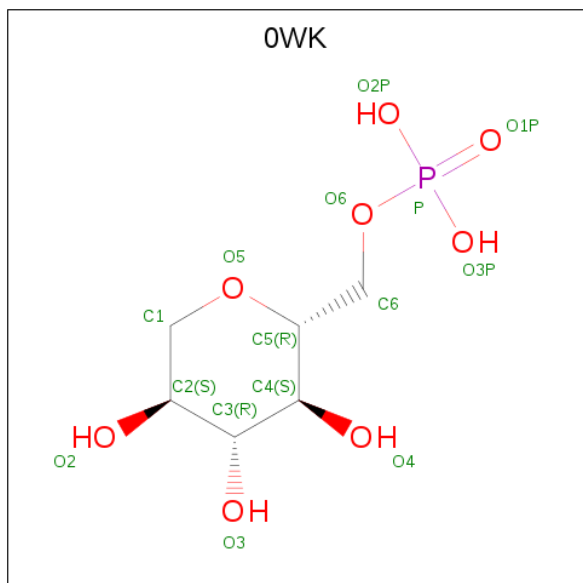
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

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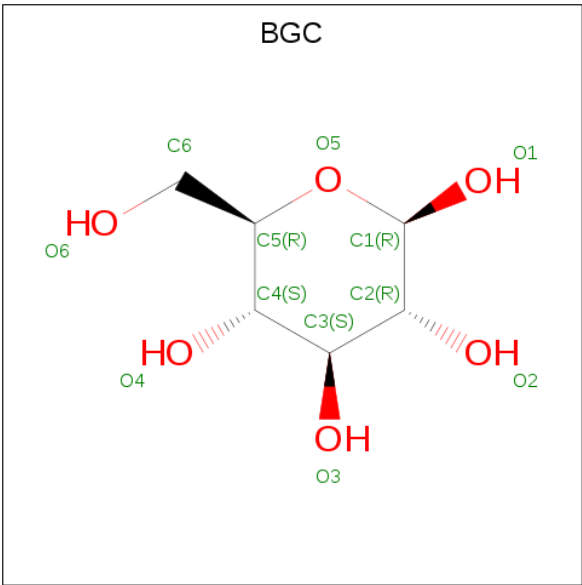
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is 1,5-anhydro-6-O-phosphono-D-glucitol (three-letter code: 0WK) (formula: $C_6H_{13}O_8P$).



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

- Molecule 7 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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

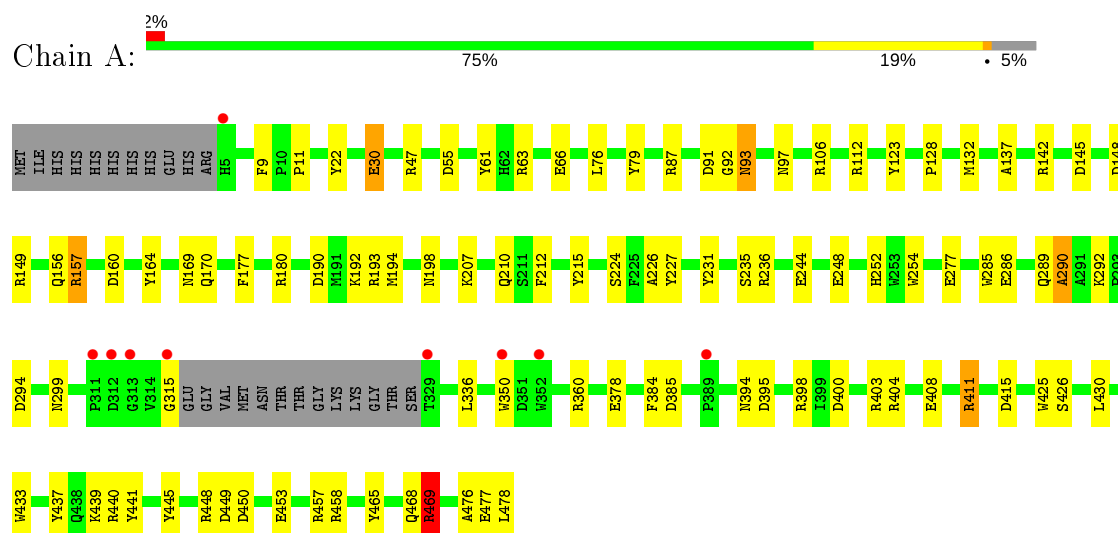
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	640	Total	O	0	0
			640	640		
8	B	638	Total	O	0	0
			638	638		
8	C	692	Total	O	0	0
			692	692		
8	D	608	Total	O	0	0
			608	608		

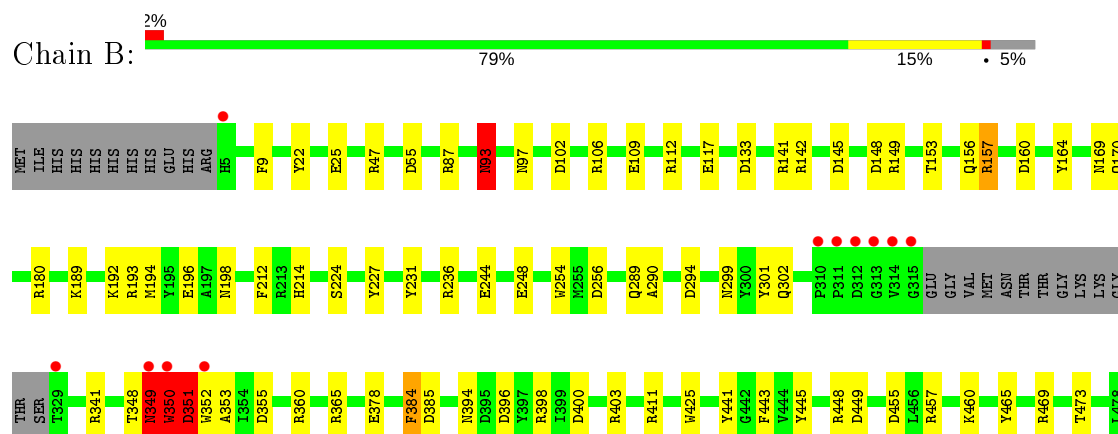
3 Residue-property plots [i](#)

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.

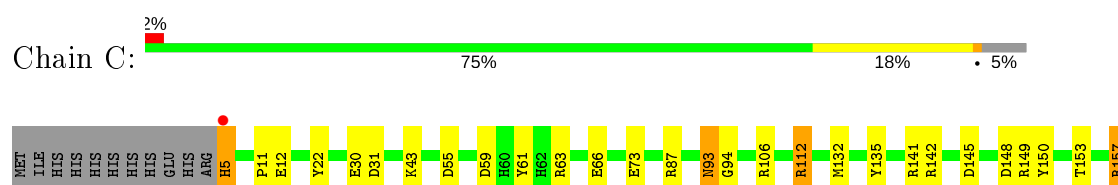
- Molecule 1: Putative 6-phospho-beta-galactobiosidase

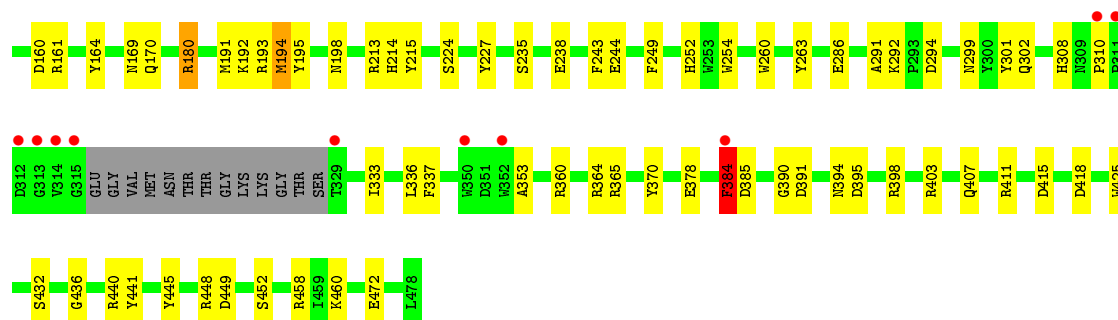


- Molecule 1: Putative 6-phospho-beta-galactobiosidase

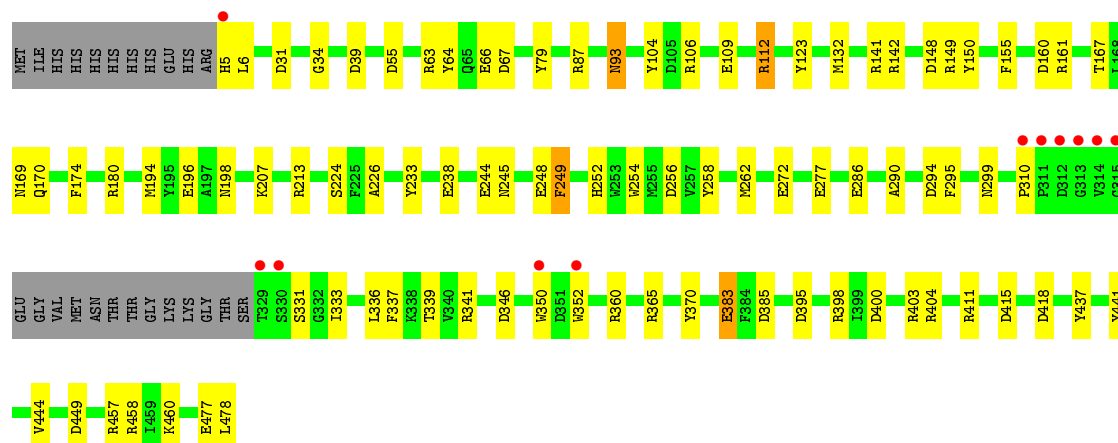
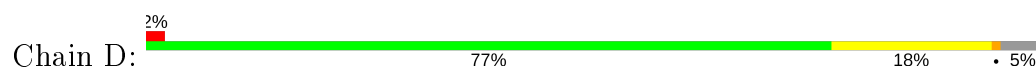


- Molecule 1: Putative 6-phospho-beta-galactobiosidase





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



● Molecule 2: 1,5-anhydro-6-O-phosphono-D-glucitol-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.59Å 97.47Å 105.27Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	22.37 – 1.40 22.36 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (22.37-1.40) 98.7 (22.36-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.130 , 0.158 0.131 , 0.159	Depositor DCC
R_{free} test set	19771 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.7	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	18396	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 69.56 % 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 3.6228e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BGC, IMD, BG6, 0WK

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	1.49	31/4146 (0.7%)	1.50	65/5630 (1.2%)
1	B	1.47	25/4087 (0.6%)	1.59	80/5558 (1.4%)
1	C	1.44	25/4107 (0.6%)	1.56	84/5581 (1.5%)
1	D	1.44	18/4050 (0.4%)	1.61	78/5509 (1.4%)
All	All	1.46	99/16390 (0.6%)	1.57	307/22278 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	1
1	D	0	1
All	All	0	8

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286[A]	GLU	CD-OE1	9.52	1.36	1.25
1	A	286[B]	GLU	CD-OE1	9.52	1.36	1.25
1	B	350[A]	TRP	CB-CG	9.51	1.67	1.50
1	B	350[B]	TRP	CB-CG	9.51	1.67	1.50
1	A	441	TYR	CE2-CZ	-9.49	1.26	1.38

The worst 5 of 307 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	398	ARG	NE-CZ-NH2	20.91	130.75	120.30
1	B	141	ARG	NE-CZ-NH1	-18.47	111.07	120.30
1	D	411	ARG	NE-CZ-NH2	-15.06	112.77	120.30
1	C	180[A]	ARG	NE-CZ-NH2	-14.26	113.17	120.30
1	C	180[B]	ARG	NE-CZ-NH2	-14.26	113.17	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ALA	Mainchain
1	A	469[B]	ARG	Mainchain
1	B	290	ALA	Mainchain
1	B	349[B]	ASN	Peptide
1	B	351[A]	ASP	Mainchain

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	3945	0	3833	42	0
1	B	3911	0	3750	31	0
1	C	3914	0	3770	48	0
1	D	3875	0	3706	30	0
2	E	27	0	20	3	0
3	A	16	0	10	0	0
3	B	16	0	10	0	0
4	A	30	0	40	3	0
4	B	12	0	16	0	0
4	C	24	0	32	1	0
4	D	6	0	8	0	0
5	A	5	0	5	1	0
5	C	5	0	5	0	0
5	D	5	0	5	1	0
6	C	15	0	9	1	0
7	C	12	0	10	4	0
8	A	640	0	0	20	0
8	B	638	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	692	0	0	21	0
8	D	608	0	0	18	0
All	All	18396	0	15229	150	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 5.

The worst 5 of 150 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:400:ASP:HB2	8:A:838:HOH:O	1.37	1.19
1:C:170:GLN:HE22	7:C:507:BGC:H6C2	1.12	1.08
1:A:132[A]:MET:HE3	8:A:1072:HOH:O	1.56	1.05
1:C:132[A]:MET:HE3	8:C:1116:HOH:O	1.60	1.00
1:D:132[A]:MET:HE3	8:D:1075:HOH:O	1.65	0.96

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	484/485 (100%)	468 (97%)	16 (3%)	0	100	100
1	B	478/485 (99%)	460 (96%)	18 (4%)	0	100	100
1	C	481/485 (99%)	464 (96%)	16 (3%)	1 (0%)	47	21
1	D	475/485 (98%)	457 (96%)	16 (3%)	2 (0%)	34	12
All	All	1918/1940 (99%)	1849 (96%)	66 (3%)	3 (0%)	47	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	167	THR
1	D	310	PRO
1	C	310	PRO

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	418/412 (102%)	416 (100%)	2 (0%)	88	74
1	B	412/412 (100%)	407 (99%)	5 (1%)	71	47
1	C	415/412 (101%)	413 (100%)	2 (0%)	88	74
1	D	409/412 (99%)	407 (100%)	2 (0%)	88	74
All	All	1654/1648 (100%)	1643 (99%)	11 (1%)	86	66

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	350[B]	TRP
1	B	351[A]	ASP
1	C	93	ASN
1	B	350[A]	TRP
1	C	5	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	379	ASN
1	C	171	GLN
1	D	252	HIS
1	B	435	ASN
1	C	129	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 ⓘ

2 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	0.73	0	17,17,17	2.10	7 (41%)
2	0WK	E	2	2	15,15,15	1.98	4 (26%)	22,22,22	2.92	7 (31%)

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	0WK	E	2	2	-	1/6/23/23	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	0WK	O2-C2	-4.61	1.33	1.43
2	E	2	0WK	P-O3P	-3.63	1.40	1.54
2	E	2	0WK	O3-C3	3.55	1.51	1.43
2	E	2	0WK	C4-C3	2.04	1.57	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	2	0WK	O3-C3-C4	7.38	127.41	110.35
2	E	2	0WK	C1-C2-C3	6.40	117.54	109.67
2	E	2	0WK	O3-C3-C2	-5.56	99.35	109.99
2	E	2	0WK	O2-C2-C1	-5.20	98.52	109.15
2	E	1	BGC	C1-C2-C3	-3.56	102.93	110.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

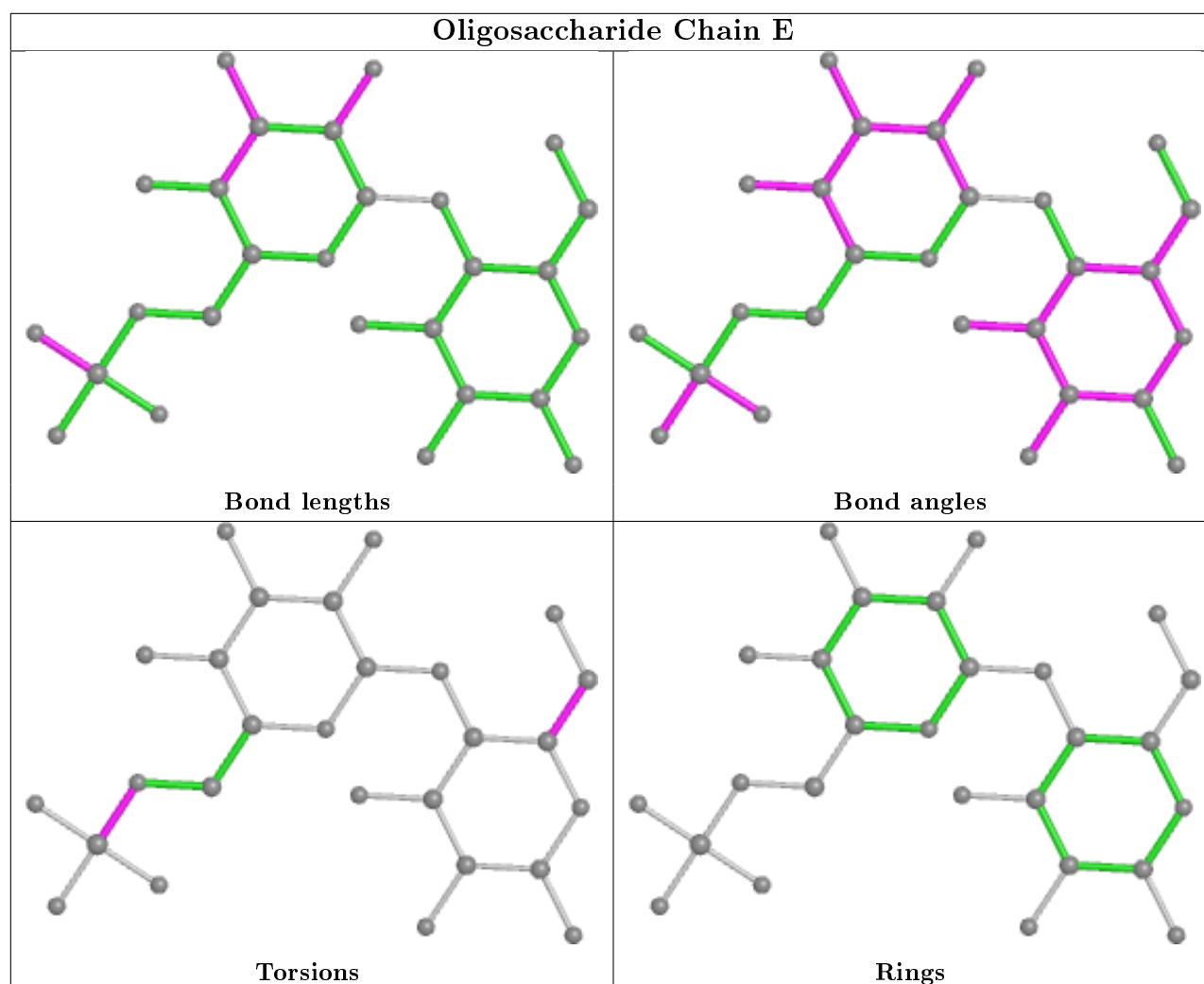
Mol	Chain	Res	Type	Atoms
2	E	1	BGC	O5-C5-C6-O6
2	E	2	0WK	C6-O6-P-O2P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	BGC	3	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](#)

19 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
3	BG6	B	501	-	16,16,16	2.18	4 (25%)	24,24,24	3.38	12 (50%)
4	GOL	A	502	-	5,5,5	0.36	0	5,5,5	0.96	0
4	GOL	C	502	-	5,5,5	1.05	1 (20%)	5,5,5	1.22	0
6	0WK	C	506	-	15,15,15	2.15	5 (33%)	22,22,22	4.45	10 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	503	-	5,5,5	0.41	0	5,5,5	1.02	0
4	GOL	A	503	-	5,5,5	0.29	0	5,5,5	1.54	1 (20%)
4	GOL	C	504	-	5,5,5	0.78	0	5,5,5	1.46	1 (20%)
4	GOL	C	503	-	5,5,5	0.72	0	5,5,5	0.95	0
4	GOL	A	504	-	5,5,5	1.00	0	5,5,5	1.51	1 (20%)
7	BGC	C	507	-	12,12,12	1.25	1 (8%)	17,17,17	3.37	12 (70%)
5	IMD	D	502	-	3,5,5	0.25	0	4,5,5	0.22	0
5	IMD	C	505	-	3,5,5	0.44	0	4,5,5	0.45	0
4	GOL	B	502	-	5,5,5	0.77	0	5,5,5	1.06	0
4	GOL	D	501	-	5,5,5	0.33	0	5,5,5	0.73	0
4	GOL	A	505	-	5,5,5	0.86	0	5,5,5	1.42	1 (20%)
3	BG6	A	501	-	16,16,16	2.25	4 (25%)	24,24,24	3.06	7 (29%)
4	GOL	C	501	-	5,5,5	0.97	0	5,5,5	1.73	2 (40%)
4	GOL	A	506	-	5,5,5	0.30	0	5,5,5	1.18	0
5	IMD	A	507	-	3,5,5	0.31	0	4,5,5	1.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BG6	B	501	-	-	1/6/26/26	0/1/1/1
4	GOL	A	502	-	-	0/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-
6	0WK	C	506	-	-	1/6/23/23	0/1/1/1
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	C	504	-	-	2/4/4/4	-
4	GOL	C	503	-	-	0/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
7	BGC	C	507	-	-	2/2/22/22	0/1/1/1
5	IMD	D	502	-	-	-	0/1/1/1
5	IMD	C	505	-	-	-	0/1/1/1
4	GOL	B	502	-	-	0/4/4/4	-
4	GOL	D	501	-	-	2/4/4/4	-
4	GOL	A	505	-	-	0/4/4/4	-
3	BG6	A	501	-	-	1/6/26/26	0/1/1/1
4	GOL	C	501	-	-	0/4/4/4	-
4	GOL	A	506	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	A	507	-	-	-	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	BG6	O2-C2	-5.41	1.30	1.43
3	B	501	BG6	O2-C2	-4.99	1.31	1.43
6	C	506	0WK	O2-C2	-4.84	1.33	1.43
3	A	501	BG6	O3-C3	4.81	1.54	1.43
3	B	501	BG6	O3-C3	4.50	1.53	1.43

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	506	0WK	O3P-P-O6	-11.50	76.14	106.73
3	A	501	BG6	O3-C3-C4	9.90	133.24	110.35
6	C	506	0WK	C1-C2-C3	9.51	121.36	109.67
3	B	501	BG6	O3-C3-C4	9.19	131.59	110.35
6	C	506	0WK	O3-C3-C4	8.43	129.84	110.35

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

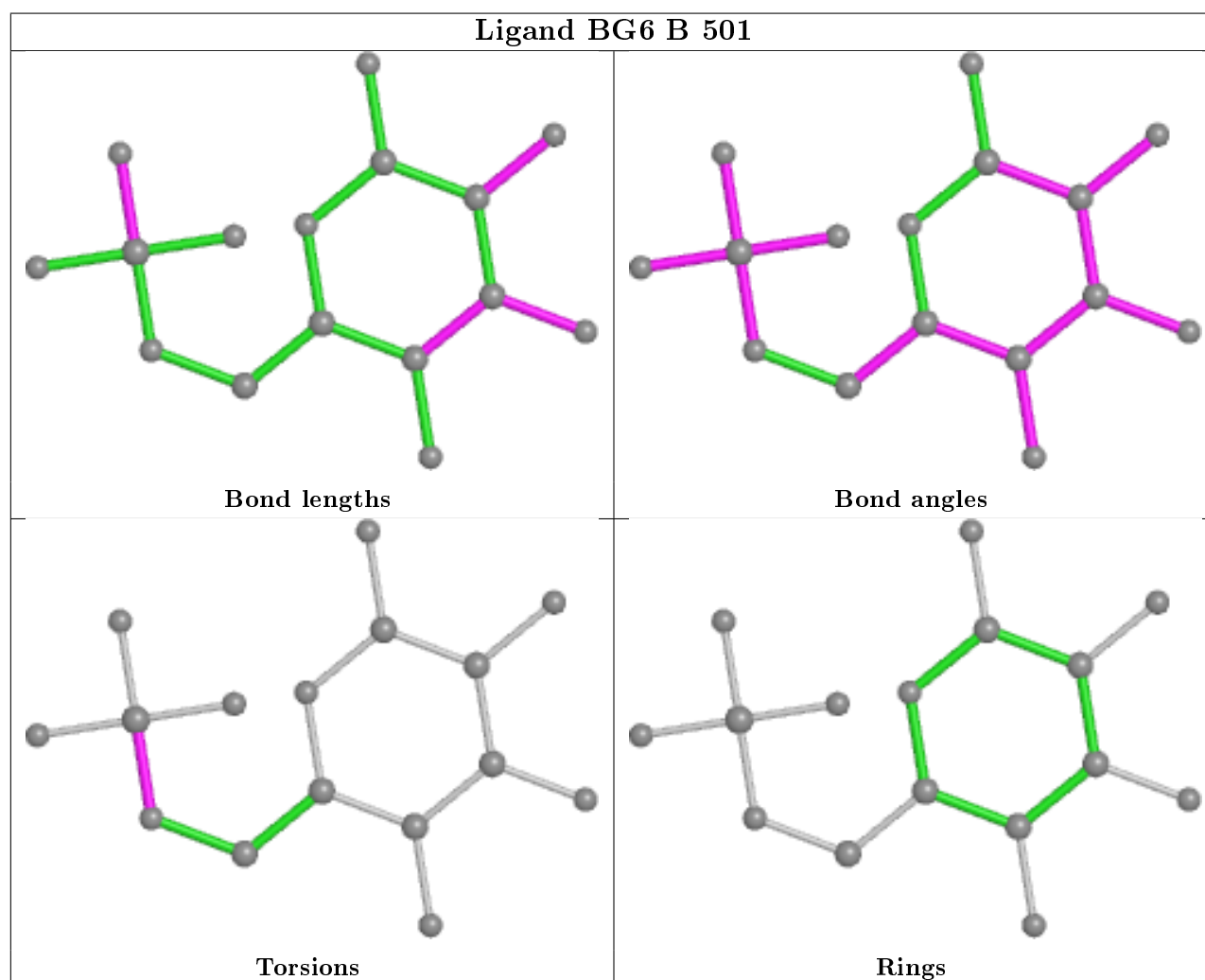
Mol	Chain	Res	Type	Atoms
4	B	503	GOL	O1-C1-C2-C3
4	C	504	GOL	C1-C2-C3-O3
4	C	504	GOL	O2-C2-C3-O3
4	A	506	GOL	C1-C2-C3-O3
7	C	507	BGC	O5-C5-C6-O6

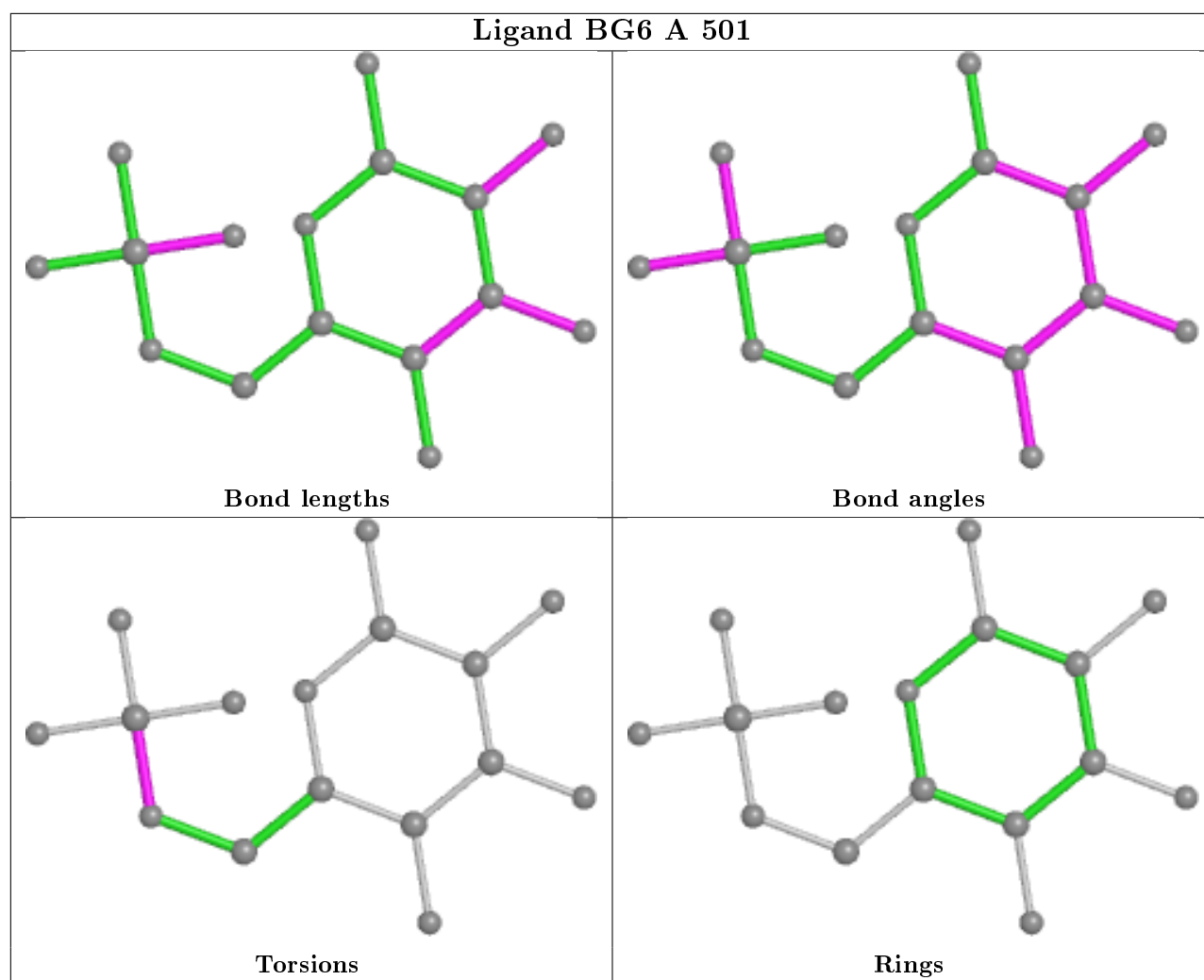
There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	506	0WK	1	0
4	C	504	GOL	1	0
7	C	507	BGC	4	0
5	D	502	IMD	1	0
4	A	505	GOL	1	0
4	A	506	GOL	2	0
5	A	507	IMD	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 ⓘ

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	461/485 (95%)	-0.34	9 (1%) 65 65	6, 11, 27, 74	0
1	B	461/485 (95%)	-0.38	11 (2%) 59 58	6, 10, 24, 61	0
1	C	461/485 (95%)	-0.42	11 (2%) 59 58	5, 10, 22, 68	0
1	D	461/485 (95%)	-0.36	11 (2%) 59 58	6, 11, 25, 76	0
All	All	1844/1940 (95%)	-0.37	42 (2%) 60 60	5, 11, 25, 76	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	329	THR	7.5
1	A	329	THR	7.2
1	A	350	TRP	7.1
1	B	329	THR	6.2
1	C	329	THR	5.7

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

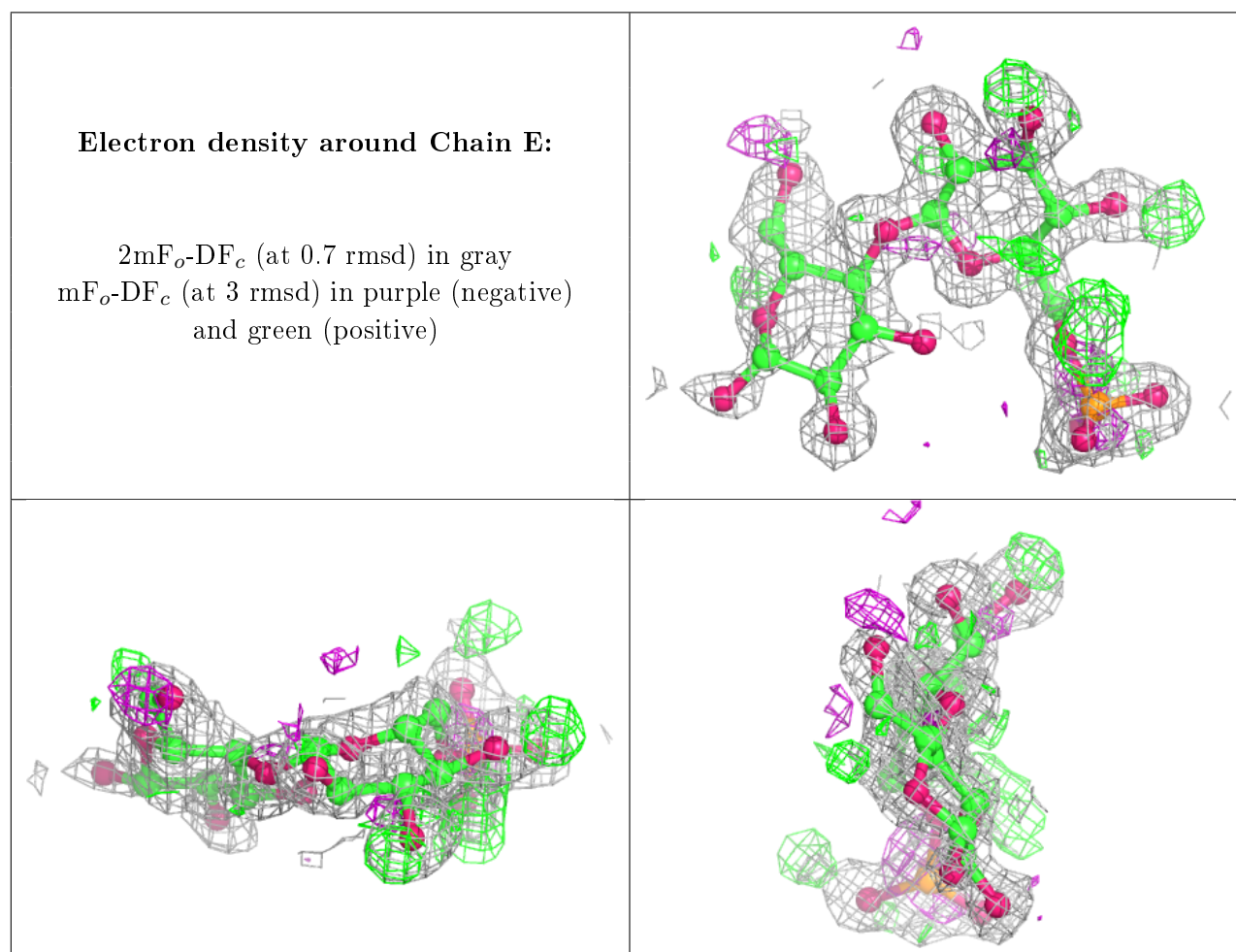
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.80	0.23	21,36,42,50	12
2	0WK	E	2	15/15	0.87	0.14	10,17,23,27	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 ⓘ

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
7	BGC	C	507	12/12	0.70	0.27	24,42,54,60	12
4	GOL	D	501	6/6	0.73	0.16	39,40,43,50	0
6	0WK	C	506	15/15	0.78	0.17	10,20,39,42	15
4	GOL	B	503	6/6	0.80	0.13	31,40,44,47	0
5	IMD	D	502	5/5	0.82	0.16	17,21,23,25	5
4	GOL	C	503	6/6	0.82	0.15	30,38,43,54	0
4	GOL	A	505	6/6	0.82	0.15	31,42,49,50	0
3	BG6	B	501	16/16	0.84	0.20	9,26,41,43	16

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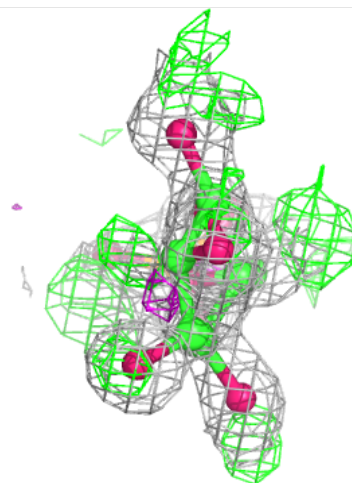
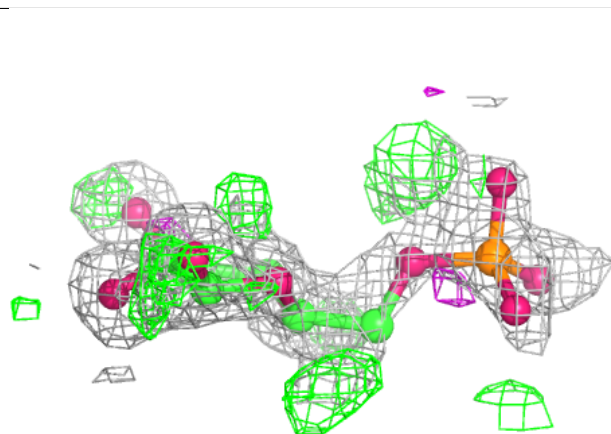
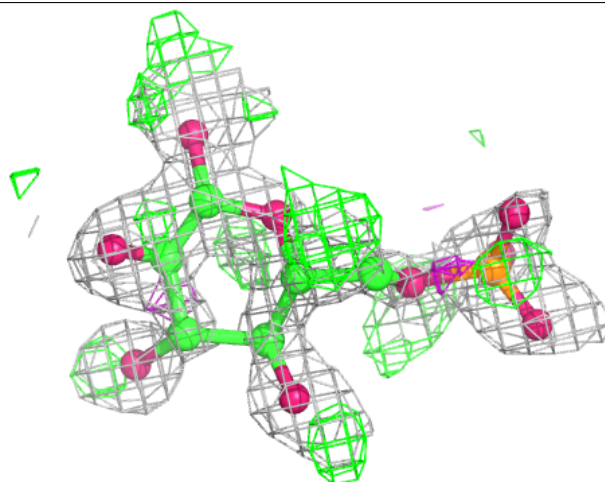
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IMD	A	507	5/5	0.84	0.16	25,28,32,32	0
4	GOL	A	502	6/6	0.85	0.10	36,36,40,42	0
3	BG6	A	501	16/16	0.85	0.18	8,28,41,44	16
4	GOL	C	504	6/6	0.85	0.25	37,44,46,59	0
5	IMD	C	505	5/5	0.89	0.18	23,29,30,32	0
4	GOL	B	502	6/6	0.90	0.12	25,41,43,46	0
4	GOL	A	506	6/6	0.93	0.15	36,40,44,45	0
4	GOL	A	504	6/6	0.94	0.12	13,19,24,26	0
4	GOL	C	502	6/6	0.94	0.10	15,18,21,26	0
4	GOL	C	501	6/6	0.95	0.12	13,17,24,27	0
4	GOL	A	503	6/6	0.96	0.09	14,19,23,27	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.

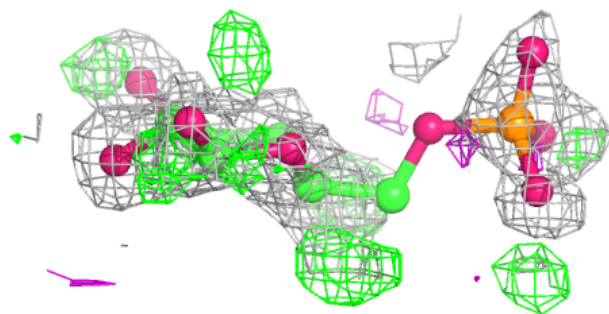
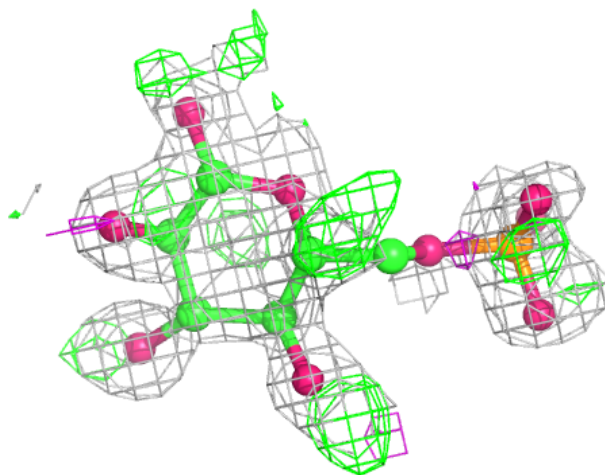
Electron density around BG6 B 501:

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.