Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 06:00 AM EDT

PDB ID	:	3W3J
Title	:	Crystal structure of human TLR8 in complex with CL097
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2012-12-22
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

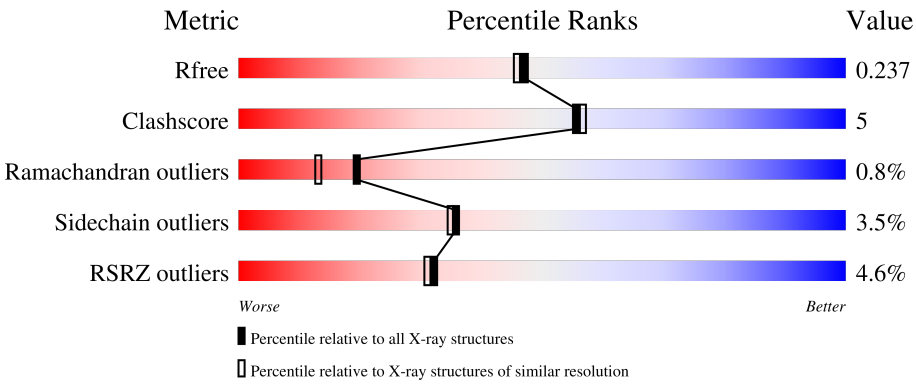
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	811	6%, 76%, 14%, • 8%
1	B	811	3%, 79%, 12%, • 8%
2	C	4	25%, 50%, 25%
2	F	4	75%, 25%
3	D	2	50%, 50%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
4	E	3	33% 67%
4	H	3	33% 67%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13299 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 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	747	5988	3832	1018	1119	19	0	0	0
1	B	746	5982	3830	1017	1116	19	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

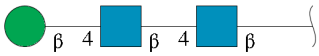
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	4	50	28	2	20	0	0	0
2	F	4	50	28	2	20	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.

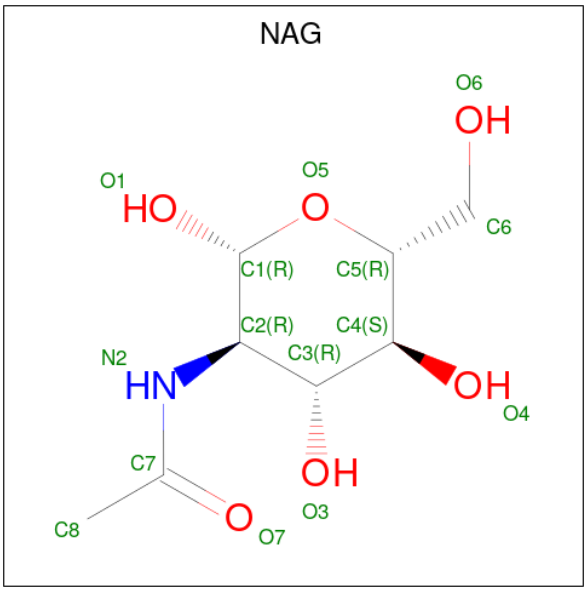
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0

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



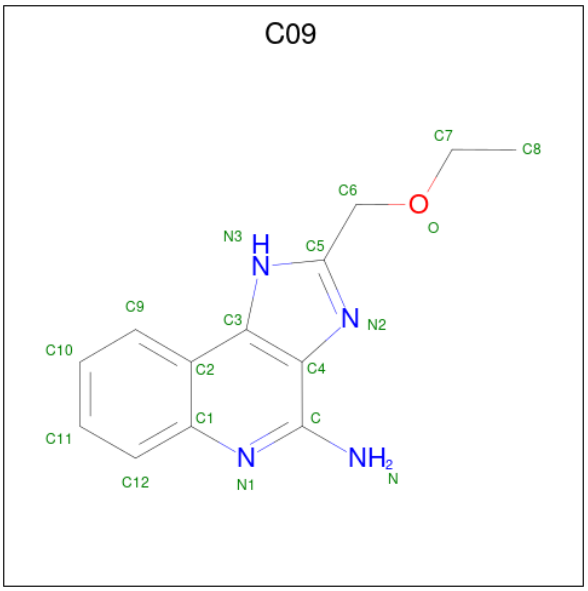
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	3	39	22	2	15	0	0	0
4	H	3	39	22	2	15	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



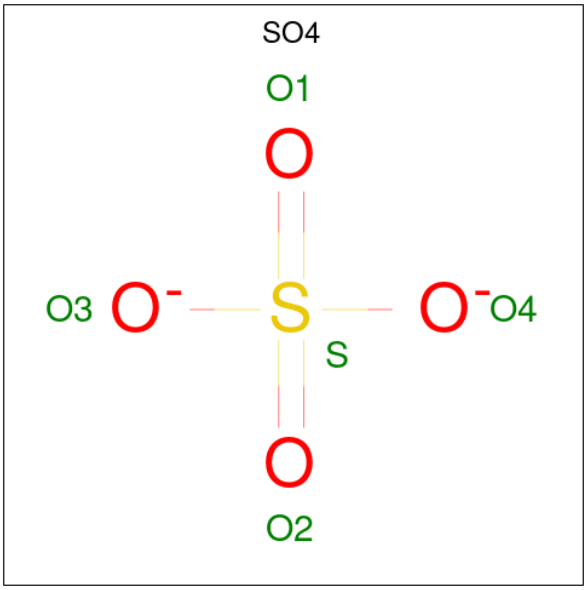
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total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

- Molecule 6 is 2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-4-amine (three-letter code: C09) (formula: $C_{13}H_{14}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	18	13	4	1	0	0
			Total	C	N	O		
6	B	1	18	13	4	1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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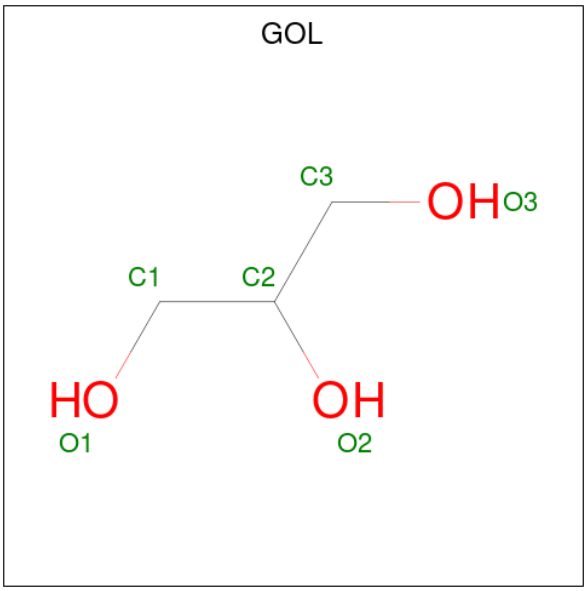
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

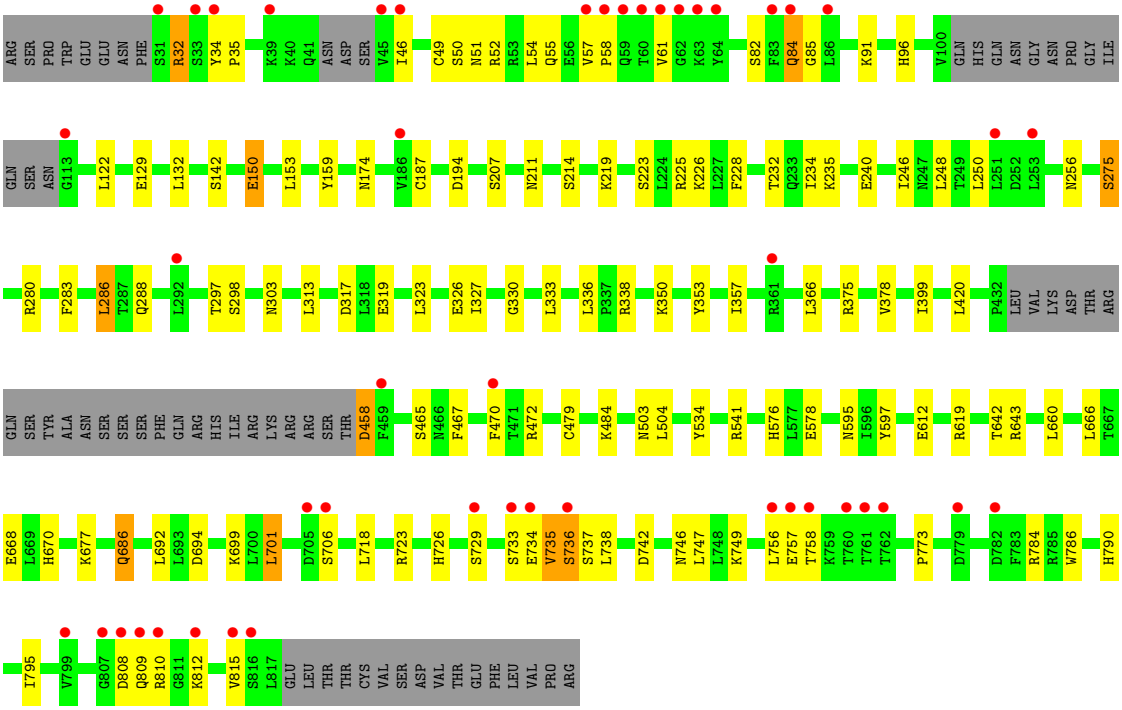
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	438	438	438	0	0
			Total	O		
9	B	423	423	423	0	0

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.

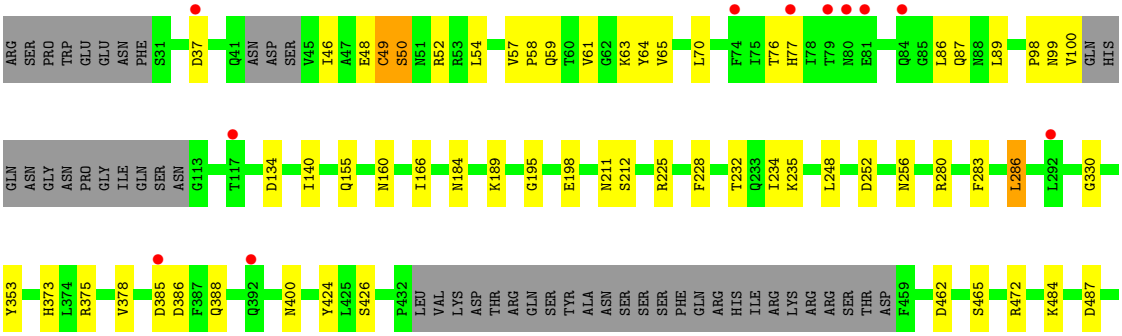
- Molecule 1: Toll-like receptor 8

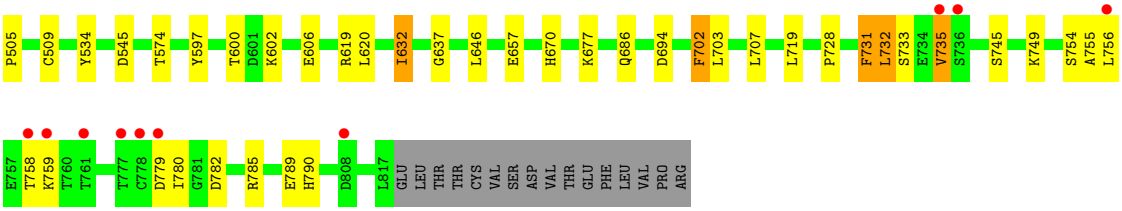
Chain A:



- Molecule 1: Toll-like receptor 8

Chain B:





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

Chain C: 25% 50% 25%

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

Chain F: 75% 25%

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

Chain D: 50% 50%

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

Chain G: 100%

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

Chain E: 33% 67%

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

Chain H: 33% 67%

NAG1
NAG2
BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.38Å 148.75Å 85.77Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	40.43 – 2.00 40.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.43-2.00) 97.9 (40.43-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.191 , 0.237 0.193 , 0.237	Depositor DCC
R_{free} test set	5748 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13299	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: GOL, SO4, BMA, NAG, MAN, C09

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	0.32	0/6112	0.50	0/8290
1	B	0.33	0/6106	0.51	0/8282
All	All	0.33	0/12218	0.50	0/16572

There are no bond length outliers.

There are no bond angle outliers.

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	5988	0	5937	73	0
1	B	5982	0	5940	51	0
2	C	50	0	43	1	0
2	F	50	0	43	1	0
3	D	28	0	25	1	0
3	G	28	0	25	0	0
4	E	39	0	34	0	0
4	H	39	0	34	0	0
5	A	56	0	52	0	0
5	B	56	0	52	0	1
6	A	18	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	14	0	0
7	A	40	0	0	4	0
7	B	40	0	0	2	0
8	B	6	0	8	0	0
9	A	438	0	0	15	1
9	B	423	0	0	10	0
All	All	13299	0	12221	125	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 (125) 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:386:ASP:OD2	9:B:1204:HOH:O	2.06	0.73
1:B:782:ASP:OD1	1:B:785:ARG:NH2	2.23	0.71
1:A:280:ARG:HD2	1:A:303:ASN:HD21	1.55	0.70
1:B:52:ARG:NH2	9:B:1320:HOH:O	2.24	0.70
1:A:150:GLU:HG2	1:A:174:ASN:HB2	1.77	0.67
1:A:194:ASP:OD1	1:A:219:LYS:NZ	2.24	0.67
1:A:375:ARG:NH2	9:A:1514:HOH:O	2.26	0.67
1:A:503:ASN:OD1	9:A:1320:HOH:O	2.13	0.65
1:A:55:GLN:NE2	9:A:1490:HOH:O	2.29	0.65
1:A:91:LYS:HG2	1:A:129:GLU:HB3	1.78	0.64
1:A:338:ARG:NH1	9:A:1177:HOH:O	2.30	0.64
1:B:677:LYS:O	9:B:1371:HOH:O	2.14	0.64
1:B:789:GLU:HG3	1:B:790:HIS:ND1	2.13	0.64
1:A:756:LEU:O	1:A:758:THR:N	2.31	0.64
1:A:223:SER:O	1:A:225:ARG:NH1	2.31	0.64
1:A:726:HIS:ND1	7:A:1022:SO4:O2	2.30	0.62
1:A:735:VAL:HG13	1:A:738:LEU:HB2	1.81	0.62
1:A:810:ARG:NH1	9:A:1277:HOH:O	2.33	0.61
1:B:37:ASP:OD2	1:B:52:ARG:NH2	2.31	0.61
1:A:326:GLU:OE2	9:A:1461:HOH:O	2.15	0.60
1:B:375:ARG:NH2	7:B:917:SO4:O3	2.27	0.59
1:A:91:LYS:NZ	1:A:129:GLU:OE1	2.32	0.58
7:A:1016:SO4:O3	9:A:1538:HOH:O	2.11	0.58
1:B:785:ARG:O	1:B:789:GLU:HG2	2.04	0.57
1:B:606:GLU:HG2	1:B:637:GLY:HA3	1.87	0.57
1:A:458:ASP:OD1	1:A:458:ASP:N	2.37	0.57
1:A:288:GLN:OE1	9:A:1474:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:LYS:NZ	7:B:920:SO4:O2	2.40	0.55
1:B:375:ARG:HD2	1:B:400:ASN:HD21	1.70	0.55
1:A:49:CYS:HA	1:A:52:ARG:HE	1.72	0.54
1:B:462:ASP:OD2	2:F:4:MAN:O6	2.19	0.54
1:A:234:ILE:O	1:A:256:ASN:HB3	2.08	0.54
1:B:49:CYS:HB3	1:B:70:LEU:HD23	1.90	0.54
1:B:632:ILE:HD11	1:B:657:GLU:HB3	1.90	0.53
1:B:234:ILE:O	1:B:256:ASN:HB3	2.08	0.53
1:A:333:LEU:HD22	1:A:366:LEU:HD11	1.90	0.53
1:B:702:PHE:O	9:B:1055:HOH:O	2.18	0.53
1:B:597:TYR:HB3	1:B:619:ARG:HB2	1.90	0.53
1:A:350:LYS:NZ	9:A:1316:HOH:O	2.38	0.53
1:B:225:ARG:NH1	9:B:1137:HOH:O	2.42	0.53
1:B:487:ASP:OD2	9:B:1266:HOH:O	2.19	0.53
1:B:48:GLU:OE1	1:B:50:SER:HB3	2.09	0.52
1:A:701:LEU:O	9:A:1308:HOH:O	2.19	0.51
1:A:458:ASP:N	9:A:1534:HOH:O	2.43	0.51
1:A:211:ASN:O	1:A:232:THR:HA	2.11	0.51
1:B:86:LEU:HB3	1:B:89:LEU:HG	1.91	0.51
1:A:207:SER:HA	1:A:228:PHE:HB2	1.93	0.50
1:B:211:ASN:O	1:B:232:THR:HA	2.11	0.50
1:B:98:PRO:O	1:B:100:VAL:N	2.41	0.49
1:B:283:PHE:HA	1:B:286:LEU:HD22	1.94	0.49
1:A:283:PHE:HA	1:A:286:LEU:HD22	1.95	0.49
1:A:84:GLN:HG2	1:A:85:GLY:N	2.27	0.49
1:B:61:VAL:HG13	1:B:65:VAL:HG21	1.95	0.49
1:B:728:PRO:HG2	1:B:731:PHE:HB2	1.95	0.48
1:A:668:GLU:HG3	1:A:692:LEU:HD22	1.95	0.48
1:B:732:LEU:HB2	1:B:755:ALA:O	2.13	0.48
1:A:677:LYS:HE3	1:A:699:LYS:HD3	1.95	0.48
1:B:195:GLY:O	1:B:198:GLU:HG2	2.15	0.47
1:A:541:ARG:HD2	9:A:1529:HOH:O	2.13	0.47
1:A:256:ASN:O	1:A:297:THR:HA	2.15	0.47
1:B:184:ASN:ND2	9:B:1259:HOH:O	2.37	0.47
1:A:34:TYR:CD1	1:A:35:PRO:HA	2.51	0.46
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.97	0.46
1:A:723:ARG:NH2	7:A:1020:SO4:O2	2.39	0.46
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.96	0.46
1:B:620:LEU:HD11	1:B:646:LEU:HD22	1.96	0.46
1:A:733:SER:O	1:A:736:SER:OG	2.28	0.46
1:B:707:LEU:HD23	1:B:735:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:CE1	1:A:187:CYS:HB2	2.50	0.45
1:A:32:ARG:NH2	1:A:790:HIS:O	2.50	0.45
1:B:670:HIS:HA	1:B:694:ASP:HB3	1.98	0.45
1:A:735:VAL:O	1:A:737:SER:N	2.40	0.45
1:B:484:LYS:NZ	9:B:1274:HOH:O	2.50	0.45
1:A:84:GLN:HG2	1:A:85:GLY:H	1.81	0.45
1:A:275:SER:HA	1:A:298:SER:HB2	1.99	0.45
1:A:323:LEU:O	1:A:327:ILE:HG13	2.17	0.45
1:B:703:LEU:HD11	1:B:719:LEU:HD13	1.99	0.45
1:A:275:SER:HB2	1:A:298:SER:O	2.17	0.44
1:A:784:ARG:HD3	1:A:815:VAL:HA	1.99	0.44
1:A:467:PHE:HB3	2:C:1:NAG:H81	1.99	0.44
1:A:479:CYS:HB2	3:D:1:NAG:H81	1.97	0.44
1:B:545:ASP:OD1	1:B:574:THR:OG1	2.25	0.44
1:B:140:ILE:HD13	1:B:166:ILE:HG12	1.98	0.44
1:B:76:THR:HG23	1:B:77:HIS:ND1	2.33	0.44
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.18	0.44
1:A:597:TYR:HB3	1:A:619:ARG:HB2	1.99	0.44
1:B:134:ASP:HA	1:B:155:GLN:O	2.18	0.44
1:A:317:ASP:OD1	1:A:319:GLU:HG3	2.18	0.43
1:A:749:LYS:HA	1:A:773:PRO:O	2.18	0.43
1:B:189:LYS:HA	1:B:212:SER:OG	2.17	0.43
1:A:809:GLN:O	1:A:812:LYS:HB3	2.19	0.43
1:B:745:SER:OG	9:B:1299:HOH:O	2.21	0.43
1:B:600:THR:O	1:B:602:LYS:N	2.48	0.43
1:A:207:SER:OG	7:A:1021:SO4:O3	2.32	0.43
1:A:58:PRO:HB2	1:A:61:VAL:HG23	2.01	0.42
1:B:733:SER:HB2	1:B:758:THR:N	2.34	0.42
1:B:57:VAL:O	1:B:59:GLN:NE2	2.50	0.42
1:A:756:LEU:HD13	1:A:786:TRP:HB2	2.02	0.42
1:A:465:SER:HB3	9:A:1323:HOH:O	2.18	0.42
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.87	0.42
1:A:357:ILE:HG22	9:A:1179:HOH:O	2.19	0.42
1:A:718:LEU:HA	1:A:742:ASP:HB3	2.02	0.41
1:A:49:CYS:SG	1:A:54:LEU:HD11	2.60	0.41
1:A:313:LEU:HD23	1:A:336:LEU:HD22	2.01	0.41
1:A:50:SER:O	1:A:52:ARG:HG3	2.20	0.41
1:A:132:LEU:HB2	1:A:153:LEU:HD23	2.02	0.41
1:B:385:ASP:HA	1:B:388:GLN:HG2	2.03	0.41
1:A:746:ASN:HB3	1:A:747:LEU:H	1.75	0.41
1:A:32:ARG:NH1	1:A:795:ILE:HG12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LYS:NZ	9:A:1517:HOH:O	2.53	0.41
1:B:505:PRO:HD3	9:B:1041:HOH:O	2.19	0.41
1:A:735:VAL:HG12	1:A:736:SER:N	2.36	0.41
1:A:280:ARG:HD2	1:A:303:ASN:ND2	2.29	0.41
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.91	0.41
1:A:612:GLU:OE2	1:A:643:ARG:NH1	2.54	0.41
1:B:54:LEU:HD13	1:B:58:PRO:HG3	2.03	0.41
1:B:63:LYS:HE3	1:B:64:TYR:CZ	2.56	0.41
1:B:424:TYR:CZ	1:B:426:SER:HB3	2.56	0.41
1:A:49:CYS:HA	1:A:52:ARG:NE	2.36	0.40
1:A:670:HIS:HA	1:A:694:ASP:HB3	2.03	0.40
1:A:226:LYS:HG2	1:A:250:LEU:HB3	2.02	0.40
1:B:228:PHE:HA	1:B:252:ASP:HB3	2.03	0.40
1:A:57:VAL:HG21	1:A:82:SER:HB3	2.03	0.40
1:A:642:THR:HA	1:A:666:LEU:HA	2.03	0.40
1:B:779:ASP:OD1	1:B:779:ASP:N	2.52	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)
5:B:914:NAG:O3	9:A:1474:HOH:O[1_655]	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	739/811 (91%)	698 (94%)	34 (5%)	7 (1%)	17 11
1	B	738/811 (91%)	688 (93%)	45 (6%)	5 (1%)	22 16
All	All	1477/1622 (91%)	1386 (94%)	79 (5%)	12 (1%)	19 13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	735	VAL
1	A	736	SER
1	A	757	GLU
1	A	734	GLU
1	B	99	ASN
1	B	731	PHE
1	B	759	LYS
1	A	214	SER
1	A	330	GLY
1	A	378	VAL
1	B	378	VAL
1	B	330	GLY

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	683/755 (90%)	657 (96%)	26 (4%)	33	31
1	B	683/755 (90%)	661 (97%)	22 (3%)	39	38
All	All	1366/1510 (90%)	1318 (96%)	48 (4%)	36	35

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	46	ILE
1	A	51	ASN
1	A	84	GLN
1	A	96	HIS
1	A	122	LEU
1	A	142	SER
1	A	150	GLU
1	A	235	LYS
1	A	240	GLU
1	A	246	ILE

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Mol	Chain	Res	Type
1	A	248	LEU
1	A	275	SER
1	A	286	LEU
1	A	353	TYR
1	A	399	ILE
1	A	458	ASP
1	A	470	PHE
1	A	472	ARG
1	A	534	TYR
1	A	595	ASN
1	A	686	GLN
1	A	701	LEU
1	A	706	SER
1	A	729	SER
1	A	808	ASP
1	B	46	ILE
1	B	49	CYS
1	B	50	SER
1	B	87	GLN
1	B	160	ASN
1	B	235	LYS
1	B	248	LEU
1	B	280	ARG
1	B	286	LEU
1	B	353	TYR
1	B	465	SER
1	B	472	ARG
1	B	509	CYS
1	B	534	TYR
1	B	632	ILE
1	B	686	GLN
1	B	702	PHE
1	B	732	LEU
1	B	735	VAL
1	B	754	SER
1	B	756	LEU
1	B	780	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS

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Mol	Chain	Res	Type
1	B	87	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)

18 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	NAG	C	1	2,1	14,14,15	0.65	0	17,19,21	0.96	1 (5%)
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	0.84	0
2	BMA	C	3	2	11,11,12	0.90	1 (9%)	15,15,17	1.00	0
2	MAN	C	4	2	11,11,12	0.49	0	15,15,17	2.08	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.61	0	17,19,21	1.14	2 (11%)
3	NAG	D	2	3	14,14,15	0.62	0	17,19,21	0.63	0
4	NAG	E	1	4,1	14,14,15	0.63	0	17,19,21	1.12	3 (17%)
4	NAG	E	2	4	14,14,15	0.58	0	17,19,21	1.04	1 (5%)
4	BMA	E	3	4	11,11,12	0.74	0	15,15,17	0.63	0
2	NAG	F	1	2,1	14,14,15	0.64	0	17,19,21	1.39	1 (5%)
2	NAG	F	2	2	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
2	BMA	F	3	2	11,11,12	1.30	1 (9%)	15,15,17	1.42	3 (20%)
2	MAN	F	4	2	11,11,12	0.52	0	15,15,17	1.79	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.94	1 (7%)	17,19,21	1.40	1 (5%)
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	H	1	4,1	14,14,15	0.64	0	17,19,21	0.90	1 (5%)
4	NAG	H	2	4	14,14,15	0.53	0	17,19,21	0.82	0
4	BMA	H	3	4	11,11,12	1.05	1 (9%)	15,15,17	0.97	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	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	1/1/1/1
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	BMA	O5-C1	-3.41	1.38	1.43
3	G	1	NAG	O5-C1	-2.95	1.38	1.43
4	H	3	BMA	O5-C5	2.46	1.48	1.43
2	C	3	BMA	O5-C1	-2.14	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	C1-O5-C5	7.12	121.72	112.19
2	F	4	MAN	C1-O5-C5	6.09	120.35	112.19
2	F	1	NAG	C1-O5-C5	4.76	118.57	112.19
3	G	1	NAG	C1-O5-C5	3.93	117.45	112.19
3	D	1	NAG	O5-C1-C2	-2.92	106.77	111.29
2	F	3	BMA	C3-C4-C5	2.88	115.46	110.23
3	G	2	NAG	C1-O5-C5	2.80	115.94	112.19
4	H	3	BMA	C1-O5-C5	2.67	115.77	112.19
2	F	3	BMA	C1-O5-C5	2.56	115.62	112.19
3	G	2	NAG	C2-N2-C7	-2.31	119.80	122.90
2	C	1	NAG	O5-C1-C2	-2.30	107.73	111.29
2	F	2	NAG	C1-O5-C5	2.25	115.20	112.19
3	D	1	NAG	C2-N2-C7	2.19	125.84	122.90
4	E	1	NAG	O5-C1-C2	-2.17	107.93	111.29
4	E	1	NAG	C1-O5-C5	2.17	115.09	112.19
4	H	1	NAG	C1-O5-C5	2.12	115.03	112.19
2	F	3	BMA	C2-C3-C4	2.05	114.47	110.86
4	E	1	NAG	O7-C7-C8	-2.04	118.43	122.05
4	E	2	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	3	BMA	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

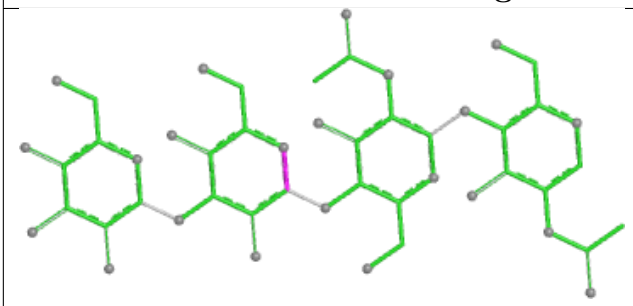
Mol	Chain	Res	Type	Atoms
2	F	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

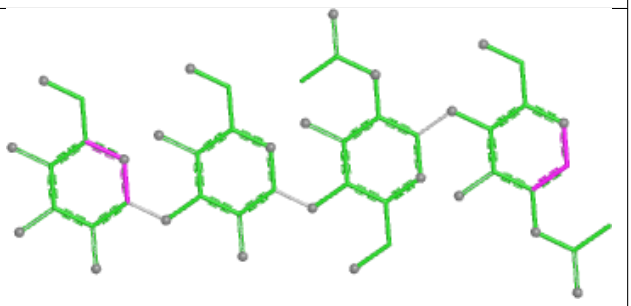
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	MAN	1	0
2	C	1	NAG	1	0
3	D	1	NAG	1	0

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

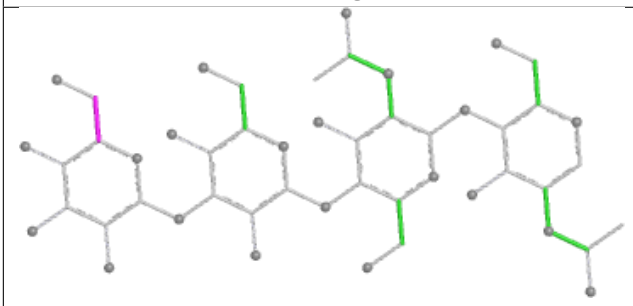
Oligosaccharide Chain C



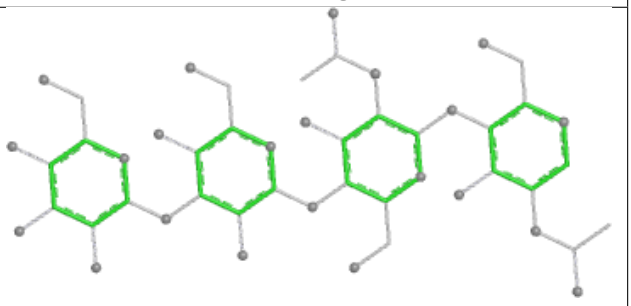
Bond lengths



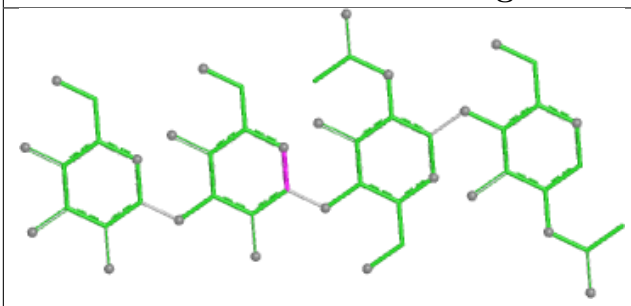
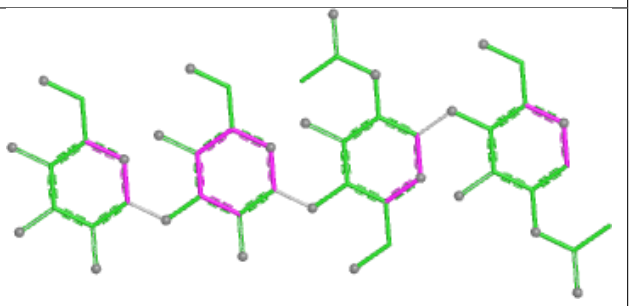
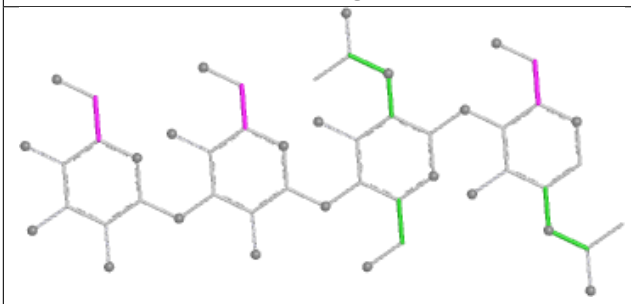
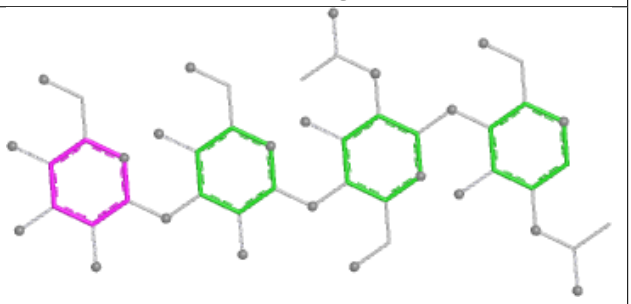
Bond angles



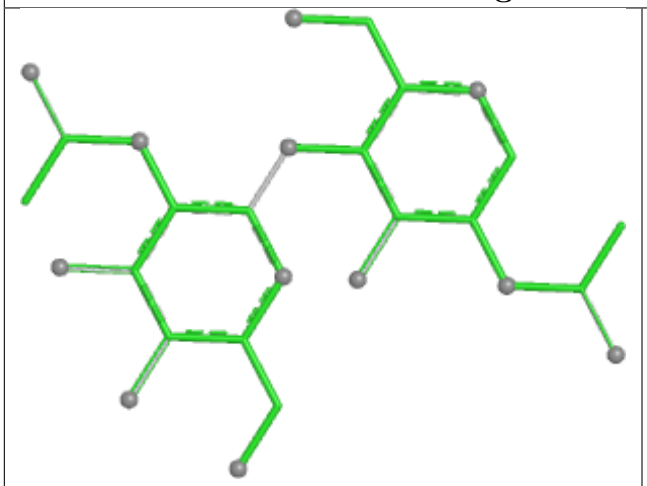
Torsions



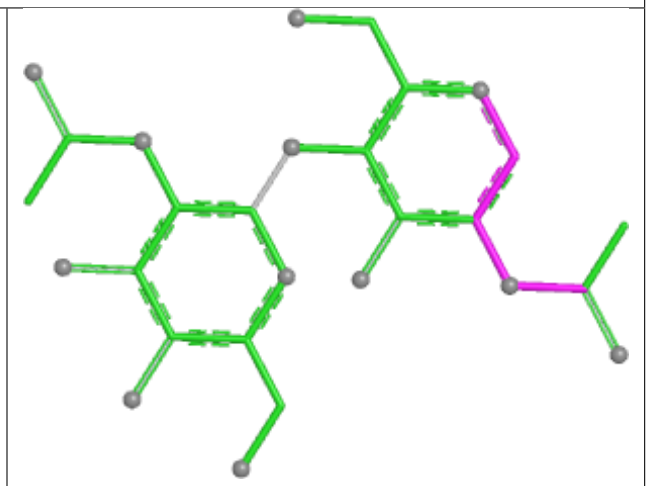
Rings

Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

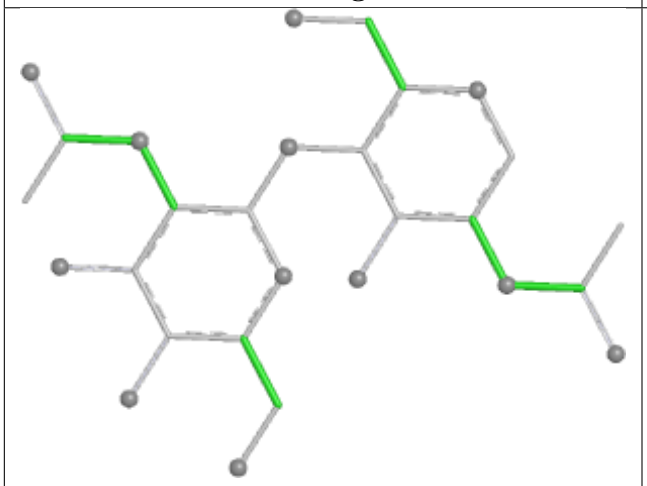
Oligosaccharide Chain D



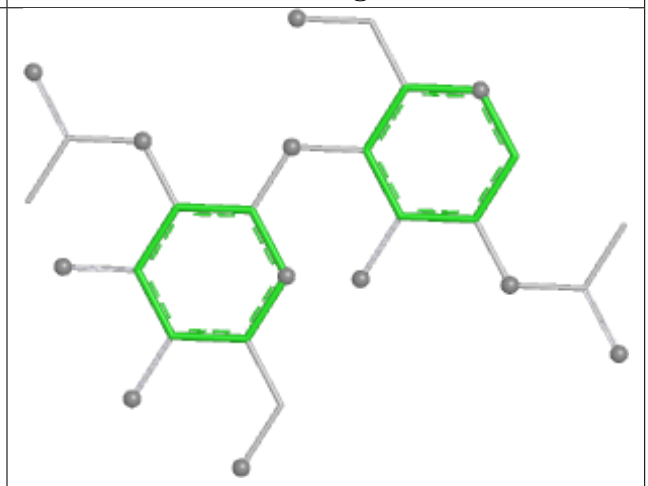
Bond lengths



Bond angles

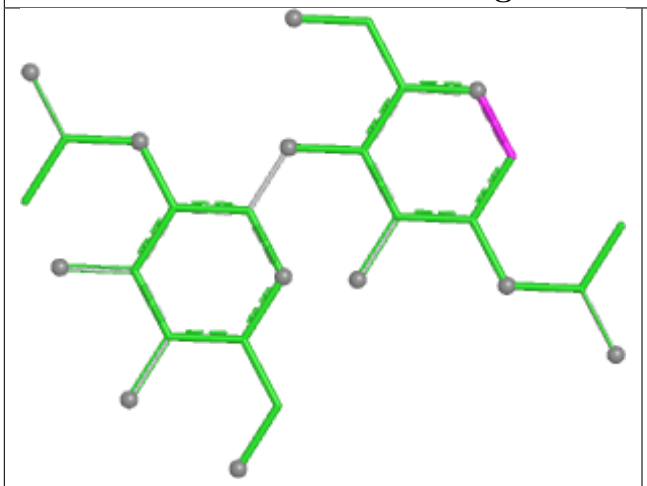


Torsions

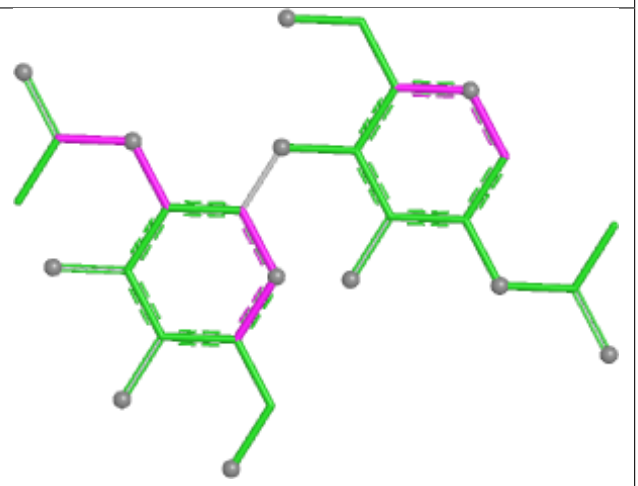


Rings

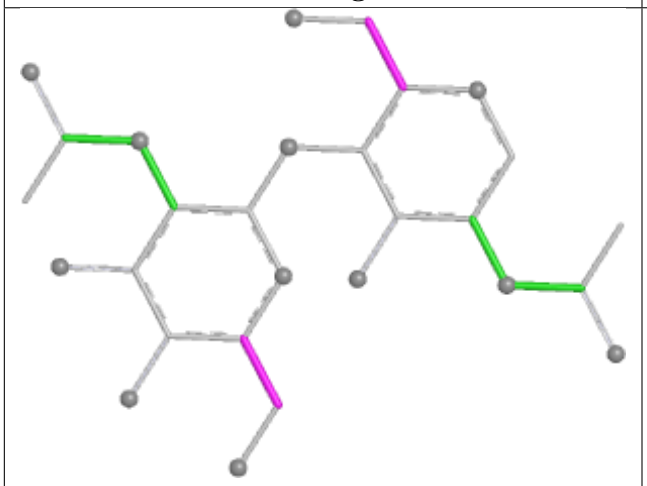
Oligosaccharide Chain G



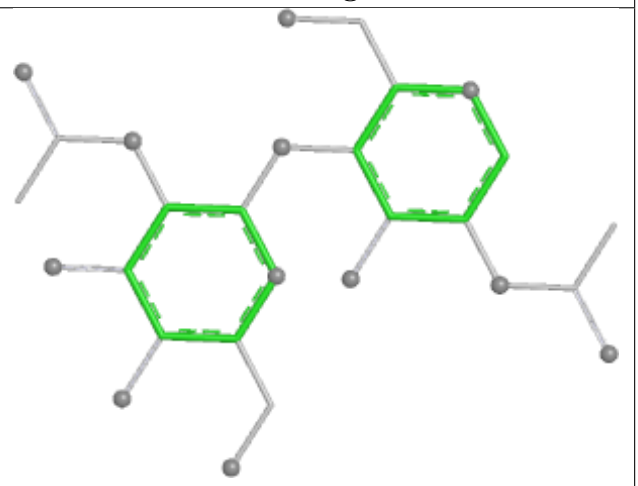
Bond lengths



Bond angles

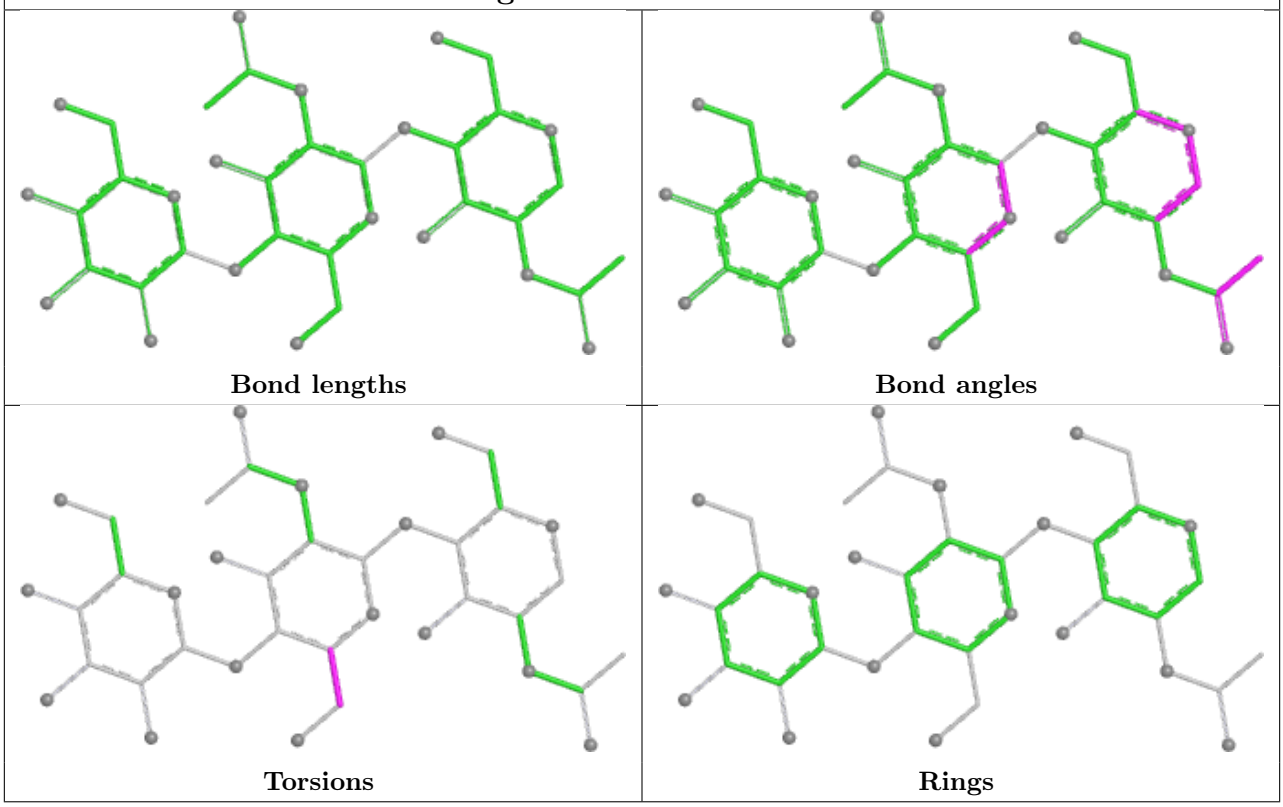


Torsions

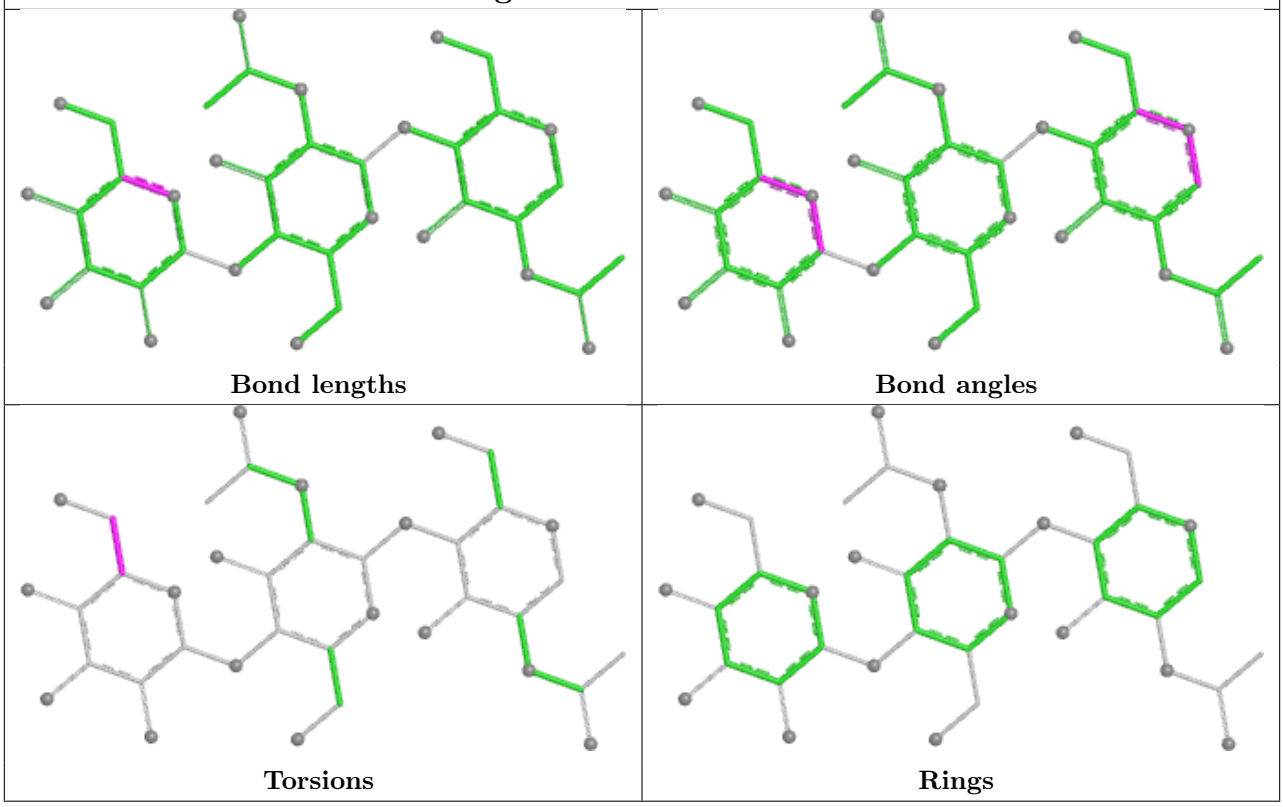


Rings

Oligosaccharide Chain E



Oligosaccharide Chain H



5.6 Ligand geometry (i)

27 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	$\#\|Z\| > 2$
5	NAG	B	913	1	14,14,15	0.52	0	17,19,21	0.88	0
7	SO4	A	1020	-	4,4,4	0.22	0	6,6,6	0.09	0
5	NAG	A	1013	1	14,14,15	0.56	0	17,19,21	0.68	0
7	SO4	A	1018	-	4,4,4	0.23	0	6,6,6	0.11	0
5	NAG	A	1007	1	14,14,15	0.58	0	17,19,21	0.98	1 (5%)
7	SO4	B	916	-	4,4,4	0.23	0	6,6,6	0.08	0
7	SO4	A	1015	-	4,4,4	0.19	0	6,6,6	0.14	0
7	SO4	B	920	-	4,4,4	0.23	0	6,6,6	0.06	0
6	C09	A	1014	-	16,20,20	1.61	2 (12%)	20,28,28	1.32	1 (5%)
7	SO4	A	1021	-	4,4,4	0.22	0	6,6,6	0.17	0
7	SO4	B	921	-	4,4,4	0.22	0	6,6,6	0.09	0
7	SO4	B	922	-	4,4,4	0.23	0	6,6,6	0.10	0
5	NAG	A	1011	1	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
7	SO4	B	917	-	4,4,4	0.23	0	6,6,6	0.08	0
6	C09	B	901	-	16,20,20	1.67	2 (12%)	20,28,28	1.44	5 (25%)
5	NAG	B	914	1	14,14,15	0.53	0	17,19,21	0.99	1 (5%)
7	SO4	A	1016	-	4,4,4	0.28	0	6,6,6	0.11	0
5	NAG	A	1012	1	14,14,15	0.55	0	17,19,21	0.76	1 (5%)
7	SO4	A	1019	-	4,4,4	0.23	0	6,6,6	0.08	0
7	SO4	B	919	-	4,4,4	0.24	0	6,6,6	0.11	0
7	SO4	B	915	-	4,4,4	0.25	0	6,6,6	0.13	0
7	SO4	B	918	-	4,4,4	0.24	0	6,6,6	0.08	0
7	SO4	A	1017	-	4,4,4	0.25	0	6,6,6	0.09	0
5	NAG	B	912	1	14,14,15	0.61	0	17,19,21	0.68	0
7	SO4	A	1022	-	4,4,4	0.31	0	6,6,6	0.13	0
8	GOL	B	923	-	5,5,5	0.38	0	5,5,5	0.37	0
5	NAG	B	908	1	14,14,15	0.61	0	17,19,21	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
5	NAG	B	912	1	-	0/6/23/26	0/1/1/1
5	NAG	B	908	1	-	2/6/23/26	0/1/1/1
6	C09	B	901	-	-	0/2/4/4	0/3/3/3
6	C09	A	1014	-	-	0/2/4/4	0/3/3/3
5	NAG	B	913	1	-	1/6/23/26	0/1/1/1
5	NAG	B	914	1	-	0/6/23/26	0/1/1/1
8	GOL	B	923	-	-	0/4/4/4	-
5	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1013	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1011	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)
6	A	1014	C09	C2-C1	4.15	1.49	1.41
6	B	901	C09	C2-C1	4.01	1.48	1.41
6	B	901	C09	C2-C3	-3.73	1.37	1.45
6	A	1014	C09	C2-C3	-3.42	1.38	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1011	NAG	C1-O5-C5	2.93	116.11	112.19
6	B	901	C09	O-C6-C5	-2.59	103.68	110.94
6	A	1014	C09	O-C6-C5	-2.55	103.81	110.94
5	B	914	NAG	C1-O5-C5	2.46	115.49	112.19
5	A	1012	NAG	C1-O5-C5	2.34	115.33	112.19
6	B	901	C09	C9-C2-C1	2.19	120.65	117.58
6	B	901	C09	C4-C-N1	-2.13	118.32	120.84
5	A	1007	NAG	O5-C1-C2	-2.11	108.03	111.29
6	B	901	C09	C3-C2-C1	-2.06	116.82	118.58
6	B	901	C09	C-N1-C1	2.01	123.72	118.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1007	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	A	1007	NAG	O7-C7-N2-C2
5	B	908	NAG	C8-C7-N2-C2
5	B	908	NAG	O7-C7-N2-C2
5	A	1011	NAG	C8-C7-N2-C2
5	A	1011	NAG	O7-C7-N2-C2
5	B	913	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1020	SO4	1	0
7	B	920	SO4	1	0
7	A	1021	SO4	1	0
7	B	917	SO4	1	0
5	B	914	NAG	0	1
7	A	1016	SO4	1	0
7	A	1022	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	747/811 (92%)	0.16	47 (6%)	20	19	16, 36, 71, 92	0
1	B	746/811 (91%)	0.04	21 (2%)	53	51	16, 34, 64, 91	0
All	All	1493/1622 (92%)	0.10	68 (4%)	32	31	16, 35, 69, 92	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	758	THR	9.7
1	B	759	LYS	6.7
1	A	62	GLY	5.8
1	A	64	TYR	5.4
1	A	758	THR	5.1
1	A	83	PHE	4.9
1	A	59	GLN	4.7
1	A	61	VAL	4.6
1	A	34	TYR	4.2
1	A	757	GLU	4.1
1	A	807	GLY	4.1
1	A	60	THR	4.0
1	A	31	SER	4.0
1	A	86	LEU	3.9
1	A	33	SER	3.9
1	B	736	SER	3.7
1	B	79	THR	3.7
1	B	756	LEU	3.6
1	B	81	GLU	3.4
1	A	812	LYS	3.4
1	A	84	GLN	3.2
1	A	761	THR	3.2
1	A	63	LYS	3.1
1	A	729	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	809	GLN	3.0
1	B	735	VAL	3.0
1	A	779	ASP	3.0
1	B	385	ASP	2.9
1	A	251	LEU	2.9
1	B	777	THR	2.9
1	A	470	PHE	2.8
1	B	74	PHE	2.8
1	A	810	ARG	2.8
1	A	756	LEU	2.8
1	A	46	ILE	2.7
1	A	361	ARG	2.7
1	B	80	ASN	2.6
1	A	58	PRO	2.6
1	A	39	LYS	2.6
1	A	186	VAL	2.6
1	A	733	SER	2.6
1	A	459	PHE	2.6
1	B	778	CYS	2.5
1	A	45	VAL	2.5
1	B	779	ASP	2.4
1	A	706	SER	2.4
1	A	113	GLY	2.4
1	A	799	VAL	2.4
1	A	734	GLU	2.4
1	A	57	VAL	2.3
1	B	808	ASP	2.3
1	A	808	ASP	2.3
1	B	77	HIS	2.3
1	A	736	SER	2.3
1	B	84	GLN	2.3
1	A	816	SER	2.3
1	B	392	GLN	2.2
1	A	253	LEU	2.2
1	B	761	THR	2.2
1	A	782	ASP	2.2
1	A	815	VAL	2.2
1	A	705	ASP	2.1
1	A	292	LEU	2.1
1	A	760	THR	2.1
1	B	292	LEU	2.1
1	A	762	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	37	ASP	2.0
1	B	117	THR	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)

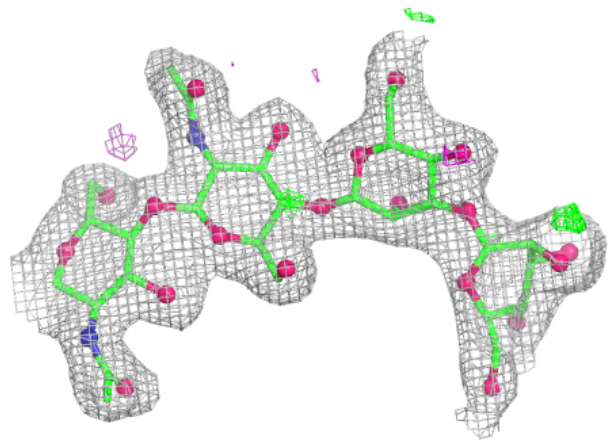
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

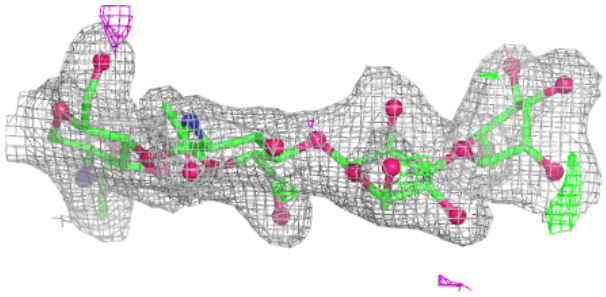
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	2	14/15	0.74	0.29	44,52,62,65	0
2	MAN	C	4	11/12	0.82	0.12	54,56,58,58	0
2	MAN	F	4	11/12	0.83	0.27	54,58,60,63	0
2	BMA	F	3	11/12	0.86	0.14	34,46,54,54	0
3	NAG	G	2	14/15	0.86	0.19	42,52,61,66	0
4	BMA	H	3	11/12	0.86	0.19	48,54,59,59	0
2	BMA	C	3	11/12	0.88	0.10	44,48,53,53	0
4	BMA	E	3	11/12	0.91	0.20	45,52,55,56	0
3	NAG	D	1	14/15	0.94	0.11	17,22,29,36	0
2	NAG	F	1	14/15	0.94	0.11	18,20,29,34	0
4	NAG	H	2	14/15	0.94	0.11	23,26,36,42	0
3	NAG	G	1	14/15	0.94	0.12	15,24,30,39	0
4	NAG	E	1	14/15	0.95	0.10	16,21,26,27	0
2	NAG	F	2	14/15	0.95	0.09	21,25,30,33	0
4	NAG	E	2	14/15	0.96	0.13	22,25,39,46	0
4	NAG	H	1	14/15	0.96	0.10	18,22,28,30	0
2	NAG	C	1	14/15	0.97	0.15	21,27,31,32	0
2	NAG	C	2	14/15	0.97	0.12	23,31,35,40	0

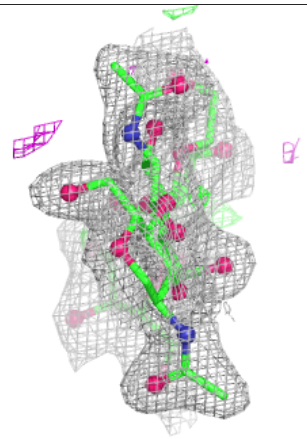
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

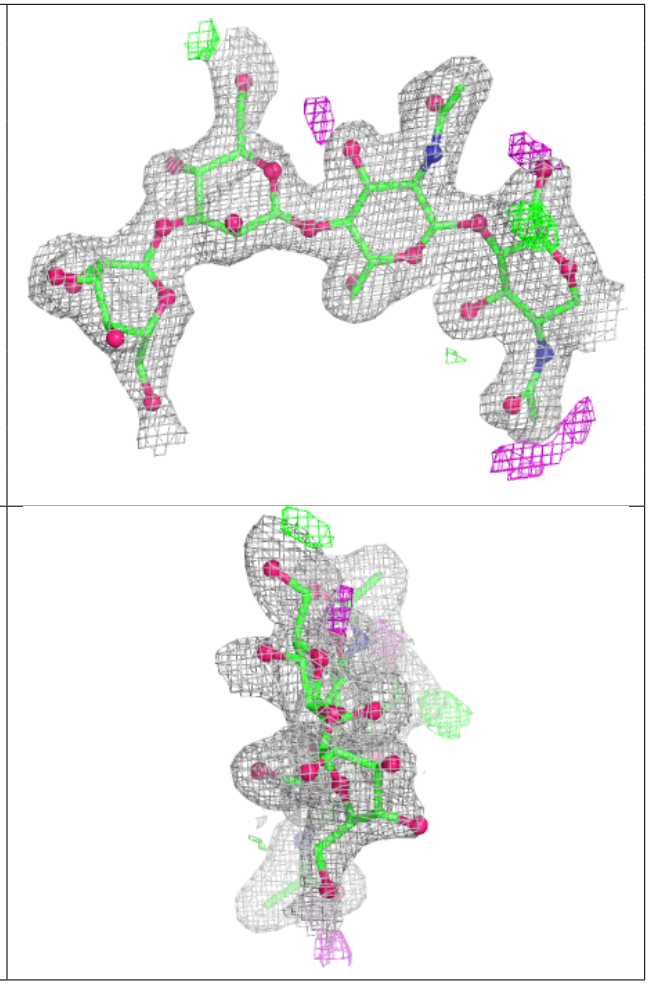






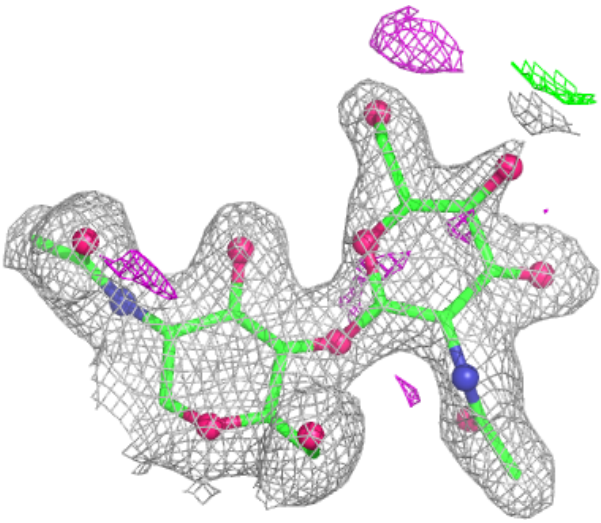
Electron density around Chain F:

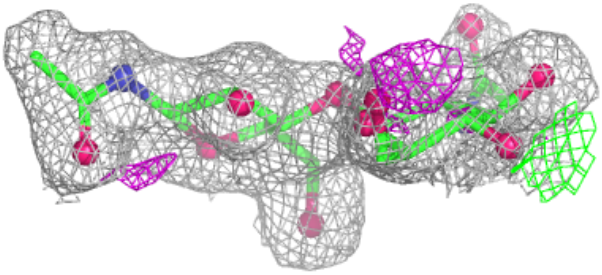
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

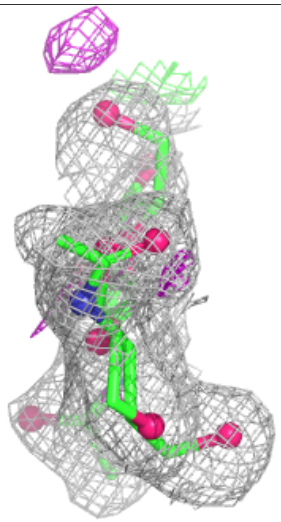


Electron density around Chain D:

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

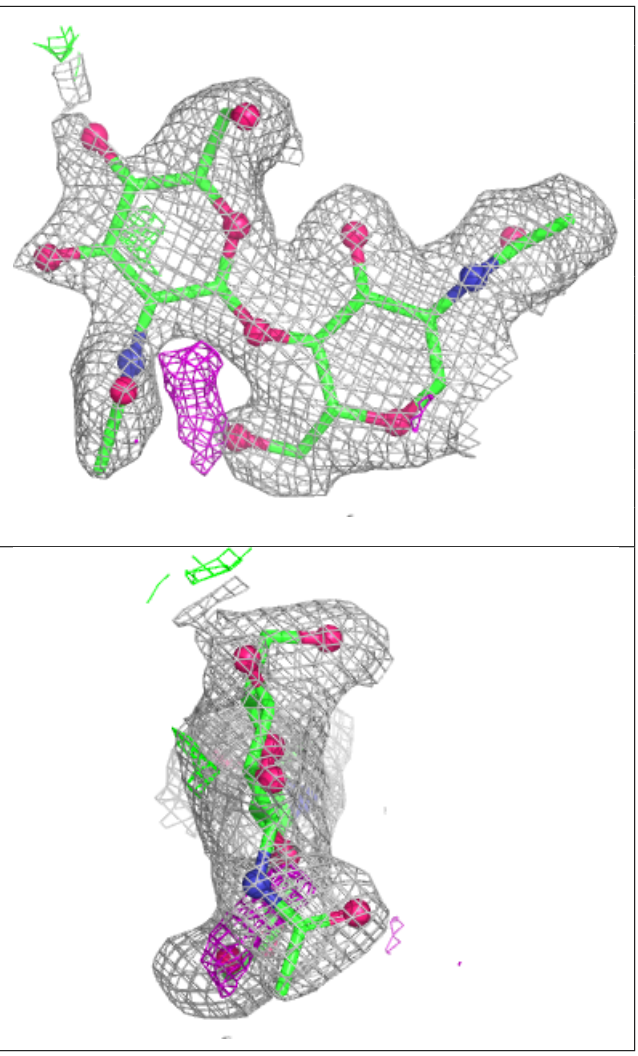






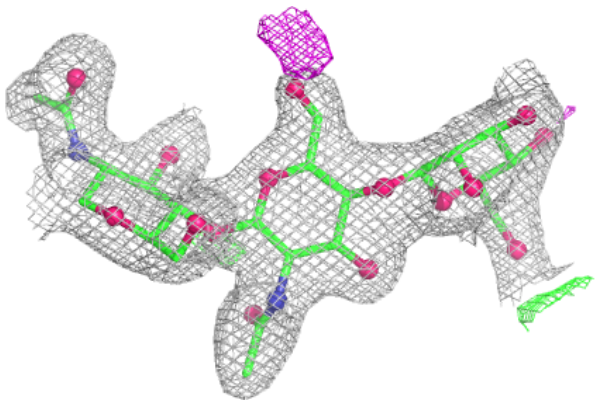
Electron density around Chain G:

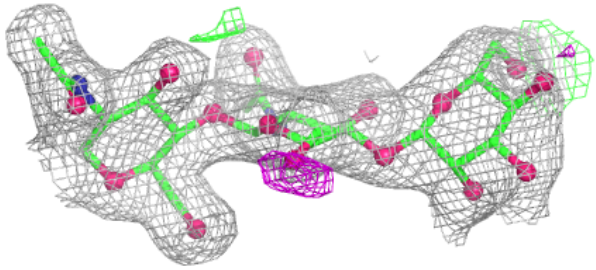
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

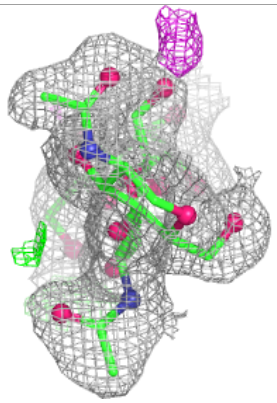


Electron density around Chain E:

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

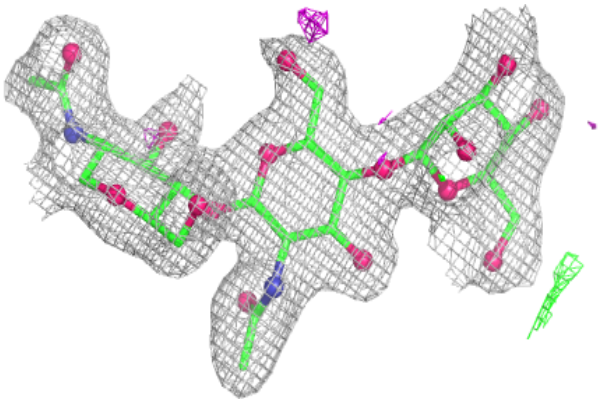


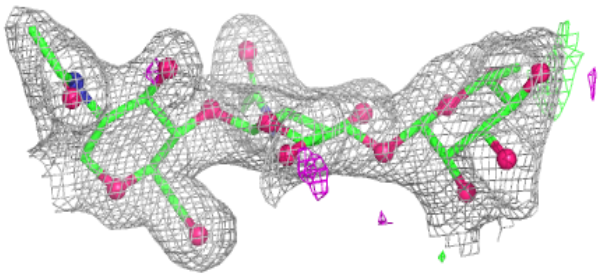


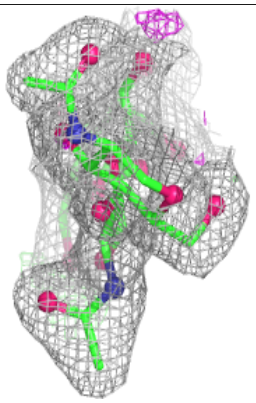


Electron density around Chain H:

$2mF_o$-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
8	GOL	B	923	6/6	0.81	0.18	38,43,46,50	0
5	NAG	B	908	14/15	0.84	0.21	49,58,67,71	0
5	NAG	A	1011	14/15	0.86	0.31	52,57,65,67	0
5	NAG	B	912	14/15	0.87	0.16	50,57,61,62	0
7	SO4	B	919	5/5	0.89	0.17	85,85,86,87	0
7	SO4	A	1021	5/5	0.90	0.17	82,83,85,85	0
5	NAG	A	1012	14/15	0.90	0.14	38,45,49,49	0
7	SO4	B	922	5/5	0.90	0.21	85,85,86,87	0
7	SO4	A	1020	5/5	0.90	0.32	95,97,97,99	0
5	NAG	B	913	14/15	0.91	0.16	38,41,46,47	0
7	SO4	B	921	5/5	0.92	0.18	89,89,90,92	0
7	SO4	A	1019	5/5	0.92	0.23	84,84,85,86	0
5	NAG	A	1007	14/15	0.92	0.15	40,49,61,67	0
5	NAG	B	914	14/15	0.93	0.12	32,46,60,63	0
5	NAG	A	1013	14/15	0.94	0.11	43,50,56,61	0
7	SO4	B	918	5/5	0.94	0.08	84,87,88,89	0
7	SO4	B	917	5/5	0.95	0.13	63,64,66,67	0
7	SO4	A	1018	5/5	0.95	0.25	91,92,93,94	0
7	SO4	A	1017	5/5	0.96	0.10	67,68,70,71	0
7	SO4	A	1022	5/5	0.96	0.22	78,79,82,82	0
7	SO4	B	915	5/5	0.97	0.11	38,41,52,53	0
7	SO4	B	920	5/5	0.97	0.12	65,65,68,70	0
7	SO4	B	916	5/5	0.97	0.08	54,56,59,61	0
6	C09	A	1014	18/18	0.97	0.13	15,21,32,32	0
6	C09	B	901	18/18	0.97	0.13	17,22,27,29	0
7	SO4	A	1016	5/5	0.98	0.07	42,46,50,57	0
7	SO4	A	1015	5/5	0.98	0.13	34,40,46,50	0

6.5 Other polymers (i)

There are no such residues in this entry.