Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 01:42 AM EDT

PDB ID	:	6HA9
Title	:	Structure of an endo-Xyloglucanase from Cellvibrio japonicus complexed with XXXG(2F)-beta-DNP
Authors	:	Offen, W.A.; Davies, G.J.
Deposited on	:	2018-08-07
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

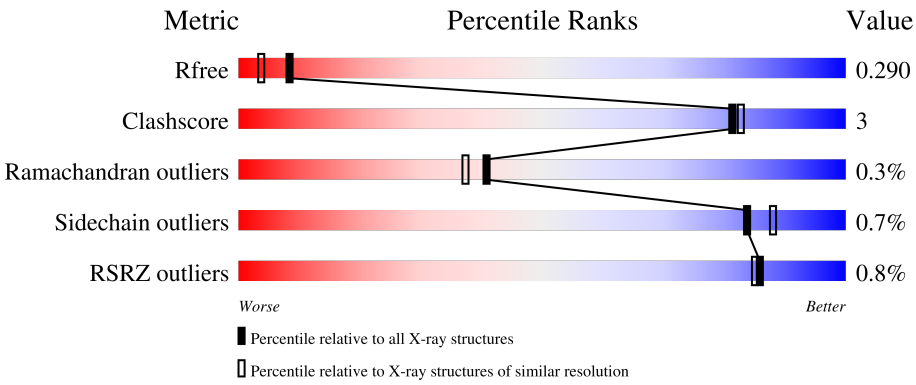
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	396	86% 7% 7%
1	B	396	% 87% 6% • 7%
2	C	6	100%
3	D	7	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6291 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 Cellulase, putative, cel5D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2954	1873	501	569	11	0	4	0
1	B	370	2916	1848	496	562	10	0	3	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	MET	-	initiating methionine	UNP B3PD52
A	74	GLY	-	expression tag	UNP B3PD52
A	75	SER	-	expression tag	UNP B3PD52
A	76	SER	-	expression tag	UNP B3PD52
A	77	HIS	-	expression tag	UNP B3PD52
A	78	HIS	-	expression tag	UNP B3PD52
A	79	HIS	-	expression tag	UNP B3PD52
A	80	HIS	-	expression tag	UNP B3PD52
A	81	HIS	-	expression tag	UNP B3PD52
A	82	HIS	-	expression tag	UNP B3PD52
A	83	SER	-	expression tag	UNP B3PD52
A	84	SER	-	expression tag	UNP B3PD52
A	85	GLY	-	expression tag	UNP B3PD52
A	86	LEU	-	expression tag	UNP B3PD52
A	87	VAL	-	expression tag	UNP B3PD52
A	88	PRO	-	expression tag	UNP B3PD52
A	89	ARG	-	expression tag	UNP B3PD52
A	90	GLY	-	expression tag	UNP B3PD52
A	91	SER	-	expression tag	UNP B3PD52
A	92	HIS	-	expression tag	UNP B3PD52
A	93	MET	-	expression tag	UNP B3PD52
A	94	ALA	-	expression tag	UNP B3PD52
A	95	SER	-	expression tag	UNP B3PD52
A	255	ALA	GLU	engineered mutation	UNP B3PD52
B	73	MET	-	initiating methionine	UNP B3PD52

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Chain	Residue	Modelled	Actual	Comment	Reference
B	74	GLY	-	expression tag	UNP B3PD52
B	75	SER	-	expression tag	UNP B3PD52
B	76	SER	-	expression tag	UNP B3PD52
B	77	HIS	-	expression tag	UNP B3PD52
B	78	HIS	-	expression tag	UNP B3PD52
B	79	HIS	-	expression tag	UNP B3PD52
B	80	HIS	-	expression tag	UNP B3PD52
B	81	HIS	-	expression tag	UNP B3PD52
B	82	HIS	-	expression tag	UNP B3PD52
B	83	SER	-	expression tag	UNP B3PD52
B	84	SER	-	expression tag	UNP B3PD52
B	85	GLY	-	expression tag	UNP B3PD52
B	86	LEU	-	expression tag	UNP B3PD52
B	87	VAL	-	expression tag	UNP B3PD52
B	88	PRO	-	expression tag	UNP B3PD52
B	89	ARG	-	expression tag	UNP B3PD52
B	90	GLY	-	expression tag	UNP B3PD52
B	91	SER	-	expression tag	UNP B3PD52
B	92	HIS	-	expression tag	UNP B3PD52
B	93	MET	-	expression tag	UNP B3PD52
B	94	ALA	-	expression tag	UNP B3PD52
B	95	SER	-	expression tag	UNP B3PD52
B	255	ALA	GLU	engineered mutation	UNP B3PD52

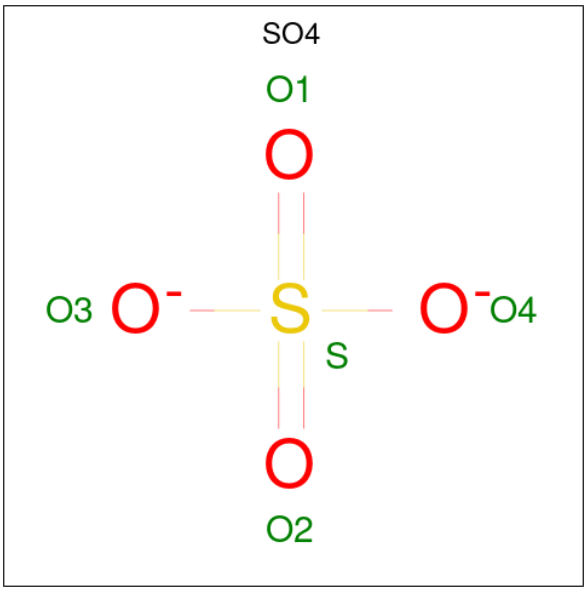
- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
2	C	6	75	40	1	2	32	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside.

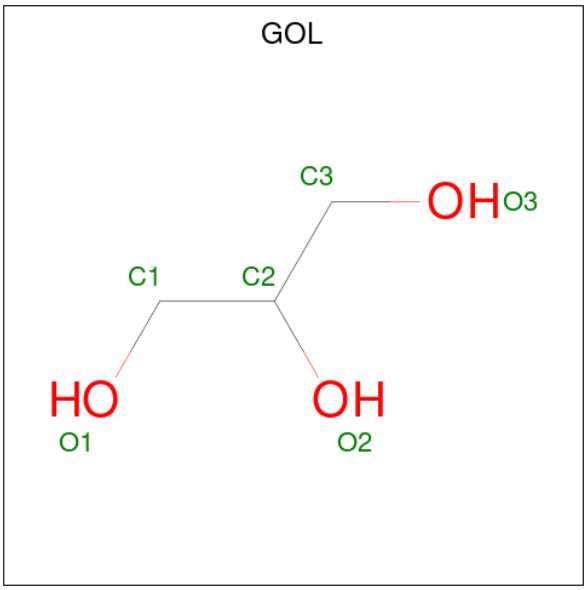
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
3	D	7	84	45	1	2	36	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



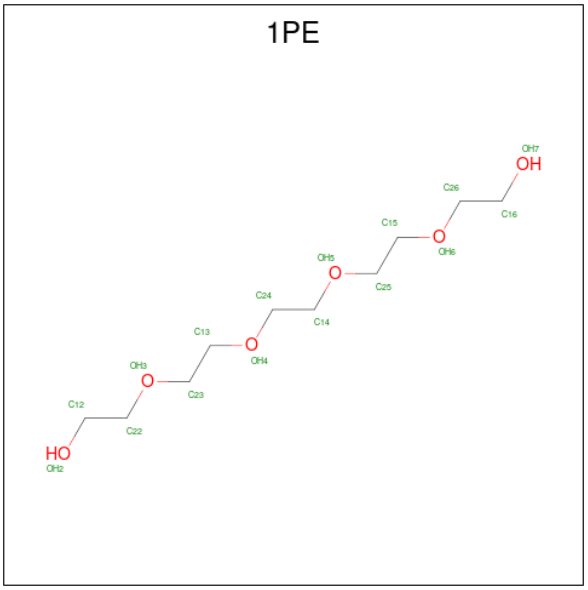
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	16	10	6	0	0

- Molecule 7 is water.

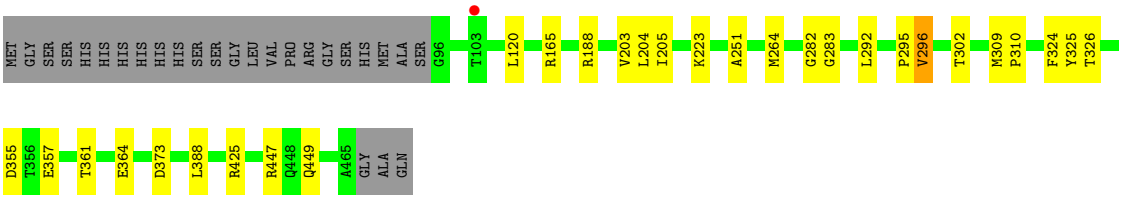
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	112	112	112	0	0
			Total	O		
7	B	97	97	97	0	0

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.

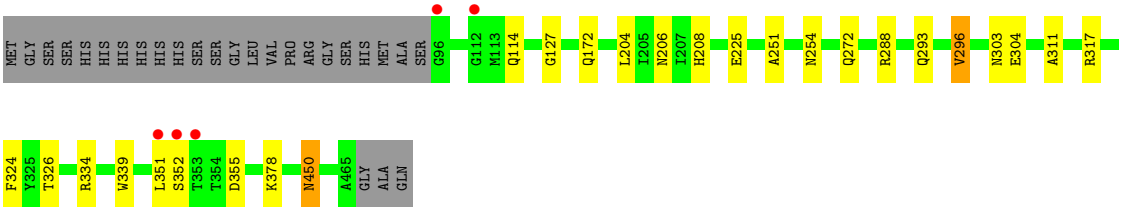
• Molecule 1: Cellulase, putative, cel5D

Chain A:



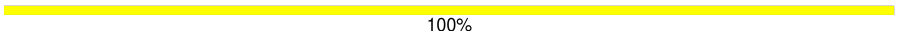
• Molecule 1: Cellulase, putative, cel5D

Chain B:



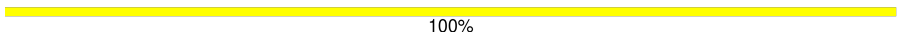
• Molecule 2: beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside

Chain C:



• Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.48Å 97.81Å 158.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.19 – 2.00 79.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.19-2.00) 99.8 (79.06-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.219 , 0.287 0.227 , 0.290	Depositor DCC
R_{free} test set	2960 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6291	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: XYS, 1PE, BGC, NFG, GOL, SO4

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	0.88	0/3027	0.87	4/4124 (0.1%)
1	B	0.83	4/2989 (0.1%)	0.84	0/4078
All	All	0.85	4/6016 (0.1%)	0.85	4/8202 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	GLU	CD-OE2	-6.77	1.18	1.25
1	B	127	GLY	N-CA	6.38	1.55	1.46
1	B	172	GLN	N-CA	5.69	1.57	1.46
1	B	304	GLU	CD-OE1	5.62	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	TYR	CB-CG-CD2	6.09	124.65	121.00
1	A	447	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	188	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	282	GLY	C-N-CA	-5.09	111.60	122.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	283	GLY	Peptide
1	B	288	ARG	Sidechain
1	B	317	ARG	Sidechain
1	B	334	ARG	Sidechain

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	2954	0	2784	17	0
1	B	2916	0	2717	13	0
2	C	75	0	54	0	0
3	D	84	0	61	0	0
4	A	5	0	0	1	0
4	B	20	0	0	2	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	16	0	22	2	0
7	A	112	0	0	3	0
7	B	97	0	0	1	0
All	All	6291	0	5654	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (31) 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:223:LYS:CE	4:A:501:SO4:O2	2.16	0.92
1:A:309:MET:HG3	1:A:310:PRO:HD2	1.72	0.72
1:A:264:MET:HE1	1:A:295:PRO:HB3	1.71	0.71
1:B:352:SER:CB	1:B:355[A]:ASP:OD1	2.44	0.66
1:A:364:GLU:OE1	7:A:601:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:HD2	1:A:302:THR:OG1	1.99	0.63
4:B:502:SO4:O1	7:B:601:HOH:O	2.17	0.54
1:A:324:PHE:CZ	1:A:326:THR:HB	2.46	0.51
1:A:361:THR:OG1	7:A:602:HOH:O	2.19	0.51
1:A:355:ASP:OD1	1:A:357:GLU:OE2	2.29	0.51
1:B:324:PHE:CZ	1:B:326:THR:HB	2.46	0.51
1:A:203:VAL:HG12	1:A:205:ILE:HD12	1.96	0.47
1:A:373:ASP:OD1	1:A:425:ARG:NE	2.44	0.47
1:A:373:ASP:OD2	7:A:603:HOH:O	2.20	0.47
1:B:272:GLN:NE2	1:B:311:ALA:O	2.40	0.47
1:B:204:LEU:HD11	1:B:251:ALA:HB2	1.96	0.46
1:A:324:PHE:HB2	1:A:388:LEU:HD11	1.98	0.45
1:B:114:GLN:HG2	4:B:504:SO4:O4	2.14	0.45
1:A:264:MET:HE1	1:A:295:PRO:CB	2.43	0.45
1:B:450:ASN:HD22	1:B:450:ASN:HA	1.68	0.45
1:B:351:LEU:O	1:B:352:SER:C	2.56	0.44
1:A:204:LEU:HD11	1:A:251:ALA:HB2	2.00	0.44
1:B:206:ASN:OD1	1:B:206:ASN:C	2.54	0.43
1:A:292:LEU:HD13	1:A:310:PRO:HD2	2.01	0.42
1:A:203:VAL:HG12	1:A:205:ILE:CD1	2.49	0.42
1:B:303:ASN:HA	1:B:378:LYS:HE3	2.02	0.42
1:B:208:HIS:HA	1:B:254:ASN:HB2	2.01	0.41
1:B:293:GLN:N	1:B:293:GLN:CD	2.74	0.41
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.93	0.41
1:B:339:TRP:CE3	6:B:513:1PE:H122	2.56	0.41
1:B:339:TRP:CZ3	6:B:513:1PE:H122	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/396 (94%)	350 (94%)	21 (6%)	1 (0%)	41	37
1	B	371/396 (94%)	350 (94%)	20 (5%)	1 (0%)	41	37
All	All	743/792 (94%)	700 (94%)	41 (6%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	VAL
1	A	296	VAL

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	303/326 (93%)	301 (99%)	2 (1%)	84	88
1	B	294/326 (90%)	292 (99%)	2 (1%)	84	88
All	All	597/652 (92%)	593 (99%)	4 (1%)	84	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	VAL
1	A	449	GLN
1	B	296	VAL
1	B	450	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	B	114	GLN
1	B	450	ASN
1	B	456	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 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	NFG	C	1	2	25,25,25	3.24	7 (28%)	28,36,36	1.72	6 (21%)
2	BGC	C	2	2	11,11,12	1.42	2 (18%)	15,15,17	1.96	5 (33%)
2	BGC	C	3	2	11,11,12	1.37	2 (18%)	15,15,17	0.86	0
2	BGC	C	4	2	11,11,12	1.16	1 (9%)	15,15,17	1.91	5 (33%)
2	XYS	C	5	2	9,9,10	1.14	1 (11%)	10,12,14	1.88	4 (40%)
2	XYS	C	6	2	9,9,10	1.20	0	10,12,14	2.65	3 (30%)
3	NFG	D	1	3	25,25,25	2.95	7 (28%)	28,36,36	1.33	3 (10%)
3	BGC	D	2	3	11,11,12	1.62	3 (27%)	15,15,17	2.52	5 (33%)
3	BGC	D	3	3	11,11,12	1.32	2 (18%)	15,15,17	0.88	0
3	BGC	D	4	3	11,11,12	0.96	0	15,15,17	1.14	1 (6%)
3	XYS	D	5	3	9,9,10	0.67	0	10,12,14	2.37	4 (40%)
3	XYS	D	6	3	9,9,10	1.80	3 (33%)	10,12,14	1.38	1 (10%)
3	XYS	D	7	3	9,9,10	0.93	0	10,12,14	1.61	1 (10%)

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	NFG	C	1	2	-	0/10/34/34	0/2/2/2
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	1/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	XYS	C	5	2	-	-	0/1/1/1
2	XYS	C	6	2	-	-	0/1/1/1
3	NFG	D	1	3	-	0/10/34/34	0/2/2/2
3	BGC	D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	D	4	3	-	0/2/19/22	0/1/1/1
3	XYS	D	5	3	-	-	0/1/1/1
3	XYS	D	6	3	-	-	0/1/1/1
3	XYS	D	7	3	-	-	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NFG	O22-N2	9.87	1.39	1.22
3	D	1	NFG	O12-N1	9.25	1.38	1.22
2	C	1	NFG	O12-N1	8.84	1.38	1.22
3	D	1	NFG	O22-N2	8.15	1.36	1.22
2	C	1	NFG	C12-C11	4.76	1.49	1.40
2	C	1	NFG	C12-N1	-4.04	1.38	1.45
2	C	1	NFG	C2-C3	3.93	1.56	1.52
3	D	1	NFG	C12-C11	3.73	1.47	1.40
3	D	2	BGC	C2-C3	3.21	1.57	1.52
3	D	3	BGC	O5-C1	3.14	1.49	1.43
3	D	6	XYS	O5-C5	3.09	1.48	1.43
2	C	2	BGC	C2-C3	2.96	1.57	1.52
3	D	1	NFG	O3-C3	2.89	1.50	1.43
2	C	4	BGC	C2-C3	2.89	1.56	1.52
3	D	6	XYS	C4-C3	2.81	1.56	1.52
3	D	2	BGC	O5-C5	2.77	1.48	1.43
3	D	1	NFG	C2-C1	2.67	1.55	1.52
3	D	1	NFG	C14-N2	-2.63	1.38	1.45
3	D	6	XYS	O2-C2	-2.51	1.38	1.43
2	C	2	BGC	O5-C1	2.50	1.47	1.43
3	D	3	BGC	C2-C3	2.47	1.56	1.52
2	C	5	XYS	O5-C1	2.37	1.47	1.43
2	C	1	NFG	O1-C1	2.36	1.44	1.41
2	C	3	BGC	O2-C2	2.24	1.48	1.43
2	C	3	BGC	C2-C3	2.18	1.55	1.52
3	D	1	NFG	C12-N1	-2.10	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NFG	O3-C3	2.07	1.48	1.43
3	D	2	BGC	O4-C4	2.03	1.48	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	BGC	C1-O5-C5	6.53	120.94	112.19
2	C	6	XYS	C5-C4-C3	5.25	117.28	109.64
2	C	6	XYS	O3-C3-C2	-5.07	99.72	110.05
3	D	5	XYS	C5-O5-C1	5.06	119.58	111.42
2	C	2	BGC	C1-O5-C5	4.80	118.61	112.19
2	C	4	BGC	C1-C2-C3	4.64	116.40	109.64
3	D	2	BGC	C1-C2-C3	4.52	116.22	109.64
2	C	1	NFG	F-C2-C3	-3.84	105.48	108.81
3	D	2	BGC	O5-C1-C2	3.70	119.61	110.79
3	D	4	BGC	C1-O5-C5	3.58	116.99	112.19
2	C	5	XYS	C4-C3-C2	-3.52	106.73	110.92
2	C	1	NFG	O22-N2-C14	3.48	123.60	118.82
2	C	4	BGC	O2-C2-C1	-3.41	101.42	109.22
3	D	1	NFG	C15-C14-N2	3.28	122.20	119.34
3	D	1	NFG	C3-C4-C5	3.24	116.10	110.23
2	C	6	XYS	C4-C3-C2	3.19	114.71	110.92
3	D	5	XYS	O4-C4-C5	-2.95	102.47	109.22
2	C	2	BGC	O4-C4-C3	2.94	117.30	110.38
2	C	1	NFG	C1-C2-C3	2.90	114.78	110.54
3	D	7	XYS	O3-C3-C4	-2.82	104.30	110.05
3	D	6	XYS	O4-C4-C3	-2.72	104.52	110.15
2	C	5	XYS	O2-C2-C3	2.71	115.76	110.15
2	C	2	BGC	C1-C2-C3	2.67	113.54	109.64
2	C	1	NFG	C15-C14-N2	2.64	121.64	119.34
3	D	1	NFG	C13-C14-N2	-2.54	116.55	118.74
2	C	2	BGC	O5-C1-C2	2.53	116.83	110.79
3	D	5	XYS	C1-C2-C3	-2.49	106.02	109.64
2	C	1	NFG	O1-C1-C2	2.47	111.31	107.29
2	C	5	XYS	C5-C4-C3	2.39	113.12	109.64
3	D	5	XYS	O3-C3-C4	2.39	114.92	110.05
3	D	2	BGC	O4-C4-C5	2.38	115.19	109.32
2	C	1	NFG	C14-C13-C12	2.33	122.34	119.26
2	C	4	BGC	C1-O5-C5	-2.24	109.18	112.19
2	C	5	XYS	O4-C4-C5	2.04	113.89	109.22
2	C	4	BGC	O3-C3-C2	2.04	114.21	110.05
3	D	2	BGC	O2-C2-C1	-2.03	104.57	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	BGC	O3-C3-C2	-2.02	105.93	110.05
2	C	4	BGC	C2-C3-C4	-2.01	107.32	110.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

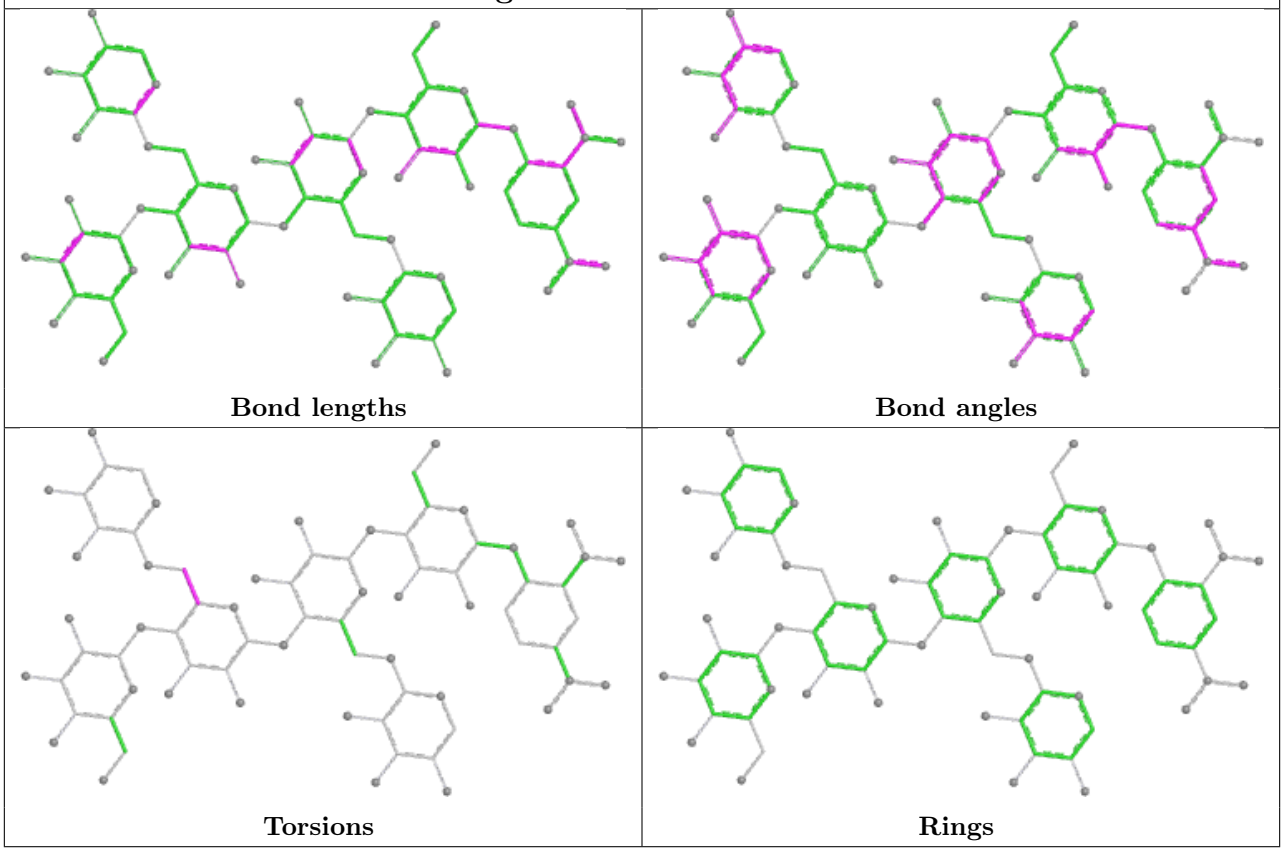
Mol	Chain	Res	Type	Atoms
2	C	3	BGC	C4-C5-C6-O6

There are no ring outliers.

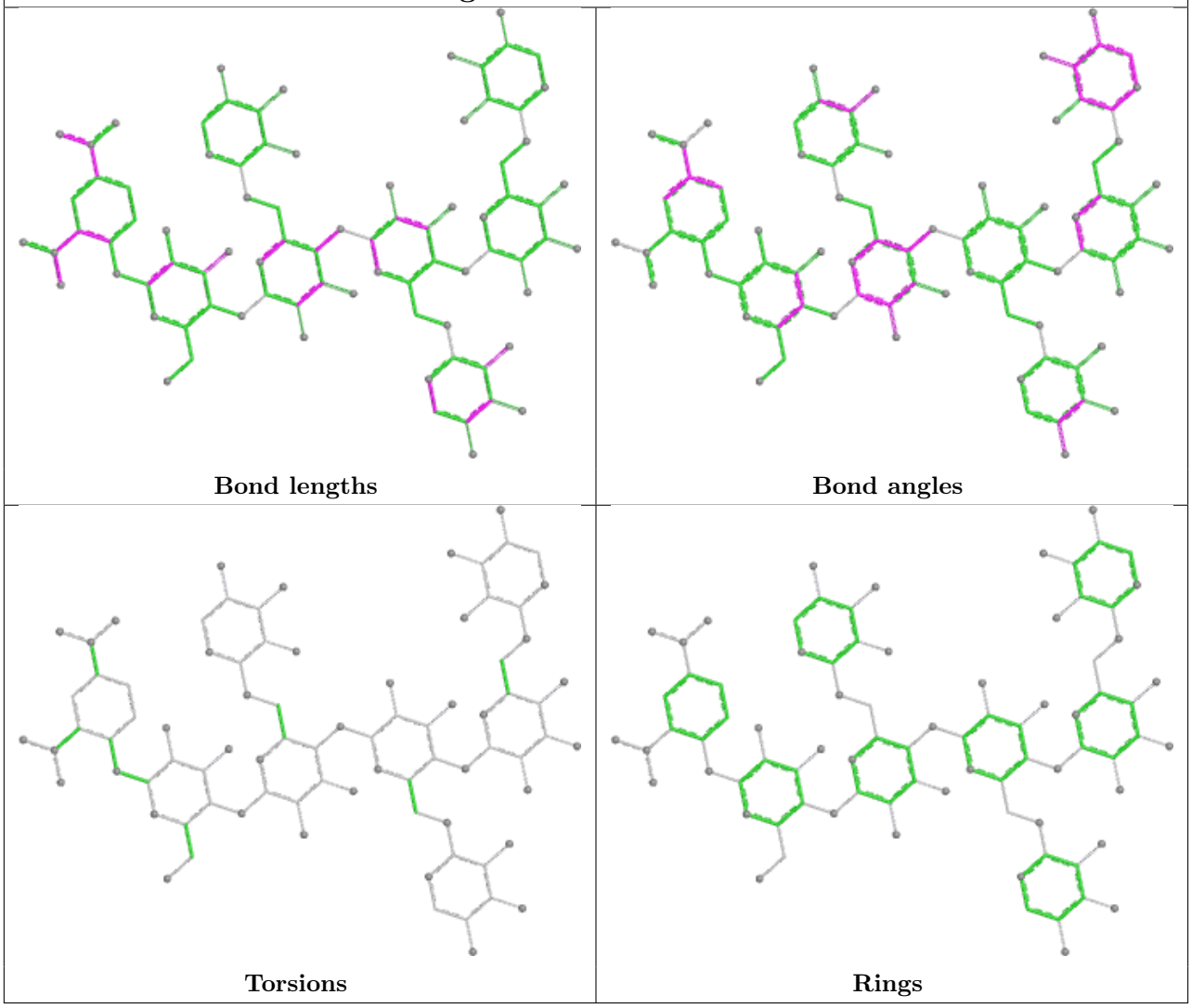
No monomer is involved in short contacts.

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

8 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	SO4	B	504	-	4,4,4	0.45	0	6,6,6	0.19	0
5	GOL	A	508	-	5,5,5	0.40	0	5,5,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	503	-	4,4,4	0.40	0	6,6,6	0.87	0
4	SO4	B	502	-	4,4,4	0.69	0	6,6,6	0.87	0
6	1PE	B	513	-	15,15,15	0.46	0	14,14,14	0.65	0
4	SO4	B	501	-	4,4,4	0.36	0	6,6,6	0.79	0
4	SO4	A	501	-	4,4,4	0.49	0	6,6,6	0.35	0
5	GOL	B	512	-	5,5,5	0.48	0	5,5,5	0.98	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	GOL	A	508	-	-	4/4/4/4	-
6	1PE	B	513	-	-	10/13/13/13	-
5	GOL	B	512	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	GOL	C1-C2-C3-O3
5	B	512	GOL	O1-C1-C2-O2
5	B	512	GOL	O1-C1-C2-C3
6	B	513	1PE	OH4-C13-C23-OH3
5	A	508	GOL	O1-C1-C2-C3
6	B	513	1PE	OH5-C14-C24-OH4
5	A	508	GOL	O2-C2-C3-O3
6	B	513	1PE	OH7-C16-C26-OH6
6	B	513	1PE	OH2-C12-C22-OH3
5	A	508	GOL	O1-C1-C2-O2
6	B	513	1PE	C16-C26-OH6-C15
6	B	513	1PE	C24-C14-OH5-C25
6	B	513	1PE	C15-C25-OH5-C14
6	B	513	1PE	C13-C23-OH3-C22
6	B	513	1PE	OH6-C15-C25-OH5
6	B	513	1PE	C12-C22-OH3-C23

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	SO4	1	0
4	B	502	SO4	1	0
6	B	513	1PE	2	0
4	A	501	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	370/396 (93%)	-0.10	1 (0%)	94	93	26, 39, 52, 67	10 (2%)
1	B	370/396 (93%)	0.02	5 (1%)	75	74	27, 44, 62, 68	29 (7%)
All	All	740/792 (93%)	-0.04	6 (0%)	86	85	26, 41, 58, 68	39 (5%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	SER	8.1
1	B	353	THR	2.7
1	B	112	GLY	2.5
1	B	96	GLY	2.1
1	A	103	THR	2.0
1	B	351	LEU	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(Å^2)	Q<0.9
3	XYS	D	5	9/10	0.85	0.30	41,43,46,48	9
2	XYS	C	6	9/10	0.87	0.23	24,25,27,28	9
3	XYS	D	7	9/10	0.90	0.27	21,26,33,35	9

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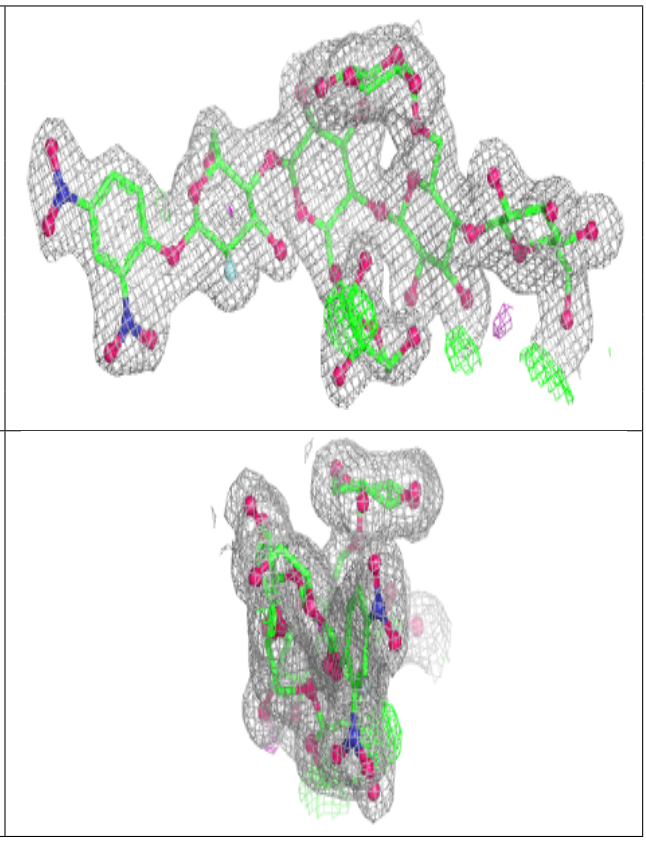
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	D	4	11/12	0.91	0.10	41,46,52,56	0
3	BGC	D	3	11/12	0.94	0.10	30,35,39,39	0
2	BGC	C	4	11/12	0.94	0.09	33,37,39,40	0
3	NFG	D	1	24/24	0.95	0.12	31,37,43,47	0
2	NFG	C	1	24/24	0.96	0.13	32,37,43,52	0
2	BGC	C	2	11/12	0.96	0.10	28,30,34,35	0
2	BGC	C	3	11/12	0.96	0.08	28,32,37,38	0
3	XYS	D	6	9/10	0.96	0.08	31,34,38,40	0
3	BGC	D	2	11/12	0.96	0.09	29,33,40,41	0
2	XYS	C	5	9/10	0.97	0.10	28,32,35,35	0

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.

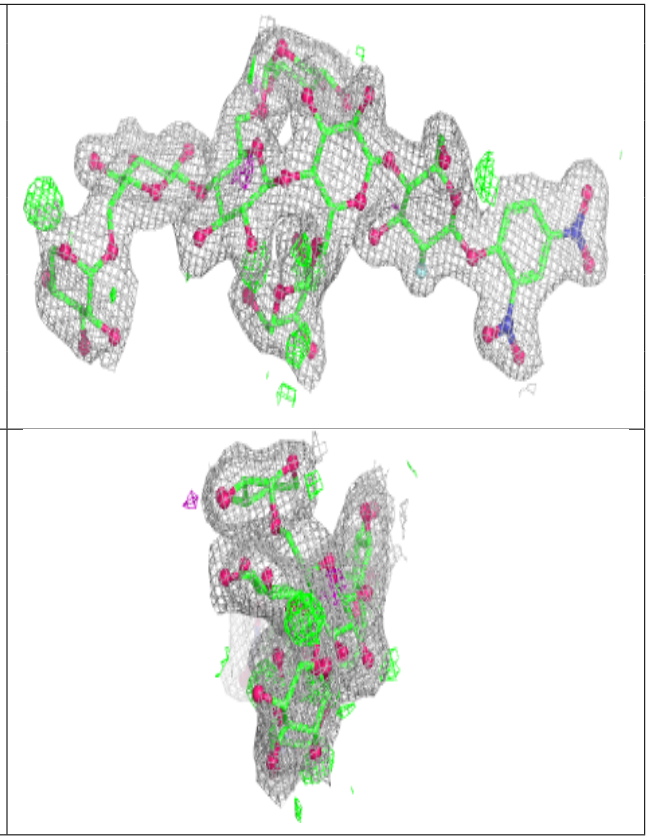
Electron density around Chain C:

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 Chain D:

$2mF_o$-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
4	SO4	A	501	5/5	0.74	0.26	52,55,57,61	5
5	GOL	A	508	6/6	0.83	0.25	29,33,35,42	6
5	GOL	B	512	6/6	0.83	0.25	40,45,48,49	6
4	SO4	B	502	5/5	0.85	0.23	40,45,52,52	5
4	SO4	B	503	5/5	0.85	0.27	40,41,47,50	5
4	SO4	B	504	5/5	0.90	0.30	52,55,57,64	5
6	1PE	B	513	16/16	0.91	0.30	35,44,51,53	16
4	SO4	B	501	5/5	0.94	0.12	39,41,43,43	5

6.5 Other polymers (i)

There are no such residues in this entry.