Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 01:10 AM EDT

PDB ID	:	3CX4
Title	:	Crystal Structure of E.coli GS mutant E377A in complex with ADP and oligosaccharides
Authors	:	Sheng, F.; Geiger, J.H.
Deposited on	:	2008-04-23
Resolution	:	2.29 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:

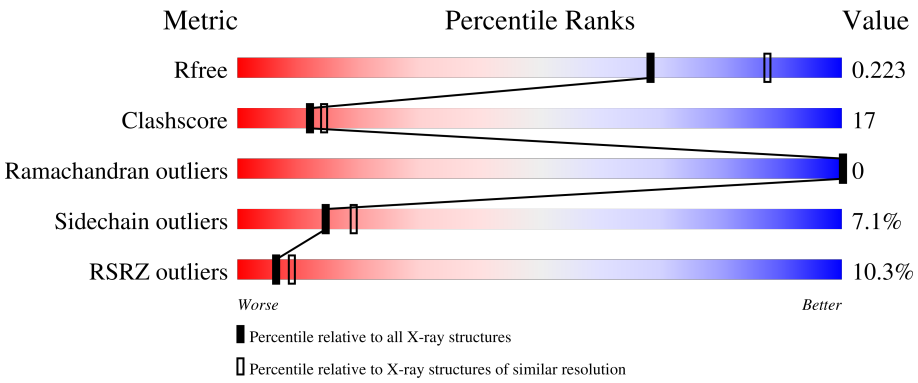
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	485	10%, 76%, 20%, • •
2	B	3	67%, 33%
3	C	2	50%, 50%
4	D	5	20%, 80%
5	E	6	67%, 33%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	C	2	-	-	-	X
4	GLC	D	1	-	-	-	X
9	ETE	A	521	-	-	X	-
9	ETE	A	522	-	-	X	X
9	ETE	A	527	-	-	-	X
9	ETE	A	528	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 4285 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.

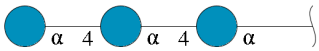
- Molecule 1 is a protein called Glycogen synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	3751	2415	656	666	14	13	4	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	ALA	GLU	engineered mutation	UNP P0A6U8
A	478	LEU	-	expression tag	UNP P0A6U8
A	479	GLU	-	expression tag	UNP P0A6U8
A	480	HIS	-	expression tag	UNP P0A6U8
A	481	HIS	-	expression tag	UNP P0A6U8
A	482	HIS	-	expression tag	UNP P0A6U8
A	483	HIS	-	expression tag	UNP P0A6U8
A	484	HIS	-	expression tag	UNP P0A6U8
A	485	HIS	-	expression tag	UNP P0A6U8

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

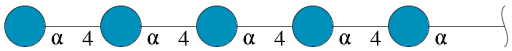


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	3	34	18	16	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

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

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	D	5	56	30	26	0	0	0

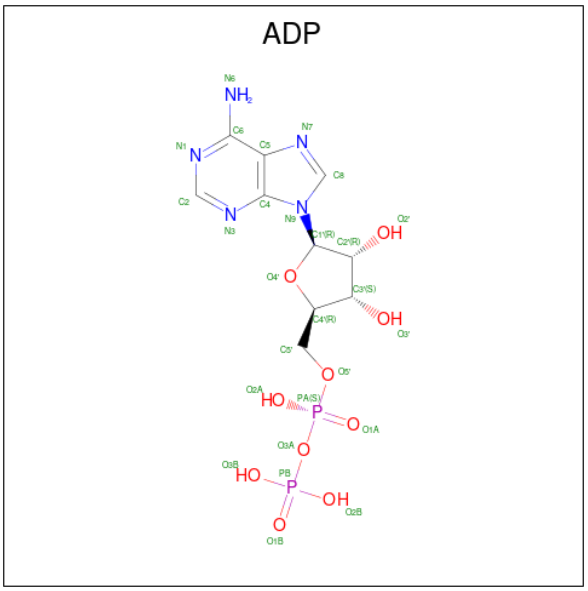
- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
5	E	6	67	36	31	0	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

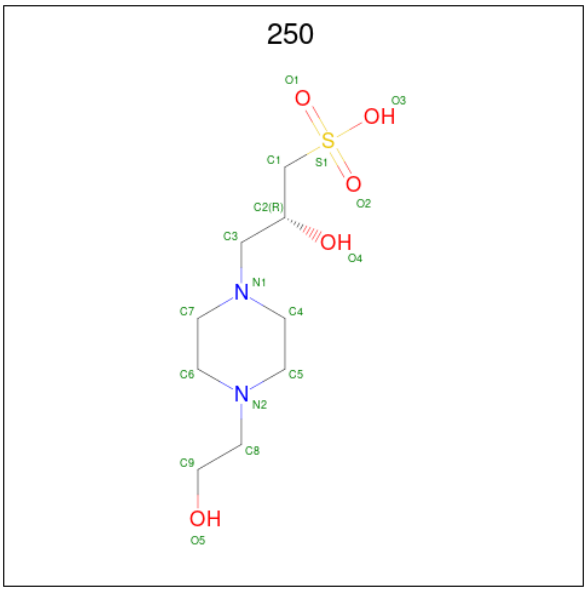
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	2	2	2	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



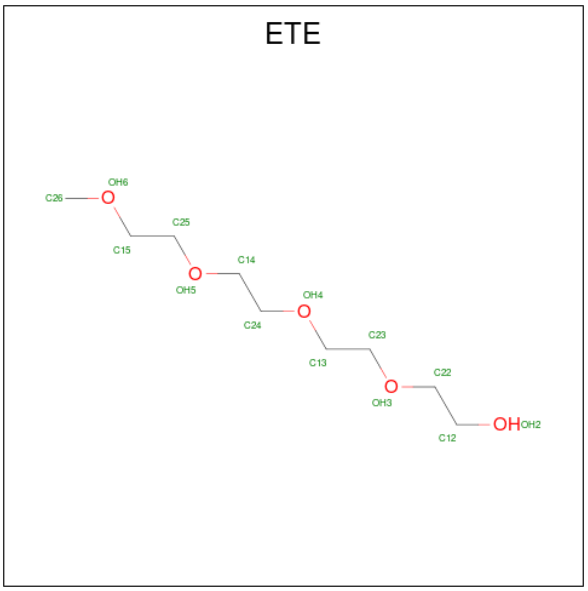
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	27	10	5	10	2	0	0

- Molecule 8 is (2R)-2-hydroxy-3-[4-(2-hydroxyethyl)piperazin-1-yl]propane-1-sulfonic acid (three-letter code: 250) (formula: $C_9H_{20}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	A	1	17	9	2	5	1	0	0

- Molecule 9 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: $C_9H_{20}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	14	9	5	0	0
			Total	C	O		
9	A	1	11	7	4	0	0
			Total	C	O		
9	A	1	14	9	5	0	0
			Total	C	O		
9	A	1	12	8	4	0	0
			Total	C	O		
9	A	1	6	4	2	0	0
			Total	C	O		
9	A	1	4	2	2	0	0
			Total	C	O		
9	A	1	5	3	2	0	0
			Total	C	O		
9	A	1	11	8	3	0	0
			Total	C	O		
9	A	1	8	5	3	0	0
			Total	C	O		
9	A	1	6	4	2	0	0
			Total	C	O		
9	A	1	10	7	3	0	0
			Total	C	O		
9	A	1	6	4	2	0	0

- Molecule 10 is water.

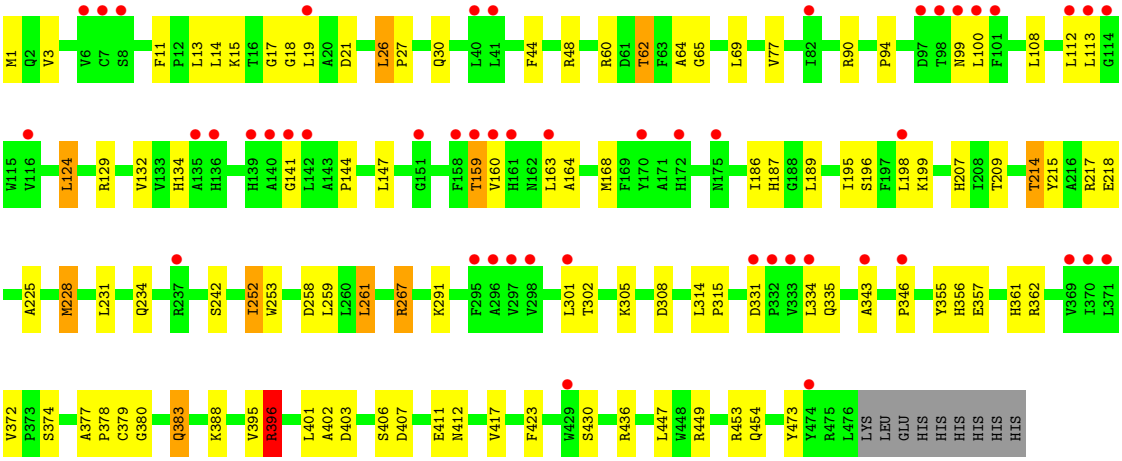
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	201	201	201	0	0

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: Glycogen synthase

Chain A: 10% 76% 20%



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain B: 67% 33%

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C: 50% 50%

• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D: 20% 80%

• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	126.32Å 126.32Å 152.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.31 – 2.29 32.61 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (9.31-2.29) 99.9 (32.61-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.221 0.190 , 0.223	Depositor DCC
R_{free} test set	2728 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4285	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: 250, ETE, GLC, NA, ADP, BGC

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	0.55	0/3865	0.68	3/5258 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	267	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	48	ARG	NE-CZ-NH2	-5.90	117.35	120.30

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	3751	0	3698	128	0
2	B	34	0	30	4	0
3	C	23	0	21	0	0
4	D	56	0	48	1	0
5	E	67	0	57	3	0
6	A	2	0	0	0	0
7	A	27	0	12	0	0
8	A	17	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	107	0	123	56	0
10	A	201	0	0	12	0
All	All	4285	0	4009	139	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 17.

All (139) 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)
8:A:517:250:H42	9:A:527:ETE:H132	1.23	1.16
1:A:252:ILE:CD1	9:A:528:ETE:H141	1.79	1.12
1:A:380:GLY:H	9:A:521:ETE:H242	1.16	1.10
1:A:252:ILE:HD11	9:A:528:ETE:H141	1.22	1.09
1:A:21:ASP:OD1	9:A:528:ETE:H252	1.58	1.01
1:A:1:MET:HE3	1:A:132:VAL:HG23	1.44	0.99
1:A:379:CYS:H	9:A:521:ETE:H241	1.24	0.98
1:A:357:GLU:OE1	9:A:528:ETE:C24	2.21	0.88
1:A:380:GLY:N	9:A:521:ETE:H242	1.88	0.88
1:A:252:ILE:HG12	9:A:528:ETE:C15	2.03	0.87
1:A:383:GLN:HE21	1:A:383:GLN:H	1.21	0.86
9:A:520:ETE:H263	10:A:730:HOH:O	1.75	0.86
1:A:214:THR:HG23	1:A:403:ASP:OD1	1.76	0.85
1:A:69:LEU:HD22	1:A:124:LEU:HD13	1.57	0.85
1:A:62:THR:CG2	1:A:64:ALA:H	1.90	0.85
1:A:1:MET:CE	1:A:132:VAL:HG23	2.07	0.84
1:A:62:THR:HG22	1:A:64:ALA:H	1.43	0.83
1:A:134:HIS:NE2	1:A:159:THR:CG2	2.43	0.82
1:A:357:GLU:OE1	9:A:528:ETE:H242	1.79	0.81
5:E:1:BGC:H6C2	5:E:2:GLC:H5	1.61	0.81
1:A:1:MET:CE	1:A:132:VAL:CG2	2.59	0.80
1:A:252:ILE:HG12	9:A:528:ETE:H152	1.63	0.80
1:A:21:ASP:OD1	9:A:528:ETE:C25	2.31	0.79
1:A:234:GLN:HG2	10:A:655:HOH:O	1.83	0.77
1:A:214:THR:CG2	1:A:403:ASP:OD1	2.33	0.77
1:A:252:ILE:HG12	9:A:528:ETE:H151	1.68	0.75
1:A:357:GLU:OE1	9:A:528:ETE:H241	1.84	0.74
1:A:17:GLY:HA3	2:B:3:GLC:C6	2.18	0.74
8:A:517:250:H42	9:A:527:ETE:C13	2.13	0.73
1:A:1:MET:HE3	1:A:132:VAL:CG2	2.17	0.73
1:A:21:ASP:CG	9:A:528:ETE:H252	2.10	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLY:H	9:A:521:ETE:C24	1.98	0.72
5:E:1:BGC:H6C2	5:E:2:GLC:C5	2.19	0.72
1:A:302:THR:HB	9:A:527:ETE:C12	2.19	0.71
1:A:168:MET:HG2	9:A:526:ETE:H151	1.72	0.71
1:A:379:CYS:N	9:A:521:ETE:H241	2.04	0.71
1:A:305:LYS:NZ	9:A:521:ETE:H232	2.06	0.70
1:A:11:PHE:CZ	9:A:528:ETE:H142	2.27	0.70
1:A:62:THR:HG22	1:A:64:ALA:N	2.06	0.69
1:A:234:GLN:CG	10:A:655:HOH:O	2.39	0.69
1:A:234:GLN:CD	10:A:655:HOH:O	2.31	0.69
1:A:267:ARG:HD2	1:A:453:ARG:O	1.92	0.68
1:A:454:GLN:HE22	9:A:523:ETE:H141	1.59	0.68
1:A:214:THR:HG23	1:A:403:ASP:CG	2.14	0.67
1:A:252:ILE:CD1	9:A:528:ETE:C14	2.66	0.66
1:A:380:GLY:C	1:A:383:GLN:HE22	1.99	0.65
1:A:196:SER:HB3	1:A:199:LYS:HB2	1.80	0.64
1:A:407:ASP:H	9:A:522:ETE:H252	1.63	0.64
1:A:252:ILE:CG1	9:A:528:ETE:H141	2.28	0.64
1:A:402:ALA:O	9:A:522:ETE:H261	1.98	0.64
1:A:252:ILE:HD12	1:A:361:HIS:HE1	1.65	0.62
9:A:530:ETE:H231	9:A:531:ETE:C26	2.30	0.62
8:A:517:250:C4	9:A:527:ETE:H132	2.14	0.61
1:A:252:ILE:CG1	9:A:528:ETE:H151	2.29	0.61
1:A:362:ARG:HD2	10:A:727:HOH:O	1.99	0.61
1:A:159:THR:HB	1:A:209:THR:OG1	2.01	0.61
1:A:1:MET:CE	1:A:132:VAL:HG21	2.31	0.61
1:A:199:LYS:HG2	1:A:228:MET:HE1	1.84	0.60
1:A:62:THR:HB	1:A:65:GLY:O	2.03	0.58
1:A:1:MET:CE	1:A:473:TYR:HB3	2.34	0.58
1:A:134:HIS:NE2	1:A:159:THR:HG23	2.17	0.58
1:A:1:MET:HE1	1:A:132:VAL:CG2	2.33	0.57
1:A:383:GLN:HE21	1:A:383:GLN:N	1.96	0.57
1:A:356[B]:HIS:CE1	10:A:728:HOH:O	2.57	0.57
1:A:412:ASN:HD21	9:A:522:ETE:C14	2.18	0.56
1:A:60:ARG:NE	10:A:620:HOH:O	2.32	0.56
1:A:343:ALA:O	1:A:346:PRO:HD3	2.06	0.56
1:A:252:ILE:HD11	9:A:528:ETE:C14	2.15	0.55
1:A:301:LEU:HB3	1:A:334:LEU:HD12	1.89	0.55
1:A:62:THR:HG21	1:A:112:LEU:HD13	1.90	0.54
1:A:406:SER:HA	9:A:522:ETE:H251	1.89	0.54
1:A:305:LYS:HZ3	9:A:521:ETE:H232	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:NE2	1:A:159:THR:HG21	2.21	0.53
1:A:383:GLN:H	1:A:383:GLN:NE2	2.00	0.53
1:A:258:ASP:HB3	1:A:261:LEU:HD22	1.90	0.53
1:A:361:HIS:NE2	9:A:528:ETE:OH4	2.35	0.53
1:A:11:PHE:CG	9:A:528:ETE:H251	2.44	0.53
1:A:26:LEU:HD22	1:A:30:GLN:HG3	1.91	0.53
1:A:129[A]:ARG:HG3	10:A:714:HOH:O	2.08	0.52
1:A:331:ASP:O	1:A:335:GLN:HG3	2.08	0.52
1:A:252:ILE:HD12	1:A:361:HIS:CE1	2.43	0.52
9:A:526:ETE:H152	10:A:637:HOH:O	2.09	0.52
1:A:209:THR:HA	1:A:242:SER:O	2.10	0.51
1:A:1:MET:HE2	1:A:473:TYR:HB3	1.92	0.51
1:A:214:THR:HB	1:A:217:ARG:NH1	2.24	0.51
1:A:314:LEU:HB3	1:A:315:PRO:HD3	1.93	0.51
1:A:14:LEU:HD12	1:A:15:LYS:N	2.27	0.50
1:A:1:MET:HE1	1:A:132:VAL:HG21	1.92	0.50
1:A:374:SER:O	1:A:396:ARG:HD3	2.10	0.50
1:A:99:ASN:O	1:A:100:LEU:HB2	2.12	0.50
1:A:3:VAL:HG21	1:A:473:TYR:CE2	2.46	0.50
1:A:305:LYS:HZ1	9:A:521:ETE:H232	1.78	0.49
1:A:15:LYS:HE2	1:A:355:TYR:OH	2.12	0.49
5:E:1:BGC:C6	5:E:2:GLC:H5	2.39	0.49
1:A:207:HIS:HE1	1:A:242:SER:OG	1.96	0.49
1:A:17:GLY:HA3	2:B:3:GLC:H62	1.94	0.48
1:A:252:ILE:HG13	1:A:253:TRP:CD1	2.48	0.48
1:A:301:LEU:HB3	1:A:334:LEU:CD1	2.43	0.48
1:A:62:THR:HG23	1:A:64:ALA:H	1.73	0.47
1:A:252:ILE:HD12	1:A:252:ILE:O	2.15	0.47
1:A:44:PHE:CZ	1:A:94:PRO:HB3	2.50	0.47
1:A:407:ASP:H	9:A:522:ETE:C25	2.28	0.47
1:A:163:LEU:HD23	1:A:225:ALA:HA	1.96	0.46
1:A:291:LYS:NZ	9:A:520:ETE:H152	2.31	0.46
1:A:377:ALA:HA	9:A:521:ETE:H131	1.98	0.46
1:A:186:ILE:HG23	1:A:187:HIS:CD2	2.51	0.46
1:A:380:GLY:HA2	9:A:521:ETE:H231	1.98	0.46
9:A:522:ETE:H263	9:A:522:ETE:H242	1.98	0.46
9:A:524:ETE:H251	4:D:2:GLC:H5	1.97	0.46
1:A:252:ILE:CD1	1:A:361:HIS:CE1	2.99	0.45
1:A:305:LYS:HZ3	9:A:521:ETE:C23	2.29	0.45
1:A:412:ASN:HD21	9:A:522:ETE:H141	1.79	0.45
1:A:378:PRO:HD2	9:A:521:ETE:H131	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLY:N	9:A:521:ETE:C24	2.68	0.45
1:A:372:VAL:HB	1:A:395:VAL:HG12	1.98	0.45
1:A:141:GLY:O	1:A:144:PRO:HD2	2.17	0.44
1:A:252:ILE:HD12	1:A:252:ILE:C	2.38	0.44
1:A:395:VAL:HB	1:A:401:LEU:HD13	1.98	0.44
1:A:449:ARG:NH2	9:A:520:ETE:H221	2.33	0.44
1:A:60:ARG:HD2	10:A:620:HOH:O	2.18	0.44
1:A:412:ASN:HD21	9:A:522:ETE:H142	1.80	0.44
1:A:308:ASP:N	1:A:308:ASP:OD1	2.52	0.43
1:A:3:VAL:HG22	1:A:132:VAL:HB	1.99	0.43
1:A:168:MET:HA	1:A:195:ILE:O	2.19	0.43
1:A:215:TYR:CG	1:A:378:PRO:HA	2.54	0.43
1:A:396:ARG:HG3	1:A:423:PHE:CE1	2.54	0.42
1:A:17:GLY:HA3	2:B:3:GLC:H61	1.96	0.42
1:A:17:GLY:CA	2:B:3:GLC:C6	2.94	0.42
1:A:60:ARG:CD	10:A:620:HOH:O	2.68	0.42
1:A:228:MET:HG3	10:A:650:HOH:O	2.19	0.42
1:A:11:PHE:CE1	9:A:528:ETE:H142	2.55	0.41
1:A:18:GLY:HA3	9:A:521:ETE:H252	2.01	0.41
1:A:1:MET:HE1	1:A:473:TYR:HB3	2.03	0.41
1:A:13:LEU:HA	1:A:13:LEU:HD23	1.80	0.41
1:A:26:LEU:HB3	1:A:27:PRO:HD3	2.02	0.41
1:A:214:THR:O	1:A:218:GLU:HG3	2.21	0.41
1:A:164:ALA:HB1	9:A:527:ETE:H231	2.02	0.40
1:A:252:ILE:HG12	9:A:528:ETE:H141	2.04	0.40
1:A:252:ILE:HD13	9:A:528:ETE:OH4	2.21	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	478/485 (99%)	457 (96%)	21 (4%)	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	384/389 (99%)	357 (93%)	27 (7%)	15	19

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	26	LEU
1	A	62	THR
1	A	77	VAL
1	A	90	ARG
1	A	108	LEU
1	A	113	LEU
1	A	124	LEU
1	A	147	LEU
1	A	159	THR
1	A	160	VAL
1	A	189	LEU
1	A	198	LEU
1	A	214	THR
1	A	228	MET
1	A	231	LEU
1	A	252	ILE
1	A	259	LEU
1	A	261	LEU
1	A	383	GLN
1	A	388	LYS
1	A	396	ARG
1	A	411	GLU

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Mol	Chain	Res	Type
1	A	417	VAL
1	A	430	SER
1	A	436	ARG
1	A	447	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	175	ASN
1	A	187	HIS
1	A	192	ASN
1	A	194	GLN
1	A	207	HIS
1	A	223	GLN
1	A	233	GLN
1	A	246	ASN
1	A	279	GLN
1	A	281	GLN
1	A	383	GLN
1	A	412	ASN
1	A	454	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)

16 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	GLC	B	1	2	12,12,12	0.61	0	17,17,17	1.02	1 (5%)
2	GLC	B	2	2	11,11,12	0.61	0	15,15,17	1.76	3 (20%)
2	GLC	B	3	2	11,11,12	0.62	0	15,15,17	1.73	4 (26%)
3	GLC	C	1	3	12,12,12	0.64	0	17,17,17	1.33	3 (17%)
3	GLC	C	2	3	11,11,12	0.59	0	15,15,17	0.80	0
4	GLC	D	1	4	12,12,12	0.56	0	17,17,17	0.70	0
4	GLC	D	2	4	11,11,12	0.67	0	15,15,17	0.73	0
4	GLC	D	3	4	11,11,12	0.78	0	15,15,17	1.18	2 (13%)
4	GLC	D	4	4	11,11,12	0.65	0	15,15,17	1.03	1 (6%)
4	GLC	D	5	4	11,11,12	0.52	0	15,15,17	0.93	1 (6%)
5	BGC	E	1	5	12,12,12	0.59	0	17,17,17	1.56	4 (23%)
5	GLC	E	2	5	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
5	GLC	E	3	5	11,11,12	0.69	0	15,15,17	1.04	1 (6%)
5	GLC	E	4	5	11,11,12	0.82	0	15,15,17	1.28	2 (13%)
5	GLC	E	5	5	11,11,12	0.48	0	15,15,17	1.24	2 (13%)
5	GLC	E	6	5	11,11,12	0.76	0	15,15,17	1.20	1 (6%)

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	GLC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	2/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1
3	GLC	C	1	3	-	0/2/22/22	0/1/1/1
3	GLC	C	2	3	-	2/2/19/22	0/1/1/1
4	GLC	D	1	4	-	0/2/22/22	0/1/1/1
4	GLC	D	2	4	-	0/2/19/22	0/1/1/1
4	GLC	D	3	4	-	0/2/19/22	0/1/1/1
4	GLC	D	4	4	-	2/2/19/22	0/1/1/1
4	GLC	D	5	4	-	2/2/19/22	0/1/1/1
5	BGC	E	1	5	-	1/2/22/22	0/1/1/1
5	GLC	E	2	5	-	0/2/19/22	0/1/1/1
5	GLC	E	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	E	4	5	-	0/2/19/22	0/1/1/1
5	GLC	E	5	5	-	0/2/19/22	0/1/1/1
5	GLC	E	6	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GLC	C1-O5-C5	4.60	118.42	112.19
5	E	2	GLC	C1-O5-C5	3.37	116.75	112.19
5	E	1	BGC	O5-C5-C4	3.34	115.76	109.69
3	C	1	GLC	O5-C5-C4	3.22	115.54	109.69
5	E	1	BGC	C3-C4-C5	3.18	115.92	110.24
2	B	3	GLC	C1-O5-C5	3.17	116.49	112.19
2	B	3	GLC	C2-C3-C4	-2.98	105.74	110.89
2	B	2	GLC	O2-C2-C3	2.85	115.84	110.14
2	B	3	GLC	O4-C4-C5	2.83	116.33	109.30
5	E	4	GLC	O5-C5-C6	2.80	111.59	107.20
3	C	1	GLC	C3-C4-C5	2.76	115.16	110.24
4	D	3	GLC	O5-C5-C6	2.73	111.48	107.20
4	D	4	GLC	O5-C5-C6	2.70	111.43	107.20
5	E	4	GLC	O5-C1-C2	-2.66	106.67	110.77
2	B	3	GLC	O3-C3-C4	-2.53	104.50	110.35
5	E	1	BGC	C1-C2-C3	-2.52	105.09	110.31
5	E	6	GLC	C1-C2-C3	2.51	112.75	109.67
5	E	1	BGC	O5-C1-C2	-2.50	105.83	110.28
2	B	2	GLC	O5-C1-C2	2.45	114.56	110.77
5	E	3	GLC	O5-C1-C2	-2.44	107.00	110.77
2	B	1	GLC	O5-C5-C6	2.42	112.45	106.44
4	D	3	GLC	C3-C4-C5	-2.29	106.16	110.24
3	C	1	GLC	C1-O5-C5	2.28	117.97	113.66
5	E	5	GLC	O5-C5-C6	2.12	110.53	107.20
4	D	5	GLC	O5-C1-C2	-2.12	107.49	110.77
5	E	5	GLC	O4-C4-C3	2.01	114.99	110.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	GLC	O5-C5-C6-O6
4	D	5	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	2	GLC	C4-C5-C6-O6
4	D	5	GLC	C4-C5-C6-O6
4	D	4	GLC	C4-C5-C6-O6
4	D	4	GLC	O5-C5-C6-O6
5	E	1	BGC	C4-C5-C6-O6
3	C	2	GLC	C4-C5-C6-O6
3	C	2	GLC	O5-C5-C6-O6

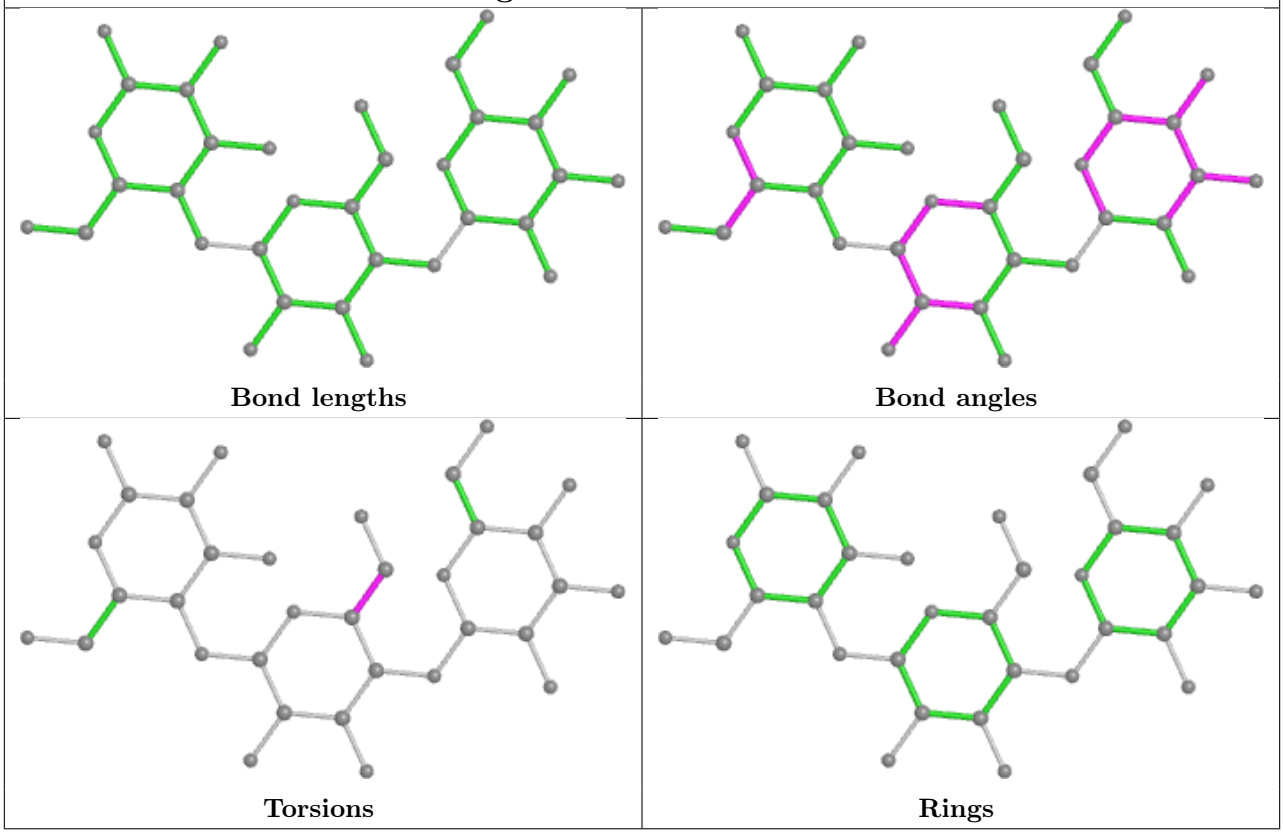
There are no ring outliers.

4 monomers are involved in 8 short contacts:

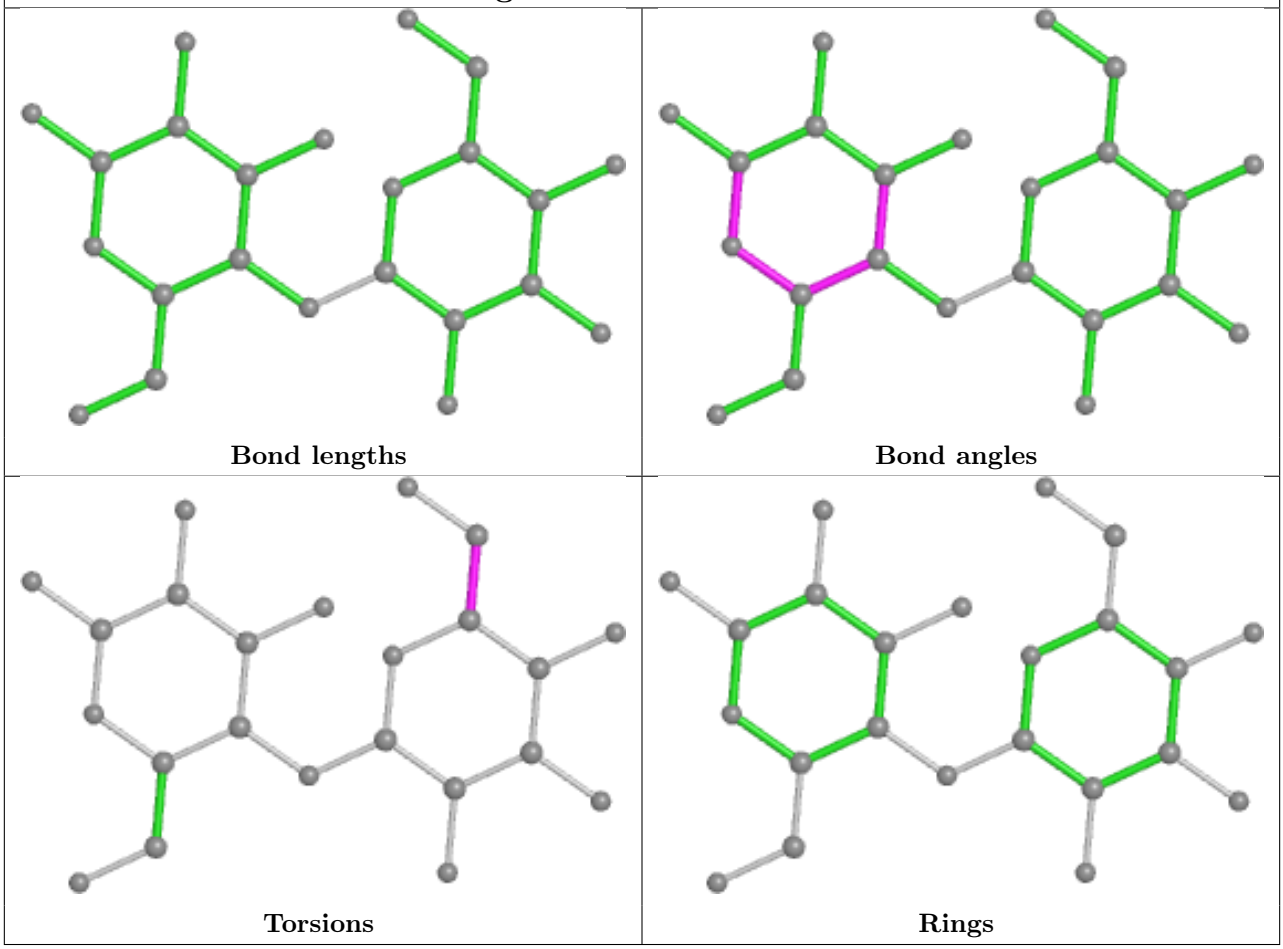
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	BGC	3	0
2	B	3	GLC	4	0
4	D	2	GLC	1	0
5	E	2	GLC	3	0

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

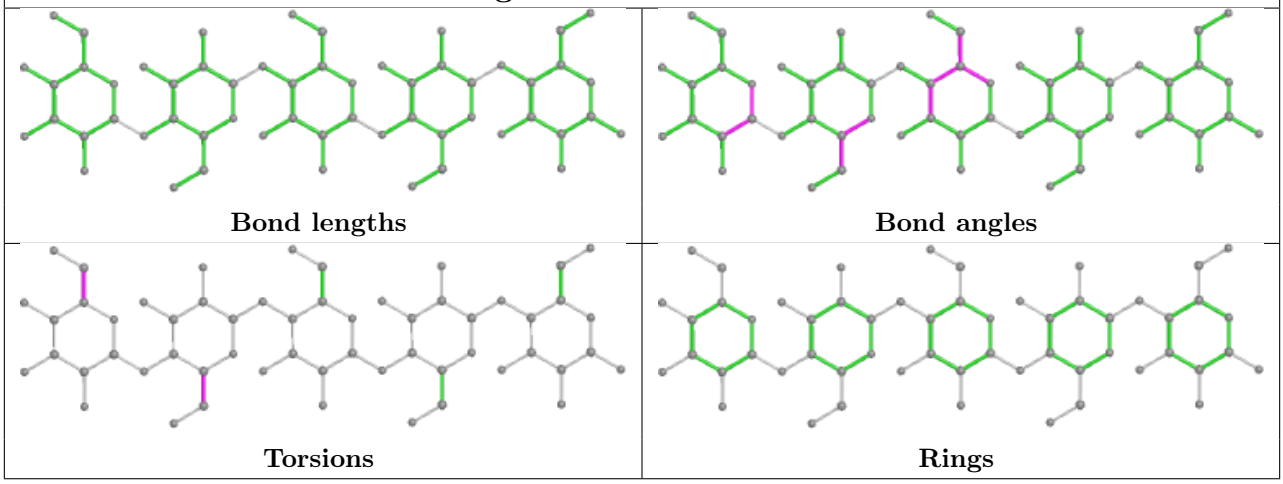
Oligosaccharide Chain B



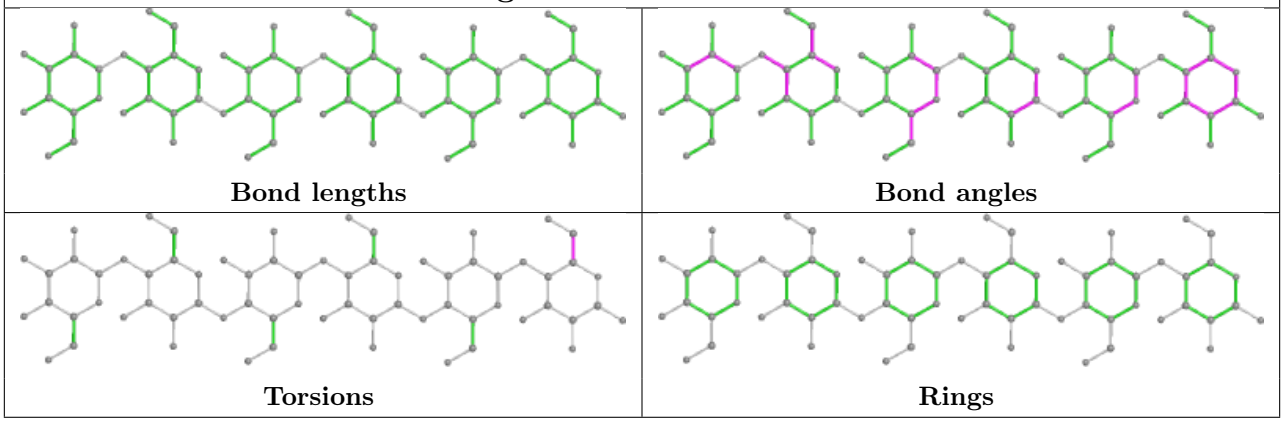
Oligosaccharide Chain C



Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
9	ETE	A	520	-	13,13,13	0.46	0	12,12,12	0.33	0
9	ETE	A	527	-	10,10,13	0.52	0	9,9,12	0.24	0
9	ETE	A	530	-	9,9,13	0.57	0	8,8,12	0.15	0
9	ETE	A	525	-	3,3,13	0.43	0	2,2,12	0.32	0
9	ETE	A	522	-	13,13,13	0.59	0	12,12,12	0.20	0
7	ADP	A	500	6	24,29,29	0.83	0	29,45,45	1.23	2 (6%)
9	ETE	A	526	-	4,4,13	0.49	0	3,3,12	0.25	0
9	ETE	A	521	-	10,10,13	0.52	0	9,9,12	0.33	0
8	250	A	517	-	17,17,17	0.87	1 (5%)	21,23,23	2.57	11 (52%)
9	ETE	A	524	-	5,5,13	0.49	0	4,4,12	0.23	0
9	ETE	A	529	-	5,5,13	0.51	0	4,4,12	0.32	0
9	ETE	A	528	-	7,7,13	0.51	0	6,6,12	0.64	0
9	ETE	A	531	-	5,5,13	0.52	0	4,4,12	0.09	0
9	ETE	A	523	-	11,11,13	0.55	0	10,10,12	0.21	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
9	ETE	A	520	-	-	5/11/11/11	-
9	ETE	A	527	-	-	5/8/8/11	-
9	ETE	A	530	-	-	4/7/7/11	-
9	ETE	A	525	-	-	1/1/1/11	-
9	ETE	A	522	-	-	8/11/11/11	-
7	ADP	A	500	6	-	4/12/32/32	0/3/3/3
9	ETE	A	526	-	-	1/2/2/11	-
9	ETE	A	521	-	-	5/8/8/11	-
8	250	A	517	-	-	4/12/22/22	0/1/1/1
9	ETE	A	524	-	-	1/3/3/11	-
9	ETE	A	529	-	-	2/3/3/11	-
9	ETE	A	528	-	-	5/5/5/11	-
9	ETE	A	531	-	-	3/3/3/11	-
9	ETE	A	523	-	-	6/9/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	517	250	C1-S1	-2.66	1.67	1.77

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	517	250	C5-N2-C6	4.94	119.95	108.83
7	A	500	ADP	N3-C2-N1	-4.70	121.34	128.68
8	A	517	250	C4-N1-C7	4.13	118.12	108.83
8	A	517	250	C8-N2-C6	3.77	120.88	111.23
8	A	517	250	C7-N1-C3	3.65	121.81	111.20
8	A	517	250	O1-S1-C1	3.23	110.78	106.94
8	A	517	250	C8-N2-C5	3.10	119.16	111.23
8	A	517	250	C4-N1-C3	3.05	120.05	111.20
8	A	517	250	C4-C5-N2	-2.79	104.91	110.64
8	A	517	250	C6-C7-N1	-2.46	105.59	110.64
7	A	500	ADP	O2B-PB-O1B	2.41	120.11	110.68
8	A	517	250	C5-C4-N1	-2.32	105.87	110.64
8	A	517	250	O2-S1-C1	2.18	109.53	106.94

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	520	ETE	C14-C24-OH4-C13
9	A	522	ETE	OH4-C13-C23-OH3
9	A	520	ETE	OH4-C13-C23-OH3
9	A	520	ETE	OH6-C15-C25-OH5
9	A	530	ETE	OH5-C14-C24-OH4
9	A	522	ETE	OH6-C15-C25-OH5
9	A	521	ETE	OH5-C14-C24-OH4
9	A	522	ETE	OH5-C14-C24-OH4
9	A	523	ETE	OH4-C13-C23-OH3
9	A	522	ETE	OH2-C12-C22-OH3
8	A	517	250	C2-C3-N1-C4
9	A	526	ETE	OH6-C15-C25-OH5
9	A	521	ETE	OH4-C13-C23-OH3
9	A	521	ETE	C15-C25-OH5-C14
9	A	528	ETE	OH5-C14-C24-OH4
9	A	525	ETE	OH6-C15-C25-OH5
9	A	528	ETE	C15-C25-OH5-C14
7	A	500	ADP	C3'-C4'-C5'-O5'
9	A	528	ETE	OH6-C15-C25-OH5
7	A	500	ADP	PA-O3A-PB-O1B
7	A	500	ADP	O4'-C4'-C5'-O5'
9	A	527	ETE	OH4-C13-C23-OH3
9	A	523	ETE	C12-C22-OH3-C23
9	A	522	ETE	C25-C15-OH6-C26
9	A	530	ETE	C13-C23-OH3-C22
7	A	500	ADP	PB-O3A-PA-O5'
9	A	520	ETE	OH2-C12-C22-OH3
9	A	521	ETE	C23-C13-OH4-C24
9	A	530	ETE	C14-C24-OH4-C13
9	A	523	ETE	C13-C23-OH3-C22
9	A	527	ETE	C13-C23-OH3-C22
9	A	522	ETE	C15-C25-OH5-C14
8	A	517	250	S1-C1-C2-O4
9	A	523	ETE	C15-C25-OH5-C14
9	A	523	ETE	C23-C13-OH4-C24
9	A	521	ETE	C13-C23-OH3-C22
9	A	529	ETE	OH6-C15-C25-OH5
9	A	527	ETE	C12-C22-OH3-C23
9	A	529	ETE	C24-C14-OH5-C25
8	A	517	250	N2-C8-C9-O5
9	A	527	ETE	C14-C24-OH4-C13
9	A	522	ETE	C13-C23-OH3-C22
9	A	531	ETE	C25-C15-OH6-C26

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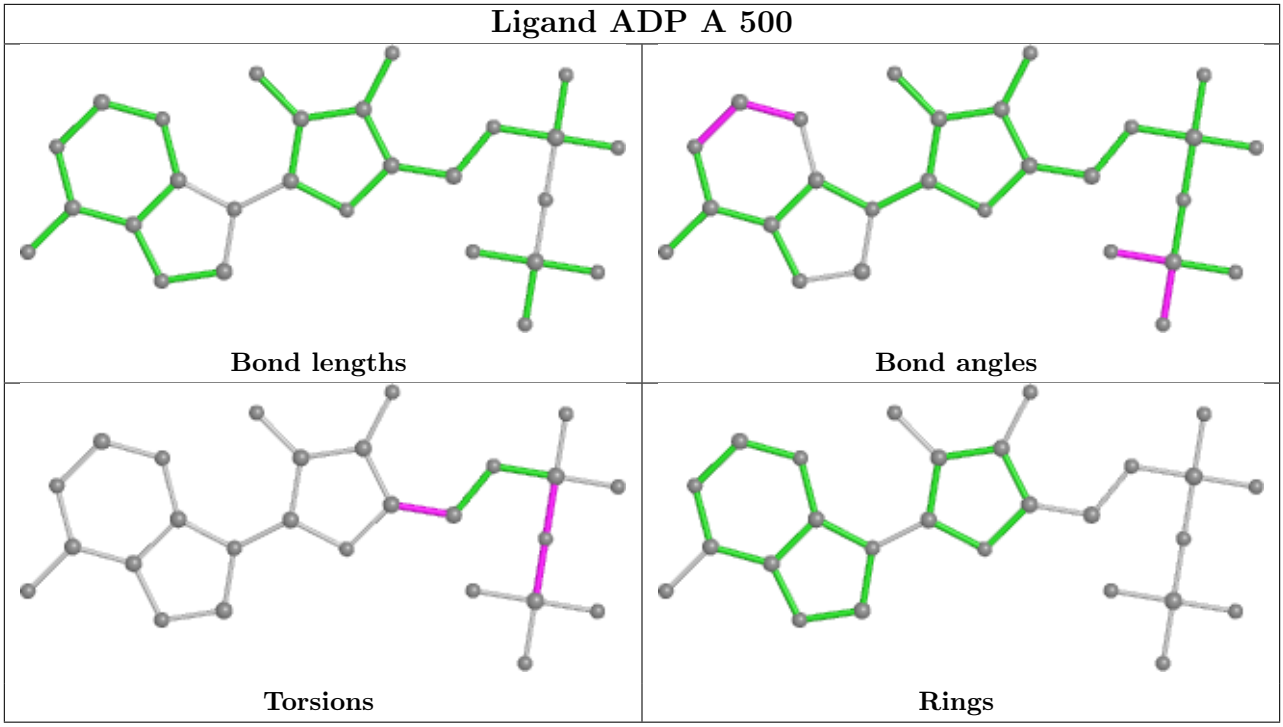
Mol	Chain	Res	Type	Atoms
9	A	524	ETE	OH5-C14-C24-OH4
9	A	531	ETE	OH6-C15-C25-OH5
9	A	528	ETE	C14-C24-OH4-C13
9	A	531	ETE	C15-C25-OH5-C14
9	A	528	ETE	C24-C14-OH5-C25
9	A	523	ETE	OH5-C14-C24-OH4
9	A	530	ETE	C24-C14-OH5-C25
8	A	517	250	S1-C1-C2-C3
9	A	522	ETE	C23-C13-OH4-C24
9	A	527	ETE	C24-C14-OH5-C25
9	A	520	ETE	OH5-C14-C24-OH4

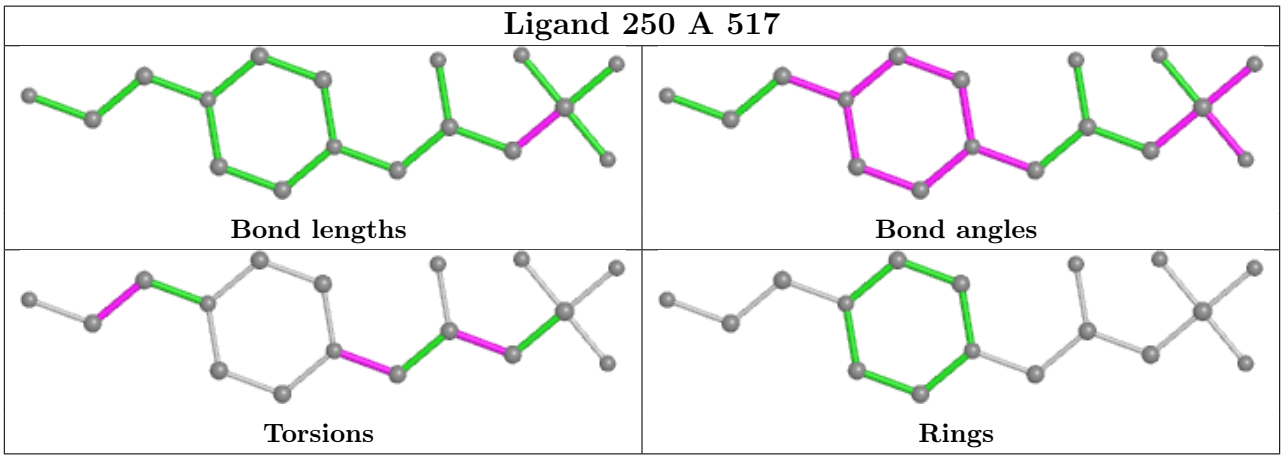
There are no ring outliers.

11 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	520	ETE	3	0
9	A	527	ETE	5	0
9	A	530	ETE	1	0
9	A	522	ETE	8	0
9	A	526	ETE	2	0
9	A	521	ETE	14	0
8	A	517	250	3	0
9	A	524	ETE	1	0
9	A	528	ETE	21	0
9	A	531	ETE	1	0
9	A	523	ETE	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 then 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	476/485 (98%)	0.34	49 (10%) 6 9	35, 47, 68, 80	34 (7%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	THR	6.4
1	A	99	ASN	6.2
1	A	6	VAL	4.7
1	A	113	LEU	4.4
1	A	135	ALA	4.1
1	A	140	ALA	4.1
1	A	198	LEU	4.1
1	A	370	ILE	3.8
1	A	101	PHE	3.7
1	A	136	HIS	3.4
1	A	297	VAL	3.4
1	A	158	PHE	3.4
1	A	371	LEU	3.4
1	A	100	LEU	3.4
1	A	159	THR	3.3
1	A	7	CYS	3.2
1	A	40	LEU	3.2
1	A	301	LEU	2.9
1	A	343	ALA	2.9
1	A	369	VAL	2.9
1	A	82	ILE	2.9
1	A	346	PRO	2.9
1	A	142	LEU	2.8
1	A	334	LEU	2.8
1	A	139	HIS	2.7
1	A	8	SER	2.7
1	A	175	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	160	VAL	2.6
1	A	237	ARG	2.6
1	A	332	PRO	2.6
1	A	298	VAL	2.5
1	A	151	GLY	2.5
1	A	116	VAL	2.5
1	A	19	LEU	2.5
1	A	295	PHE	2.4
1	A	296	ALA	2.4
1	A	172	HIS	2.4
1	A	97	ASP	2.4
1	A	331	ASP	2.3
1	A	41	LEU	2.3
1	A	170	TYR	2.2
1	A	141	GLY	2.2
1	A	114	GLY	2.2
1	A	474	TYR	2.2
1	A	112	LEU	2.1
1	A	161	HIS	2.1
1	A	429	TRP	2.1
1	A	163	LEU	2.1
1	A	333	VAL	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	GLC	C	1	12/12	0.77	0.30	90,91,91,92	1
3	GLC	C	2	11/12	0.78	0.47	92,93,95,95	0
4	GLC	D	1	12/12	0.79	0.50	66,67,68,68	12
2	GLC	B	1	12/12	0.82	0.36	50,51,51,52	12
2	GLC	B	2	11/12	0.84	0.21	50,52,55,57	0
5	BGC	E	1	12/12	0.88	0.28	72,75,75,76	12

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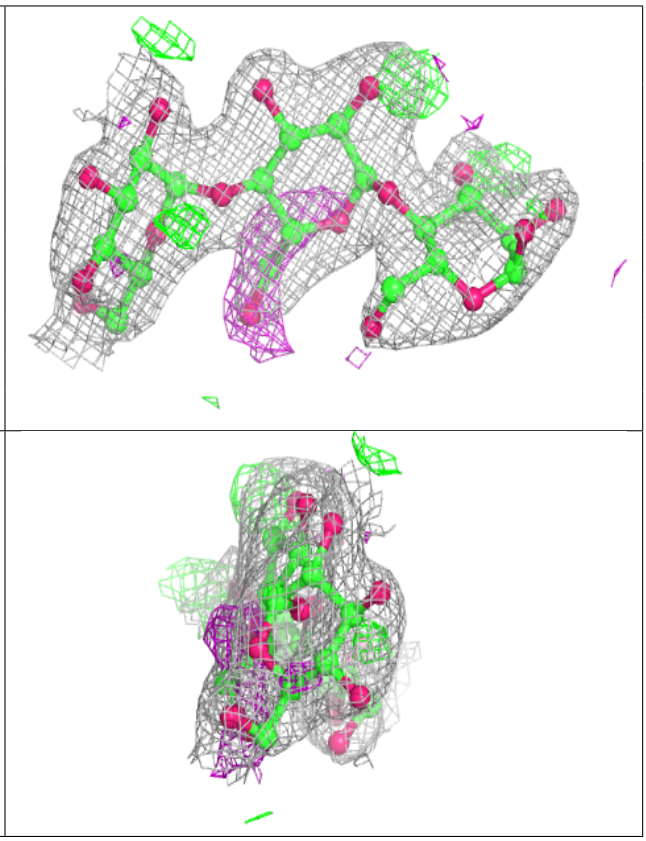
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLC	D	5	11/12	0.91	0.34	79,81,82,83	0
4	GLC	D	4	11/12	0.91	0.22	67,69,74,76	0
4	GLC	D	2	11/12	0.92	0.21	60,62,63,64	0
5	GLC	E	3	11/12	0.93	0.26	66,68,68,68	0
2	GLC	B	3	11/12	0.94	0.18	54,55,56,57	0
5	GLC	E	4	11/12	0.94	0.26	62,63,64,65	0
4	GLC	D	3	11/12	0.95	0.14	58,60,64,65	0
5	GLC	E	5	11/12	0.95	0.15	56,58,59,60	0
5	GLC	E	2	11/12	0.96	0.22	69,70,71,71	11
5	GLC	E	6	11/12	0.96	0.15	55,56,56,57	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.

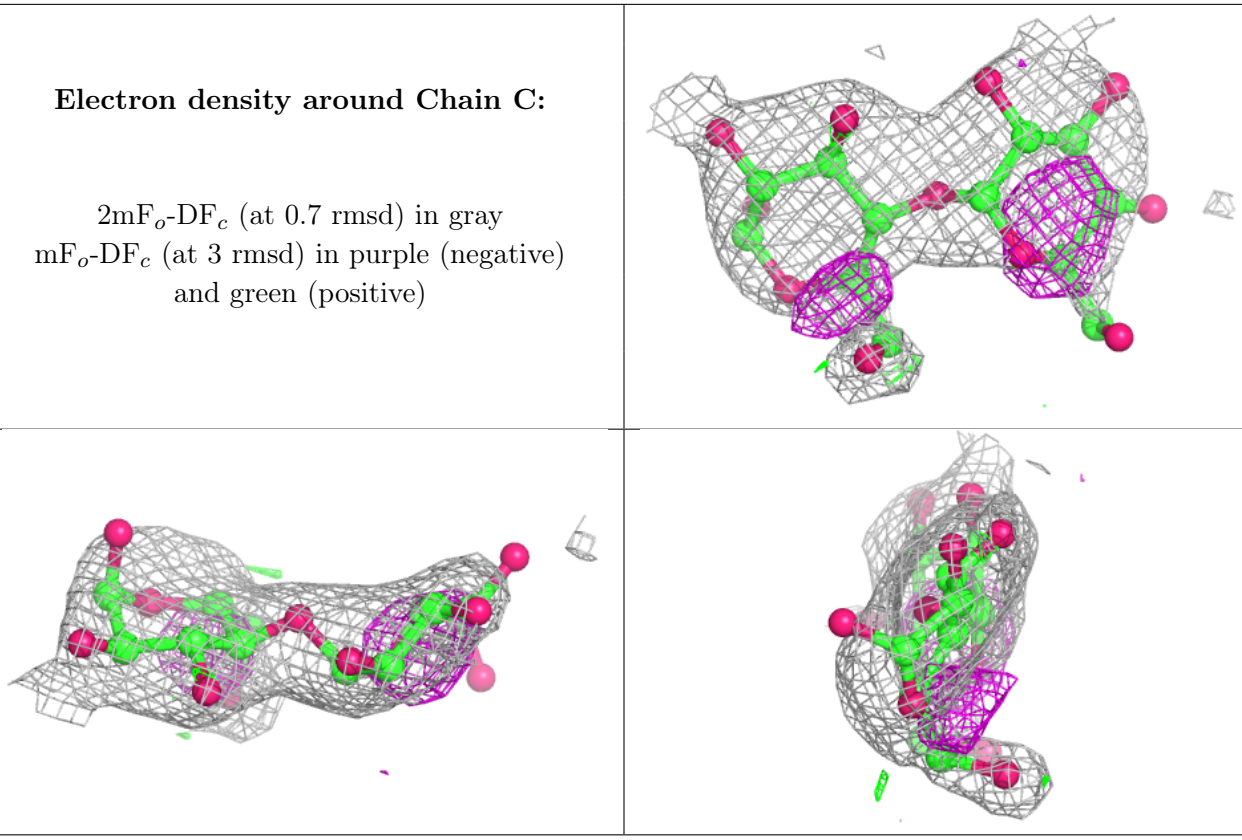
Electron density around Chain B:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



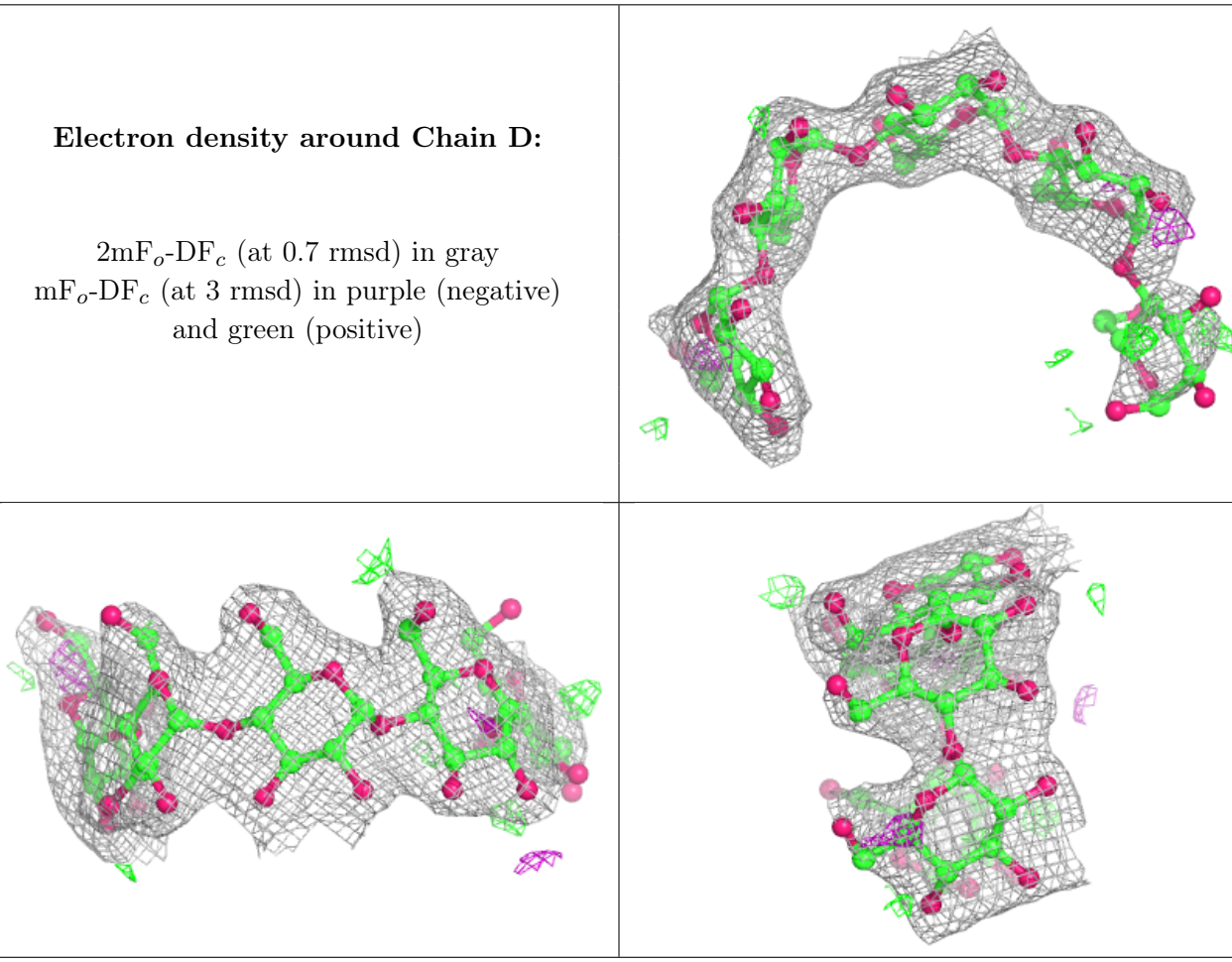
Electron density around Chain C:

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



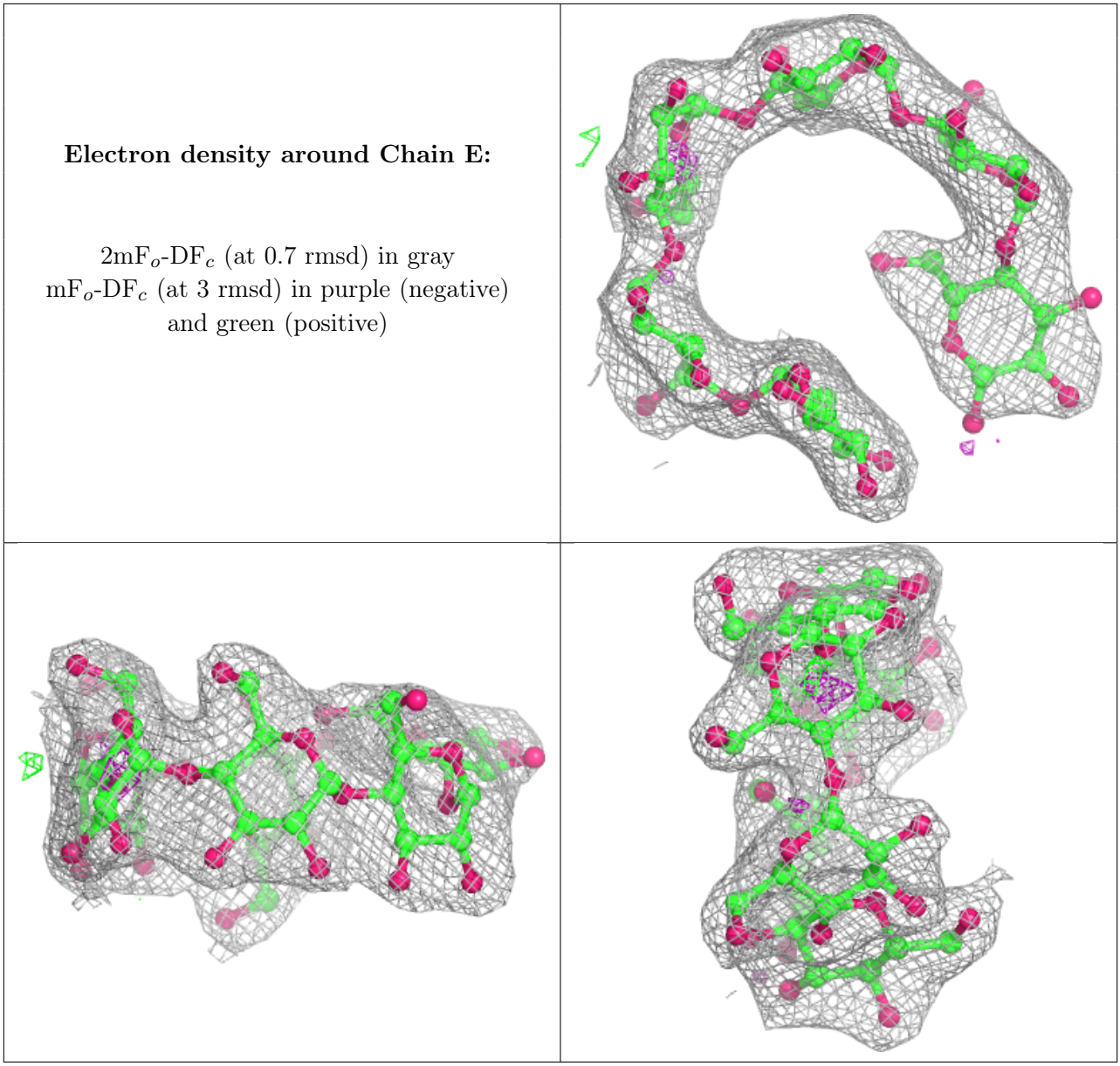
Electron density around Chain D:

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



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
9	ETE	A	522	14/14	0.60	0.42	52,59,68,68	10
9	ETE	A	529	6/14	0.64	0.23	82,83,84,84	1
9	ETE	A	525	4/14	0.66	0.33	96,96,96,96	0
9	ETE	A	523	12/14	0.67	0.32	78,79,80,80	8
9	ETE	A	527	11/14	0.75	0.73	89,89,90,90	11

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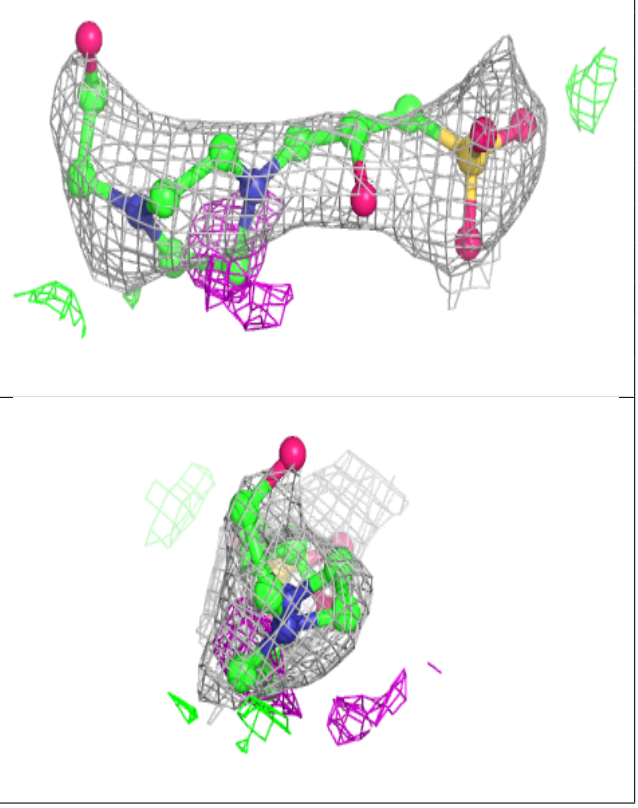
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	ETE	A	531	6/14	0.77	0.23	93,94,95,95	0
9	ETE	A	530	10/14	0.80	0.23	100,101,103,103	0
8	250	A	517	17/17	0.80	0.24	99,101,103,103	5
9	ETE	A	526	5/14	0.82	0.37	86,87,87,88	0
9	ETE	A	521	11/14	0.85	0.55	55,58,61,61	5
9	ETE	A	520	14/14	0.86	0.18	69,70,75,75	9
9	ETE	A	528	8/14	0.88	0.39	8,10,12,12	8
9	ETE	A	524	6/14	0.92	0.34	94,94,94,94	0
7	ADP	A	500	27/27	0.96	0.13	43,47,48,49	0
6	NA	A	518	1/1	0.96	0.42	58,58,58,58	0
6	NA	A	519	1/1	0.97	0.19	58,58,58,58	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.

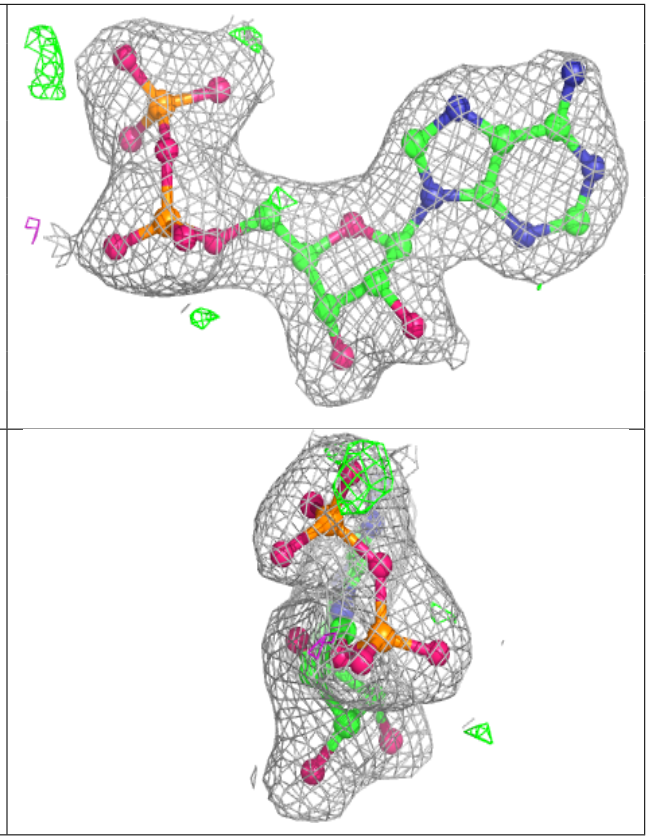
Electron density around 250 A 517:

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 ADP A 500:

$2mF_o$-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.