Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 11:39 PM JST

PDB ID	:	7C6H
Title	:	Crystal structure of beta-glycosides-binding protein (W177X) of ABC transporter in an open-liganded state bound to laminaribiose
Authors	:	Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.
Deposited on	:	2020-05-21
Resolution	:	1.85 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:

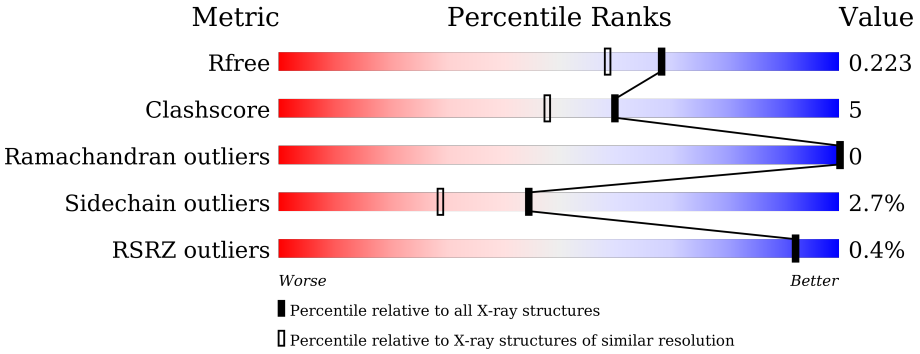
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	422	88% 11%
1	B	422	90% 9% ••
2	C	2	100%
2	D	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PGO	B	505	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7189 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 Sugar ABC transporter, periplasmic sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3260	2092	570	587	11	0	7	0
1	B	417	3205	2057	561	577	10	0	2	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q53W80
A	174	ARG	LYS	engineered mutation	UNP Q53W80
A	175	THR	ASN	engineered mutation	UNP Q53W80
A	176	PRO	SER	engineered mutation	UNP Q53W80
A	?	-	TRP	deletion	UNP Q53W80
A	177	ARG	ASP	engineered mutation	UNP Q53W80
A	178	THR	VAL	engineered mutation	UNP Q53W80
A	416	HIS	-	expression tag	UNP Q53W80
A	417	HIS	-	expression tag	UNP Q53W80
A	418	HIS	-	expression tag	UNP Q53W80
A	419	HIS	-	expression tag	UNP Q53W80
A	420	HIS	-	expression tag	UNP Q53W80
A	421	HIS	-	expression tag	UNP Q53W80
B	0	MET	-	initiating methionine	UNP Q53W80
B	174	ARG	LYS	engineered mutation	UNP Q53W80
B	175	THR	ASN	engineered mutation	UNP Q53W80
B	176	PRO	SER	engineered mutation	UNP Q53W80
B	?	-	TRP	deletion	UNP Q53W80
B	177	ARG	ASP	engineered mutation	UNP Q53W80
B	178	THR	VAL	engineered mutation	UNP Q53W80
B	416	HIS	-	expression tag	UNP Q53W80
B	417	HIS	-	expression tag	UNP Q53W80
B	418	HIS	-	expression tag	UNP Q53W80
B	419	HIS	-	expression tag	UNP Q53W80
B	420	HIS	-	expression tag	UNP Q53W80

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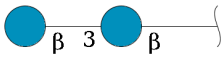
Chain	Residue	Modelled	Actual	Comment	Reference
B	421	HIS	-	expression tag	UNP Q53W80

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.

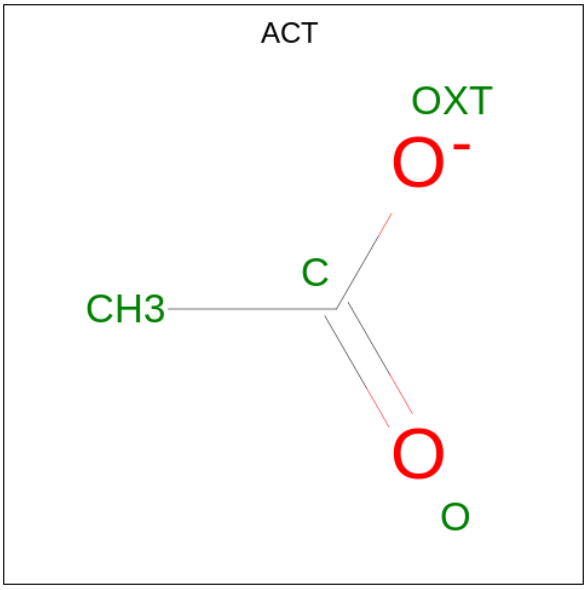


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	2	23	12	11	0	0	0
			Total	C	O			
2	D	2	23	12	11	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

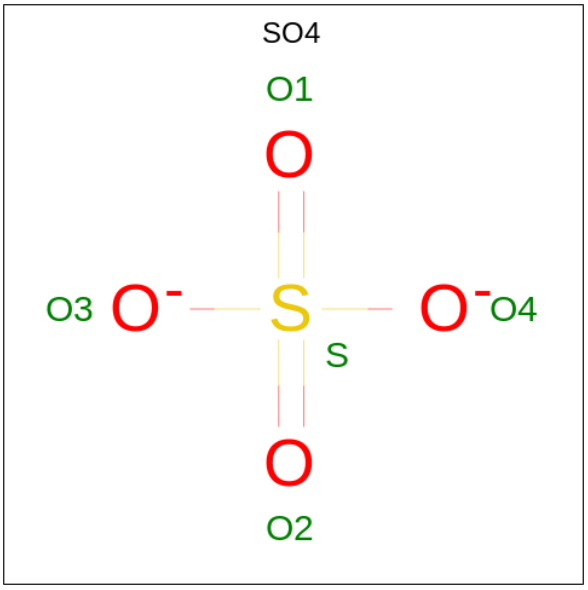
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
			Total	Cl		
3	B	1	1	1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



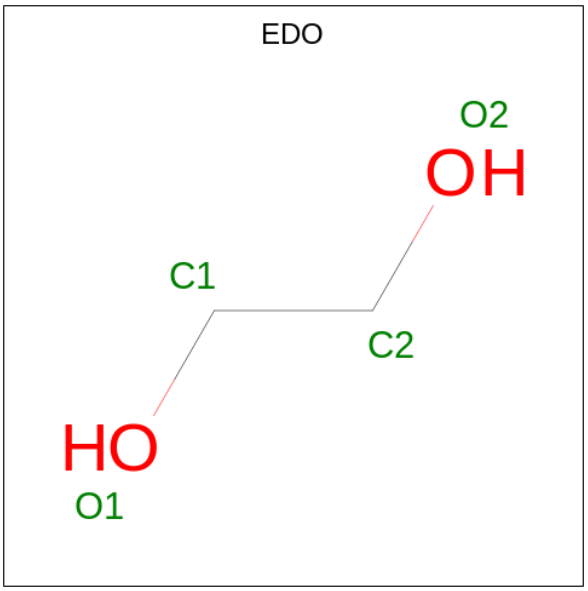
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



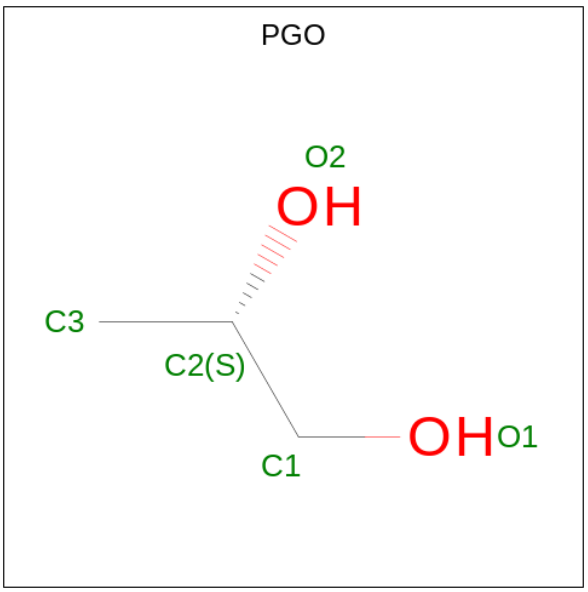
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



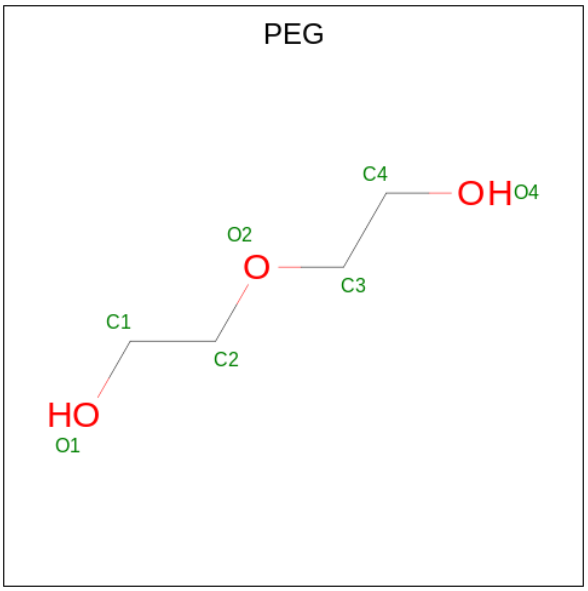
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	B	1	4	2	2	0	0
			Total	C	O		
6	B	1	4	2	2	0	0

- Molecule 7 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	5	3	2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	7	4	3	0	0

- Molecule 9 is water.

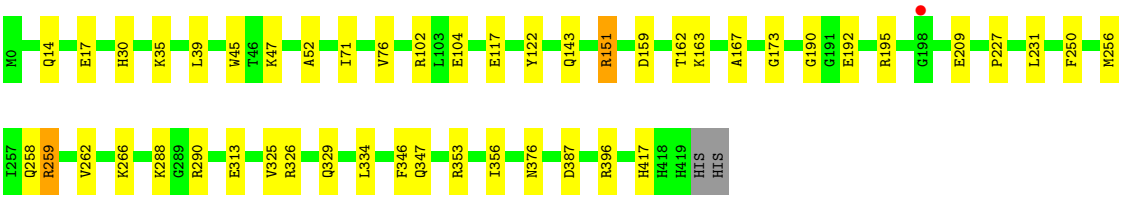
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	300	300	300	0	0
			Total	O		
9	B	330	330	330	0	0

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.

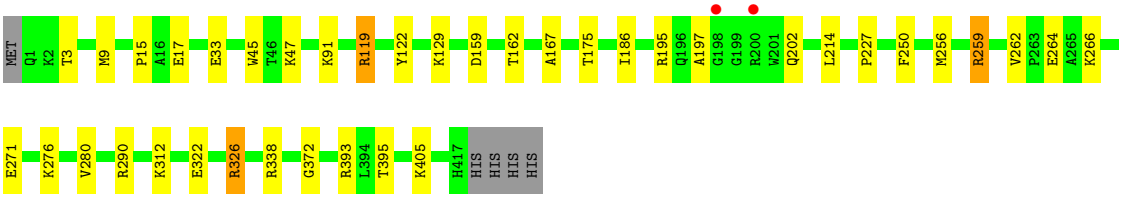
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain A:



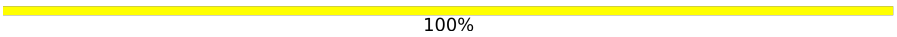
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain B:



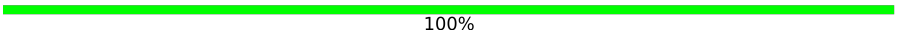
• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain C:



• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.51Å 92.25Å 69.78Å 90.00° 112.42° 90.00°	Depositor
Resolution (Å)	54.62 – 1.85 54.62 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.62-1.85) 100.0 (54.62-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.168 , 0.217 0.177 , 0.223	Depositor DCC
R_{free} test set	3076 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: BGC, SO4, CL, EDO, PEG, PGO, ACT

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	3/3372 (0.1%)	0.95	4/4587 (0.1%)
1	B	0.86	0/3300	1.00	7/4491 (0.2%)
All	All	0.87	3/6672 (0.0%)	0.97	11/9078 (0.1%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLU	CD-OE1	9.10	1.35	1.25
1	A	104	GLU	CD-OE1	6.80	1.33	1.25
1	A	209	GLU	CD-OE1	5.05	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	ARG	NE-CZ-NH1	-11.76	114.42	120.30
1	B	290	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	A	259	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	B	259	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	B	290	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	119	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	290	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	290	ARG	CG-CD-NE	-6.20	98.78	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	326	ARG	CG-CD-NE	5.60	123.57	111.80
1	A	259	ARG	CG-CD-NE	-5.22	100.83	111.80
1	B	119	ARG	CG-CD-NE	5.07	122.45	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	197	ALA	Peptide

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	3260	0	3238	33	0
1	B	3205	0	3182	24	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	3	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	12	0	18	5	0
6	B	8	0	12	4	0
7	B	5	0	8	1	0
8	B	7	0	10	3	0
9	A	300	0	0	8	1
9	B	330	0	0	8	1
All	All	7189	0	6513	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 5.

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:B:395:THR:HB	7:B:505:PGO:H11	1.53	0.89
1:A:417:HIS:HB3	9:A:603:HOH:O	1.76	0.85
1:A:39:LEU:HD22	1:A:47:LYS:HD2	1.65	0.79
1:A:258[A]:GLN:HG2	9:A:706:HOH:O	1.85	0.77
8:B:506:PEG:O4	9:B:601:HOH:O	1.99	0.77
8:B:506:PEG:H31	9:B:866:HOH:O	1.86	0.76
1:A:347:GLN:O	1:A:353:ARG:HD3	1.87	0.74
1:A:326[B]:ARG:NH2	9:A:601:HOH:O	2.16	0.72
1:A:396:ARG:H	6:A:506:EDO:H12	1.58	0.68
1:A:35:LYS:NZ	9:A:602:HOH:O	2.27	0.66
1:B:393:ARG:HH22	6:B:504:EDO:H12	1.61	0.64
1:A:151:ARG:CG	1:A:151:ARG:HH21	2.11	0.63
1:B:372:GLY:HA3	6:B:503:EDO:H12	1.80	0.63
1:B:45:TRP:CE2	6:B:503:EDO:H21	2.37	0.59
6:A:504:EDO:H21	9:A:814:HOH:O	2.04	0.56
1:A:39:LEU:HD22	1:A:47:LYS:CD	2.34	0.56
1:A:45:TRP:CZ3	1:A:71:ILE:HD11	2.40	0.55
1:B:405:LYS:NZ	9:B:605:HOH:O	2.36	0.55
1:A:262:VAL:CG1	1:A:266:LYS:HB2	2.37	0.54
6:A:504:EDO:C2	9:A:814:HOH:O	2.56	0.54
1:A:52:ALA:HB1	1:A:76:VAL:HG21	1.90	0.53
1:B:122:TYR:CD1	1:B:280:VAL:HG22	2.44	0.53
1:B:167:ALA:HB1	1:B:227:PRO:HD3	1.92	0.52
1:B:271:GLU:O	1:B:276:LYS:NZ	2.42	0.52
1:B:262:VAL:CG1	1:B:266:LYS:HB2	2.40	0.51
1:B:262:VAL:HG13	1:B:266:LYS:HB2	1.93	0.50
1:A:262:VAL:HG13	1:A:266:LYS:HB2	1.94	0.50
1:A:102:ARG:NE	9:A:613:HOH:O	2.44	0.50
1:B:129:LYS:HE3	9:B:892:HOH:O	2.10	0.50
1:B:91:LYS:HB2	9:B:675:HOH:O	2.12	0.49
6:B:503:EDO:H22	9:B:861:HOH:O	2.12	0.48
1:B:15:PRO:HD2	8:B:506:PEG:H12	1.95	0.48
1:A:346:PHE:HB3	1:A:356:ILE:HD11	1.96	0.48
1:A:151:ARG:HH21	1:A:151:ARG:HG3	1.78	0.47
1:A:329[A]:GLN:HE22	1:A:346:PHE:HZ	1.61	0.47
1:A:122:TYR:CZ	1:A:256:MET:HB2	2.50	0.46
1:A:190:GLY:HA3	1:A:288:LYS:HD3	1.97	0.46
1:B:312:LYS:NZ	9:B:620:HOH:O	2.49	0.46
1:A:376:ASN:ND2	1:B:338:ARG:HH12	2.14	0.45
1:A:417:HIS:CB	9:A:603:HOH:O	2.50	0.45
1:A:325:VAL:O	1:A:329[A]:GLN:NE2	2.36	0.44
1:A:173:GLY:HA3	1:A:231:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:HH21	1:A:151:ARG:HG2	1.80	0.43
1:A:167:ALA:HB1	1:A:227:PRO:HD3	2.01	0.43
1:A:14:GLN:HB3	1:A:17[A]:GLU:HB3	2.00	0.43
1:B:326:ARG:HH21	1:B:326:ARG:HG3	1.83	0.43
1:A:334:LEU:HD12	1:A:334:LEU:HA	1.78	0.43
1:B:122:TYR:CE1	1:B:280:VAL:HG22	2.53	0.43
1:A:159:ASP:HB3	1:A:162:THR:OG1	2.19	0.43
1:B:3:THR:HG22	1:B:33:GLU:HB3	2.00	0.42
1:A:17[B]:GLU:HG3	6:A:504:EDO:O2	2.19	0.42
1:B:122:TYR:CZ	1:B:256:MET:HB2	2.55	0.42
1:A:30:HIS:CE1	1:A:313[B]:GLU:OE1	2.73	0.41
1:A:376:ASN:HD21	1:B:338:ARG:HH12	1.68	0.41
1:A:151:ARG:CG	1:A:151:ARG:NH2	2.79	0.41
1:B:322:GLU:HG3	9:B:818:HOH:O	2.19	0.41
1:B:159:ASP:HB3	1:B:162:THR:OG1	2.20	0.41
1:A:396:ARG:H	6:A:506:EDO:C1	2.28	0.41
1:B:264:GLU:HG3	1:B:271:GLU:OE1	2.20	0.41
1:B:186:ILE:HD11	1:B:214:LEU:HD21	2.03	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)
9:A:797:HOH:O	9:B:891:HOH:O[1_556]	2.06	0.14

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	425/422 (101%)	422 (99%)	3 (1%)	0	100	100
1	B	417/422 (99%)	411 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	842/844 (100%)	833 (99%)	9 (1%)	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	326/321 (102%)	318 (98%)	8 (2%)	47	31
1	B	318/321 (99%)	309 (97%)	9 (3%)	43	27
All	All	644/642 (100%)	627 (97%)	17 (3%)	44	30

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	151	ARG
1	A	163	LYS
1	A	192	GLU
1	A	195	ARG
1	A	250	PHE
1	A	259	ARG
1	A	387	ASP
1	B	9	MET
1	B	17	GLU
1	B	47	LYS
1	B	119	ARG
1	B	175	THR
1	B	195	ARG
1	B	202	GLN
1	B	250	PHE
1	B	259	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	C	1	2	12,12,12	0.51	0	17,17,17	1.20	1 (5%)
2	BGC	C	2	2	11,11,12	0.84	0	15,15,17	1.09	2 (13%)
2	BGC	D	1	2	12,12,12	0.69	0	17,17,17	0.66	0
2	BGC	D	2	2	11,11,12	0.93	0	15,15,17	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	BGC	O5-C1-C2	-2.63	105.59	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	BGC	O2-C2-C3	-2.23	105.67	110.14
2	C	2	BGC	O5-C5-C6	2.22	110.69	107.20

There are no chirality outliers.

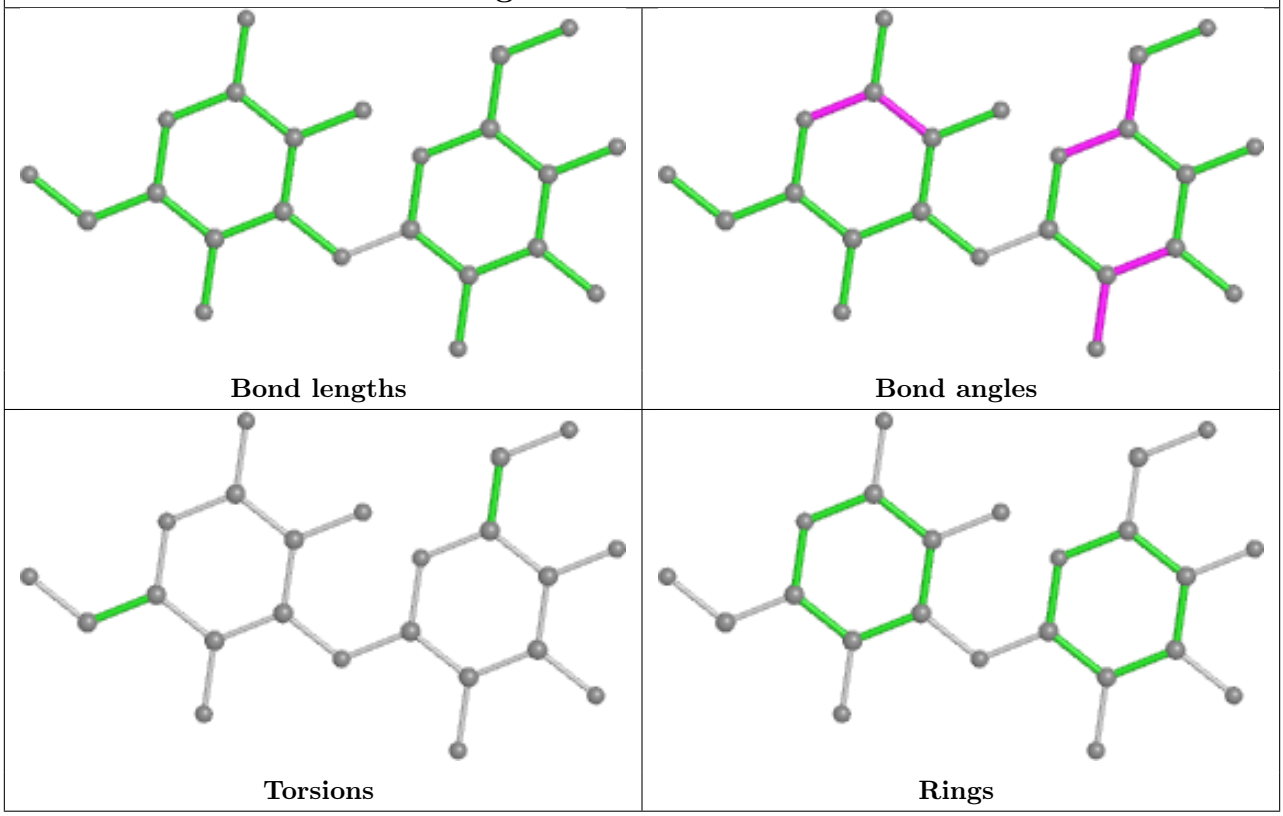
There are no torsion outliers.

There are no ring outliers.

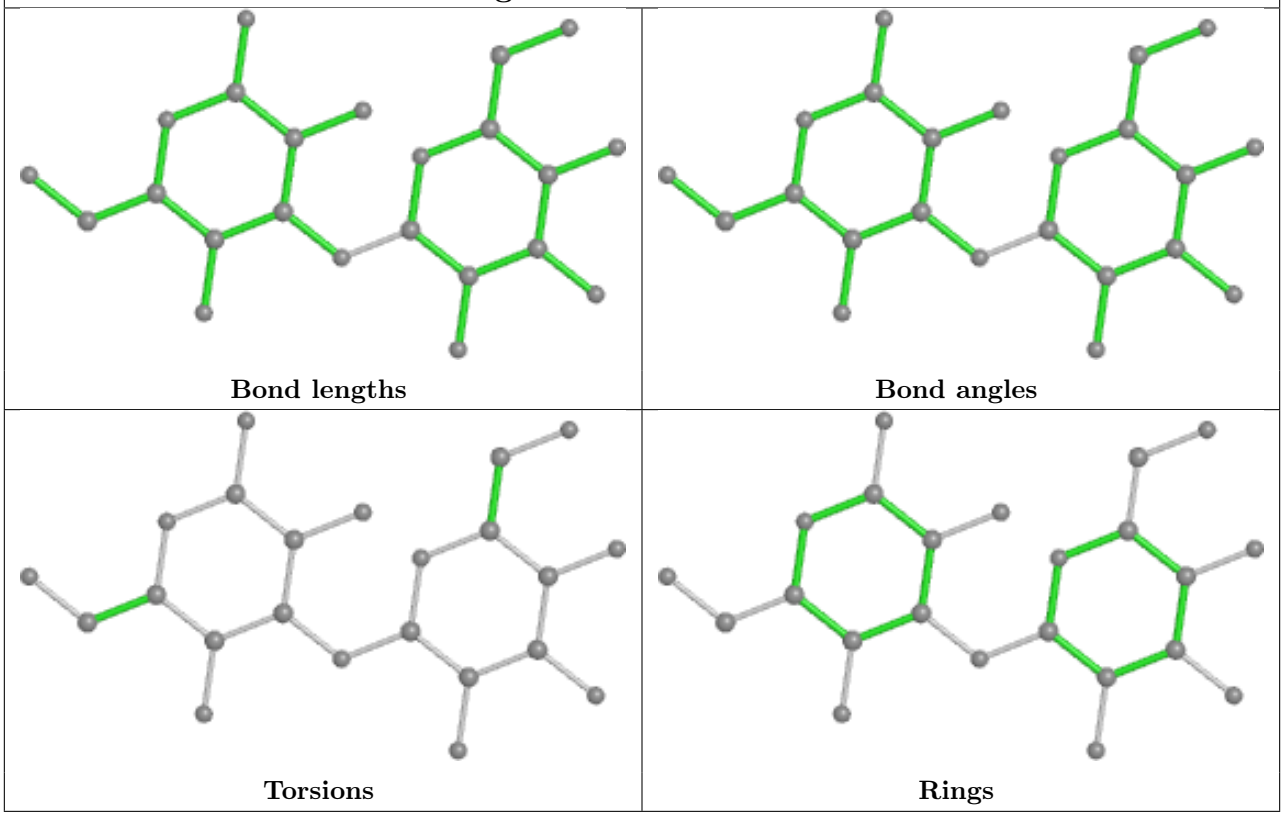
No monomer is involved in short contacts.

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)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	A	502	-	3,3,3	0.95	0	3,3,3	0.82	0
8	PEG	B	506	-	6,6,6	0.32	0	5,5,5	0.17	0
7	PGO	B	505	-	3,4,4	0.24	0	1,4,4	0.60	0
6	EDO	A	505	-	3,3,3	0.18	0	2,2,2	0.41	0
6	EDO	B	504	-	3,3,3	0.15	0	2,2,2	0.08	0
5	SO4	B	502	-	4,4,4	0.38	0	6,6,6	0.19	0
6	EDO	A	504	-	3,3,3	0.22	0	2,2,2	0.32	0
6	EDO	A	506	-	3,3,3	0.42	0	2,2,2	0.25	0
6	EDO	B	503	-	3,3,3	0.17	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	A	503	-	4,4,4	0.42	0	6,6,6	0.24	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
8	PEG	B	506	-	-	2/4/4/4	-
7	PGO	B	505	-	1/1/1/1	2/2/2/2	-
6	EDO	A	505	-	-	1/1/1/1	-
6	EDO	B	504	-	-	0/1/1/1	-
6	EDO	A	506	-	-	1/1/1/1	-
6	EDO	A	504	-	-	1/1/1/1	-
6	EDO	B	503	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	505	PGO	C2

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	505	PGO	O1-C1-C2-C3
7	B	505	PGO	O1-C1-C2-O2
8	B	506	PEG	C4-C3-O2-C2
8	B	506	PEG	O2-C3-C4-O4
6	A	505	EDO	O1-C1-C2-O2
6	A	506	EDO	O1-C1-C2-O2
6	A	504	EDO	O1-C1-C2-O2
6	B	503	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	506	PEG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	505	PGO	1	0
6	B	504	EDO	1	0
6	A	504	EDO	3	0
6	A	506	EDO	2	0
6	B	503	EDO	3	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	420/422 (99%)	-0.49	1 (0%)	95	94	12, 22, 39, 54	0
1	B	417/422 (98%)	-0.50	2 (0%)	91	91	13, 21, 40, 59	0
All	All	837/844 (99%)	-0.49	3 (0%)	92	92	12, 22, 40, 59	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	GLY	3.1
1	B	200	ARG	2.6
1	A	198	GLY	2.1

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)

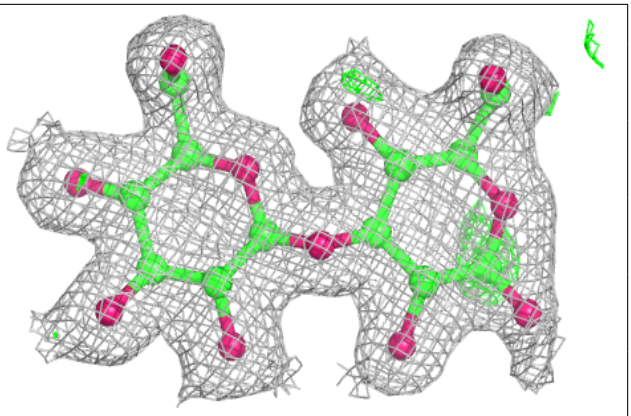
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

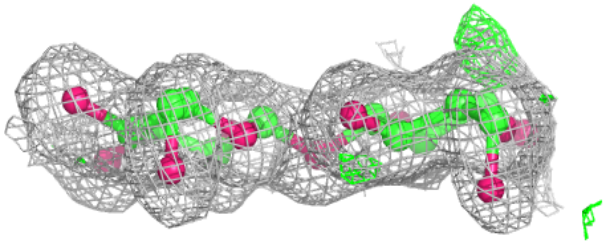
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	D	1	12/12	0.92	0.10	19,22,29,31	0
2	BGC	C	1	12/12	0.94	0.09	16,18,27,30	0
2	BGC	C	2	11/12	0.96	0.07	13,13,15,15	0
2	BGC	D	2	11/12	0.97	0.07	15,16,17,18	0

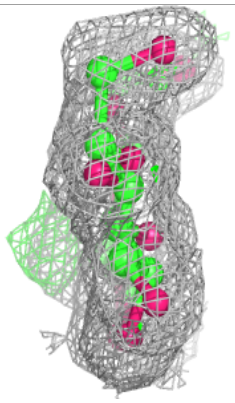
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

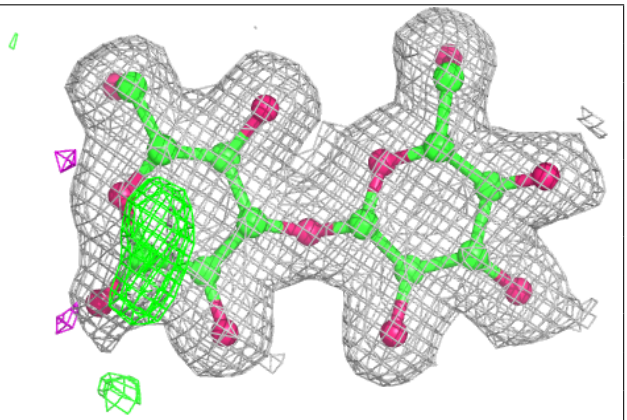


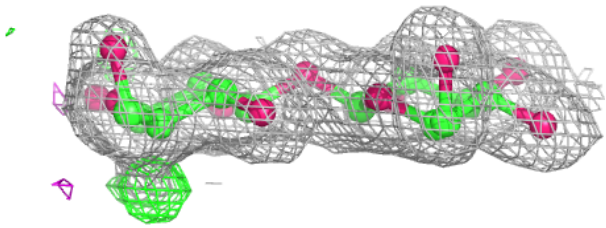


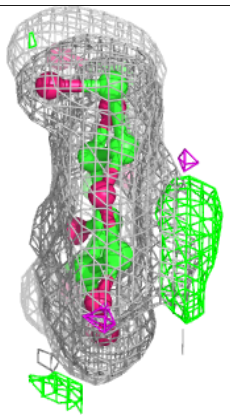


Electron density around Chain D:

$2mF_o$-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
6	EDO	B	503	4/4	0.79	0.11	36,36,38,39	0
4	ACT	A	502	4/4	0.82	0.13	39,43,44,49	0
6	EDO	B	504	4/4	0.82	0.10	42,42,43,44	0
6	EDO	A	505	4/4	0.83	0.12	33,33,35,35	0
7	PGO	B	505	5/5	0.83	0.11	26,30,32,32	0
6	EDO	A	506	4/4	0.86	0.10	28,29,30,31	0
8	PEG	B	506	7/7	0.86	0.15	33,36,37,37	0
6	EDO	A	504	4/4	0.90	0.11	34,35,40,43	0
5	SO4	B	502	5/5	0.97	0.10	37,38,42,47	0
5	SO4	A	503	5/5	0.99	0.06	22,24,29,31	0
3	CL	B	501	1/1	0.99	0.06	25,25,25,25	0
3	CL	A	501	1/1	0.99	0.06	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.