Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 02:17 PM JST

PDB ID	:	5ZSC
Title	:	Crystal structure of monkey TLR7 in complex with IMDQ and CCUUCC
Authors	:	Zhang, Z.; Ohto, U.; Shimizu, T.
Deposited on	:	2018-04-28
Resolution	:	2.20 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:

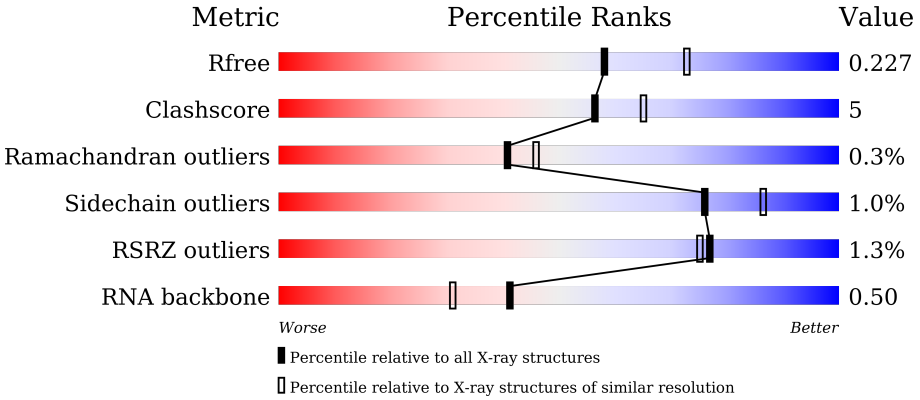
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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	823	2%, 82%, 12%, 6%
1	B	823	84%, 10%, 6%
2	C	6	17%, 50%, 33%
2	D	6	17%, 50%, 33%

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Mol	Chain	Length	Quality of chain
3	E	2	50% 50%
3	F	2	50% 50%
3	G	2	50% 50%

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
6	SO4	A	1010	-	-	X	-
6	SO4	B	1012	-	-	X	-
6	SO4	B	1018	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13897 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	775	6281	4027	1071	1153	30	0	0	0
1	A	774	6266	4015	1069	1152	30	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	440	LEU	SER	see sequence details	UNP B3Y653
B	441	VAL	GLU	see sequence details	UNP B3Y653
B	442	PRO	VAL	see sequence details	UNP B3Y653
B	443	ARG	GLY	see sequence details	UNP B3Y653
B	444	GLY	PHE	see sequence details	UNP B3Y653
B	445	SER	CYS	see sequence details	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653
B	840	GLU	-	expression tag	UNP B3Y653
B	841	PHE	-	expression tag	UNP B3Y653
B	842	LEU	-	expression tag	UNP B3Y653
B	843	VAL	-	expression tag	UNP B3Y653
B	844	PRO	-	expression tag	UNP B3Y653
B	845	ARG	-	expression tag	UNP B3Y653
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653

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Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	440	LEU	SER	see sequence details	UNP B3Y653
A	441	VAL	GLU	see sequence details	UNP B3Y653
A	442	PRO	VAL	see sequence details	UNP B3Y653
A	443	ARG	GLY	see sequence details	UNP B3Y653
A	444	GLY	PHE	see sequence details	UNP B3Y653
A	445	SER	CYS	see sequence details	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
A	840	GLU	-	expression tag	UNP B3Y653
A	841	PHE	-	expression tag	UNP B3Y653
A	842	LEU	-	expression tag	UNP B3Y653
A	843	VAL	-	expression tag	UNP B3Y653
A	844	PRO	-	expression tag	UNP B3Y653
A	845	ARG	-	expression tag	UNP B3Y653

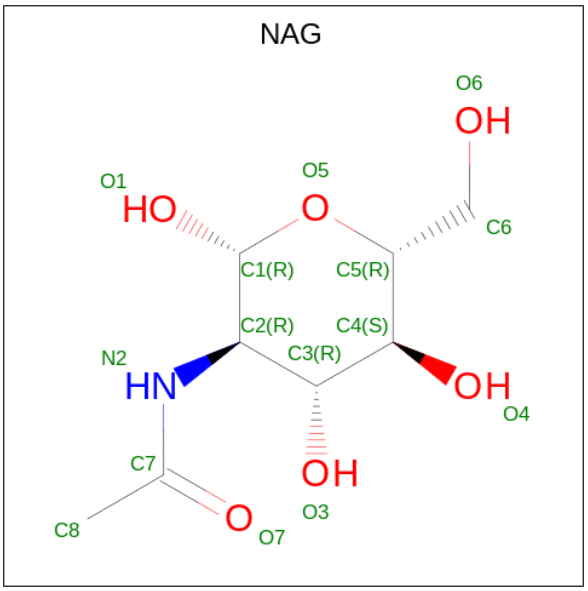
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	4	64	27	7	26	4	0	0	0
2	D	4	64	27	7	26	4	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

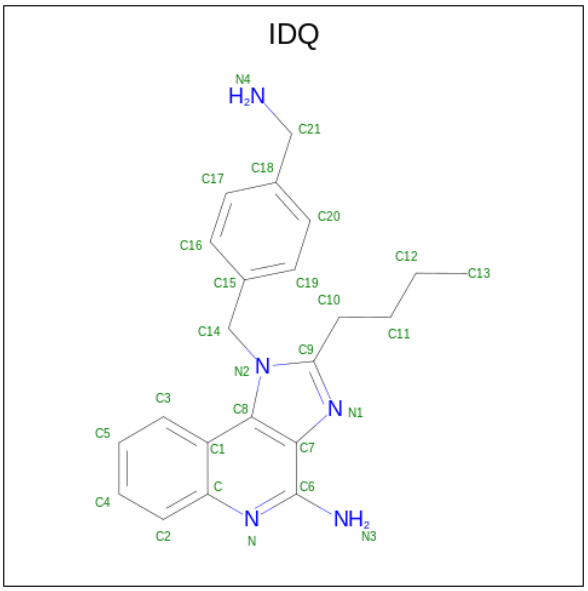
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



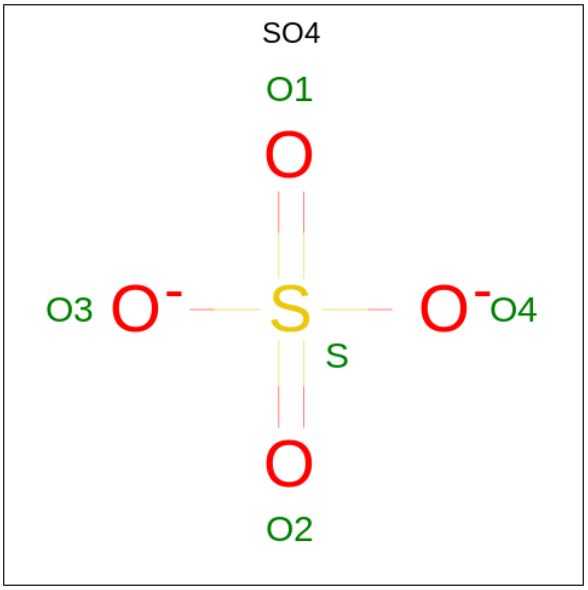
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0

- Molecule 5 is 1-[[4-(aminomethyl)phenyl]methyl]-2-butyl-imidazo[4,5-c]quinolin-4-amine (three-letter code: IDQ) (formula: $C_{22}H_{25}N_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N 27 22 5	0	0
5	A	1	Total C N 27 22 5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 7 is water.

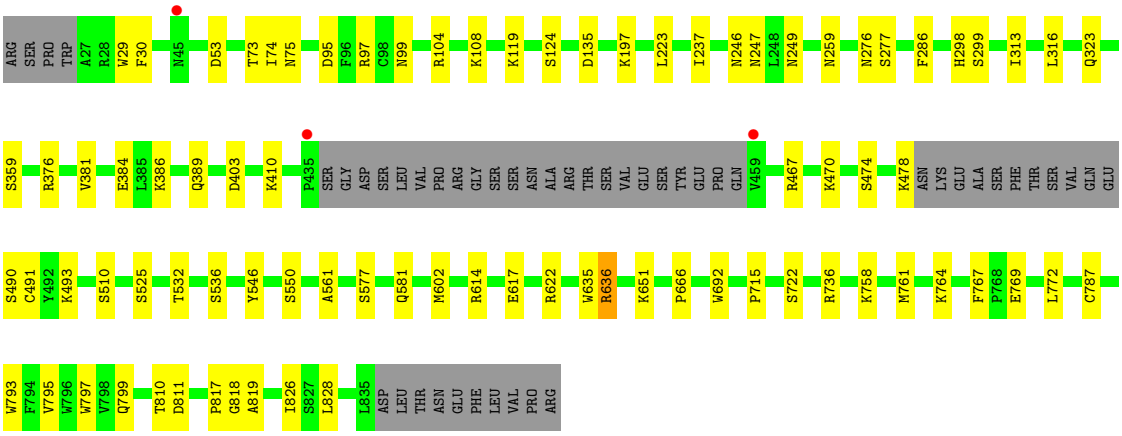
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	493	Total O 493 493	0	0
7	A	348	Total O 348 348	0	0
7	C	5	Total O 5 5	0	0
7	D	4	Total O 4 4	0	0

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.

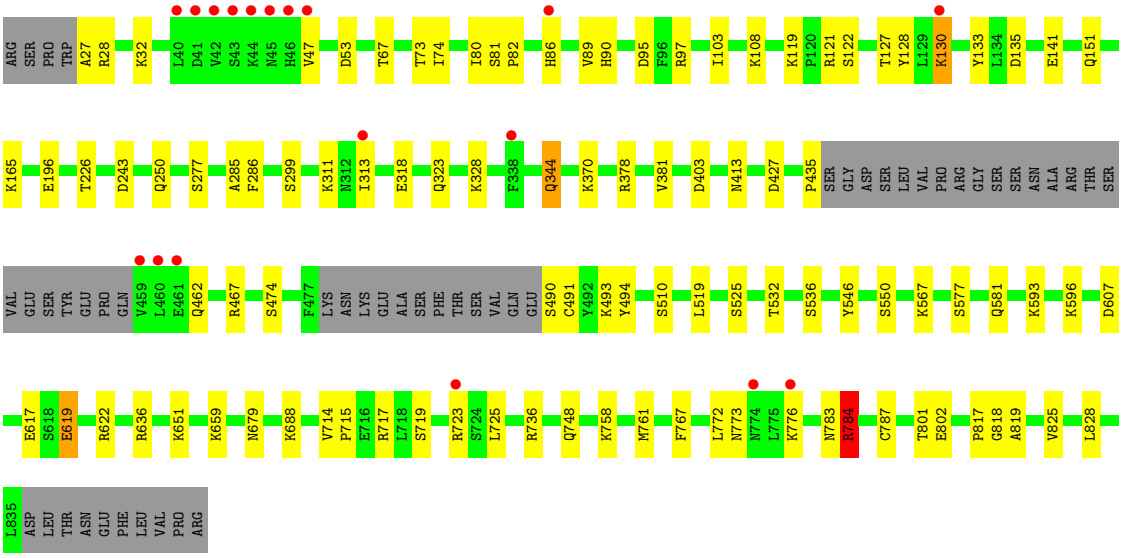
• Molecule 1: Toll-like receptor 7

Chain B: 84% 10% 6%

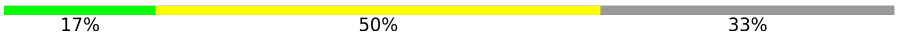


• Molecule 1: Toll-like receptor 7

Chain A: 2% 82% 12% 6%



• Molecule 2: RNA (5'-R(P*UP*UP*CP*A)-3')

Chain C: 

• Molecule 2: RNA (5'-R(P*UP*UP*CP*A)-3')

Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.57Å 138.83Å 149.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.20 49.29 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.28-2.20) 99.4 (49.29-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.191 , 0.227 0.191 , 0.227	Depositor DCC
R_{free} test set	5132 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13897	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 5.42% 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: IDQ, SO4, NAG

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	0.46	4/6397 (0.1%)	0.73	10/8667 (0.1%)
1	B	0.44	0/6413	0.64	6/8687 (0.1%)
2	C	0.59	0/69	1.15	0/105
2	D	0.51	0/69	1.06	0/105
All	All	0.46	4/12948 (0.0%)	0.69	16/17564 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	LYS	CD-CE	7.40	1.69	1.51
1	A	619	GLU	CB-CG	5.27	1.62	1.52
1	A	776	LYS	CD-CE	5.23	1.64	1.51
1	A	784	ARG	CB-CG	-5.22	1.38	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	784	ARG	NE-CZ-NH2	-17.62	111.49	120.30
1	A	784	ARG	NE-CZ-NH1	13.39	127.00	120.30
1	A	784	ARG	CG-CD-NE	-9.57	91.71	111.80
1	A	344	GLN	CA-CB-CG	7.08	128.97	113.40
1	A	723	ARG	CB-CG-CD	-6.90	93.67	111.60
1	A	328	LYS	CB-CG-CD	6.75	129.14	111.60
1	B	602	MET	CG-SD-CE	-6.61	89.62	100.20
1	B	636	ARG	CB-CG-CD	-5.98	96.04	111.60
1	A	311	LYS	CG-CD-CE	-5.97	93.98	111.90
1	B	636	ARG	CA-CB-CG	5.94	126.47	113.40
1	A	776	LYS	CB-CG-CD	5.92	127.00	111.60
1	A	784	ARG	CD-NE-CZ	5.83	131.77	123.60
1	A	130	LYS	CB-CG-CD	5.82	126.74	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	636	ARG	CG-CD-NE	5.34	123.01	111.80
1	B	769	GLU	N-CA-CB	5.33	120.20	110.60
1	B	769	GLU	CA-CB-CG	5.22	124.88	113.40

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	6266	0	6314	65	0
1	B	6281	0	6330	55	0
2	C	64	0	31	3	0
2	D	64	0	31	5	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
4	A	42	0	39	1	0
4	B	112	0	104	1	0
5	A	27	0	25	0	0
5	B	27	0	25	2	0
6	A	35	0	0	3	0
6	B	45	0	0	5	0
7	A	348	0	0	16	1
7	B	493	0	0	22	1
7	C	5	0	0	1	0
7	D	4	0	0	1	0
All	All	13897	0	12974	129	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 (129) 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:593:LYS:NZ	1:A:617:GLU:OE1	1.91	1.02
1:A:581:GLN:NE2	7:A:1101:HOH:O	1.92	0.97
1:B:617:GLU:OE1	7:B:1101:HOH:O	1.83	0.96
1:A:773:ASN:ND2	7:A:1103:HOH:O	1.98	0.95
1:B:30:PHE:O	7:B:1102:HOH:O	1.87	0.91
1:A:767:PHE:HB3	1:A:772:LEU:HD11	1.54	0.89
2:D:1:U:OP2	7:D:101:HOH:O	1.91	0.88
1:B:384:GLU:OE1	7:B:1103:HOH:O	1.90	0.88
1:B:614:ARG:NH1	7:B:1105:HOH:O	2.08	0.85
1:A:462:GLN:O	7:A:1102:HOH:O	1.98	0.81
6:B:1017:SO4:O1	7:B:1104:HOH:O	2.01	0.78
1:A:196:GLU:OE2	7:A:1105:HOH:O	2.07	0.72
1:A:490:SER:O	1:A:493:LYS:NZ	2.21	0.72
1:A:286:PHE:HB3	1:A:313:ILE:HD11	1.72	0.72
7:A:1106:HOH:O	3:G:2:NAG:O6	2.08	0.71
1:B:276:ASN:OD1	7:B:1109:HOH:O	2.09	0.70
1:B:722:SER:O	7:B:1106:HOH:O	2.08	0.70
1:B:478:LYS:O	7:B:1107:HOH:O	2.09	0.70
1:B:29:TRP:O	7:B:1108:HOH:O	2.09	0.69
1:A:97:ARG:NH2	1:A:474:SER:O	2.25	0.69
2:C:1:U:OP1	7:C:101:HOH:O	2.10	0.68
1:B:510:SER:OG	1:B:536:SER:O	2.10	0.68
1:A:141:GLU:OE1	7:A:1107:HOH:O	2.11	0.68
7:B:1449:HOH:O	1:A:688:LYS:HE3	1.94	0.67
1:B:561:ALA:O	7:B:1112:HOH:O	2.13	0.67
6:B:1012:SO4:O2	7:B:1111:HOH:O	2.13	0.67
1:A:510:SER:OG	1:A:536:SER:O	2.13	0.66
1:A:318:GLU:HG3	1:A:344:GLN:HG2	1.79	0.65
1:A:679:ASN:ND2	7:A:1120:HOH:O	2.28	0.64
1:B:97:ARG:NH2	1:B:474:SER:O	2.31	0.64
1:B:490:SER:O	1:B:493:LYS:NZ	2.32	0.63
1:B:119:LYS:NZ	7:B:1114:HOH:O	2.27	0.63
1:A:285:ALA:O	7:A:1108:HOH:O	2.16	0.63
1:A:95:ASP:OD1	1:A:97:ARG:HD3	1.98	0.62
1:A:467:ARG:HB2	2:C:4:A:OP1	1.99	0.62
1:A:127:THR:HG23	1:A:128:TYR:CD2	2.34	0.62
1:A:736:ARG:NH2	7:A:1122:HOH:O	2.30	0.62
6:B:1018:SO4:O3	7:B:1110:HOH:O	2.12	0.62
1:A:787:CYS:HB3	1:A:828:LEU:HD21	1.80	0.62
1:B:532:THR:HG23	6:A:1011:SO4:O4	2.00	0.62
1:B:491:CYS:HB3	4:B:1001:NAG:H81	1.81	0.62
1:B:95:ASP:OD1	1:B:97:ARG:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1012:SO4:O1	7:B:1111:HOH:O	2.17	0.57
1:B:470:LYS:NZ	7:B:1125:HOH:O	2.38	0.56
1:B:104:ARG:HB2	7:B:1247:HOH:O	2.05	0.56
1:B:787:CYS:HB3	1:B:828:LEU:HD21	1.87	0.56
1:A:767:PHE:CD1	1:A:772:LEU:HD21	2.41	0.56
1:A:27:ALA:HB1	1:A:802:GLU:OE2	2.07	0.55
1:A:226:THR:HA	1:A:250:GLN:OE1	2.06	0.55
1:B:197:LYS:NZ	7:B:1130:HOH:O	2.40	0.54
1:A:532:THR:HG23	6:A:1010:SO4:O4	2.08	0.54
1:A:619:GLU:HA	1:A:619:GLU:OE1	2.06	0.54
1:B:767:PHE:HB3	1:B:772:LEU:HD11	1.89	0.53
1:A:130:LYS:HE2	1:A:151:GLN:HG3	1.89	0.53
1:A:28:ARG:NH2	1:A:801:THR:O	2.39	0.53
1:A:81:SER:O	7:A:1109:HOH:O	2.18	0.53
1:A:736:ARG:HG2	1:A:758:LYS:HB2	1.90	0.52
1:B:299:SER:HA	1:B:323:GLN:O	2.09	0.52
1:A:47:VAL:HB	1:A:67:THR:HA	1.92	0.51
1:A:491:CYS:HB3	4:A:1001:NAG:H81	1.92	0.51
1:B:467:ARG:HB2	2:D:4:A:OP1	2.10	0.51
1:A:89:VAL:HG22	1:A:90:HIS:CE1	2.44	0.51
1:A:299:SER:HA	1:A:323:GLN:O	2.11	0.51
1:A:413:ASN:ND2	7:A:1129:HOH:O	2.36	0.51
1:B:286:PHE:HB3	1:B:313:ILE:HD11	1.92	0.50
1:B:386:LYS:HE2	6:B:1016:SO4:O1	2.12	0.49
1:A:717:ARG:NH2	1:A:719:SER:OG	2.40	0.49
1:B:799:GLN:HA	1:B:826:ILE:HD12	1.93	0.49
1:B:246:ASN:ND2	7:B:1134:HOH:O	2.45	0.49
1:A:370:LYS:NZ	7:A:1141:HOH:O	2.45	0.49
1:A:103:ILE:HG22	7:A:1310:HOH:O	2.13	0.49
1:B:359:SER:HB2	1:B:389:GLN:NE2	2.28	0.48
1:A:243:ASP:OD1	1:A:243:ASP:N	2.46	0.48
1:B:817:PRO:O	1:B:819:ALA:N	2.46	0.48
5:B:1011:IDQ:H23	5:B:1011:IDQ:H11	1.95	0.48
1:B:249:ASN:HB3	7:B:1554:HOH:O	2.14	0.48
1:B:635:TRP:HB3	1:B:666:PRO:HG2	1.95	0.48
1:A:725:LEU:O	1:A:748:GLN:HG2	2.14	0.47
1:B:197:LYS:HD3	1:B:197:LYS:HA	1.69	0.47
1:B:622:ARG:CZ	1:B:651:LYS:HD2	2.45	0.47
1:B:772:LEU:HD13	1:B:797:TRP:CZ2	2.49	0.47
1:B:124:SER:N	7:B:1135:HOH:O	2.47	0.47
1:B:298:HIS:CE1	1:B:323:GLN:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:NH1	2:D:3:C:H1'	2.31	0.46
1:B:73:THR:HA	1:B:97:ARG:O	2.16	0.45
1:B:761:MET:HB3	1:B:761:MET:HE2	1.58	0.45
1:A:593:LYS:O	1:A:596:LYS:HD3	2.17	0.45
1:A:277:SER:OG	7:A:1111:HOH:O	2.21	0.45
1:A:761:MET:HE2	1:A:761:MET:HB3	1.78	0.45
1:A:82:PRO:O	1:A:86:HIS:HB2	2.17	0.45
1:A:636:ARG:HH12	2:D:3:C:H3'	1.81	0.44
1:A:817:PRO:O	1:A:819:ALA:N	2.50	0.44
1:A:525:SER:HA	1:A:550:SER:O	2.18	0.44
1:B:223:LEU:O	1:B:247:ASN:ND2	2.47	0.44
1:B:474:SER:HB2	2:D:3:C:N4	2.33	0.43
1:A:532:THR:N	6:A:1010:SO4:O4	2.37	0.43
1:A:435:PRO:N	7:A:1150:HOH:O	2.50	0.43
1:A:73:THR:HA	1:A:97:ARG:O	2.18	0.43
1:B:736:ARG:HG2	1:B:758:LYS:HB2	2.00	0.43
1:A:659:LYS:HB3	1:A:659:LYS:HE2	1.79	0.43
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.87	0.43
1:A:80:ILE:HG22	1:A:122:SER:HB3	2.00	0.43
1:B:376:ARG:HA	1:B:403:ASP:HB3	2.01	0.42
1:B:577:SER:O	1:B:581:GLN:HG3	2.18	0.42
1:A:714:VAL:HB	1:A:715:PRO:HD2	2.01	0.42
1:A:577:SER:O	1:A:581:GLN:HG3	2.19	0.42
1:B:316:LEU:HD12	1:B:316:LEU:HA	1.93	0.42
1:A:378:ARG:HD2	1:A:403:ASP:OD2	2.19	0.42
1:B:410:LYS:NZ	7:B:1123:HOH:O	2.36	0.42
1:B:810:THR:HG23	1:B:811:ASP:HB2	2.00	0.42
1:A:403:ASP:HA	1:A:427:ASP:HB3	2.01	0.42
1:A:82:PRO:HG3	1:A:121:ARG:HB2	2.00	0.42
1:B:614:ARG:HH11	1:B:614:ARG:HD2	1.71	0.41
5:B:1011:IDQ:H23	5:B:1011:IDQ:C14	2.50	0.41
1:B:764:LYS:HD3	1:B:793:TRP:NE1	2.35	0.41
1:B:237:ILE:O	1:B:259:ASN:HB3	2.21	0.41
1:A:133:TYR:OH	7:A:1112:HOH:O	2.22	0.41
1:A:467:ARG:NH1	2:C:3:C:H1'	2.36	0.41
1:A:493:LYS:HG3	1:A:494:TYR:CD2	2.56	0.41
1:A:593:LYS:HE2	1:A:617:GLU:HG3	2.03	0.41
1:B:53:ASP:HA	1:B:74:ILE:O	2.21	0.41
1:A:53:ASP:HA	1:A:74:ILE:O	2.21	0.41
1:B:525:SER:HA	1:B:550:SER:O	2.21	0.40
1:B:795:VAL:HG21	1:B:828:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:TRP:CE2	1:B:715:PRO:HD3	2.56	0.40
1:A:622:ARG:CZ	1:A:651:LYS:HD2	2.52	0.40
1:A:783:ASN:HB3	1:A:784:ARG:H	1.69	0.40
1:B:75:ASN:O	1:B:99:ASN:HA	2.22	0.40
1:A:165:LYS:HE2	1:A:165:LYS:HB3	1.79	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)
7:B:1567:HOH:O	7:A:1399:HOH:O[4_545]	1.95	0.25

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	768/823 (93%)	727 (95%)	39 (5%)	2 (0%)	41	46
1	B	769/823 (93%)	729 (95%)	38 (5%)	2 (0%)	41	46
All	All	1537/1646 (93%)	1456 (95%)	77 (5%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	818	GLY
1	A	818	GLY
1	A	381	VAL
1	B	381	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	726/774 (94%)	717 (99%)	9 (1%)	71	83
1	B	728/774 (94%)	723 (99%)	5 (1%)	84	91
All	All	1454/1548 (94%)	1440 (99%)	14 (1%)	76	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	108	LYS
1	B	135	ASP
1	B	277	SER
1	B	546	TYR
1	B	636	ARG
1	A	32	LYS
1	A	108	LYS
1	A	119	LYS
1	A	135	ASP
1	A	546	TYR
1	A	567	LYS
1	A	607	ASP
1	A	784	ARG
1	A	825	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	763	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	2/6 (33%)	0	0
2	D	2/6 (33%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4/12 (33%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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)

6 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	0.46	0
3	NAG	E	2	3	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.38	0	17,19,21	0.64	0
3	NAG	F	2	3	14,14,15	0.82	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.23	0	17,19,21	0.91	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	-2.78	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C1-O5-C5	3.04	116.32	112.19
3	F	2	NAG	C1-O5-C5	3.04	116.31	112.19
3	G	2	NAG	C1-O5-C5	2.87	116.07	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

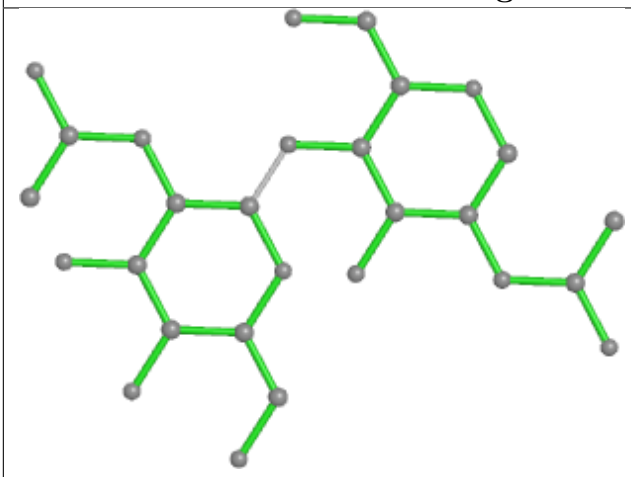
There are no ring outliers.

1 monomer is involved in 1 short contact:

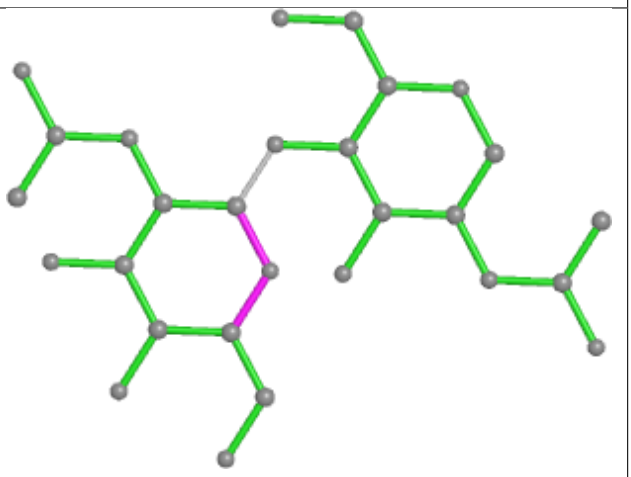
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0

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

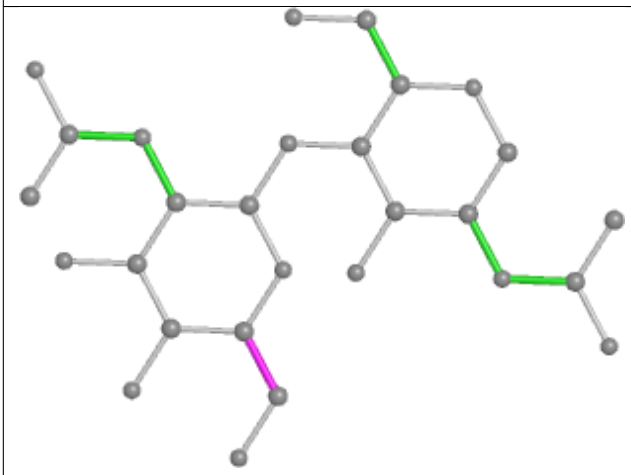
Oligosaccharide Chain E



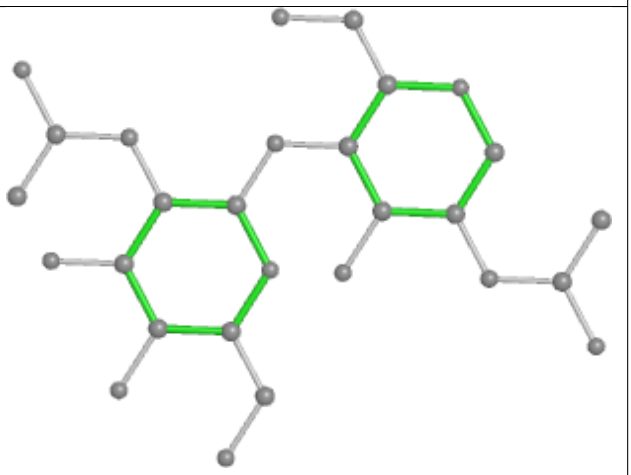
Bond lengths



Bond angles

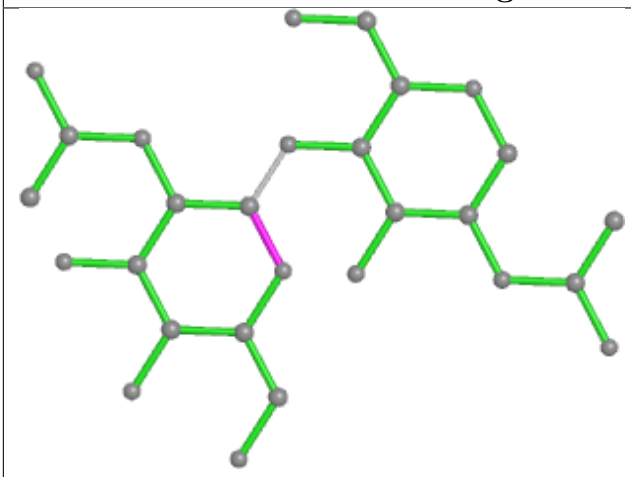


Torsions

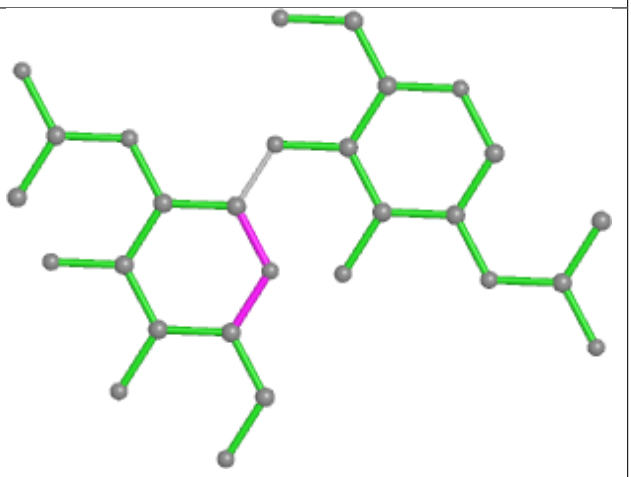


Rings

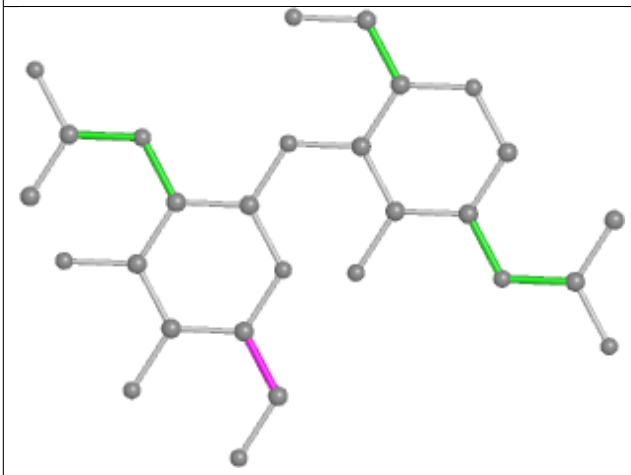
Oligosaccharide Chain F



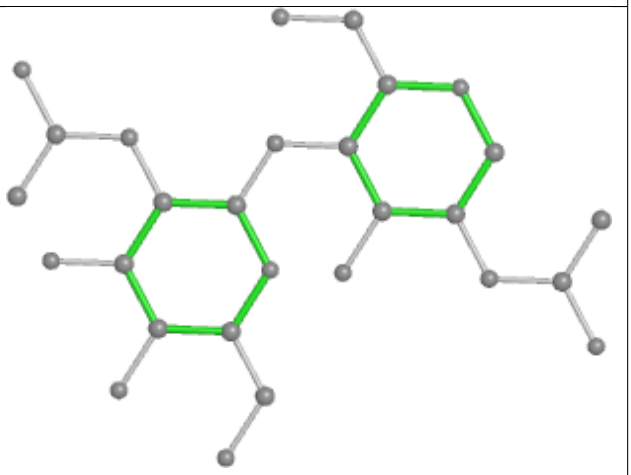
Bond lengths



Bond angles

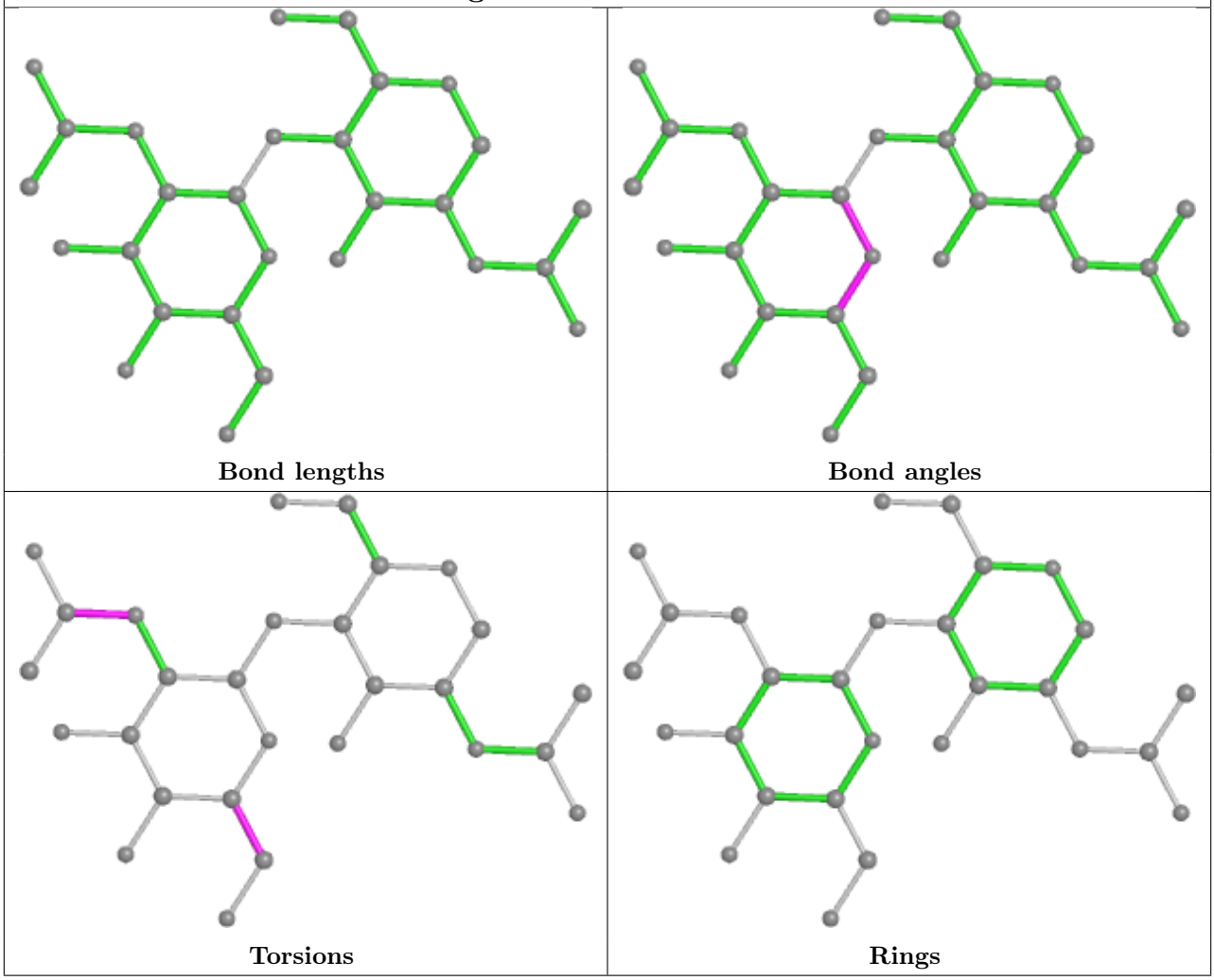


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

29 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	$\#\|Z\| > 2$
6	SO4	B	1020	-	4,4,4	0.16	0	6,6,6	0.05	0
4	NAG	B	1001	1	14,14,15	0.59	0	17,19,21	0.60	0
4	NAG	B	1008	1	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	A	1001	1	14,14,15	0.34	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	A	1013	-	4,4,4	0.26	0	6,6,6	0.39	0
4	NAG	B	1007	1	14,14,15	0.84	1 (7%)	17,19,21	0.71	0
6	SO4	B	1015	-	4,4,4	0.22	0	6,6,6	0.27	0
6	SO4	B	1018	-	4,4,4	0.20	0	6,6,6	0.11	0
6	SO4	B	1019	-	4,4,4	0.22	0	6,6,6	0.48	0
4	NAG	A	1007	1	14,14,15	0.44	0	17,19,21	0.54	0
6	SO4	A	1010	-	4,4,4	0.21	0	6,6,6	0.32	0
4	NAG	A	1006	1	14,14,15	0.53	0	17,19,21	0.52	0
6	SO4	B	1014	-	4,4,4	0.17	0	6,6,6	0.17	0
6	SO4	A	1014	-	4,4,4	0.22	0	6,6,6	0.19	0
4	NAG	B	1005	1	14,14,15	0.18	0	17,19,21	0.78	1 (5%)
6	SO4	B	1016	-	4,4,4	0.22	0	6,6,6	0.24	0
5	IDQ	B	1011	-	26,30,30	1.11	1 (3%)	33,42,42	1.29	3 (9%)
6	SO4	A	1009	-	4,4,4	0.14	0	6,6,6	0.73	0
6	SO4	B	1017	-	4,4,4	0.15	0	6,6,6	0.15	0
6	SO4	B	1012	-	4,4,4	0.11	0	6,6,6	0.39	0
5	IDQ	A	1008	-	26,30,30	1.08	1 (3%)	33,42,42	1.53	4 (12%)
6	SO4	A	1011	-	4,4,4	0.25	0	6,6,6	0.29	0
4	NAG	B	1006	1	14,14,15	0.49	0	17,19,21	0.44	0
6	SO4	A	1012	-	4,4,4	0.19	0	6,6,6	0.20	0
4	NAG	B	1002	1	14,14,15	0.73	1 (7%)	17,19,21	0.99	1 (5%)
6	SO4	A	1015	-	4,4,4	0.24	0	6,6,6	0.20	0
4	NAG	B	1009	1	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
6	SO4	B	1013	-	4,4,4	0.19	0	6,6,6	0.43	0
4	NAG	B	1010	1	14,14,15	0.45	0	17,19,21	0.51	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
4	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	1/6/23/26	0/1/1/1
5	IDQ	A	1008	-	-	2/10/10/10	0/4/4/4
4	NAG	B	1007	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
5	IDQ	B	1011	-	-	2/10/10/10	0/4/4/4
4	NAG	B	1006	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1011	IDQ	C1-C	4.26	1.49	1.41
5	A	1008	IDQ	C1-C	4.17	1.49	1.41
4	B	1007	NAG	O5-C1	-2.62	1.39	1.43
4	B	1002	NAG	O5-C1	2.45	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1008	IDQ	C15-C14-N2	-4.11	106.25	112.63
5	B	1011	IDQ	C8-C1-C	-3.94	116.65	119.65
5	A	1008	IDQ	C7-C6-N	-3.67	118.60	121.01
4	B	1002	NAG	C1-O5-C5	3.61	117.08	112.19
5	A	1008	IDQ	C11-C10-C9	-3.49	104.43	112.16
5	A	1008	IDQ	C8-C1-C	-3.34	117.11	119.65
5	B	1011	IDQ	C7-C6-N	-2.95	119.08	121.01
5	B	1011	IDQ	C15-C14-N2	-2.72	108.40	112.63
4	B	1005	NAG	C1-O5-C5	2.61	115.73	112.19
4	B	1009	NAG	C1-O5-C5	2.39	115.43	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1006	NAG	O5-C5-C6-O6
4	B	1006	NAG	C4-C5-C6-O6
4	A	1006	NAG	O5-C5-C6-O6
5	B	1011	IDQ	N2-C14-C15-C19
5	B	1011	IDQ	N2-C14-C15-C16
5	A	1008	IDQ	N2-C14-C15-C16
5	A	1008	IDQ	N2-C14-C15-C19
4	A	1007	NAG	C4-C5-C6-O6
4	A	1007	NAG	O5-C5-C6-O6

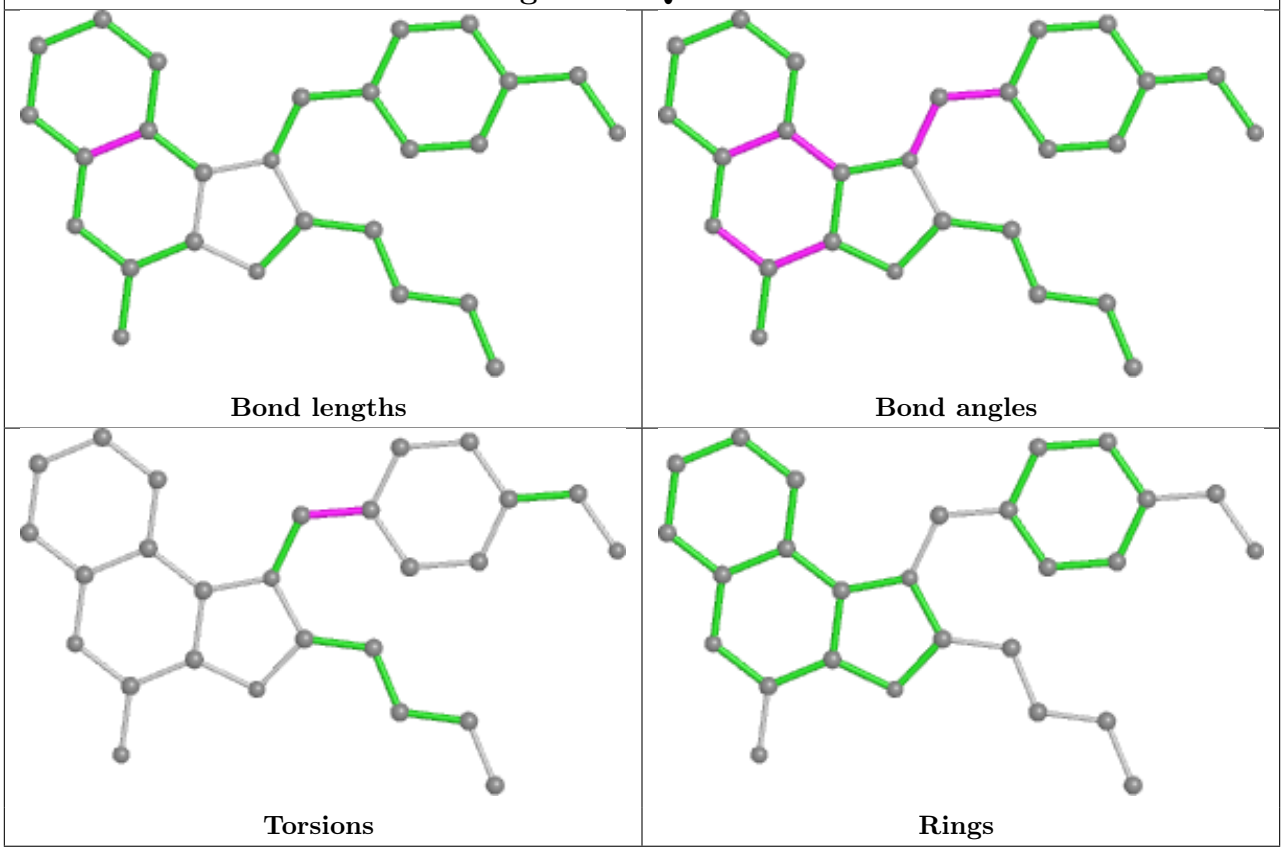
There are no ring outliers.

9 monomers are involved in 12 short contacts:

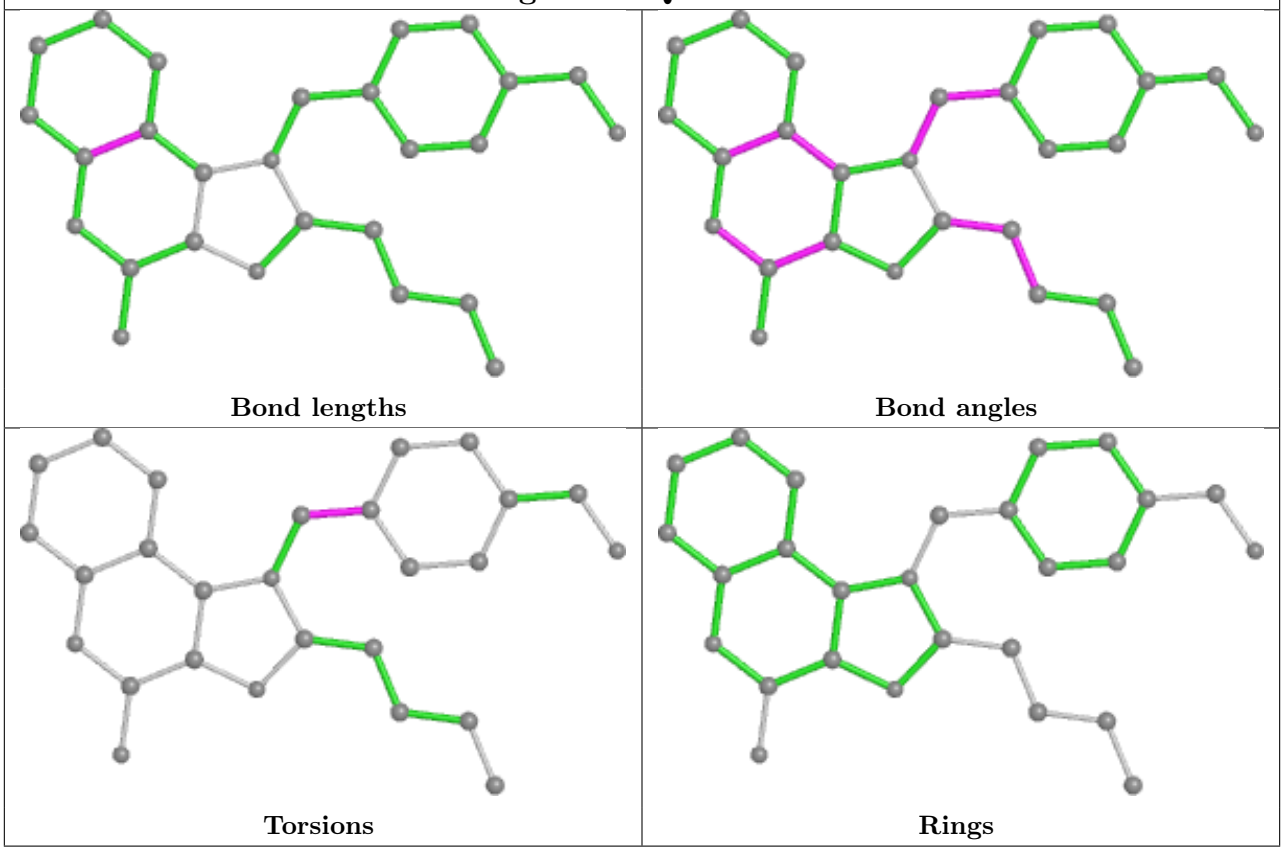
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	NAG	1	0
4	A	1001	NAG	1	0
6	B	1018	SO4	1	0
6	A	1010	SO4	2	0
6	B	1016	SO4	1	0
5	B	1011	IDQ	2	0
6	B	1017	SO4	1	0
6	B	1012	SO4	2	0
6	A	1011	SO4	1	0

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.

Ligand IDQ B 1011



Ligand IDQ A 1008



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	774/823 (94%)	-0.09	18 (2%) 60 58	28, 44, 61, 85	0
1	B	775/823 (94%)	-0.27	3 (0%) 92 91	22, 36, 52, 79	0
2	C	4/6 (66%)	-0.33	0 100 100	36, 42, 50, 52	0
2	D	4/6 (66%)	-0.44	0 100 100	37, 46, 50, 53	0
All	All	1557/1658 (93%)	-0.18	21 (1%) 77 75	22, 40, 58, 85	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	VAL	4.5
1	A	313	ILE	3.7
1	A	45	ASN	3.4
1	A	43	SER	3.4
1	A	723	ARG	3.2
1	A	41	ASP	3.1
1	B	45	ASN	3.0
1	A	40	LEU	3.0
1	B	435	PRO	2.9
1	A	47	VAL	2.8
1	B	459	VAL	2.5
1	A	461	GLU	2.5
1	A	42	VAL	2.5
1	A	130	LYS	2.5
1	A	46	HIS	2.4
1	A	776	LYS	2.4
1	A	460	LEU	2.2
1	A	44	LYS	2.1
1	A	86	HIS	2.1
1	A	338	PHE	2.1
1	A	774	ASN	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)

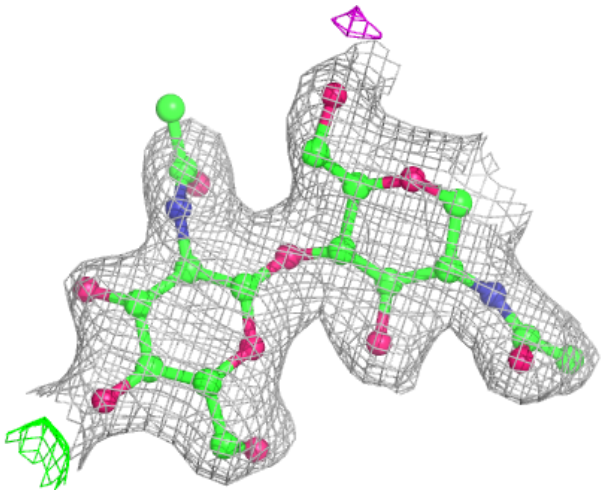
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

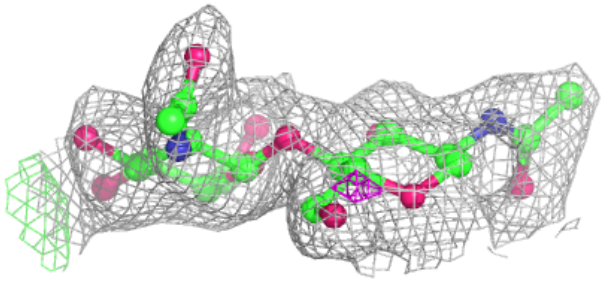
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.85	0.23	69,74,79,82	0
3	NAG	F	2	14/15	0.91	0.10	49,56,58,64	0
3	NAG	E	2	14/15	0.91	0.15	46,54,59,60	0
3	NAG	G	1	14/15	0.94	0.13	50,59,64,67	0
3	NAG	E	1	14/15	0.96	0.10	33,39,42,48	0
3	NAG	F	1	14/15	0.97	0.11	34,40,45,46	0

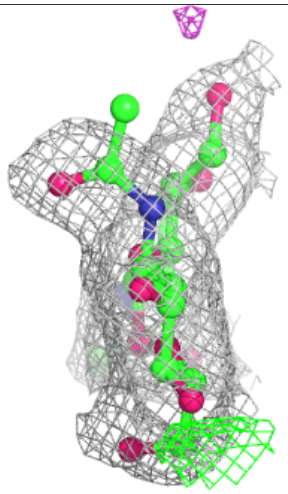
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

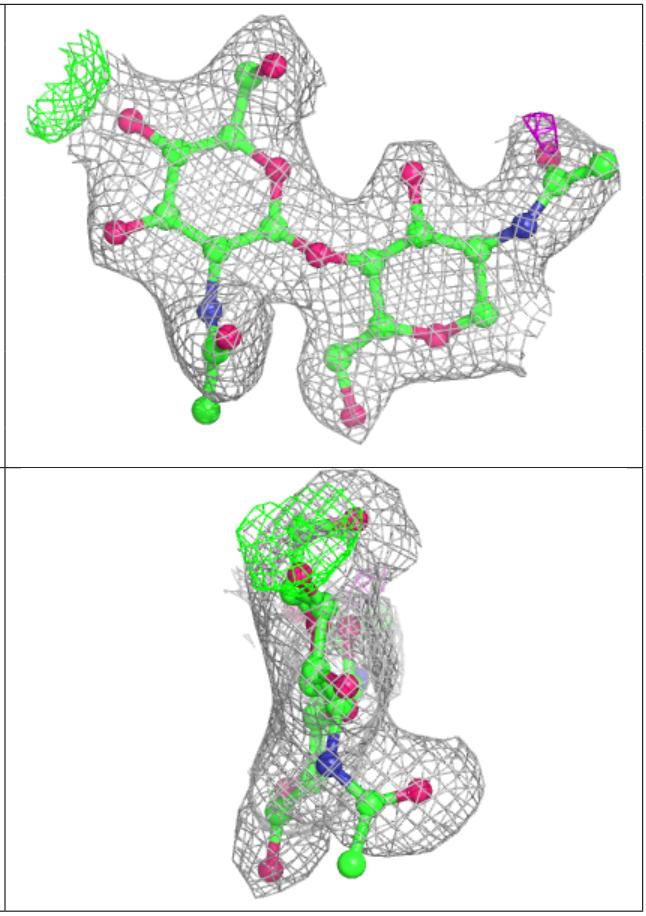






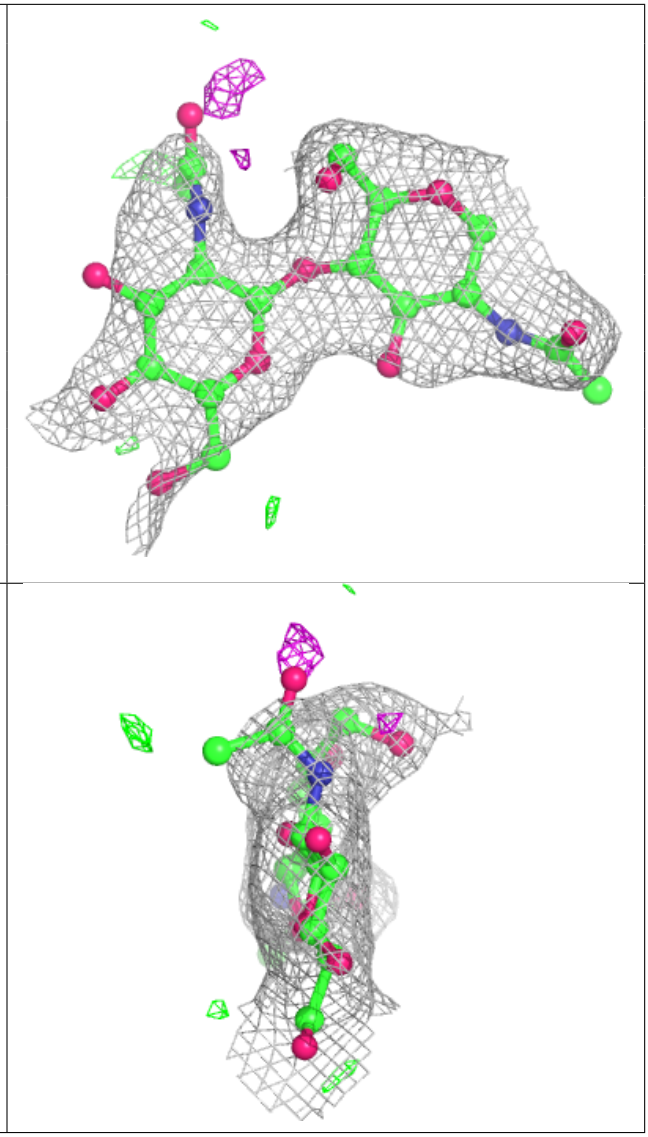
Electron density around Chain F:

$2mF_o$-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 G:

$2mF_o$-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	SO4	A	1014	5/5	0.69	0.28	70,75,96,98	0
6	SO4	B	1018	5/5	0.79	0.55	77,78,89,97	0
4	NAG	A	1007	14/15	0.80	0.24	58,70,74,76	0
6	SO4	B	1015	5/5	0.85	0.21	55,58,68,69	0
4	NAG	B	1006	14/15	0.87	0.14	42,53,56,65	0
4	NAG	B	1009	14/15	0.87	0.22	48,55,60,60	0
6	SO4	A	1012	5/5	0.88	0.22	56,61,75,82	0

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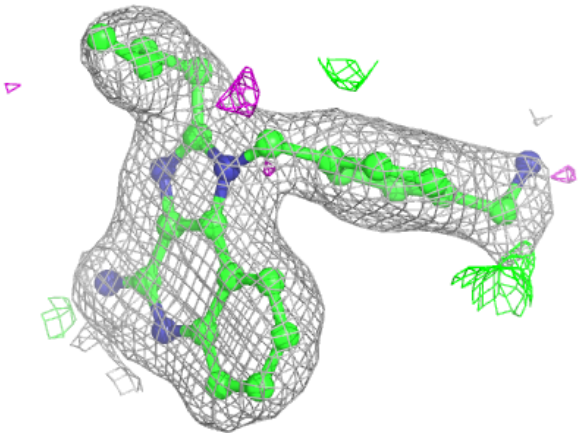
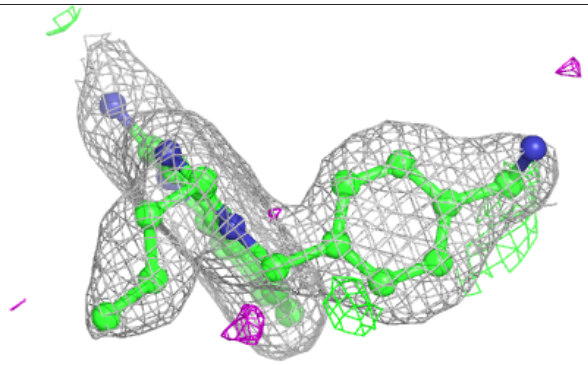
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	1009	5/5	0.89	0.13	53,56,73,77	0
6	SO4	A	1010	5/5	0.89	0.21	55,64,68,73	0
4	NAG	B	1007	14/15	0.89	0.14	50,57,64,64	0
4	NAG	B	1008	14/15	0.89	0.12	43,48,55,57	0
6	SO4	B	1017	5/5	0.90	0.22	69,69,81,86	0
4	NAG	B	1010	14/15	0.90	0.17	52,64,70,71	0
6	SO4	A	1015	5/5	0.91	0.12	57,59,71,77	0
6	SO4	A	1013	5/5	0.92	0.23	46,52,53,69	0
4	NAG	B	1005	14/15	0.92	0.12	47,55,60,64	0
6	SO4	B	1014	5/5	0.92	0.21	54,56,72,76	0
4	NAG	A	1006	14/15	0.93	0.11	55,61,64,70	0
6	SO4	B	1019	5/5	0.93	0.24	41,50,53,67	0
4	NAG	B	1001	14/15	0.94	0.10	28,33,36,37	0
6	SO4	B	1016	5/5	0.94	0.14	51,62,68,71	0
4	NAG	B	1002	14/15	0.94	0.14	41,44,49,49	0
6	SO4	B	1013	5/5	0.94	0.21	48,49,60,63	0
4	NAG	A	1001	14/15	0.94	0.12	37,41,47,49	0
6	SO4	B	1020	5/5	0.94	0.30	59,65,70,76	0
5	IDQ	A	1008	27/27	0.95	0.16	29,36,42,49	0
6	SO4	B	1012	5/5	0.96	0.09	46,50,59,63	0
6	SO4	A	1011	5/5	0.96	0.19	53,56,71,73	0
5	IDQ	B	1011	27/27	0.96	0.13	32,38,40,49	0

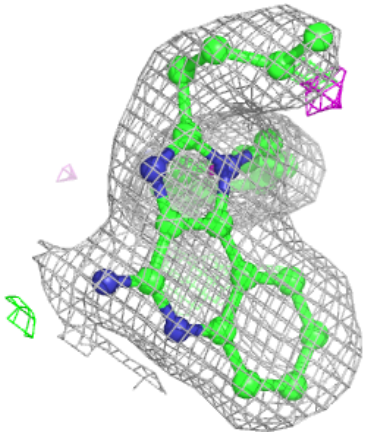
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around IDQ A 1008:

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







Electron density around IDQ B 1011:

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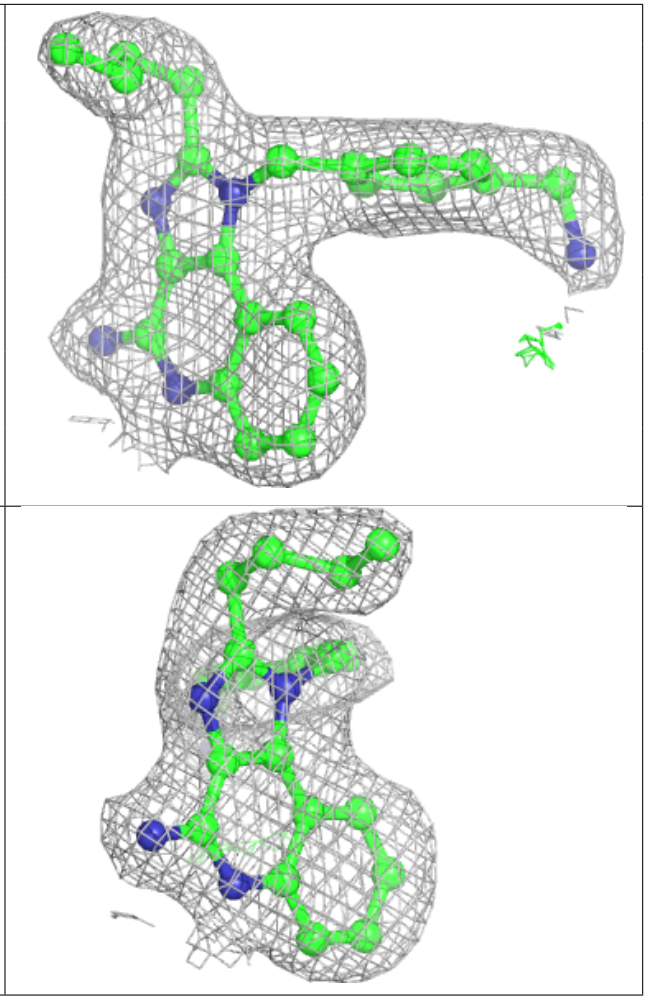
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.