Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 06:43 AM EDT

PDB ID	:	3W3L
Title	:	Crystal structure of human TLR8 in complex with Resiquimod (R848) crystal form 1
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2012-12-22
Resolution	:	2.33 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 ⓘ 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 ⓘ) were used in the production of this report:

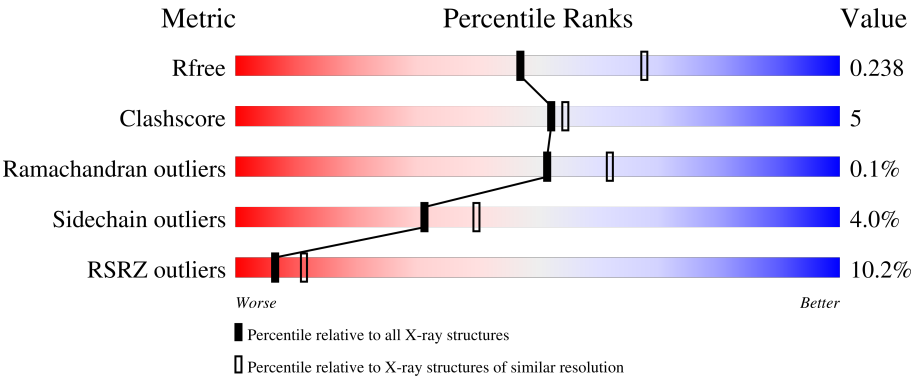
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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% 77% 14% • 7%
1	B	811	9% 77% 14% • 7%
1	C	811	12% 78% 14% • 7%
1	D	811	11% 77% 14% • 7%
2	E	5	40% 60%

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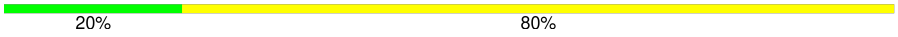
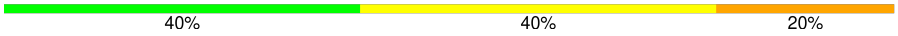
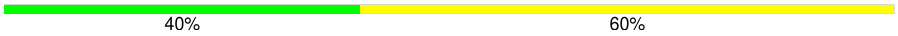
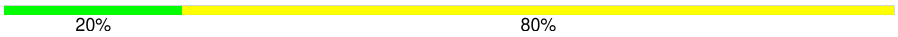
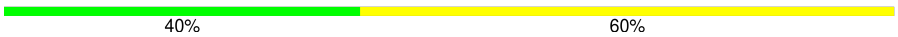
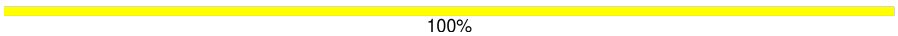
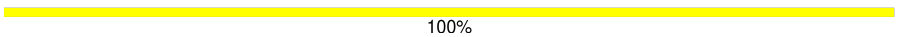
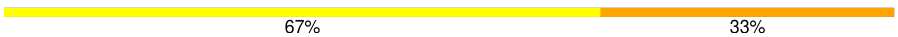
Mol	Chain	Length	Quality of chain
2	G	5	
2	H	5	
2	J	5	
2	K	5	
2	M	5	
2	N	5	
2	P	5	
3	F	3	
3	I	3	
3	L	3	
3	O	3	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 26024 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
1	A	751	Total	C	N	O	S	0	0	0
			6038	3862	1025	1132	19			
1	B	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			
1	C	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			
1	D	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			

There are 40 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
C	23	ARG	-	expression tag	UNP Q9NR97

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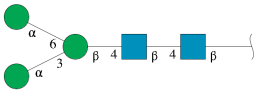
Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP Q9NR97
C	25	PRO	-	expression tag	UNP Q9NR97
C	26	TRP	-	expression tag	UNP Q9NR97
C	828	GLU	-	expression tag	UNP Q9NR97
C	829	PHE	-	expression tag	UNP Q9NR97
C	830	LEU	-	expression tag	UNP Q9NR97
C	831	VAL	-	expression tag	UNP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

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

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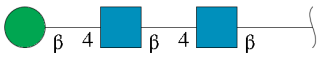
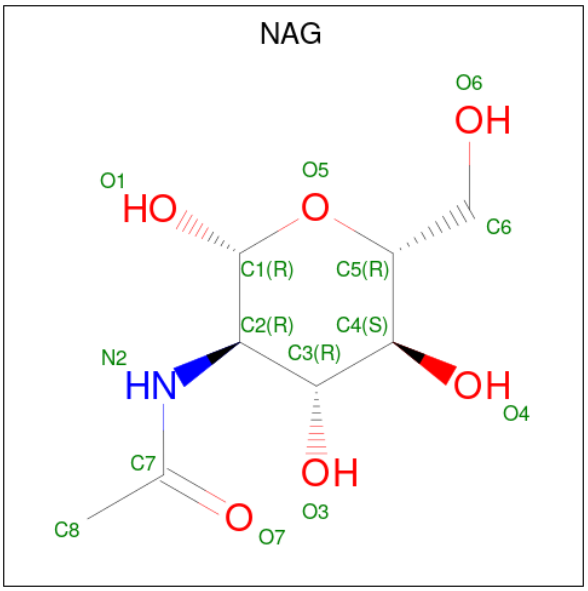
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	N	5	Total C N O 61 34 2 25	0	0	0
2	P	5	Total C N O 61 34 2 25	0	0	0

- Molecule 3 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.



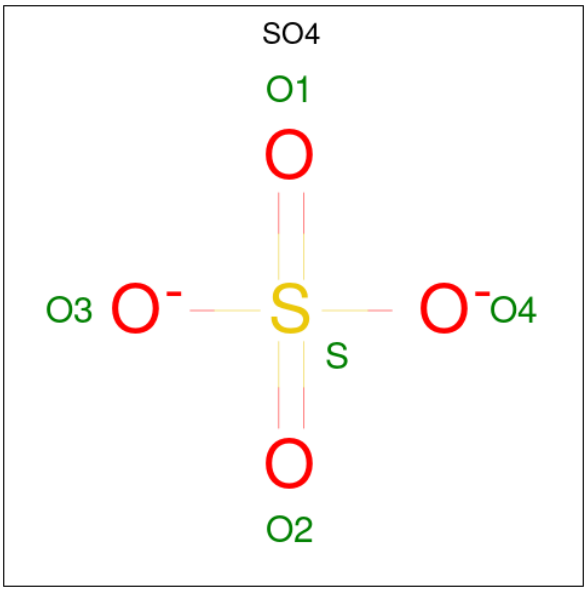
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	3	Total C N O 39 22 2 15	0	0	0
3	I	3	Total C N O 39 22 2 15	0	0	0
3	L	3	Total C N O 39 22 2 15	0	0	0
3	O	3	Total C N O 39 22 2 15	0	0	0

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



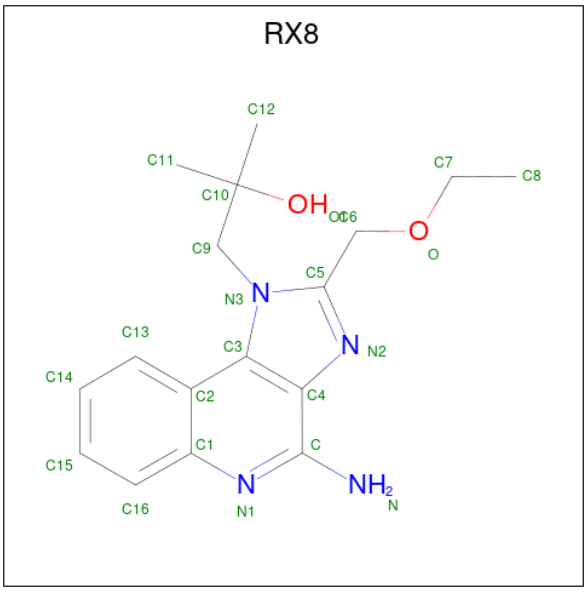
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

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



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

- Molecule 6 is 1-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-2-methylpropan-2-ol (three-letter code: RX8) (formula: $C_{17}H_{22}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 23 17 4 2	0	0
6	C	1	Total C N O 23 17 4 2	0	0
6	D	1	Total C N O 23 17 4 2	0	0
6	D	1	Total C N O 23 17 4 2	0	0

- Molecule 7 is water.

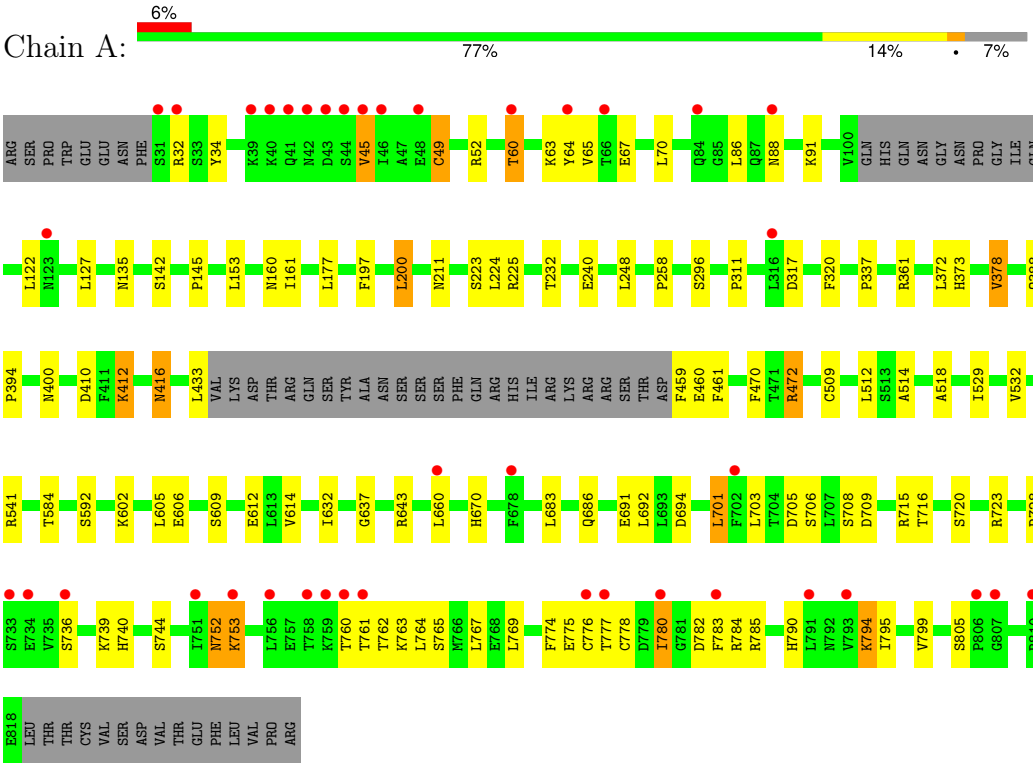
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	269	Total O 269 269	0	0
7	B	240	Total O 240 240	0	0
7	C	214	Total O 214 214	0	0
7	D	172	Total O 172 172	0	0

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.

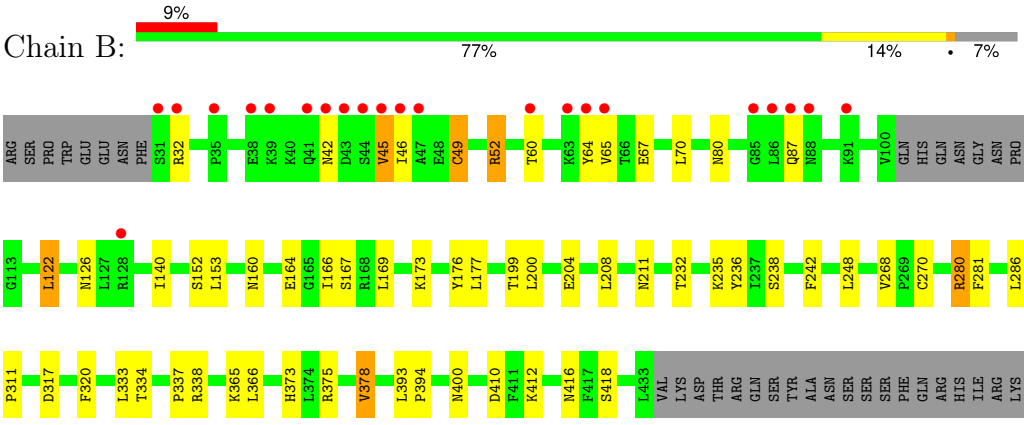
• Molecule 1: Toll-like receptor 8

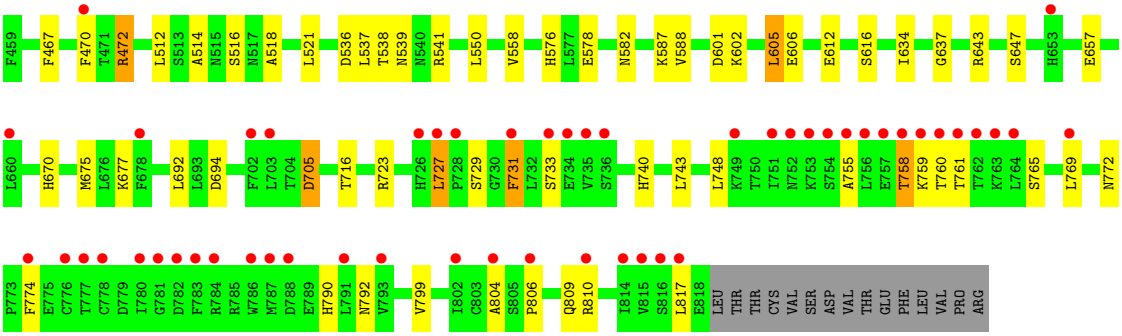
Chain A:



• Molecule 1: Toll-like receptor 8

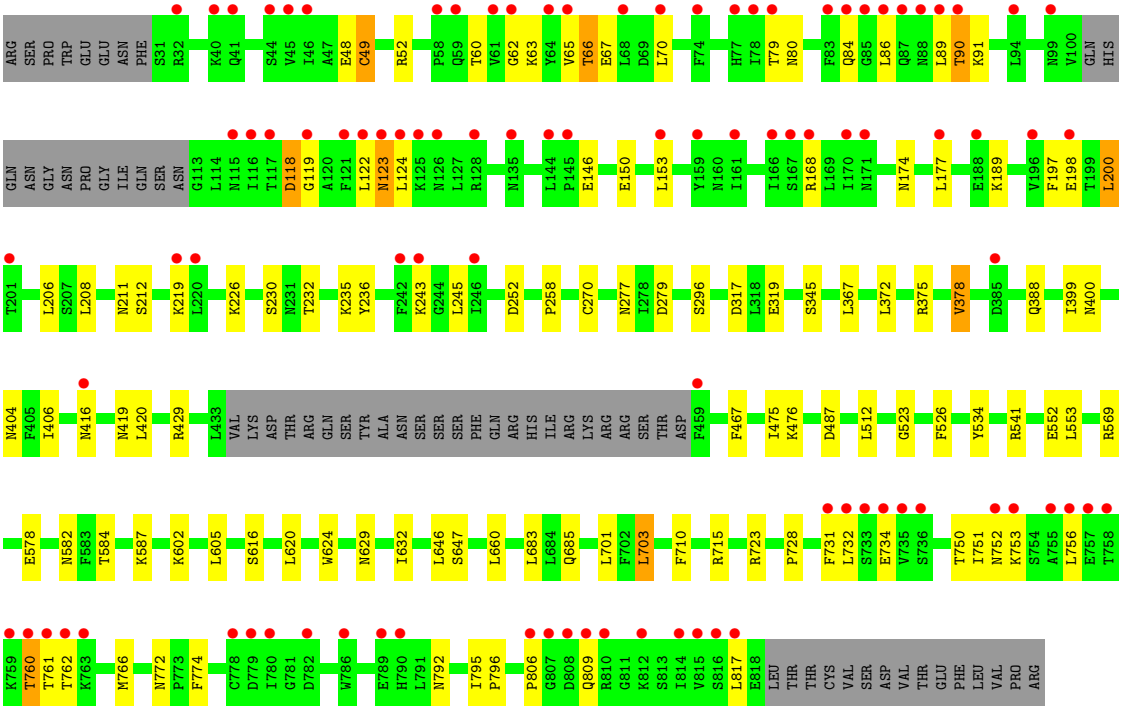
Chain B:





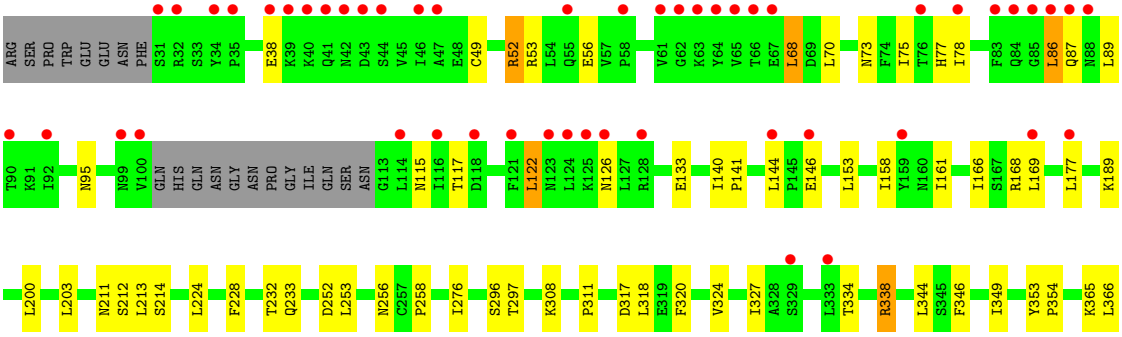
• Molecule 1: Toll-like receptor 8

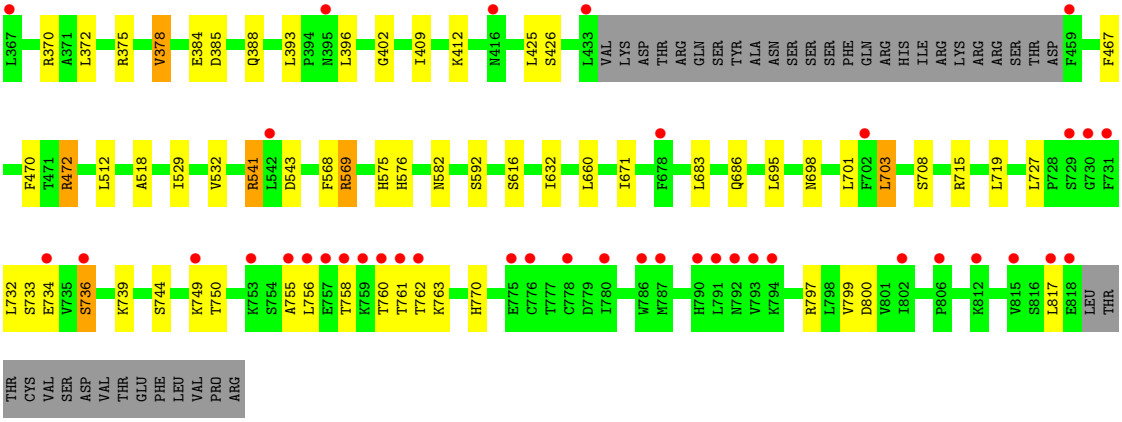
Chain C:



• Molecule 1: Toll-like receptor 8

Chain D:



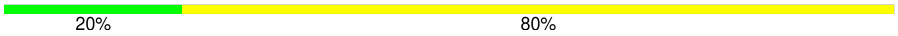


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

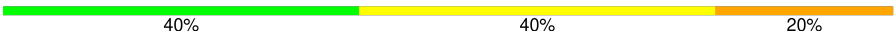
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

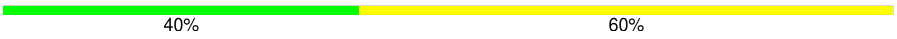


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

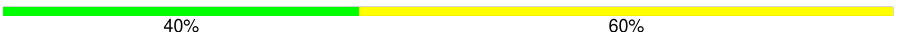
Chain M:

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

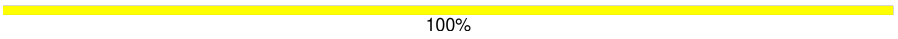
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



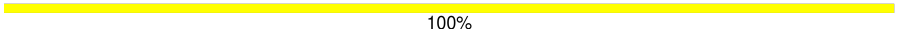
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



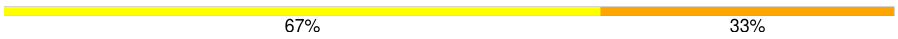
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain L:



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

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.47Å 138.87Å 169.66Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	45.08 – 2.33 45.07 – 2.33	Depositor EDS
% Data completeness (in resolution range)	93.1 (45.08-2.33) 93.1 (45.07-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.196 , 0.239 0.199 , 0.238	Depositor DCC
R_{free} test set	7995 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26024	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, SO4, RX8, 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	0.35	0/6163	0.61	1/8360 (0.0%)
1	B	0.34	0/6160	0.60	0/8356
1	C	0.33	0/6160	0.58	0/8356
1	D	0.31	0/6160	0.57	0/8356
All	All	0.33	0/24643	0.59	1/33428 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	753	LYS	CD-CE-NZ	-5.75	98.49	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6038	0	6012	65	2
1	B	6035	0	6003	73	0
1	C	6035	0	6004	66	0
1	D	6035	0	6003	68	2
2	E	61	0	52	0	0
2	G	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	61	0	52	1	0
2	J	61	0	52	0	0
2	K	61	0	52	2	0
2	M	61	0	52	0	0
2	N	61	0	52	1	0
2	P	61	0	52	0	0
3	F	39	0	34	0	0
3	I	39	0	34	0	0
3	L	39	0	34	1	0
3	O	39	0	34	0	0
4	A	56	0	52	0	0
4	B	56	0	52	0	0
4	C	42	0	39	0	0
4	D	56	0	52	0	0
5	A	10	0	0	0	0
5	B	15	0	0	1	0
5	C	5	0	0	1	0
5	D	10	0	0	0	0
6	B	23	0	22	3	0
6	C	23	0	22	2	0
6	D	46	0	44	5	0
7	A	269	0	0	3	0
7	B	240	0	0	9	0
7	C	214	0	0	4	0
7	D	172	0	0	2	0
All	All	26024	0	24857	274	2

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 (274) 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:34:TYR:O	1:A:60:THR:OG1	1.99	0.79
1:C:80:ASN:O	1:C:84:GLN:NE2	2.17	0.78
1:C:123:ASN:OD1	1:C:123:ASN:N	2.20	0.74
1:D:749:LYS:HG3	1:D:750:THR:HG22	1.71	0.73
1:D:52:ARG:HG2	1:D:799:VAL:HG21	1.70	0.73
1:C:399:ILE:HG12	1:C:420:LEU:HD21	1.70	0.72
1:A:692:LEU:HD13	1:A:716:THR:HB	1.72	0.72
1:B:286:LEU:O	7:B:1199:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:LEU:HD23	1:D:89:LEU:HD12	1.73	0.68
1:B:470:PHE:HD2	1:B:472:ARG:HG3	1.58	0.67
1:A:777:THR:O	1:A:780:ILE:HG23	1.96	0.66
1:D:569:ARG:NH2	7:D:1158:HOH:O	2.29	0.65
1:A:161:ILE:HD12	1:A:177:LEU:HD13	1.77	0.65
1:A:780:ILE:HD11	1:A:784:ARG:HG2	1.79	0.65
1:C:766:MET:SD	7:C:1205:HOH:O	2.55	0.65
1:C:89:LEU:HD11	1:C:124:LEU:HB3	1.77	0.65
1:B:164:GLU:OE1	1:B:164:GLU:N	2.29	0.64
1:A:470:PHE:CD1	1:A:472:ARG:HG3	2.33	0.64
1:A:223:SER:O	1:A:225:ARG:NH1	2.30	0.64
1:A:311:PRO:HB3	1:B:337:PRO:HB2	1.78	0.64
1:B:80:ASN:ND2	7:B:1233:HOH:O	2.30	0.63
1:A:160:ASN:ND2	7:A:1150:HOH:O	2.28	0.63
1:B:606:GLU:OE2	7:B:1266:HOH:O	2.16	0.63
1:D:213:LEU:HB2	1:D:232:THR:HB	1.81	0.63
1:B:729:SER:HA	1:B:755:ALA:HA	1.80	0.62
1:A:518:ALA:HA	1:A:541:ARG:O	1.99	0.62
1:B:32:ARG:NH2	1:B:790:HIS:O	2.33	0.62
1:C:119:GLY:HA2	1:C:122:LEU:HD13	1.79	0.62
6:C:901:RX8:H9	6:C:901:RX8:H19	1.81	0.61
6:D:901:RX8:H19	6:D:901:RX8:H9	1.83	0.61
1:A:52:ARG:HG2	1:A:799:VAL:HG21	1.82	0.60
1:C:118:ASP:OD1	1:C:118:ASP:N	2.35	0.60
1:B:470:PHE:CD2	1:B:472:ARG:HG3	2.37	0.59
1:B:705:ASP:OD1	1:B:705:ASP:N	2.22	0.59
1:C:86:LEU:HB2	1:C:89:LEU:HD23	1.84	0.59
1:B:518:ALA:HA	1:B:541:ARG:O	2.03	0.59
1:B:743:LEU:HD23	1:B:748:LEU:HD11	1.84	0.59
1:C:67:GLU:HG2	1:C:91:LYS:HB3	1.84	0.59
1:C:79:THR:HG22	1:C:80:ASN:H	1.68	0.59
1:A:775:GLU:OE1	1:A:805:SER:OG	2.15	0.59
6:D:902:RX8:H19	6:D:902:RX8:H9	1.84	0.59
1:C:723:ARG:NH1	5:C:918:SO4:O3	2.29	0.58
1:A:337:PRO:HB2	1:B:311:PRO:HB3	1.84	0.58
1:B:289:LEU:HB2	7:B:1199:HOH:O	2.04	0.57
1:C:760:THR:OG1	1:C:761:THR:N	2.37	0.57
1:D:518:ALA:HA	1:D:541:ARG:O	2.05	0.57
1:A:378:VAL:HG21	6:D:901:RX8:H8	1.87	0.57
1:B:806:PRO:HD2	1:B:809:GLN:HB2	1.86	0.57
1:B:587:LYS:NZ	7:B:1217:HOH:O	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:HD23	1:D:224:LEU:HD21	1.86	0.56
1:B:375:ARG:NH1	7:B:1200:HOH:O	2.38	0.56
1:B:612:GLU:OE2	1:B:643:ARG:NH1	2.39	0.56
1:C:578:GLU:HG2	1:C:602:LYS:HG3	1.88	0.56
1:A:769:LEU:HD23	1:A:774:PHE:HZ	1.70	0.56
1:B:87:GLN:O	1:B:126:ASN:ND2	2.33	0.55
1:B:521:LEU:HD13	1:B:550:LEU:HD21	1.89	0.55
1:A:197:PHE:HA	1:A:200:LEU:HD22	1.88	0.55
1:A:705:ASP:HB3	1:A:728:PRO:HB2	1.88	0.54
1:C:226:LYS:NZ	2:K:2:NAG:O7	2.38	0.54
1:A:153:LEU:HB2	1:A:177:LEU:HD23	1.89	0.54
1:B:334:THR:HG22	1:B:365:LYS:HD2	1.87	0.54
1:D:87:GLN:O	1:D:126:ASN:ND2	2.38	0.54
1:D:153:LEU:HD23	1:D:158:ILE:HD13	1.90	0.54
1:A:691:GLU:HG2	1:A:715:ARG:HD3	1.89	0.54
1:B:52:ARG:HG2	1:B:799:VAL:HG21	1.90	0.54
1:D:53:ARG:NH1	1:D:800:ASP:OD1	2.37	0.54
1:B:378:VAL:HG21	6:C:901:RX8:H8	1.89	0.54
1:B:242:PHE:HB3	1:B:286:LEU:HD21	1.90	0.54
1:D:727:LEU:HD23	1:D:755:ALA:HB1	1.89	0.54
1:C:728:PRO:HG2	1:C:731:PHE:HB2	1.90	0.53
6:B:1018:RX8:H19	6:B:1018:RX8:H9	1.90	0.53
1:C:236:TYR:HD1	1:C:277:ASN:HB3	1.74	0.53
7:B:1197:HOH:O	1:C:541:ARG:HD2	2.07	0.53
1:B:46:ILE:HG22	1:B:67:GLU:HB2	1.91	0.53
1:C:587:LYS:NZ	7:C:1210:HOH:O	2.34	0.53
1:D:141:PRO:HG2	1:D:144:LEU:HD11	1.91	0.53
1:B:49:CYS:HB3	1:B:70:LEU:HD23	1.90	0.52
1:D:70:LEU:O	1:D:73:ASN:ND2	2.38	0.52
1:D:327:ILE:HG12	1:D:344:LEU:HD13	1.90	0.52
1:C:89:LEU:HD12	1:C:89:LEU:O	2.09	0.52
1:B:692:LEU:HD13	1:B:716:THR:HB	1.92	0.52
1:B:727:LEU:HG	1:B:755:ALA:HB1	1.91	0.52
1:A:739:LYS:HE3	1:A:763:LYS:HE3	1.92	0.52
1:B:558:VAL:HG13	1:B:588:VAL:HB	1.90	0.52
1:D:733:SER:HA	1:D:758:THR:OG1	2.10	0.52
1:D:146:GLU:N	1:D:146:GLU:OE1	2.43	0.52
1:D:311:PRO:O	1:D:338:ARG:HG3	2.10	0.51
1:D:576:HIS:NE2	7:D:1045:HOH:O	2.34	0.51
1:A:361:ARG:NH1	7:A:1255:HOH:O	2.38	0.51
1:A:739:LYS:HA	1:A:764:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:GLU:HG2	1:B:637:GLY:HA3	1.91	0.51
1:A:63:LYS:HA	1:A:86:LEU:HD23	1.93	0.51
1:D:95:ASN:OD1	1:D:133:GLU:N	2.44	0.51
1:C:660:LEU:HD21	1:C:683:LEU:HD22	1.92	0.50
1:C:189:LYS:HA	1:C:212:SER:HB3	1.94	0.50
1:A:776:CYS:HA	1:A:780:ILE:HG21	1.94	0.50
1:B:804:ALA:O	1:B:810:ARG:NH1	2.44	0.50
1:C:715:ARG:NH1	7:C:1189:HOH:O	2.44	0.50
1:D:467:PHE:HB3	2:N:1:NAG:H81	1.93	0.50
1:B:296:SER:HA	1:B:320:PHE:O	2.12	0.49
1:D:318:LEU:HB2	1:D:344:LEU:HD23	1.94	0.49
1:A:612:GLU:HG3	1:A:643:ARG:HD3	1.93	0.49
1:D:258:PRO:HA	1:D:296:SER:O	2.11	0.49
1:B:153:LEU:HB2	1:B:177:LEU:HD23	1.95	0.49
1:A:258:PRO:HA	1:A:296:SER:O	2.11	0.49
1:A:731:PHE:CG	1:A:732:LEU:N	2.80	0.49
1:D:253:LEU:O	1:D:256:ASN:ND2	2.37	0.49
1:D:77:HIS:CE1	1:D:115:ASN:HD22	2.31	0.49
1:C:66:THR:HA	1:C:89:LEU:HA	1.95	0.49
1:D:334:THR:HG22	1:D:365:LYS:HD3	1.94	0.49
1:B:467:PHE:HB3	2:H:1:NAG:H81	1.94	0.49
1:C:79:THR:HG22	1:C:80:ASN:N	2.27	0.49
1:C:150:GLU:HG3	1:C:174:ASN:HB2	1.94	0.49
1:D:140:ILE:HD13	1:D:166:ILE:HD11	1.94	0.49
1:B:536:ASP:OD1	1:B:538:THR:HG23	2.13	0.49
1:C:734:GLU:H	1:C:760:THR:HG21	1.78	0.49
1:D:660:LEU:HD21	1:D:683:LEU:HD22	1.94	0.49
1:B:760:THR:OG1	1:B:761:THR:N	2.46	0.48
1:B:235:LYS:HG3	1:B:270:CYS:SG	2.52	0.48
6:B:1018:RX8:H2	1:C:378:VAL:HG11	1.95	0.48
1:A:49:CYS:HB3	1:A:70:LEU:HD23	1.96	0.48
1:C:388:GLN:NE2	7:C:1118:HOH:O	2.46	0.48
1:A:706:SER:OG	1:A:709:ASP:OD2	2.30	0.48
1:B:792:ASN:OD1	1:B:792:ASN:N	2.39	0.48
1:C:197:PHE:HA	1:C:200:LEU:HD22	1.96	0.48
1:B:723:ARG:NH1	5:B:1019:SO4:O1	2.38	0.48
1:D:732:LEU:HD11	1:D:756:LEU:O	2.13	0.48
1:B:211:ASN:O	1:B:232:THR:HA	2.14	0.48
1:D:695:LEU:O	1:D:698:ASN:ND2	2.45	0.48
1:B:731:PHE:HD1	1:B:731:PHE:H	1.62	0.47
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLN:OE1	1:C:84:GLN:N	2.45	0.47
1:B:152:SER:HA	1:B:176:TYR:HB2	1.97	0.47
1:D:378:VAL:HG21	6:D:902:RX8:H8	1.97	0.47
1:D:122:LEU:HD12	1:D:122:LEU:HA	1.78	0.47
1:D:734:GLU:HG2	1:D:760:THR:HG21	1.96	0.46
1:C:66:THR:OG1	1:C:90:THR:OG1	2.31	0.46
1:C:206:LEU:HG	1:C:208:LEU:HD13	1.98	0.46
1:B:733:SER:HA	1:B:758:THR:HG23	1.97	0.46
1:C:63:LYS:HA	1:C:86:LEU:HD23	1.96	0.46
1:C:198:GLU:OE1	1:C:219:LYS:HD3	2.16	0.46
1:D:214:SER:HA	1:D:233:GLN:O	2.15	0.46
1:C:49:CYS:HB3	1:C:70:LEU:HD23	1.97	0.46
1:A:410:ASP:OD1	1:A:412:LYS:HG2	2.15	0.46
1:A:606:GLU:HG2	1:A:637:GLY:HA3	1.97	0.46
1:B:670:HIS:HA	1:B:694:ASP:HB3	1.98	0.46
1:C:629:ASN:O	1:C:632:ILE:HG13	2.16	0.46
1:D:385:ASP:HA	1:D:388:GLN:HG2	1.97	0.45
1:A:753:LYS:HD3	1:A:782:ASP:HB3	1.98	0.45
1:B:601:ASP:C	1:B:602:LYS:HD2	2.37	0.45
1:D:68:LEU:HD22	1:D:70:LEU:HG	1.97	0.45
1:A:752:ASN:OD1	1:A:752:ASN:N	2.50	0.45
1:B:166:ILE:HD13	1:B:166:ILE:HA	1.77	0.45
1:B:657:GLU:OE1	1:B:657:GLU:N	2.34	0.45
1:D:708:SER:HB3	1:D:733:SER:O	2.16	0.45
1:D:736:SER:O	1:D:763:LYS:HG2	2.17	0.45
1:A:780:ILE:O	1:A:783:PHE:N	2.49	0.45
1:D:402:GLY:HA2	1:D:426:SER:O	2.16	0.45
1:A:765:SER:O	1:A:794:LYS:HG3	2.17	0.45
1:D:384:GLU:OE1	1:D:412:LYS:HE3	2.17	0.45
1:A:592:SER:HB3	1:A:614:VAL:HG12	1.99	0.45
1:C:258:PRO:HA	1:C:296:SER:O	2.17	0.45
1:D:276:ILE:CG2	1:D:297:THR:HB	2.47	0.45
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.98	0.44
1:B:582:ASN:ND2	7:B:1336:HOH:O	2.49	0.44
1:D:715:ARG:HE	1:D:739:LYS:HD2	1.81	0.44
1:A:211:ASN:O	1:A:232:THR:HA	2.18	0.44
1:D:228:PHE:HA	1:D:252:ASP:HB3	1.99	0.44
1:D:334:THR:HB	1:D:365:LYS:HE2	1.99	0.44
1:D:660:LEU:HD22	1:D:686:GLN:HG3	1.99	0.44
1:A:296:SER:HA	1:A:320:PHE:O	2.18	0.43
1:D:211:ASN:O	1:D:232:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:SER:HB2	1:C:252:ASP:OD2	2.18	0.43
1:C:750:THR:OG1	1:C:751:ILE:N	2.51	0.43
1:A:632:ILE:HD13	1:A:632:ILE:HA	1.83	0.43
1:A:705:ASP:OD1	1:A:705:ASP:N	2.42	0.43
1:B:177:LEU:HB2	1:B:208:LEU:HD23	1.99	0.43
1:C:62:GLY:O	1:C:65:VAL:HG22	2.19	0.43
1:D:324:VAL:HG21	1:D:349:ILE:HG13	2.01	0.43
1:C:620:LEU:HD11	1:C:646:LEU:HD22	2.01	0.43
1:C:752:ASN:OD1	1:C:753:LYS:N	2.50	0.43
1:D:346:PHE:N	1:D:375:ARG:O	2.30	0.43
1:D:543:ASP:OD2	6:D:901:RX8:N1	2.51	0.43
1:D:760:THR:OG1	1:D:761:THR:N	2.52	0.43
1:A:529:ILE:O	1:A:532:VAL:HG23	2.19	0.43
1:B:169:LEU:O	1:B:200:LEU:HD22	2.18	0.43
1:B:514:ALA:HA	1:B:539:ASN:O	2.19	0.43
1:D:732:LEU:HD12	1:D:758:THR:OG1	2.18	0.43
1:A:460:GLU:HG3	1:A:461:PHE:CD2	2.54	0.43
1:A:660:LEU:HD22	1:A:686:GLN:HG3	2.00	0.43
1:C:319:GLU:HG2	1:C:345:SER:HB2	2.00	0.43
1:C:732:LEU:HD13	1:C:756:LEU:HD23	2.01	0.43
1:C:467:PHE:HB3	2:K:1:NAG:H81	2.01	0.43
1:C:772:ASN:HB2	1:C:774:PHE:CE2	2.54	0.43
1:D:370:ARG:O	1:D:396:LEU:HD12	2.18	0.43
1:A:767:LEU:HG	1:A:769:LEU:HD11	2.01	0.42
1:C:404:ASN:HB2	1:C:406:ILE:HG13	2.01	0.42
1:D:161:ILE:HD12	1:D:177:LEU:HD13	2.01	0.42
1:B:769:LEU:O	1:B:772:ASN:ND2	2.42	0.42
1:C:146:GLU:HG2	1:C:168:ARG:O	2.19	0.42
1:C:620:LEU:O	1:C:624:TRP:HB2	2.19	0.42
1:D:146:GLU:OE2	1:D:168:ARG:NH2	2.52	0.42
1:A:32:ARG:NH2	1:A:790:HIS:O	2.51	0.42
1:D:70:LEU:HD23	1:D:70:LEU:HA	1.87	0.42
1:D:296:SER:HA	1:D:320:PHE:O	2.19	0.42
1:C:806:PRO:HD2	1:C:809:GLN:HB2	2.01	0.42
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.83	0.42
1:C:48:GLU:HG3	1:C:52:ARG:HH21	1.83	0.42
1:C:703:LEU:HD12	1:C:703:LEU:HA	1.87	0.42
1:D:409:ILE:HD12	1:D:425:LEU:HD13	2.00	0.42
1:A:67:GLU:HG2	1:A:91:LYS:HB3	2.01	0.42
1:C:523:GLY:O	1:C:552:GLU:HB3	2.20	0.42
1:A:412:LYS:HB3	1:A:412:LYS:HE3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LEU:HD22	1:B:634:ILE:HG12	2.02	0.42
1:D:189:LYS:HA	1:D:212:SER:HB3	2.01	0.42
6:B:1018:RX8:H21	1:C:429:ARG:NH1	2.35	0.42
1:A:114:LEU:HB3	1:A:135:ASN:HB3	2.02	0.41
1:B:716:THR:HG23	1:B:740:HIS:HB3	2.02	0.41
1:D:78:ILE:O	1:D:117:THR:HG23	2.20	0.41
1:A:45:VAL:HG22	1:A:65:VAL:HA	2.01	0.41
1:A:514:ALA:HA	1:A:539:ASN:O	2.21	0.41
1:B:576:HIS:HB3	1:B:578:GLU:OE1	2.20	0.41
1:D:568:PHE:HA	1:D:575:HIS:CD2	2.55	0.41
1:A:127:LEU:HD23	1:A:145:PRO:HG2	2.01	0.41
1:A:769:LEU:HD13	1:A:795:ILE:HD13	2.02	0.41
1:B:675:MET:HB3	1:B:677:LYS:HZ3	1.85	0.41
1:C:375:ARG:HD3	1:C:400:ASN:HD21	1.84	0.41
1:D:354:PRO:HD2	1:D:378:VAL:O	2.21	0.41
1:A:670:HIS:HA	1:A:694:ASP:HB3	2.01	0.41
1:A:720:SER:HA	1:A:744:SER:O	2.20	0.41
1:B:333:LEU:HD22	1:B:366:LEU:HD11	2.02	0.41
1:B:675:MET:HB3	1:B:677:LYS:NZ	2.35	0.41
1:D:56:GLU:HA	1:D:75:ILE:HG23	2.03	0.41
1:D:470:PHE:CD1	1:D:472:ARG:HG3	2.55	0.41
1:A:459:PHE:HB2	7:A:1337:HOH:O	2.20	0.41
1:B:616:SER:HA	1:B:647:SER:O	2.20	0.41
1:D:529:ILE:O	1:D:532:VAL:HG23	2.20	0.41
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.95	0.41
1:A:753:LYS:CD	1:A:782:ASP:HB3	2.51	0.41
1:B:236:TYR:CE2	1:B:238:SER:HB3	2.56	0.41
1:B:410:ASP:OD1	1:B:412:LYS:HG2	2.20	0.41
1:B:537:LEU:HD23	1:B:537:LEU:HA	1.92	0.41
1:C:235:LYS:HG3	1:C:270:CYS:SG	2.61	0.41
1:C:526:PHE:HB3	1:C:553:LEU:HD21	2.02	0.41
1:C:616:SER:HA	1:C:647:SER:O	2.20	0.41
1:D:276:ILE:HG21	1:D:297:THR:HB	2.03	0.41
1:D:703:LEU:HD11	1:D:719:LEU:HD13	2.01	0.41
1:A:391:MET:SD	1:A:416:ASN:HB3	2.61	0.41
1:A:584:THR:O	1:A:609:SER:HB3	2.21	0.41
1:B:45:VAL:HG11	1:B:64:TYR:HD1	1.85	0.41
1:B:140:ILE:HD13	1:B:166:ILE:HG12	2.02	0.41
1:B:167:SER:HB3	1:B:199:THR:HG21	2.03	0.41
1:D:592:SER:HA	1:D:616:SER:O	2.21	0.41
1:C:475:ILE:HD11	1:C:487:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:GLN:HG3	1:C:710:PHE:HA	2.03	0.41
1:A:537:LEU:HD23	1:A:537:LEU:HA	1.90	0.41
1:B:280:ARG:HG2	1:B:281:PHE:N	2.32	0.41
1:B:373:HIS:HA	1:B:400:ASN:HB3	2.03	0.41
1:C:153:LEU:HB2	1:C:177:LEU:HD23	2.03	0.40
1:C:476:LYS:HD2	3:L:1:NAG:H83	2.03	0.40
1:C:728:PRO:HG2	1:C:731:PHE:CD1	2.56	0.40
1:B:772:ASN:HB2	1:B:774:PHE:CE1	2.56	0.40
1:C:399:ILE:CG1	1:C:420:LEU:HD21	2.45	0.40
1:D:366:LEU:O	1:D:393:LEU:HD22	2.20	0.40
1:D:744:SER:HB2	1:D:770:HIS:O	2.21	0.40
1:B:45:VAL:HG13	1:B:65:VAL:HA	2.02	0.40
1:B:286:LEU:C	7:B:1199:HOH:O	2.56	0.40
1:C:795:ILE:HA	1:C:796:PRO:HD3	1.81	0.40
1:A:393:LEU:HA	1:A:394:PRO:HD3	1.87	0.40
1:A:701:LEU:HD23	1:A:723:ARG:HB3	2.03	0.40
1:A:716:THR:HG23	1:A:740:HIS:HB3	2.02	0.40
1:B:173:LYS:HE3	1:B:204:GLU:OE1	2.20	0.40
1:B:393:LEU:HA	1:B:394:PRO:HD3	1.87	0.40
1:C:211:ASN:O	1:C:232:THR:HA	2.22	0.40

All (2) 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)
1:A:760:THR:OG1	1:D:308:LYS:O[2_645]	2.13	0.07
1:A:708:SER:O	1:D:338:ARG:NH2[2_645]	2.18	0.02

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	745/811 (92%)	720 (97%)	24 (3%)	1 (0%)	51	62
1	B	745/811 (92%)	722 (97%)	22 (3%)	1 (0%)	51	62
1	C	745/811 (92%)	723 (97%)	21 (3%)	1 (0%)	51	62
1	D	745/811 (92%)	723 (97%)	21 (3%)	1 (0%)	51	62
All	All	2980/3244 (92%)	2888 (97%)	88 (3%)	4 (0%)	51	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	VAL
1	B	378	VAL
1	C	378	VAL
1	D	378	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	694/755 (92%)	660 (95%)	34 (5%)	25	31
1	B	693/755 (92%)	668 (96%)	25 (4%)	35	44
1	C	693/755 (92%)	666 (96%)	27 (4%)	32	41
1	D	693/755 (92%)	668 (96%)	25 (4%)	35	44
All	All	2773/3020 (92%)	2662 (96%)	111 (4%)	31	40

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	49	CYS
1	A	60	THR
1	A	64	TYR
1	A	88	ASN
1	A	122	LEU
1	A	142	SER

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Mol	Chain	Res	Type
1	A	200	LEU
1	A	240	GLU
1	A	248	LEU
1	A	317	ASP
1	A	372	LEU
1	A	388	GLN
1	A	412	LYS
1	A	416	ASN
1	A	433	LEU
1	A	472	ARG
1	A	509	CYS
1	A	512	LEU
1	A	602	LYS
1	A	605	LEU
1	A	701	LEU
1	A	703	LEU
1	A	731	PHE
1	A	736	SER
1	A	752	ASN
1	A	761	THR
1	A	762	THR
1	A	778	CYS
1	A	780	ILE
1	A	785	ARG
1	A	794	LYS
1	A	815	VAL
1	A	817	LEU
1	B	42	ASN
1	B	45	VAL
1	B	49	CYS
1	B	52	ARG
1	B	60	THR
1	B	122	LEU
1	B	160	ASN
1	B	248	LEU
1	B	268	VAL
1	B	280	ARG
1	B	317	ASP
1	B	338	ARG
1	B	416	ASN
1	B	418	SER
1	B	472	ARG

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Mol	Chain	Res	Type
1	B	512	LEU
1	B	516	SER
1	B	605	LEU
1	B	705	ASP
1	B	727	LEU
1	B	731	PHE
1	B	758	THR
1	B	759	LYS
1	B	765	SER
1	B	817	LEU
1	C	49	CYS
1	C	60	THR
1	C	66	THR
1	C	90	THR
1	C	118	ASP
1	C	123	ASN
1	C	200	LEU
1	C	243	LYS
1	C	245	LEU
1	C	279	ASP
1	C	317	ASP
1	C	367	LEU
1	C	372	LEU
1	C	416	ASN
1	C	419	ASN
1	C	512	LEU
1	C	534	TYR
1	C	569	ARG
1	C	582	ASN
1	C	584	THR
1	C	605	LEU
1	C	701	LEU
1	C	703	LEU
1	C	760	THR
1	C	762	THR
1	C	792	ASN
1	C	817	LEU
1	D	38	GLU
1	D	49	CYS
1	D	52	ARG
1	D	68	LEU
1	D	86	LEU

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Mol	Chain	Res	Type
1	D	122	LEU
1	D	169	LEU
1	D	200	LEU
1	D	317	ASP
1	D	338	ARG
1	D	353	TYR
1	D	372	LEU
1	D	472	ARG
1	D	512	LEU
1	D	541	ARG
1	D	569	ARG
1	D	582	ASN
1	D	632	ILE
1	D	671	ILE
1	D	701	LEU
1	D	703	LEU
1	D	736	SER
1	D	762	THR
1	D	797	ARG
1	D	817	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	726	HIS
1	B	160	ASN
1	B	191	ASN
1	B	581	GLN
1	C	77	HIS
1	C	595	ASN
1	D	77	HIS
1	D	160	ASN

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)

52 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	E	1	2,1	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
2	NAG	E	2	2	14,14,15	0.61	0	17,19,21	0.84	0
2	BMA	E	3	2	11,11,12	0.96	1 (9%)	15,15,17	0.99	1 (6%)
2	MAN	E	4	2	11,11,12	0.56	0	15,15,17	0.89	1 (6%)
2	MAN	E	5	2	11,11,12	0.67	0	15,15,17	0.82	0
3	NAG	F	1	1,3	14,14,15	0.52	0	17,19,21	1.06	1 (5%)
3	NAG	F	2	3	14,14,15	0.73	0	17,19,21	1.04	1 (5%)
3	BMA	F	3	3	11,11,12	0.93	1 (9%)	15,15,17	0.90	0
2	NAG	G	1	2,1	14,14,15	0.66	0	17,19,21	0.95	0
2	NAG	G	2	2	14,14,15	0.52	0	17,19,21	1.71	3 (17%)
2	BMA	G	3	2	11,11,12	1.38	1 (9%)	15,15,17	0.79	0
2	MAN	G	4	2	11,11,12	0.51	0	15,15,17	1.06	1 (6%)
2	MAN	G	5	2	11,11,12	0.70	0	15,15,17	0.95	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.60	0	17,19,21	1.05	1 (5%)
2	NAG	H	2	2	14,14,15	0.74	0	17,19,21	0.92	1 (5%)
2	BMA	H	3	2	11,11,12	0.86	1 (9%)	15,15,17	1.03	1 (6%)
2	MAN	H	4	2	11,11,12	0.58	0	15,15,17	0.59	0
2	MAN	H	5	2	11,11,12	0.62	0	15,15,17	0.69	0
3	NAG	I	1	1,3	14,14,15	0.55	0	17,19,21	1.24	2 (11%)
3	NAG	I	2	3	14,14,15	0.62	0	17,19,21	1.28	1 (5%)
3	BMA	I	3	3	11,11,12	1.07	1 (9%)	15,15,17	0.94	0
2	NAG	J	1	2,1	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
2	NAG	J	2	2	14,14,15	0.69	0	17,19,21	0.74	0
2	BMA	J	3	2	11,11,12	1.38	1 (9%)	15,15,17	0.92	1 (6%)
2	MAN	J	4	2	11,11,12	0.51	0	15,15,17	0.96	1 (6%)
2	MAN	J	5	2	11,11,12	0.69	0	15,15,17	0.72	0
2	NAG	K	1	2,1	14,14,15	0.55	0	17,19,21	1.07	0
2	NAG	K	2	2	14,14,15	0.59	0	17,19,21	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	K	3	2	11,11,12	0.92	1 (9%)	15,15,17	0.86	0
2	MAN	K	4	2	11,11,12	0.62	0	15,15,17	0.60	0
2	MAN	K	5	2	11,11,12	0.67	0	15,15,17	0.67	0
3	NAG	L	1	1,3	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
3	NAG	L	2	3	14,14,15	0.69	0	17,19,21	1.13	1 (5%)
3	BMA	L	3	3	11,11,12	0.99	1 (9%)	15,15,17	0.80	0
2	NAG	M	1	2,1	14,14,15	0.64	0	17,19,21	0.94	1 (5%)
2	NAG	M	2	2	14,14,15	0.63	0	17,19,21	0.73	0
2	BMA	M	3	2	11,11,12	1.12	1 (9%)	15,15,17	0.91	0
2	MAN	M	4	2	11,11,12	0.46	0	15,15,17	1.01	1 (6%)
2	MAN	M	5	2	11,11,12	0.69	0	15,15,17	0.92	1 (6%)
2	NAG	N	1	2,1	14,14,15	0.50	0	17,19,21	0.98	2 (11%)
2	NAG	N	2	2	14,14,15	0.55	0	17,19,21	1.00	0
2	BMA	N	3	2	11,11,12	1.24	1 (9%)	15,15,17	0.68	0
2	MAN	N	4	2	11,11,12	0.53	0	15,15,17	0.75	0
2	MAN	N	5	2	11,11,12	0.70	0	15,15,17	0.61	0
3	NAG	O	1	1,3	14,14,15	0.50	0	17,19,21	0.68	0
3	NAG	O	2	3	14,14,15	0.61	0	17,19,21	0.94	1 (5%)
3	BMA	O	3	3	11,11,12	0.83	0	15,15,17	0.67	0
2	NAG	P	1	2,1	14,14,15	0.66	0	17,19,21	1.04	1 (5%)
2	NAG	P	2	2	14,14,15	0.64	0	17,19,21	0.71	0
2	BMA	P	3	2	11,11,12	1.00	1 (9%)	15,15,17	0.74	0
2	MAN	P	4	2	11,11,12	0.50	0	15,15,17	0.84	1 (6%)
2	MAN	P	5	2	11,11,12	0.69	0	15,15,17	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	MAN	H	5	2	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	0/2/19/22	0/1/1/1
2	MAN	J	5	2	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	BMA	M	3	2	-	2/2/19/22	0/1/1/1
2	MAN	M	4	2	-	2/2/19/22	0/1/1/1
2	MAN	M	5	2	-	0/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1
2	BMA	N	3	2	-	2/2/19/22	0/1/1/1
2	MAN	N	4	2	-	0/2/19/22	0/1/1/1
2	MAN	N	5	2	-	2/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	BMA	P	3	2	-	2/2/19/22	0/1/1/1
2	MAN	P	4	2	-	0/2/19/22	0/1/1/1
2	MAN	P	5	2	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	3	BMA	O5-C1	-3.86	1.37	1.43
2	G	3	BMA	O5-C1	-3.63	1.37	1.43
2	N	3	BMA	O5-C1	-3.51	1.37	1.43
2	M	3	BMA	O5-C1	-2.62	1.39	1.43
2	E	3	BMA	O5-C1	-2.55	1.39	1.43
2	P	3	BMA	O5-C1	-2.44	1.39	1.43
3	I	3	BMA	C2-C3	2.32	1.56	1.52
3	L	3	BMA	C2-C3	2.20	1.55	1.52
2	H	3	BMA	O5-C1	-2.06	1.40	1.43
2	K	3	BMA	O5-C1	-2.05	1.40	1.43
3	F	3	BMA	C1-C2	2.00	1.57	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	C1-O5-C5	5.52	119.59	112.19
3	I	2	NAG	C2-N2-C7	-3.70	117.94	122.90
3	F	1	NAG	C2-N2-C7	-3.57	118.12	122.90
2	P	1	NAG	O5-C1-C2	-3.15	106.42	111.29
2	M	4	MAN	C1-O5-C5	3.12	116.37	112.19
3	I	1	NAG	C2-N2-C7	-3.07	118.78	122.90
2	J	4	MAN	C1-O5-C5	2.94	116.13	112.19
2	G	4	MAN	C1-O5-C5	2.93	116.11	112.19
2	H	1	NAG	O5-C1-C2	-2.82	106.92	111.29
3	L	2	NAG	C4-C3-C2	2.70	114.98	111.02
2	H	2	NAG	O5-C1-C2	-2.67	107.17	111.29
2	H	3	BMA	C1-O5-C5	2.59	115.66	112.19
2	E	3	BMA	O2-C2-C3	-2.48	105.02	110.15
2	N	1	NAG	O5-C1-C2	-2.44	107.52	111.29
2	M	5	MAN	C1-O5-C5	-2.43	108.94	112.19
3	F	2	NAG	C4-C3-C2	2.40	114.54	111.02
3	O	2	NAG	C2-N2-C7	-2.40	119.69	122.90
2	J	1	NAG	O5-C1-C2	-2.30	107.73	111.29
2	E	1	NAG	O5-C1-C2	-2.28	107.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	5	MAN	C3-C4-C5	2.25	114.31	110.23
2	G	2	NAG	C3-C4-C5	2.19	114.20	110.23
2	M	1	NAG	O5-C1-C2	-2.18	107.91	111.29
2	G	2	NAG	O5-C1-C2	2.18	114.66	111.29
2	J	3	BMA	C1-O5-C5	2.17	115.09	112.19
2	P	4	MAN	C1-O5-C5	2.15	115.06	112.19
2	E	4	MAN	C1-O5-C5	2.06	114.94	112.19
3	I	1	NAG	C6-C5-C4	-2.03	108.02	113.02
2	N	1	NAG	C2-N2-C7	-2.02	120.19	122.90
3	L	1	NAG	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	3	BMA	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	P	3	BMA	C4-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6
2	N	5	MAN	O5-C5-C6-O6
2	N	3	BMA	C4-C5-C6-O6
2	P	3	BMA	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	H	5	MAN	O5-C5-C6-O6
2	N	5	MAN	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
2	H	5	MAN	C4-C5-C6-O6
2	M	4	MAN	C4-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	M	4	MAN	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

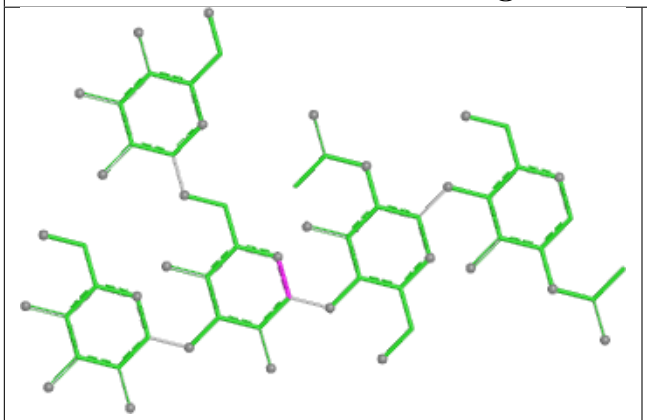
There are no ring outliers.

5 monomers are involved in 5 short contacts:

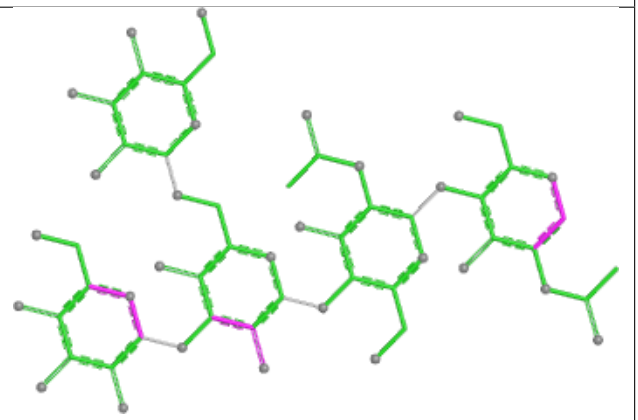
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	1	NAG	1	0
2	K	1	NAG	1	0
2	H	1	NAG	1	0
3	L	1	NAG	1	0
2	K	2	NAG	1	0

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

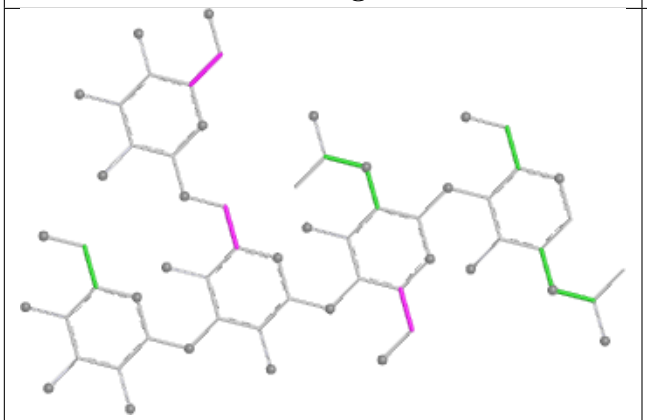
Oligosaccharide Chain E



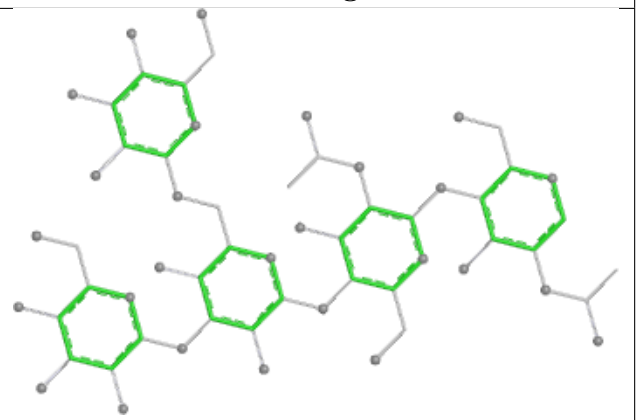
Bond lengths



Bond angles

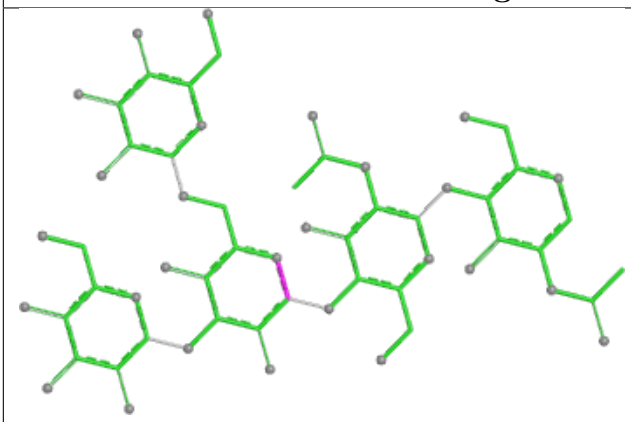


Torsions

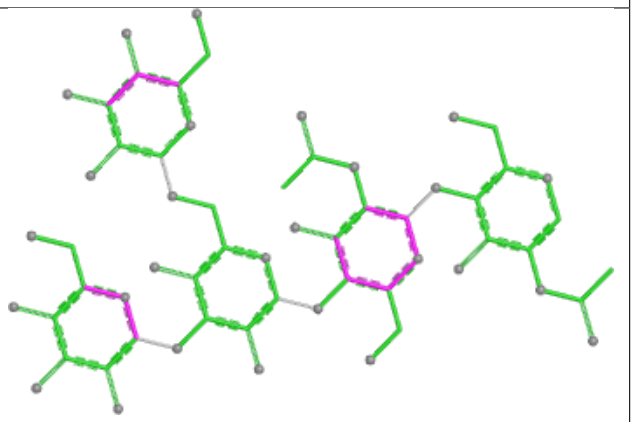


Rings

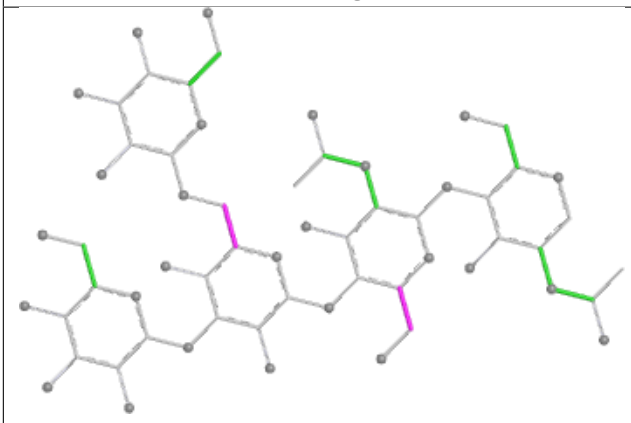
Oligosaccharide Chain G



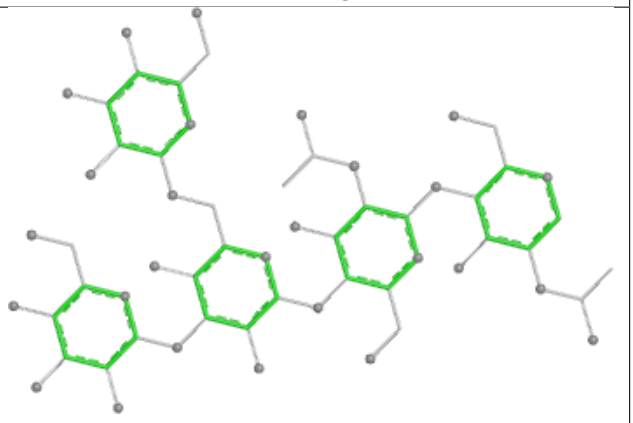
Bond lengths



Bond angles

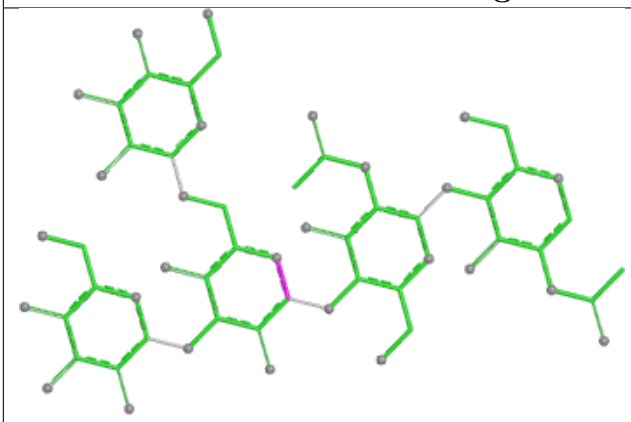


Torsions

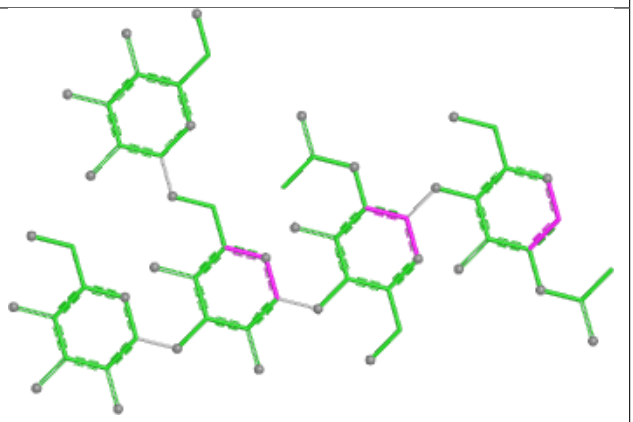


Rings

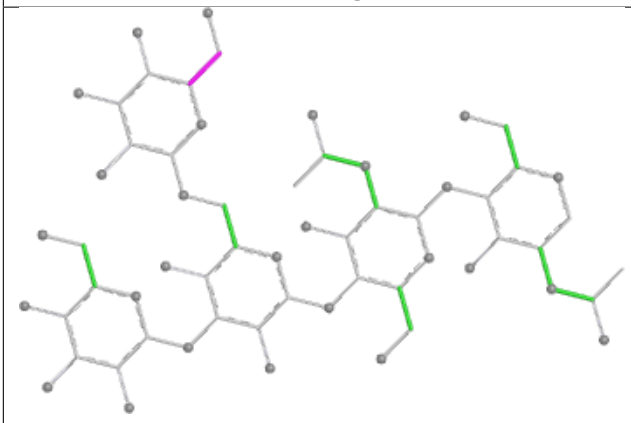
Oligosaccharide Chain H



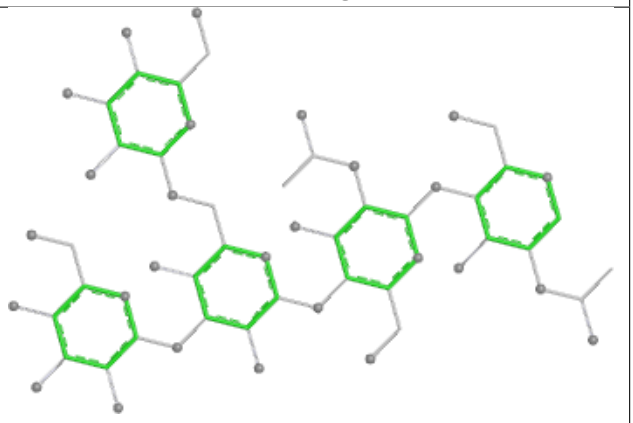
Bond lengths



Bond angles

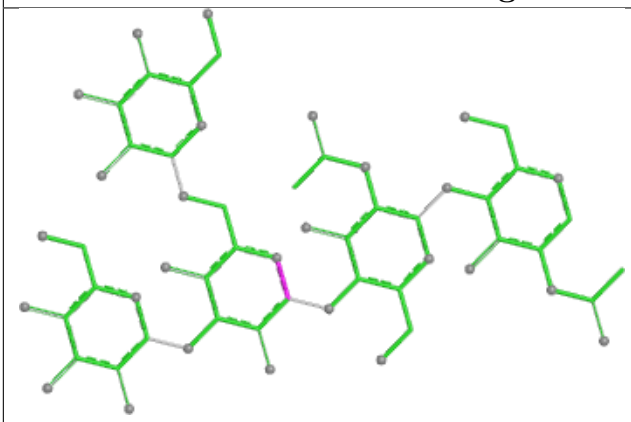


Torsions

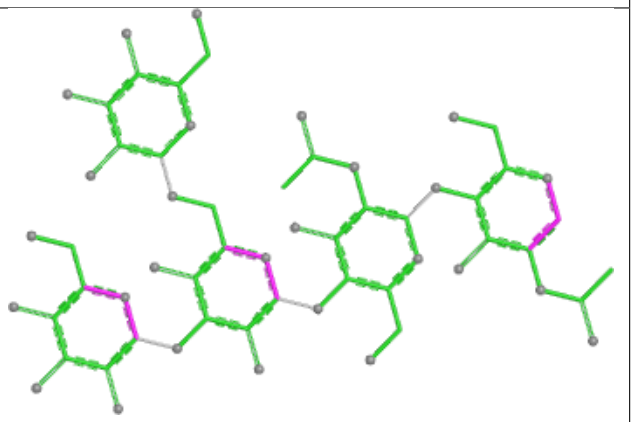


Rings

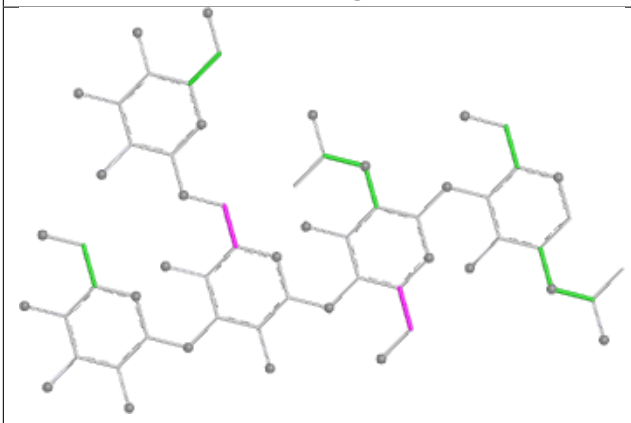
Oligosaccharide Chain J



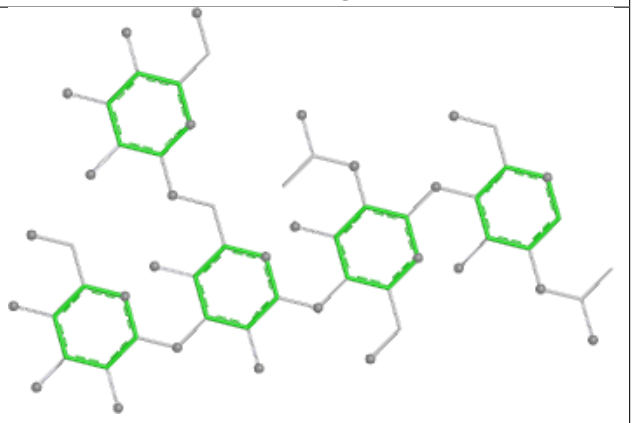
Bond lengths



Bond angles

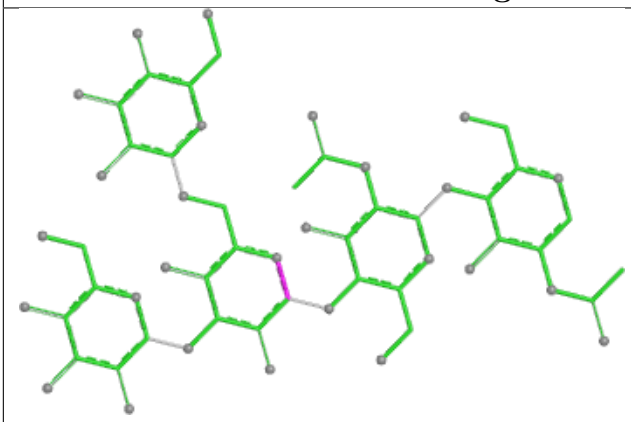


Torsions

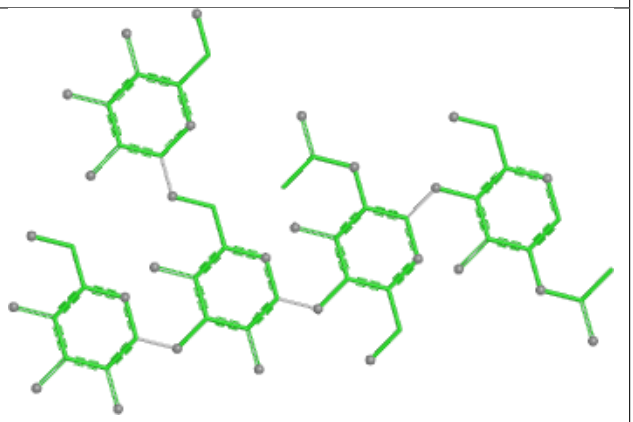


Rings

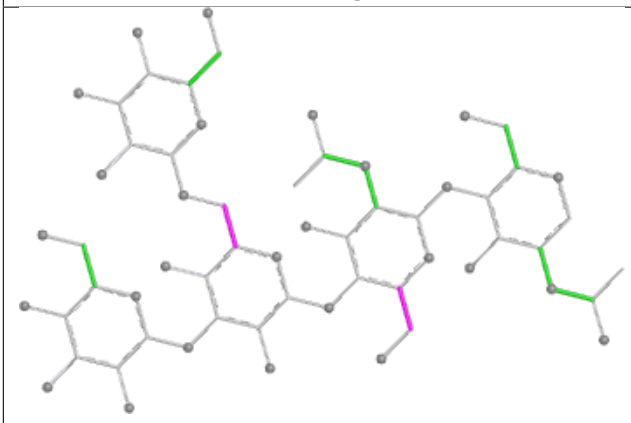
Oligosaccharide Chain K



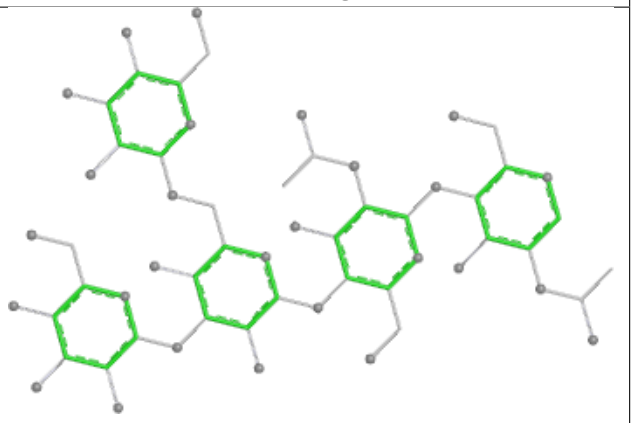
Bond lengths



Bond angles

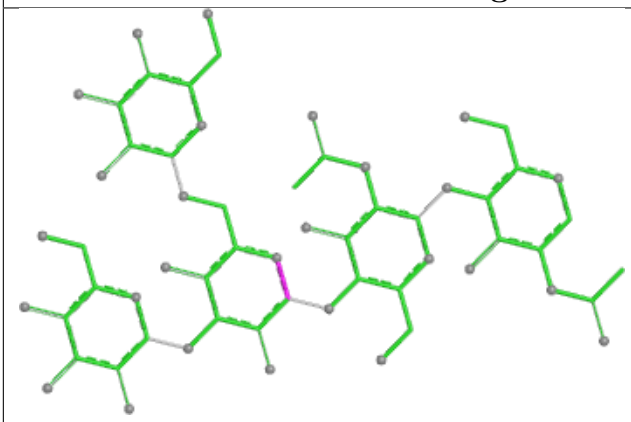


Torsions

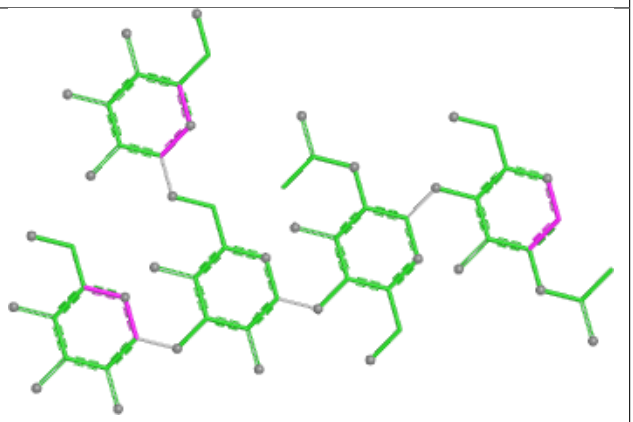


Rings

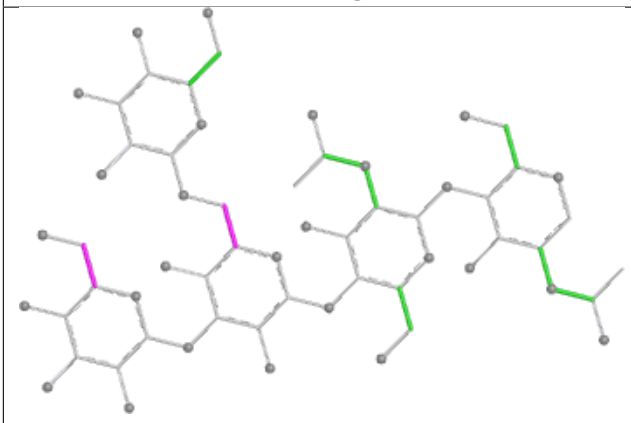
Oligosaccharide Chain M



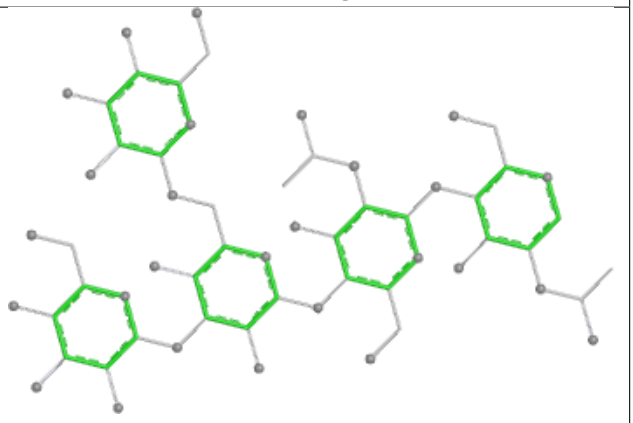
Bond lengths



Bond angles

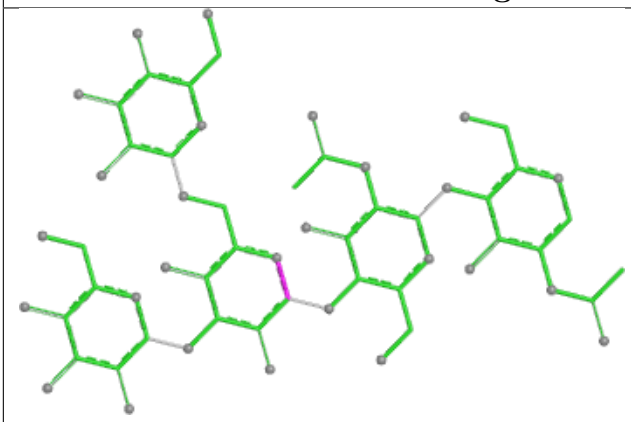


Torsions

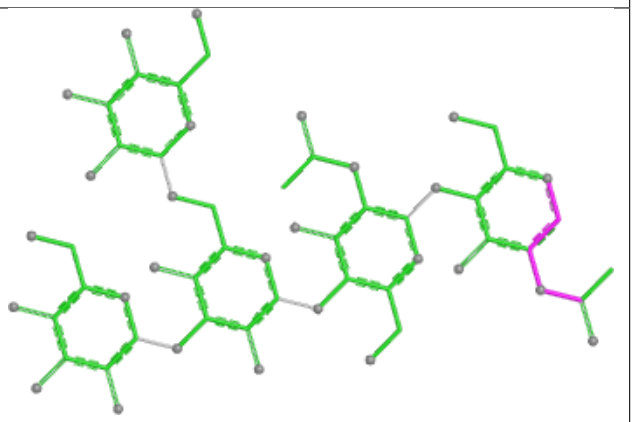


Rings

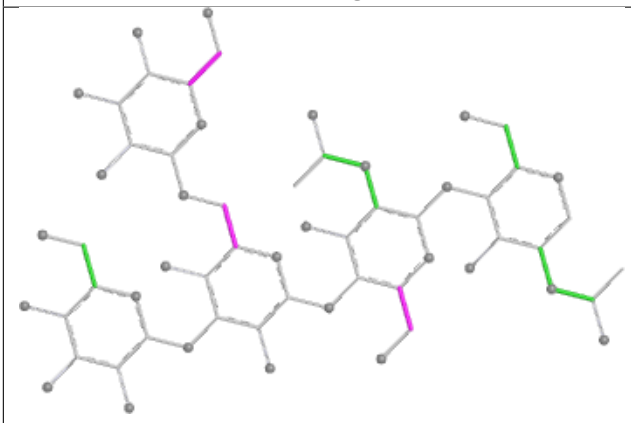
Oligosaccharide Chain N



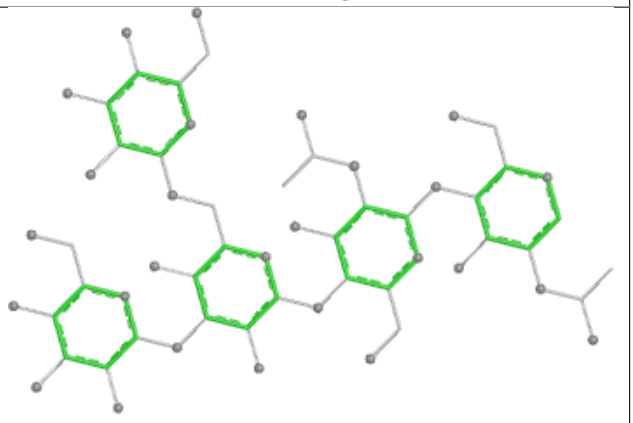
Bond lengths



Bond angles

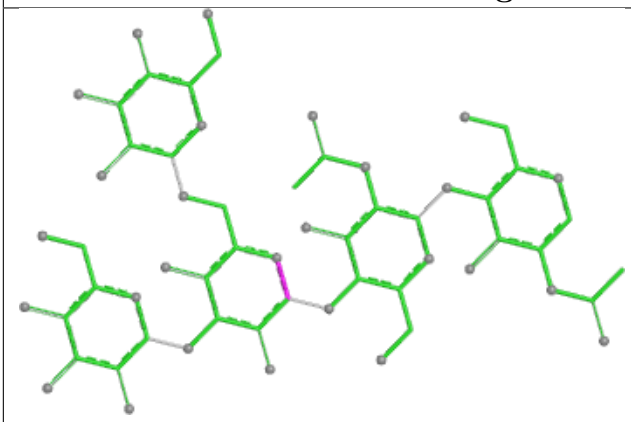


Torsions

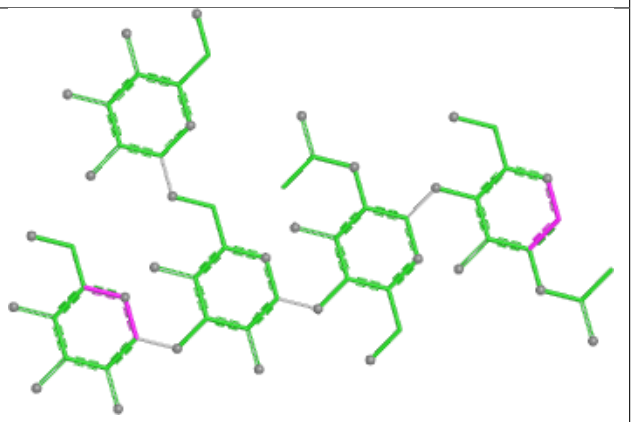


Rings

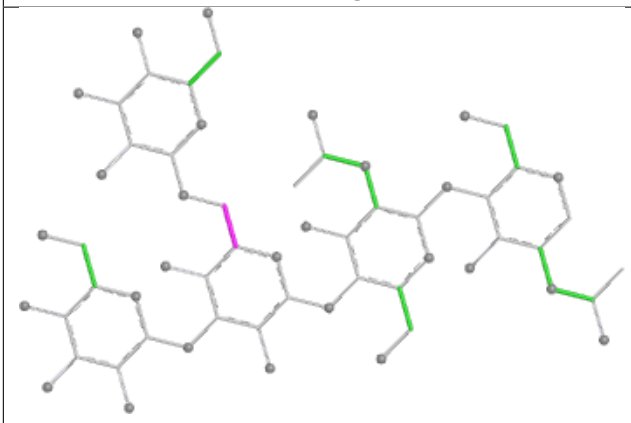
Oligosaccharide Chain P



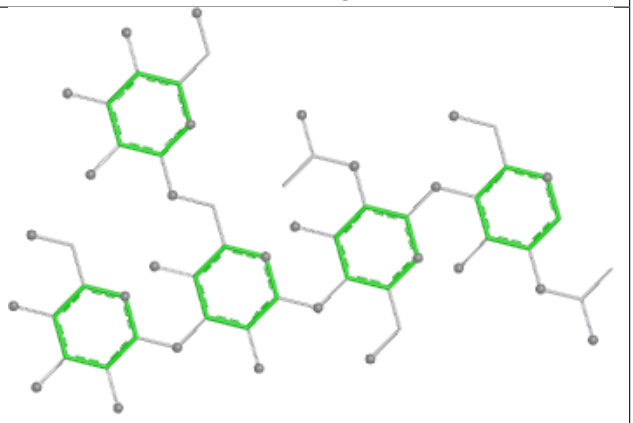
Bond lengths



Bond angles

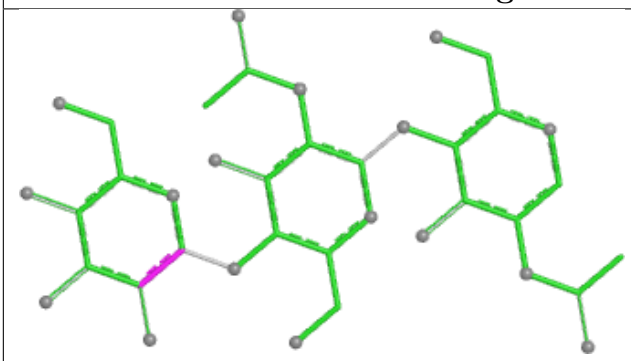


Torsions

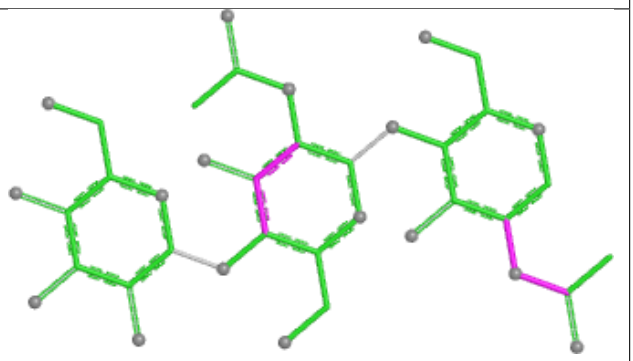


Rings

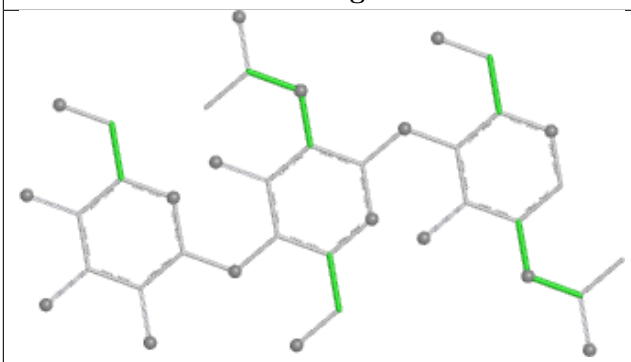
Oligosaccharide Chain F



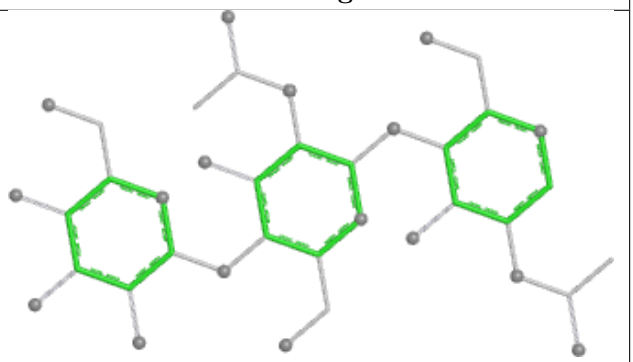
Bond lengths



Bond angles

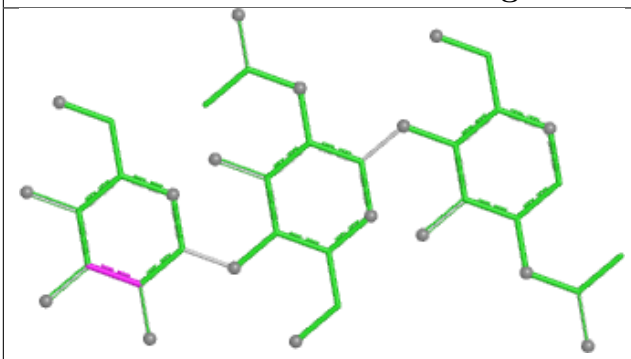


Torsions

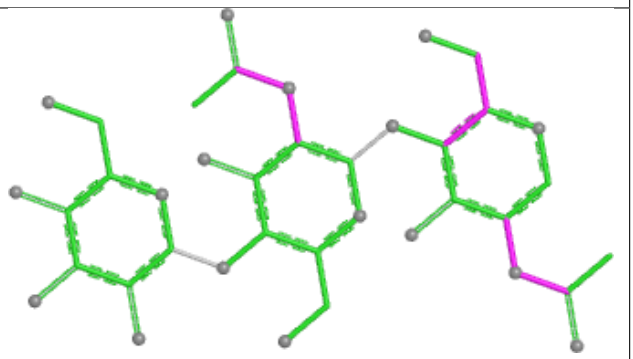


Rings

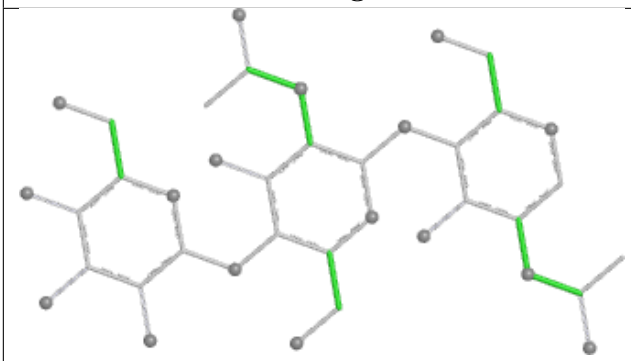
Oligosaccharide Chain I



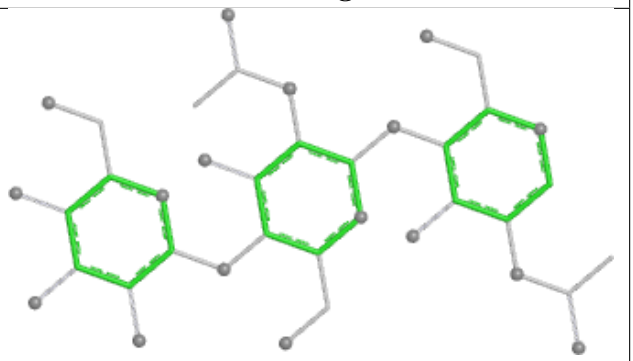
Bond lengths



Bond angles

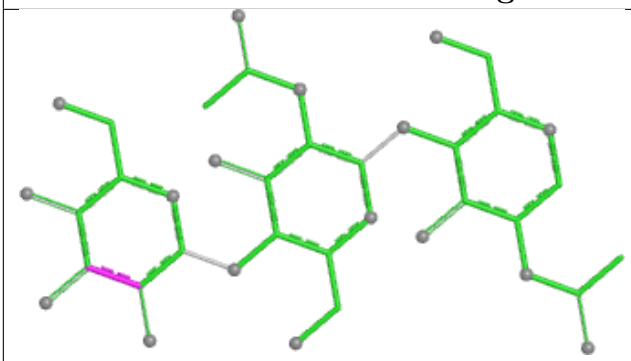


Torsions

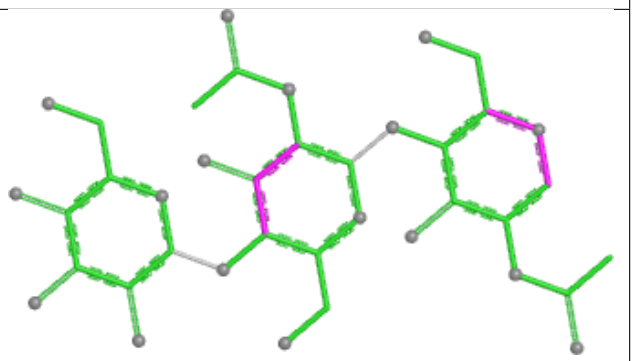


Rings

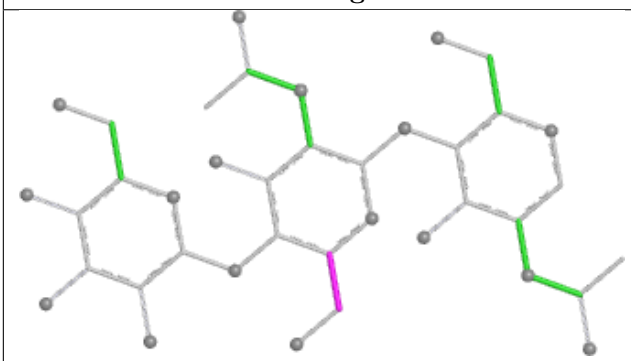
Oligosaccharide Chain L



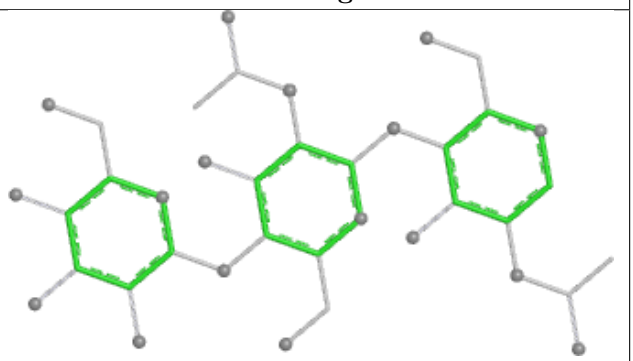
Bond lengths



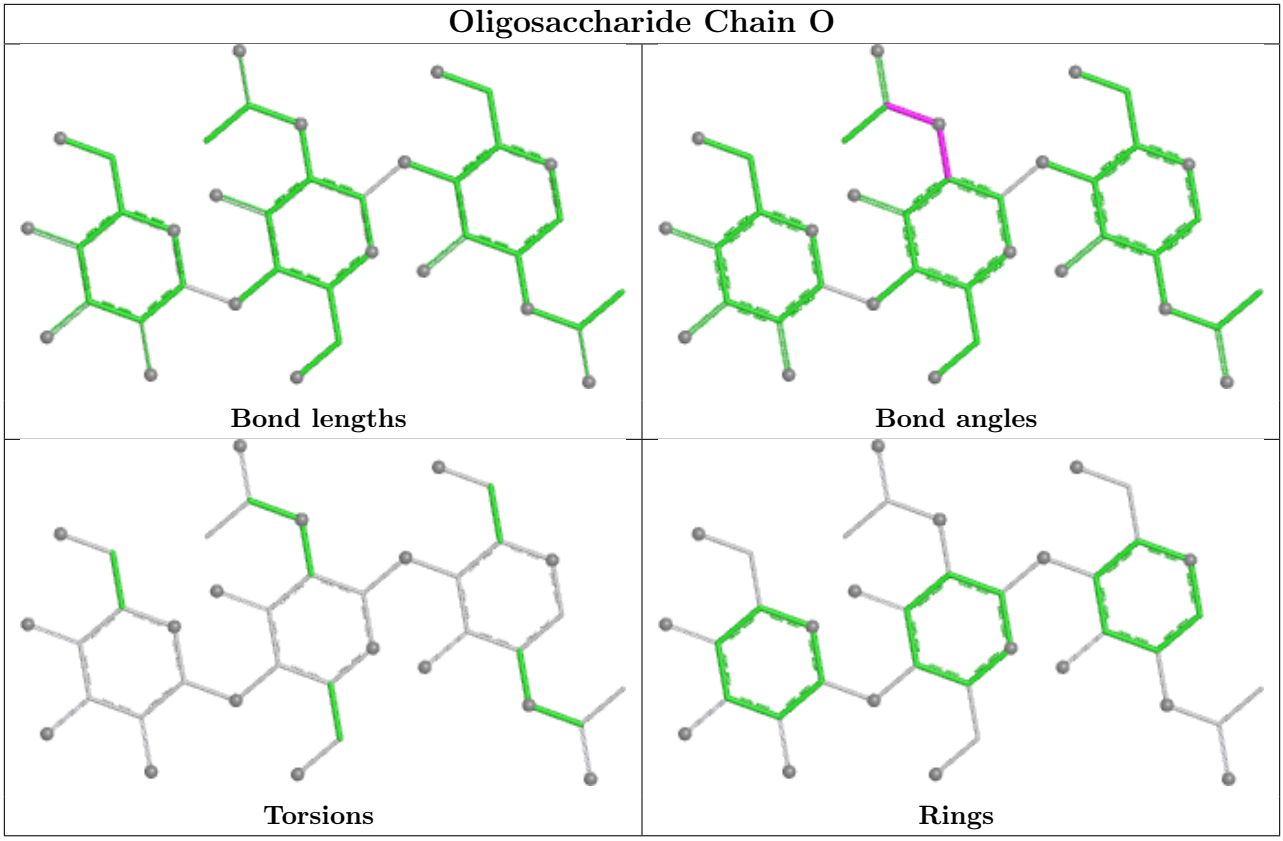
Bond angles



Torsions



Rings



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	SO4	A	1019	-	4,4,4	0.30	0	6,6,6	0.14	0
4	NAG	C	910	1	14,14,15	0.57	0	17,19,21	0.84	1 (5%)
5	SO4	B	1020	-	4,4,4	0.26	0	6,6,6	0.21	0
4	NAG	D	917	1	14,14,15	0.56	0	17,19,21	0.78	0
6	RX8	D	902	-	21,25,25	1.64	4 (19%)	28,37,37	1.18	4 (14%)
4	NAG	D	911	1	14,14,15	0.52	0	17,19,21	0.89	1 (5%)
6	RX8	C	901	-	21,25,25	1.62	4 (19%)	28,37,37	1.09	3 (10%)
5	SO4	A	1018	-	4,4,4	0.23	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	RX8	D	901	-	21,25,25	1.61	3 (14%)	28,37,37	1.20	3 (10%)
4	NAG	C	916	1	14,14,15	0.63	0	17,19,21	1.12	1 (5%)
4	NAG	B	1017	1	14,14,15	0.54	0	17,19,21	0.68	0
4	NAG	B	1015	1	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
4	NAG	D	919	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
4	NAG	B	1016	1	14,14,15	0.52	0	17,19,21	1.19	2 (11%)
4	NAG	D	918	1	14,14,15	0.46	0	17,19,21	0.96	1 (5%)
5	SO4	D	920	-	4,4,4	0.24	0	6,6,6	0.06	0
4	NAG	A	1017	1	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
4	NAG	B	1009	1	14,14,15	0.53	0	17,19,21	1.23	1 (5%)
4	NAG	A	1009	1	14,14,15	0.57	0	17,19,21	0.69	0
4	NAG	A	1015	1	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
4	NAG	A	1016	1	14,14,15	0.56	0	17,19,21	1.19	2 (11%)
5	SO4	B	1021	-	4,4,4	0.26	0	6,6,6	0.30	0
4	NAG	C	917	1	14,14,15	0.59	0	17,19,21	0.84	1 (5%)
5	SO4	C	918	-	4,4,4	0.25	0	6,6,6	0.13	0
5	SO4	B	1019	-	4,4,4	0.25	0	6,6,6	0.11	0
5	SO4	D	921	-	4,4,4	0.27	0	6,6,6	0.16	0
6	RX8	B	1018	-	21,25,25	1.69	5 (23%)	28,37,37	1.33	5 (17%)

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	C	910	1	-	2/6/23/26	0/1/1/1
4	NAG	D	917	1	-	2/6/23/26	0/1/1/1
6	RX8	D	902	-	-	4/6/9/9	0/3/3/3
4	NAG	D	911	1	-	2/6/23/26	0/1/1/1
6	RX8	C	901	-	-	4/6/9/9	0/3/3/3
6	RX8	D	901	-	-	3/6/9/9	0/3/3/3
4	NAG	C	916	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1017	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1015	1	-	2/6/23/26	0/1/1/1
4	NAG	D	919	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1016	1	-	2/6/23/26	0/1/1/1
4	NAG	D	918	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1017	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1015	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1016	1	-	2/6/23/26	0/1/1/1
4	NAG	C	917	1	-	0/6/23/26	0/1/1/1
6	RX8	B	1018	-	-	4/6/9/9	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1018	RX8	C2-C3	5.29	1.49	1.40
6	D	902	RX8	C2-C3	5.05	1.49	1.40
6	D	901	RX8	C2-C3	4.98	1.49	1.40
6	C	901	RX8	C2-C3	4.69	1.48	1.40
6	B	1018	RX8	O1-C10	-2.95	1.37	1.44
6	C	901	RX8	O1-C10	-2.83	1.37	1.44
6	D	901	RX8	O1-C10	-2.73	1.38	1.44
6	D	901	RX8	C-N	2.69	1.43	1.34
6	C	901	RX8	C-N	2.65	1.43	1.34
6	B	1018	RX8	C-N	2.62	1.43	1.34
6	D	902	RX8	O1-C10	-2.57	1.38	1.44
6	D	902	RX8	C-N	2.55	1.43	1.34
6	C	901	RX8	C2-C1	-2.20	1.37	1.41
6	D	902	RX8	C2-C1	-2.20	1.37	1.41
6	B	1018	RX8	C2-C1	-2.09	1.37	1.41
6	B	1018	RX8	C14-C13	2.02	1.41	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1018	RX8	C6-O-C7	3.98	122.77	112.82
6	D	901	RX8	C6-O-C7	3.45	121.43	112.82
4	A	1016	NAG	C1-O5-C5	3.40	116.74	112.19
4	B	1009	NAG	C1-O5-C5	3.35	116.67	112.19
6	D	902	RX8	C6-O-C7	3.18	120.76	112.82
6	C	901	RX8	C6-O-C7	3.11	120.57	112.82
4	C	916	NAG	C2-N2-C7	-2.99	118.89	122.90
4	B	1016	NAG	C1-O5-C5	2.77	115.89	112.19
4	D	911	NAG	C1-O5-C5	2.60	115.67	112.19
4	D	918	NAG	C1-O5-C5	2.60	115.66	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1016	NAG	C2-N2-C7	-2.57	119.45	122.90
4	D	919	NAG	C1-O5-C5	2.55	115.60	112.19
6	D	902	RX8	O-C6-C5	2.55	118.08	110.94
6	B	1018	RX8	C2-C1-N1	-2.53	120.62	122.98
6	B	1018	RX8	C2-C3-N3	2.49	135.68	130.42
4	C	910	NAG	C1-O5-C5	2.43	115.44	112.19
6	B	1018	RX8	O-C6-C5	2.35	117.53	110.94
6	D	901	RX8	C2-C1-N1	-2.32	120.81	122.98
4	B	1015	NAG	O5-C1-C2	-2.30	107.73	111.29
6	D	902	RX8	C2-C1-N1	-2.29	120.85	122.98
6	C	901	RX8	C2-C1-N1	-2.28	120.85	122.98
4	A	1017	NAG	C1-O5-C5	2.22	115.16	112.19
6	D	902	RX8	C2-C3-N3	2.20	135.08	130.42
4	A	1015	NAG	C1-O5-C5	2.13	115.04	112.19
6	D	901	RX8	C3-C2-C1	-2.10	118.05	119.65
6	B	1018	RX8	C2-C3-C4	-2.07	118.92	120.03
4	C	917	NAG	C2-N2-C7	-2.05	120.15	122.90
6	C	901	RX8	C3-C2-C1	-2.04	118.10	119.65
4	A	1016	NAG	C6-C5-C4	-2.02	108.05	113.02

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1009	NAG	C8-C7-N2-C2
4	A	1009	NAG	O7-C7-N2-C2
4	B	1009	NAG	C8-C7-N2-C2
4	B	1009	NAG	O7-C7-N2-C2
4	C	910	NAG	C8-C7-N2-C2
4	C	910	NAG	O7-C7-N2-C2
4	D	911	NAG	C8-C7-N2-C2
4	D	911	NAG	O7-C7-N2-C2
6	B	1018	RX8	O1-C10-C9-N3
6	B	1018	RX8	C5-C6-O-C7
6	C	901	RX8	O1-C10-C9-N3
6	C	901	RX8	C11-C10-C9-N3
6	C	901	RX8	C12-C10-C9-N3
6	C	901	RX8	C5-C6-O-C7
6	D	901	RX8	O1-C10-C9-N3
6	D	901	RX8	C11-C10-C9-N3
6	D	901	RX8	C12-C10-C9-N3
6	D	902	RX8	O1-C10-C9-N3

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Mol	Chain	Res	Type	Atoms
6	D	902	RX8	C11-C10-C9-N3
6	D	902	RX8	C12-C10-C9-N3
6	D	902	RX8	C5-C6-O-C7
4	A	1015	NAG	C4-C5-C6-O6
4	B	1015	NAG	C4-C5-C6-O6
4	A	1015	NAG	O5-C5-C6-O6
4	D	917	NAG	C4-C5-C6-O6
4	A	1016	NAG	O5-C5-C6-O6
4	B	1015	NAG	O5-C5-C6-O6
4	D	917	NAG	O5-C5-C6-O6
4	B	1016	NAG	C4-C5-C6-O6
6	B	1018	RX8	C11-C10-C9-N3
6	B	1018	RX8	C12-C10-C9-N3
4	A	1016	NAG	C4-C5-C6-O6
4	D	918	NAG	O5-C5-C6-O6
4	B	1016	NAG	O5-C5-C6-O6

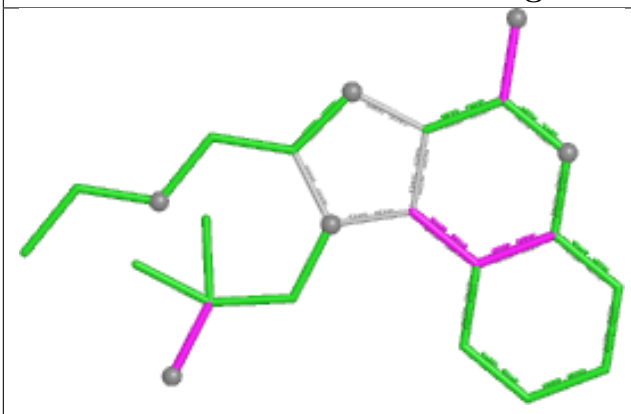
There are no ring outliers.

6 monomers are involved in 12 short contacts:

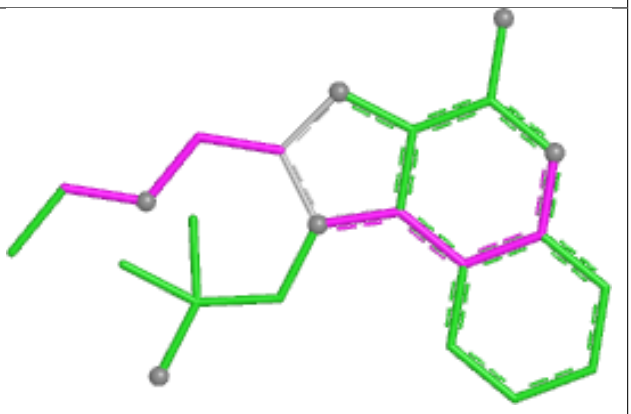
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	902	RX8	2	0
6	C	901	RX8	2	0
6	D	901	RX8	3	0
5	C	918	SO4	1	0
5	B	1019	SO4	1	0
6	B	1018	RX8	3	0

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

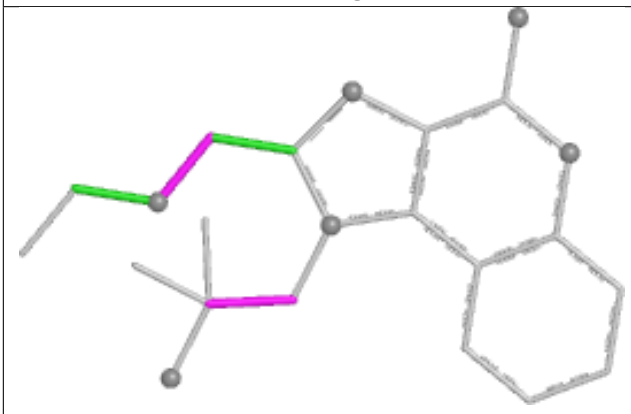
Ligand RX8 D 902



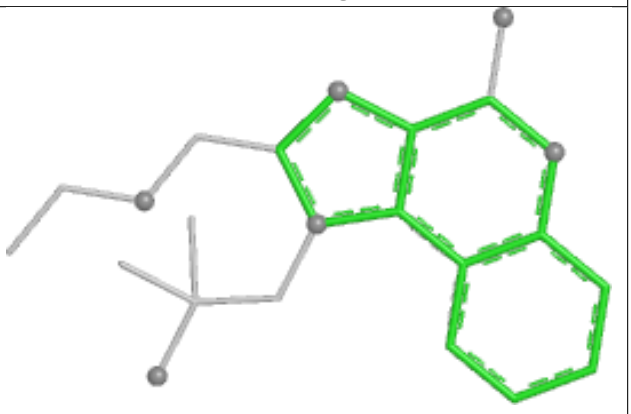
Bond lengths



Bond angles

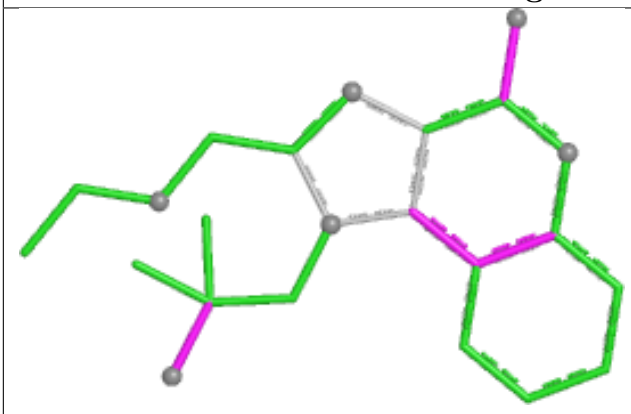


Torsions

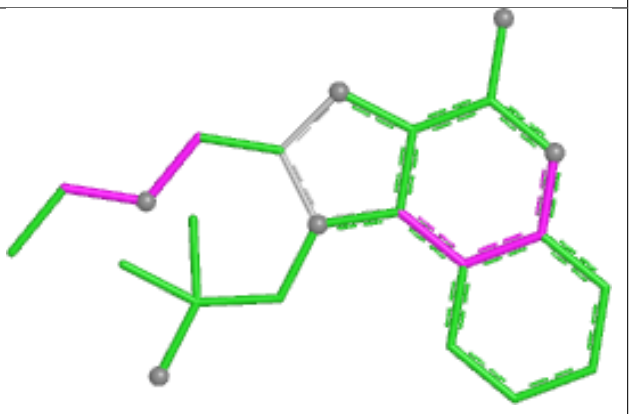


Rings

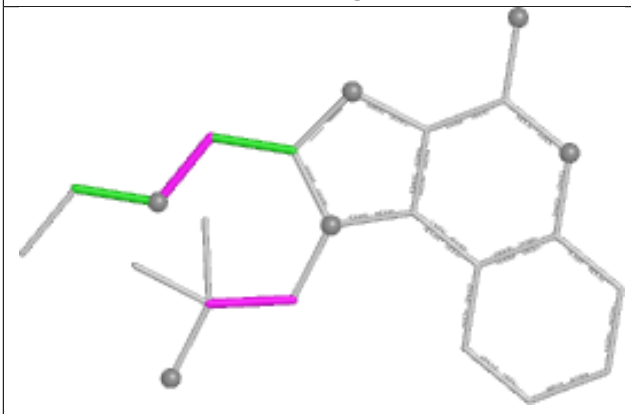
Ligand RX8 C 901



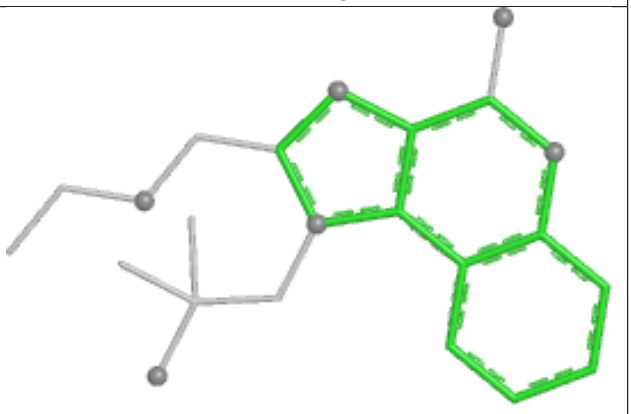
Bond lengths



Bond angles

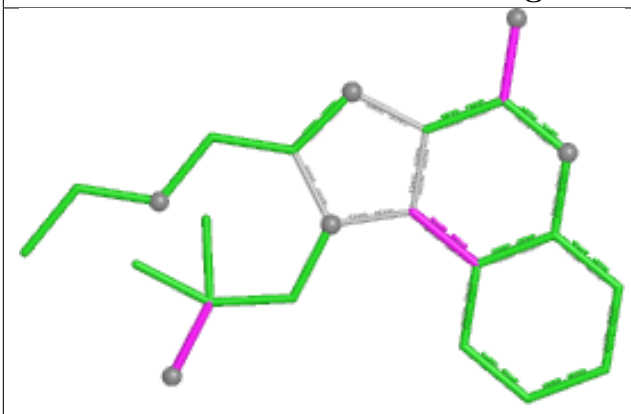


Torsions

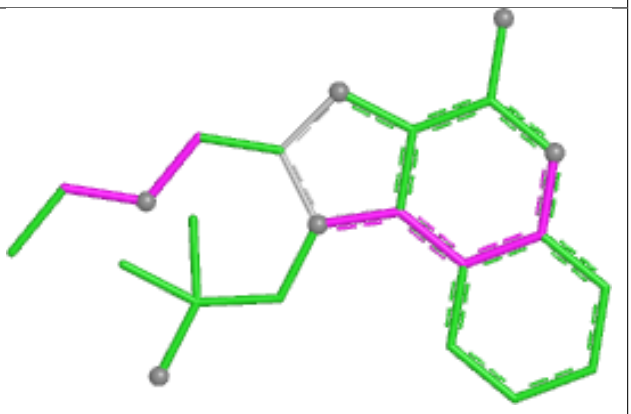


Rings

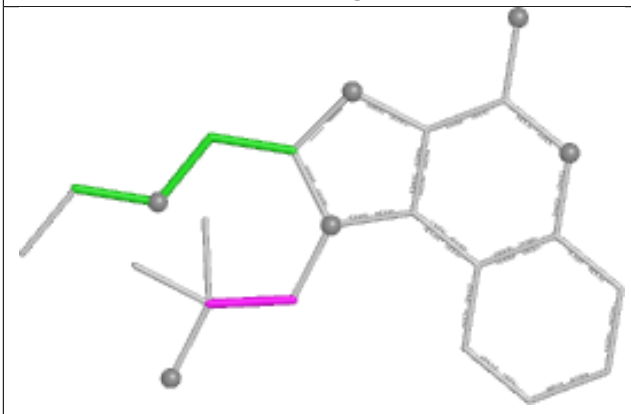
Ligand RX8 D 901



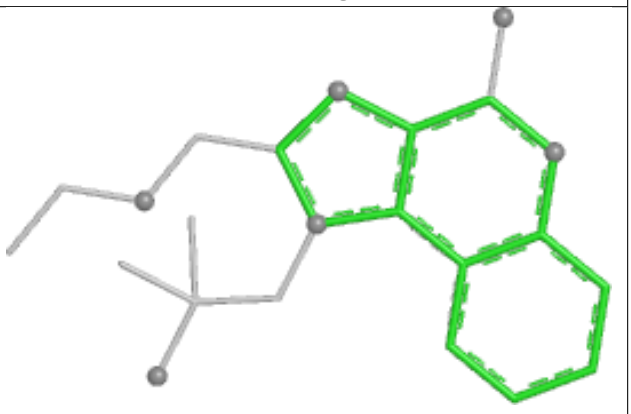
Bond lengths



Bond angles

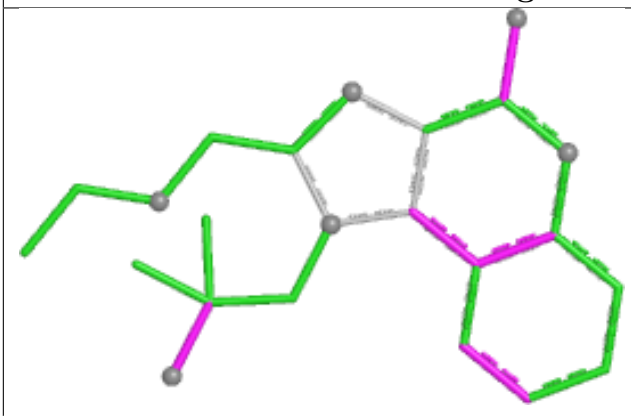


Torsions

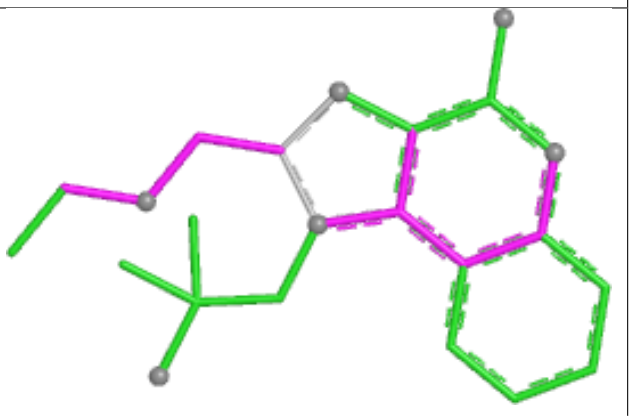


Rings

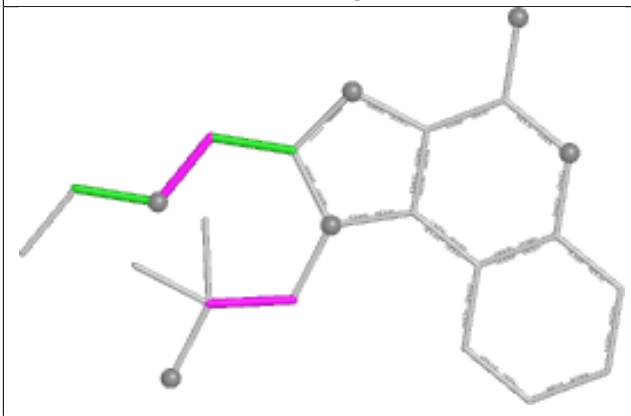
Ligand RX8 B 1018



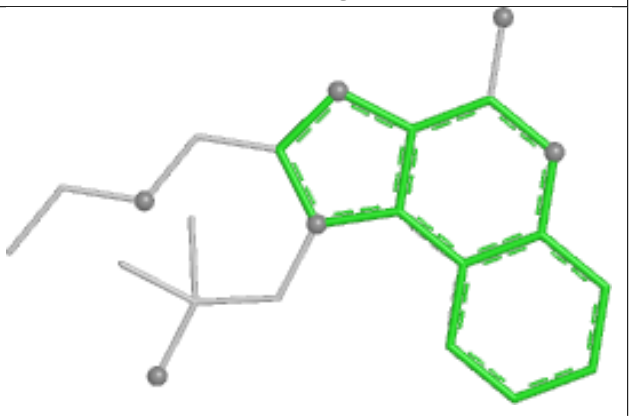
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	751/811 (92%)	0.43	45 (5%) 21 30	11, 33, 87, 120	0
1	B	751/811 (92%)	0.47	74 (9%) 7 12	9, 33, 93, 127	0
1	C	751/811 (92%)	0.66	97 (12%) 3 6	11, 43, 92, 115	0
1	D	751/811 (92%)	0.67	90 (11%) 4 7	14, 49, 91, 115	0
All	All	3004/3244 (92%)	0.56	306 (10%) 6 11	9, 39, 92, 127	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	THR	15.8
1	C	756	LEU	12.9
1	C	88	ASN	12.6
1	B	758	THR	12.1
1	C	86	LEU	11.3
1	B	733	SER	11.2
1	D	761	THR	10.7
1	D	64	TYR	10.5
1	B	760	THR	10.5
1	A	761	THR	10.2
1	B	759	LYS	10.0
1	D	756	LEU	8.9
1	B	64	TYR	8.8
1	C	760	THR	8.6
1	D	760	THR	8.4
1	C	83	PHE	8.3
1	A	756	LEU	8.2
1	A	41	GLN	8.1
1	C	758	THR	7.7
1	C	733	SER	7.6
1	B	817	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
1	C	45	VAL	7.1
1	D	46	ILE	7.0
1	B	756	LEU	6.7
1	D	42	ASN	6.6
1	B	731	PHE	6.6
1	D	41	GLN	6.6
1	C	759	LYS	6.6
1	C	78	ILE	6.3
1	D	817	LEU	6.3
1	C	734	GLU	6.3
1	C	757	GLU	6.3
1	A	40	LYS	6.2
1	D	85	GLY	6.2
1	C	166	ILE	6.1
1	A	817	LEU	6.1
1	C	85	GLY	6.0
1	C	761	THR	6.0
1	D	759	LYS	5.9
1	B	783	PHE	5.8
1	D	818	GLU	5.8
1	C	123	ASN	5.8
1	B	762	THR	5.7
1	C	65	VAL	5.7
1	A	43	ASP	5.6
1	C	116	ILE	5.6
1	B	39	LYS	5.6
1	B	45	VAL	5.4
1	A	39	LYS	5.3
1	A	733	SER	5.2
1	B	763	LYS	5.2
1	B	42	ASN	5.1
1	C	124	LEU	5.0
1	B	735	VAL	5.0
1	D	88	ASN	5.0
1	C	121	PHE	5.0
1	D	83	PHE	5.0
1	D	43	ASP	4.9
1	D	730	GLY	4.9
1	A	64	TYR	4.9
1	C	807	GLY	4.9
1	B	810	ARG	4.9
1	B	734	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	170	ILE	4.9
1	A	730	GLY	4.8
1	D	778	CYS	4.8
1	D	815	VAL	4.7
1	B	751	ILE	4.7
1	C	64	TYR	4.6
1	C	126	ASN	4.4
1	C	762	THR	4.3
1	D	758	THR	4.3
1	A	678	PHE	4.3
1	A	732	LEU	4.3
1	C	122	LEU	4.3
1	B	727	LEU	4.3
1	D	66	THR	4.2
1	B	87	GLN	4.2
1	A	807	GLY	4.2
1	B	804	ALA	4.2
1	B	787	MET	4.1
1	C	46	ILE	4.1
1	D	61	VAL	4.1
1	C	125	LYS	4.1
1	D	762	THR	4.1
1	A	123	ASN	4.1
1	D	736	SER	4.1
1	D	38	GLU	4.0
1	A	759	LYS	4.0
1	C	736	SER	4.0
1	C	806	PRO	4.0
1	D	62	GLY	4.0
1	A	42	ASN	4.0
1	C	763	LYS	4.0
1	D	65	VAL	3.9
1	B	32	ARG	3.9
1	C	40	LYS	3.9
1	D	121	PHE	3.9
1	B	815	VAL	3.9
1	D	791	LEU	3.9
1	A	44	SER	3.9
1	C	62	GLY	3.9
1	D	86	LEU	3.9
1	D	87	GLN	3.9
1	B	41	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	736	SER	3.8
1	B	802	ILE	3.8
1	A	45	VAL	3.8
1	C	786	TRP	3.8
1	B	726	HIS	3.8
1	D	793	VAL	3.7
1	B	757	GLU	3.7
1	B	728	PRO	3.7
1	C	779	ASP	3.7
1	B	793	VAL	3.6
1	C	385	ASP	3.6
1	B	774	PHE	3.6
1	D	128	ARG	3.5
1	C	99	ASN	3.5
1	B	46	ILE	3.5
1	C	94	LEU	3.5
1	B	702	PHE	3.5
1	A	84	GLN	3.4
1	B	782	ASP	3.4
1	C	41	GLN	3.4
1	D	100	VAL	3.4
1	B	788	ASP	3.4
1	A	729	SER	3.4
1	C	246	ILE	3.4
1	B	791	LEU	3.4
1	B	780	ILE	3.3
1	D	702	PHE	3.3
1	B	786	TRP	3.3
1	D	32	ARG	3.3
1	C	731	PHE	3.3
1	D	31	SER	3.3
1	A	734	GLU	3.3
1	A	760	THR	3.2
1	C	812	LYS	3.2
1	A	88	ASN	3.2
1	C	814	ILE	3.2
1	D	39	LYS	3.2
1	D	802	ILE	3.2
1	B	43	ASP	3.2
1	D	78	ILE	3.2
1	D	35	PRO	3.2
1	D	124	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	46	ILE	3.1
1	A	751	ILE	3.1
1	D	678	PHE	3.1
1	B	65	VAL	3.1
1	D	40	LYS	3.1
1	D	58	PRO	3.1
1	B	470	PHE	3.1
1	B	88	ASN	3.1
1	C	167	SER	3.1
1	A	777	THR	3.1
1	B	47	ALA	3.0
1	B	678	PHE	3.0
1	C	752	ASN	3.0
1	B	806	PRO	3.0
1	D	47	ALA	3.0
1	D	67	GLU	3.0
1	A	32	ARG	3.0
1	B	753	LYS	3.0
1	B	778	CYS	3.0
1	C	144	LEU	3.0
1	D	123	ASN	3.0
1	C	58	PRO	3.0
1	C	84	GLN	2.9
1	A	731	PHE	2.9
1	C	808	ASP	2.9
1	C	778	CYS	2.9
1	C	789	GLU	2.9
1	D	44	SER	2.9
1	C	70	LEU	2.9
1	C	159	TYR	2.9
1	D	125	LYS	2.9
1	B	60	THR	2.9
1	D	757	GLU	2.9
1	B	814	ILE	2.9
1	B	63	LYS	2.9
1	C	89	LEU	2.9
1	A	758	THR	2.8
1	B	38	GLU	2.8
1	D	459	PHE	2.8
1	D	34	TYR	2.8
1	D	731	PHE	2.8
1	D	416	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	790	HIS	2.8
1	A	31	SER	2.8
1	C	44	SER	2.8
1	D	92	ILE	2.8
1	D	159	TYR	2.8
1	D	144	LEU	2.7
1	C	79	THR	2.7
1	D	790	HIS	2.7
1	C	59	GLN	2.7
1	C	201	THR	2.7
1	C	753	LYS	2.7
1	C	755	ALA	2.7
1	C	61	VAL	2.7
1	C	809	GLN	2.7
1	C	188	GLU	2.7
1	C	153	LEU	2.7
1	C	220	LEU	2.7
1	D	63	LYS	2.7
1	B	755	ALA	2.7
1	D	734	GLU	2.7
1	D	433	LEU	2.7
1	C	816	SER	2.6
1	D	55	GLN	2.6
1	C	117	THR	2.6
1	D	329	SER	2.6
1	A	66	THR	2.6
1	C	817	LEU	2.6
1	A	806	PRO	2.6
1	D	806	PRO	2.6
1	B	85	GLY	2.6
1	B	769	LEU	2.6
1	C	145	PRO	2.6
1	B	749	LYS	2.6
1	C	243	LYS	2.5
1	D	755	ALA	2.5
1	C	77	HIS	2.5
1	B	781	GLY	2.5
1	D	780	ILE	2.5
1	B	660	LEU	2.5
1	C	68	LEU	2.5
1	D	787	MET	2.5
1	C	416	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	653	HIS	2.5
1	C	732	LEU	2.5
1	B	31	SER	2.4
1	A	810	ARG	2.4
1	D	76	THR	2.4
1	D	99	ASN	2.4
1	B	754	SER	2.4
1	B	816	SER	2.4
1	C	119	GLY	2.4
1	A	776	CYS	2.4
1	D	116	ILE	2.4
1	D	90	THR	2.4
1	C	115	ASN	2.4
1	D	114	LEU	2.4
1	A	48	GLU	2.4
1	D	729	SER	2.4
1	A	753	LYS	2.3
1	C	810	ARG	2.3
1	C	87	GLN	2.3
1	A	702	PHE	2.3
1	B	44	SER	2.3
1	C	171	ASN	2.3
1	A	660	LEU	2.3
1	C	782	ASP	2.3
1	C	177	LEU	2.3
1	C	196	VAL	2.3
1	D	333	LEU	2.3
1	D	794	LYS	2.3
1	A	316	LEU	2.3
1	D	753	LYS	2.3
1	A	60	THR	2.2
1	B	777	THR	2.2
1	C	135	ASN	2.2
1	C	242	PHE	2.2
1	C	168	ARG	2.2
1	B	776	CYS	2.2
1	A	780	ILE	2.2
1	A	791	LEU	2.2
1	C	219	LYS	2.2
1	D	792	ASN	2.2
1	B	703	LEU	2.2
1	C	735	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	459	PHE	2.2
1	D	118	ASP	2.2
1	D	177	LEU	2.2
1	D	367	LEU	2.2
1	D	775	GLU	2.2
1	B	752	ASN	2.2
1	B	764	LEU	2.2
1	D	84	GLN	2.2
1	C	815	VAL	2.1
1	C	780	ILE	2.1
1	A	736	SER	2.1
1	D	395	ASN	2.1
1	B	128	ARG	2.1
1	B	784	ARG	2.1
1	D	126	ASN	2.1
1	D	169	LEU	2.1
1	C	32	ARG	2.1
1	D	749	LYS	2.1
1	C	90	THR	2.1
1	D	776	CYS	2.1
1	C	74	PHE	2.1
1	B	35	PRO	2.1
1	C	198	GLU	2.1
1	C	128	ARG	2.1
1	B	86	LEU	2.0
1	D	146	GLU	2.0
1	A	783	PHE	2.0
1	A	793	VAL	2.0
1	D	786	TRP	2.0
1	C	161	ILE	2.0
1	D	542	LEU	2.0
1	B	91	LYS	2.0
1	D	812	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	H	5	11/12	0.78	0.21	61,65,73,76	0
2	MAN	J	5	11/12	0.79	0.27	72,75,80,81	0
2	MAN	K	5	11/12	0.80	0.15	69,72,74,74	0
2	MAN	M	5	11/12	0.80	0.16	69,76,80,82	0
2	MAN	P	5	11/12	0.80	0.20	64,74,78,78	0
3	BMA	F	3	11/12	0.80	0.19	64,72,77,79	0
3	BMA	I	3	11/12	0.80	0.17	59,64,78,78	0
2	MAN	N	4	11/12	0.82	0.12	41,51,59,59	0
3	BMA	O	3	11/12	0.82	0.19	59,64,102,102	0
3	NAG	O	2	14/15	0.83	0.19	44,56,61,61	0
3	BMA	L	3	11/12	0.83	0.17	69,72,75,75	0
2	MAN	G	5	11/12	0.85	0.18	59,66,67,68	0
2	MAN	G	4	11/12	0.85	0.23	66,72,75,76	0
2	MAN	M	4	11/12	0.86	0.15	67,68,70,70	0
2	MAN	P	4	11/12	0.86	0.23	70,74,76,76	0
2	MAN	J	4	11/12	0.87	0.18	66,69,77,77	0
2	BMA	K	3	11/12	0.88	0.10	54,59,62,65	0
2	MAN	N	5	11/12	0.88	0.21	80,82,85,88	0
2	MAN	H	4	11/12	0.88	0.13	29,41,45,48	0
2	BMA	M	3	11/12	0.90	0.13	43,55,66,67	0
3	NAG	I	2	14/15	0.90	0.17	32,43,56,63	0
2	BMA	P	3	11/12	0.90	0.11	49,57,66,72	0
2	MAN	K	4	11/12	0.92	0.09	51,57,59,60	0
2	MAN	E	5	11/12	0.92	0.10	68,70,73,74	0
2	BMA	G	3	11/12	0.92	0.16	48,52,64,64	0
2	BMA	J	3	11/12	0.92	0.12	48,55,62,69	0
2	NAG	N	2	14/15	0.94	0.14	34,44,49,57	0
2	BMA	H	3	11/12	0.94	0.10	32,36,45,52	0
3	NAG	F	2	14/15	0.94	0.12	33,46,51,58	0
3	NAG	L	2	14/15	0.95	0.10	31,46,59,66	0
2	BMA	N	3	11/12	0.95	0.11	59,61,73,77	0
2	NAG	K	2	14/15	0.96	0.13	29,41,51,55	0
2	NAG	M	1	14/15	0.96	0.15	12,14,22,23	0
2	NAG	J	1	14/15	0.96	0.12	14,17,28,32	0
2	MAN	E	4	11/12	0.96	0.11	36,40,43,44	0
2	NAG	N	1	14/15	0.97	0.16	34,37,52,54	0
3	NAG	F	1	14/15	0.97	0.12	11,16,18,26	0

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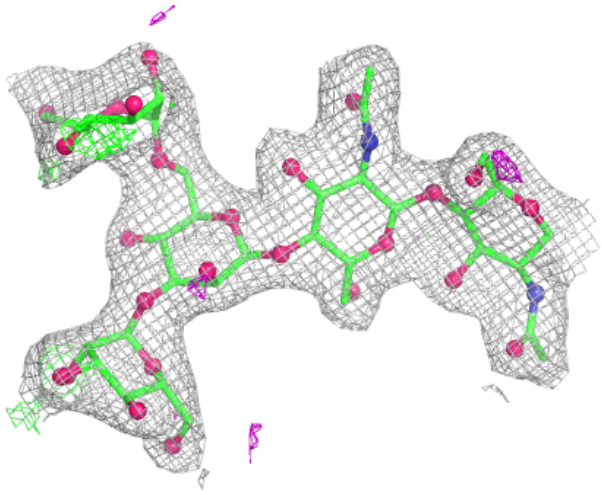
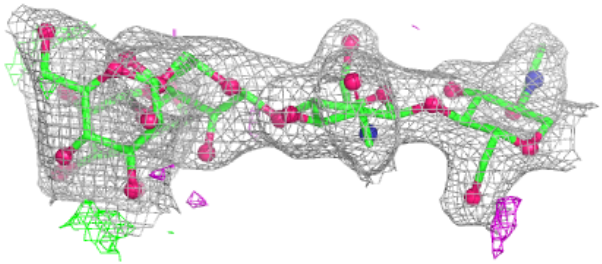
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	1	14/15	0.97	0.17	9,14,20,20	0
2	BMA	E	3	11/12	0.97	0.10	38,41,58,64	0
3	NAG	I	1	14/15	0.97	0.15	9,18,22,28	0
2	NAG	G	1	14/15	0.97	0.09	15,20,24,24	0
2	NAG	K	1	14/15	0.97	0.14	30,36,38,41	0
2	NAG	P	1	14/15	0.97	0.12	17,19,27,32	0
2	NAG	P	2	14/15	0.97	0.11	19,27,40,40	0
2	NAG	H	1	14/15	0.97	0.15	8,14,22,25	0
2	NAG	J	2	14/15	0.97	0.11	16,31,38,41	0
3	NAG	L	1	14/15	0.98	0.11	13,18,30,35	0
2	NAG	M	2	14/15	0.98	0.10	14,22,31,37	0
2	NAG	H	2	14/15	0.98	0.11	12,20,27,28	0
3	NAG	O	1	14/15	0.98	0.15	18,21,31,38	0
2	NAG	E	2	14/15	0.98	0.17	8,20,34,34	0
2	NAG	G	2	14/15	0.98	0.09	17,24,32,42	0

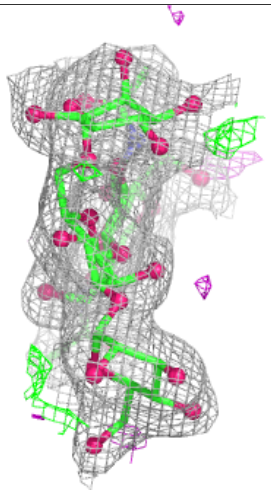
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

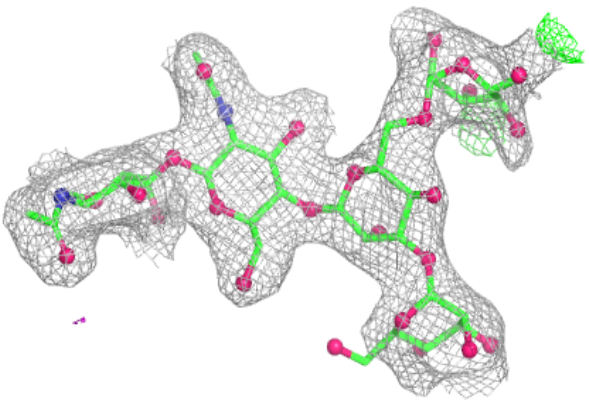


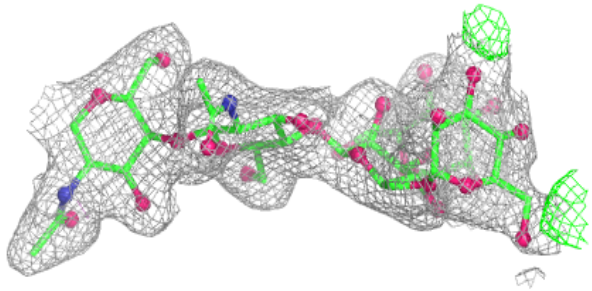


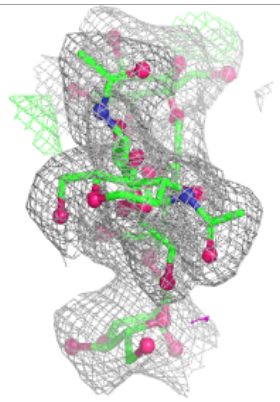


Electron density around Chain G:

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

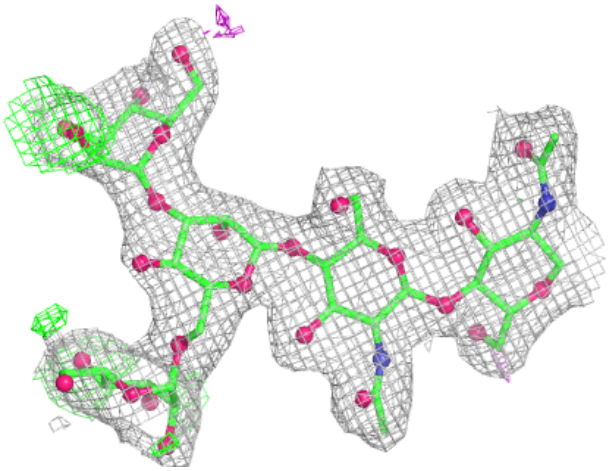


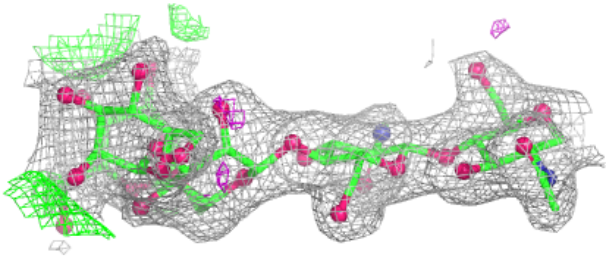


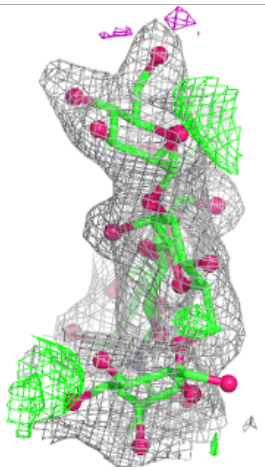


Electron density around Chain H:

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

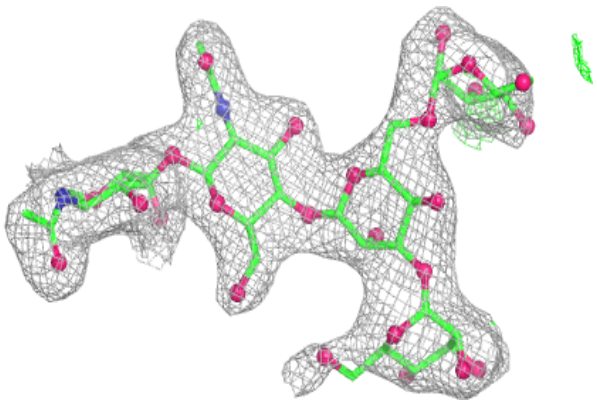


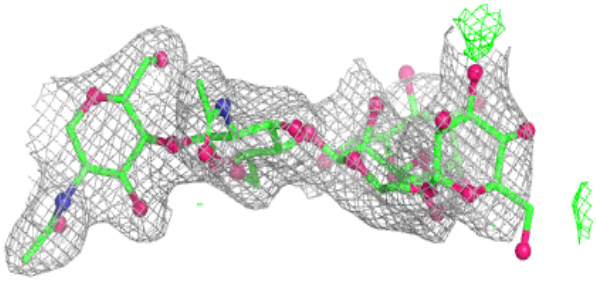


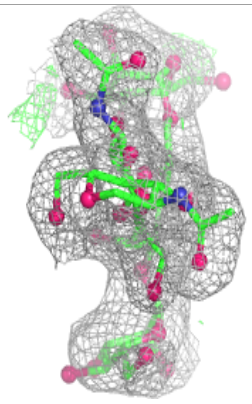


Electron density around Chain J:

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

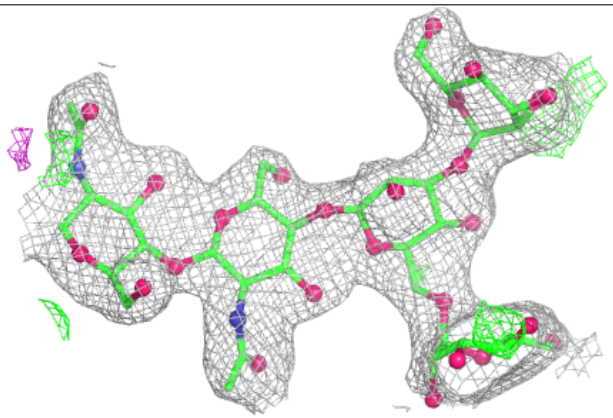


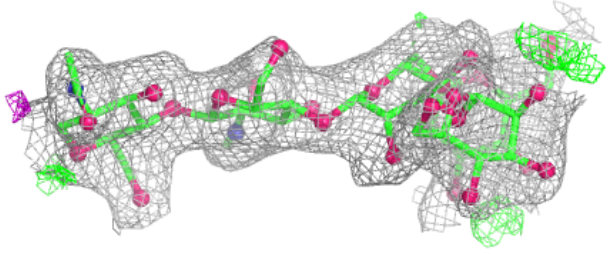




Electron density around Chain K:

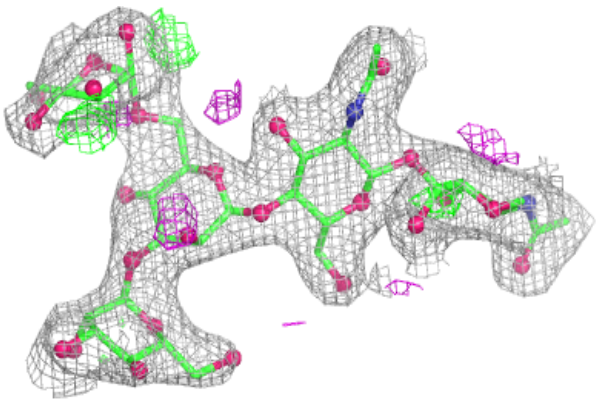
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

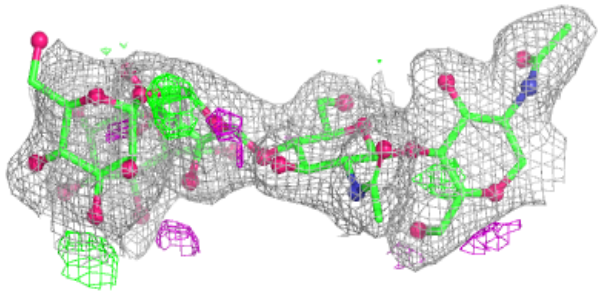


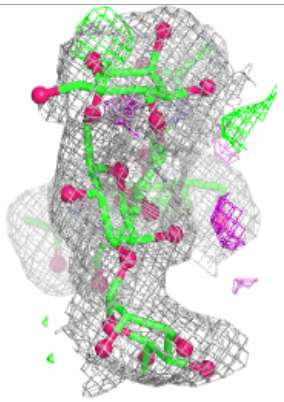


Electron density around Chain M:

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

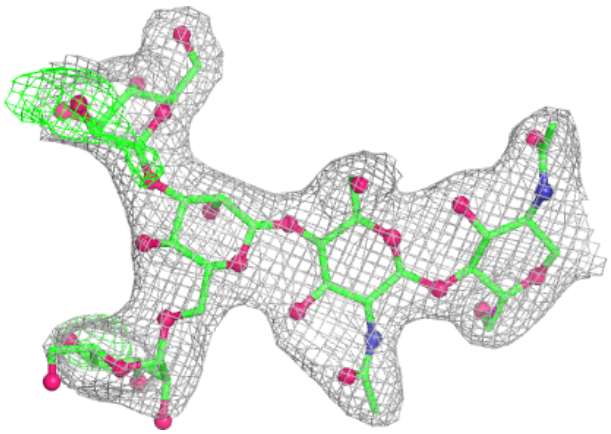


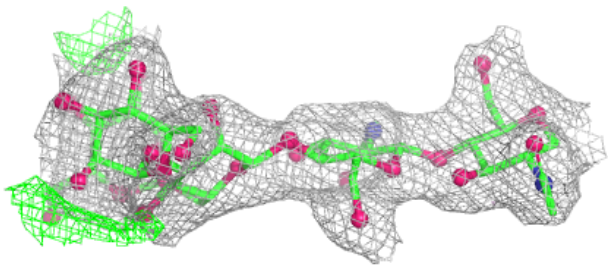


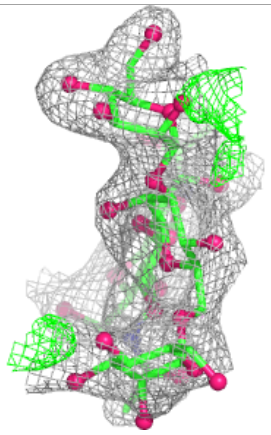


Electron density around Chain N:

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

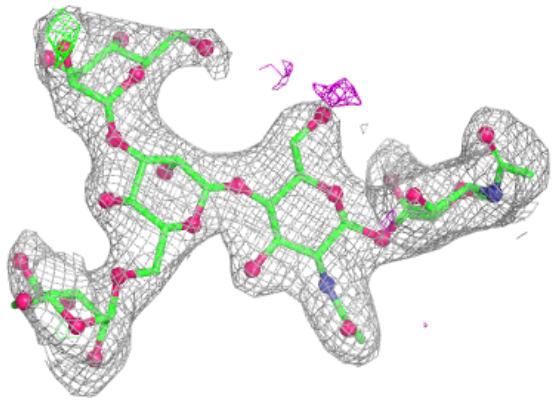


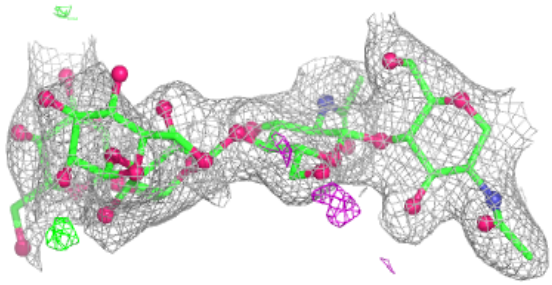


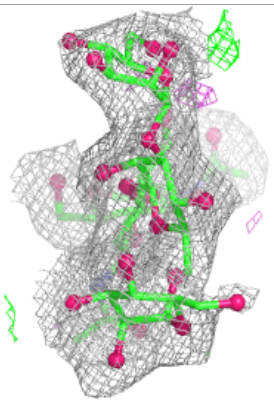


Electron density around Chain P:

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

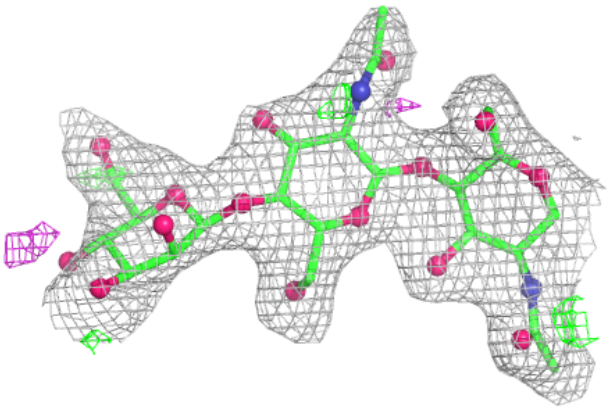


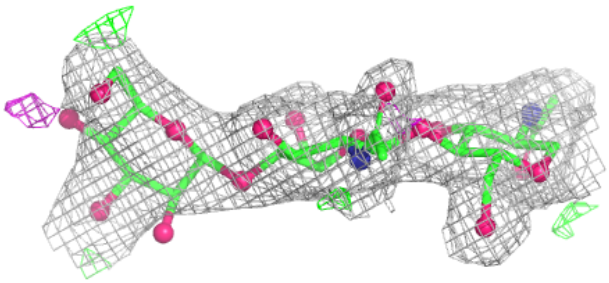


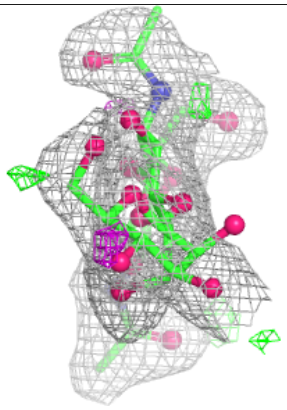


Electron density around Chain F:

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

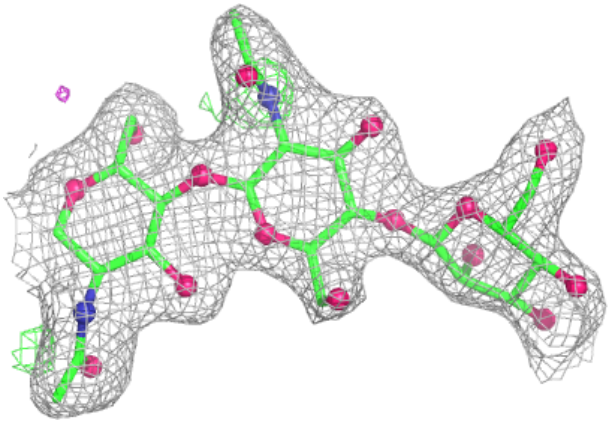


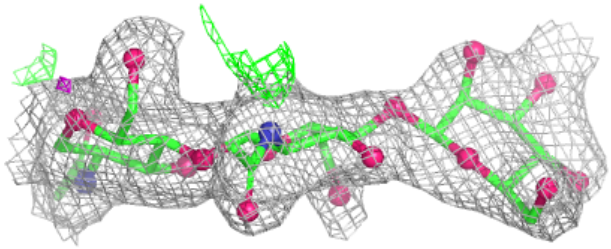


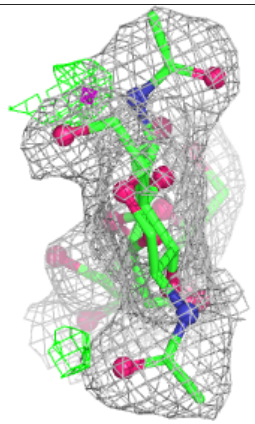


Electron density around Chain I:

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

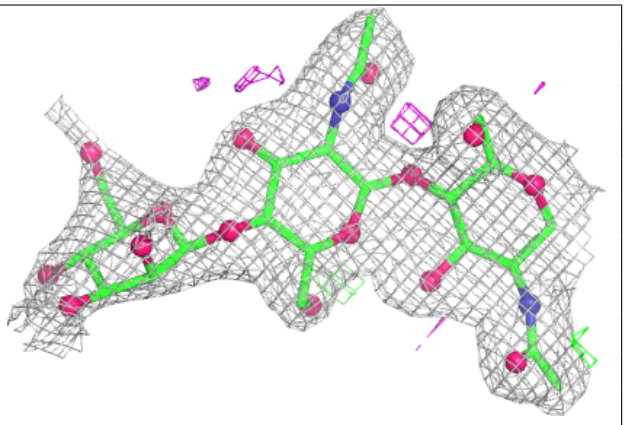


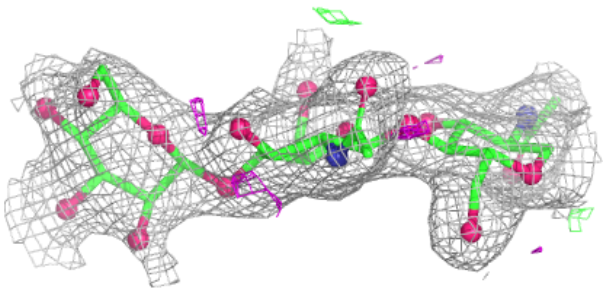


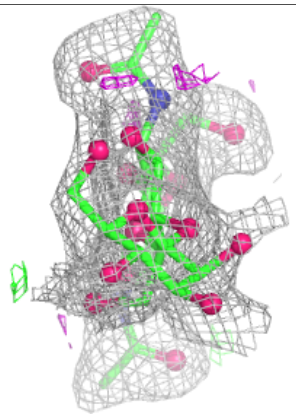


Electron density around Chain L:

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

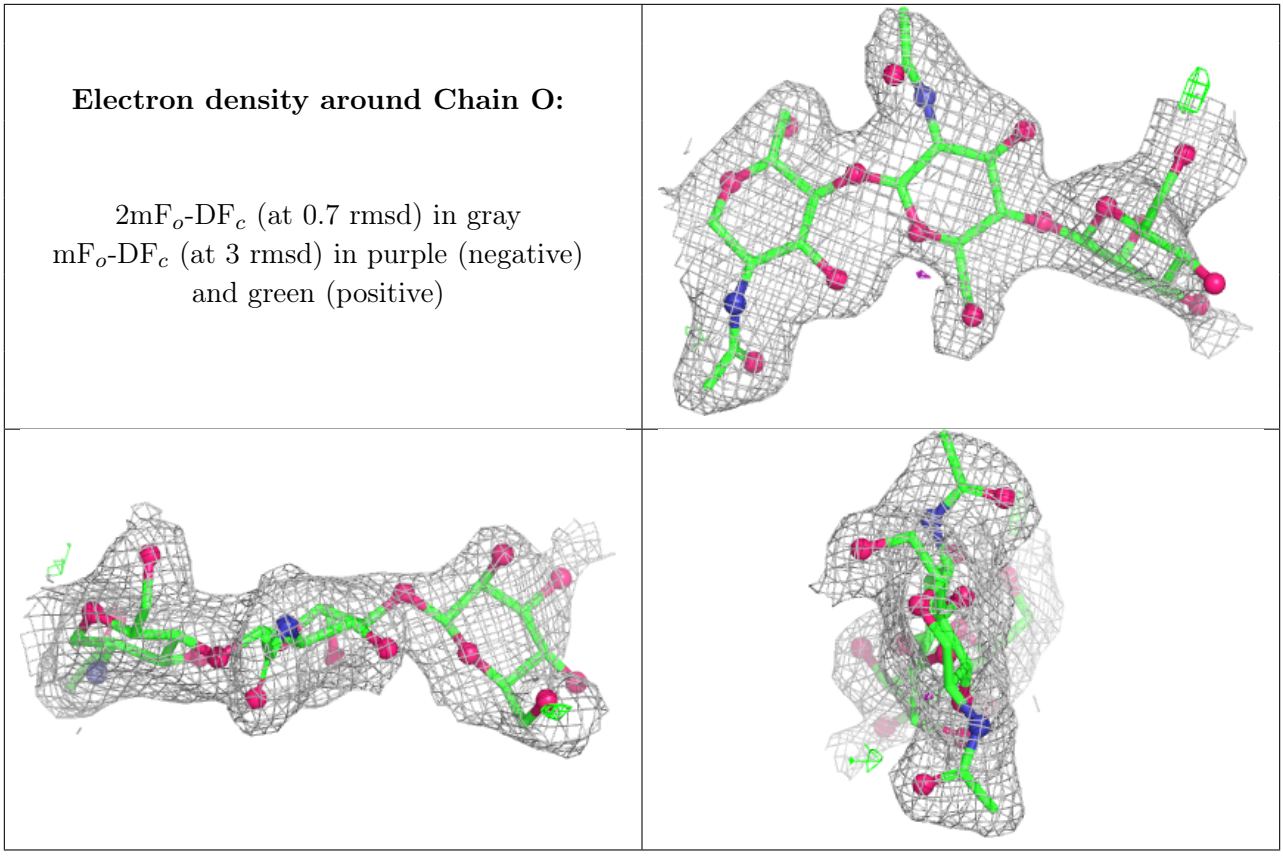






Electron density around Chain O:

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



6.4 Ligands

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, 95^{th} 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
5	SO4	B	1021	5/5	0.71	0.26	107,108,110,110	0
4	NAG	A	1017	14/15	0.84	0.20	47,64,67,70	0
5	SO4	B	1020	5/5	0.84	0.17	97,98,99,102	0
4	NAG	A	1015	14/15	0.84	0.26	63,67,69,74	0
5	SO4	D	921	5/5	0.85	0.20	106,106,107,111	0
4	NAG	D	918	14/15	0.86	0.29	66,68,71,74	0
5	SO4	D	920	5/5	0.86	0.22	104,105,106,106	0
4	NAG	B	1015	14/15	0.86	0.20	71,78,82,83	0
4	NAG	C	916	14/15	0.88	0.14	40,46,50,53	0
5	SO4	A	1019	5/5	0.89	0.21	100,102,104,105	0
4	NAG	B	1017	14/15	0.90	0.20	56,61,62,63	0
4	NAG	B	1009	14/15	0.90	0.14	48,60,68,68	0
4	NAG	C	917	14/15	0.91	0.17	50,59,62,63	0
4	NAG	D	917	14/15	0.91	0.18	58,61,68,72	0

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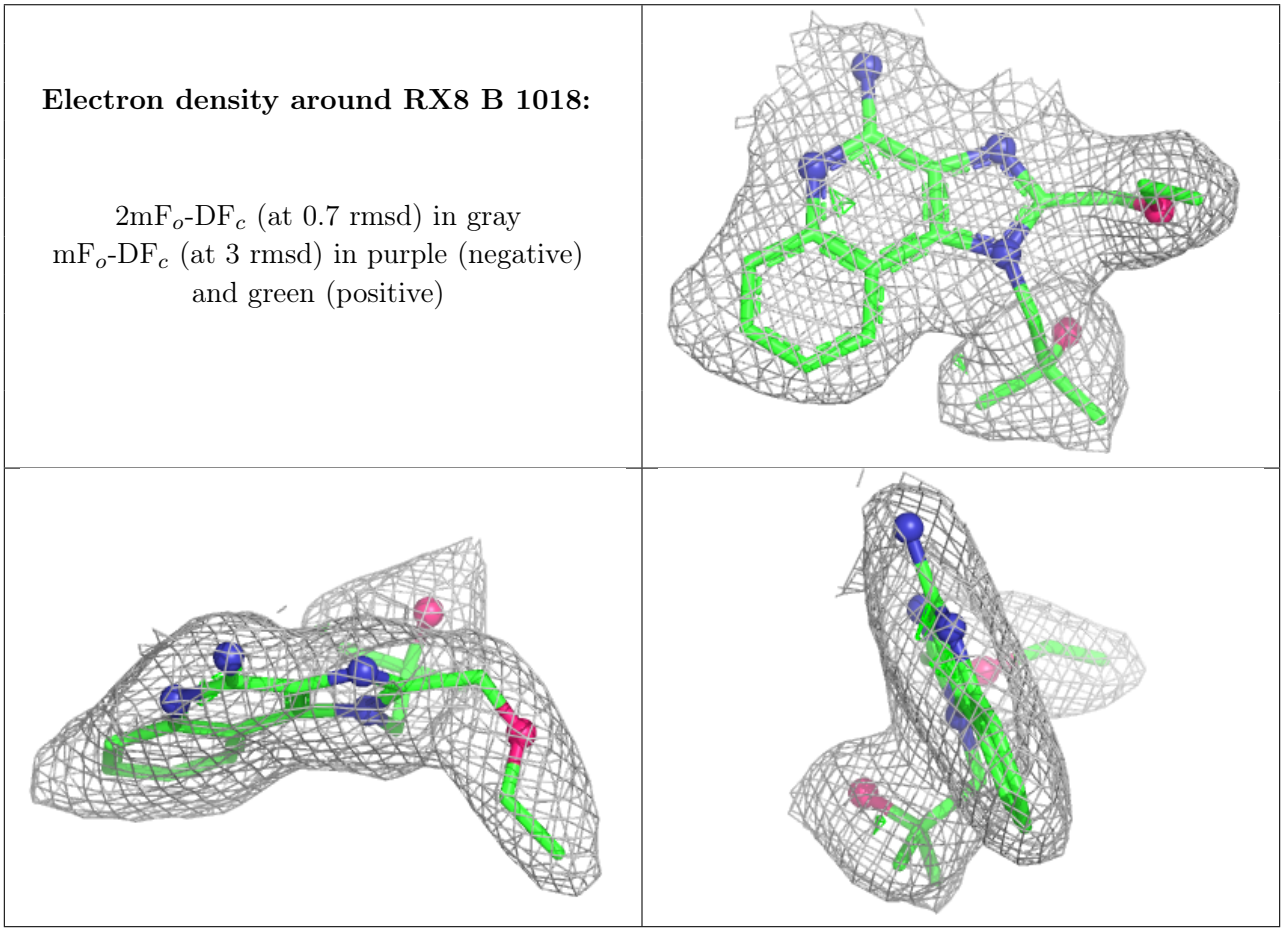
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	911	14/15	0.92	0.13	49,54,59,61	0
5	SO4	C	918	5/5	0.93	0.17	89,91,92,93	0
4	NAG	D	919	14/15	0.93	0.14	41,51,57,58	0
4	NAG	C	910	14/15	0.93	0.10	31,46,52,54	0
4	NAG	A	1009	14/15	0.94	0.10	46,56,68,71	0
5	SO4	A	1018	5/5	0.94	0.11	91,93,94,94	0
5	SO4	B	1019	5/5	0.96	0.07	86,87,88,89	0
4	NAG	B	1016	14/15	0.96	0.14	27,32,39,46	0
6	RX8	B	1018	23/23	0.97	0.17	22,25,30,88	0
6	RX8	C	901	23/23	0.97	0.17	8,14,18,21	0
6	RX8	D	901	23/23	0.97	0.18	11,17,22,23	0
4	NAG	A	1016	14/15	0.98	0.11	26,34,41,48	0
6	RX8	D	902	23/23	0.98	0.20	25,28,38,44	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.

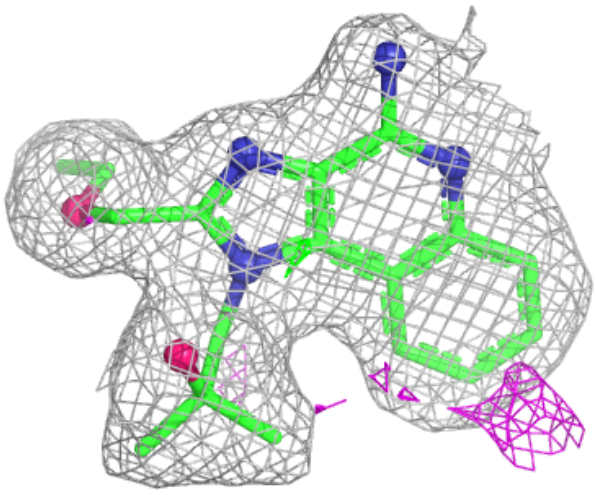
Electron density around RX8 B 1018:

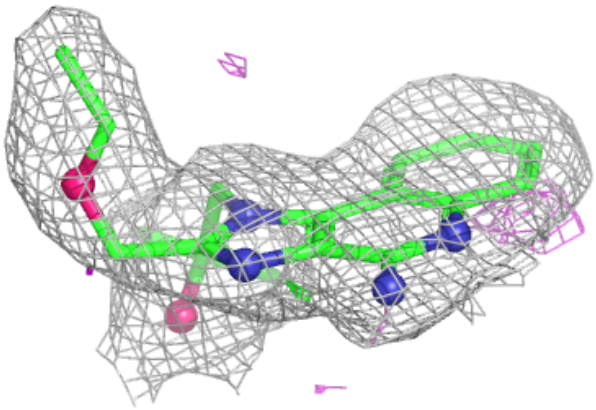
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

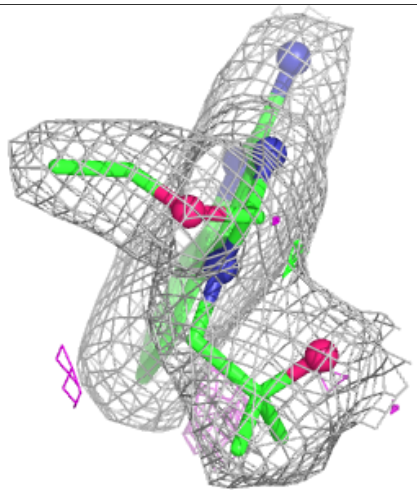


Electron density around RX8 C 901:

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

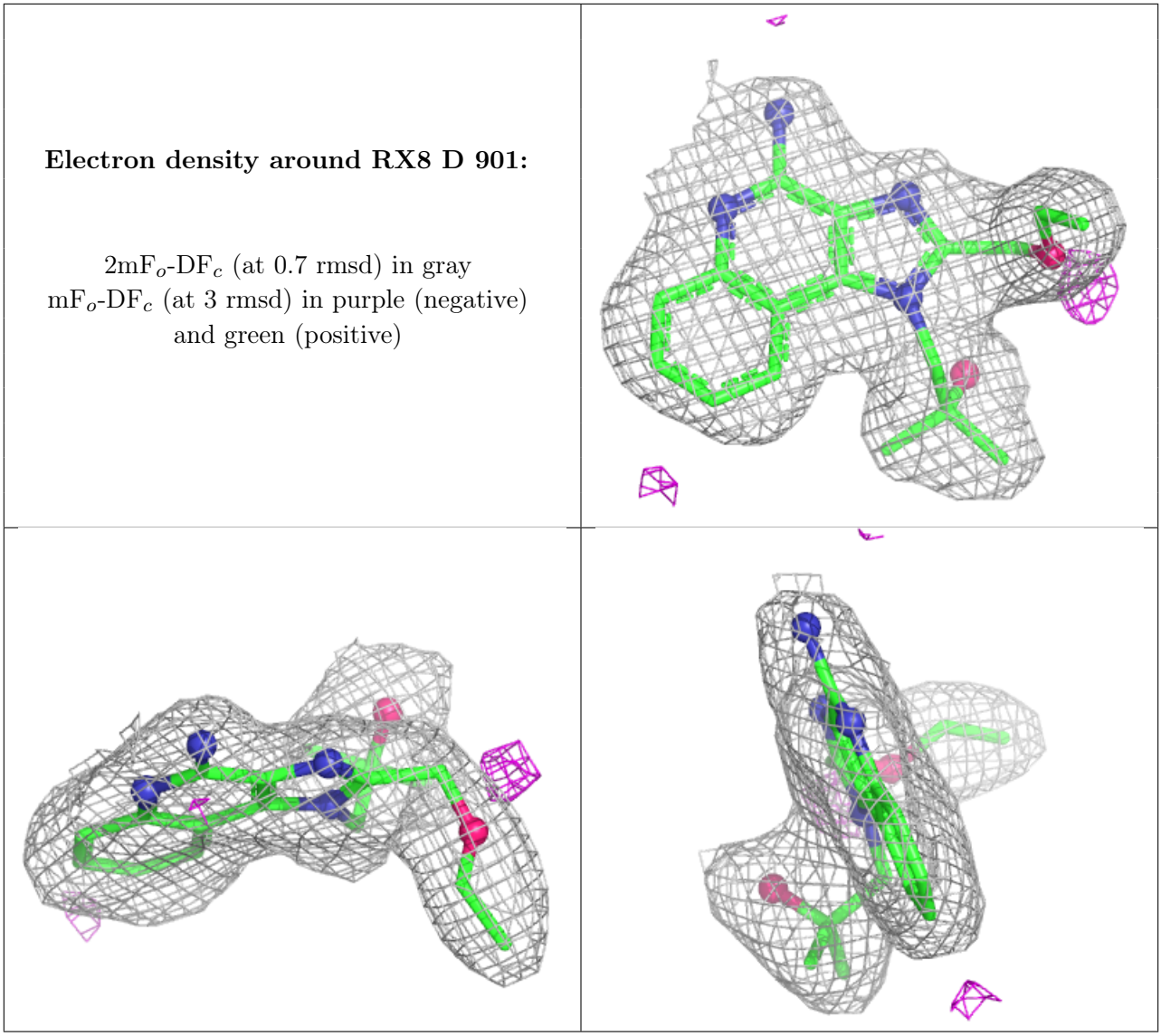






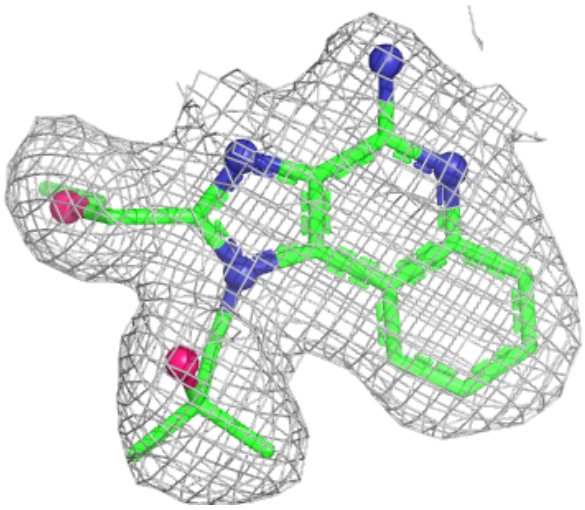
Electron density around RX8 D 901:

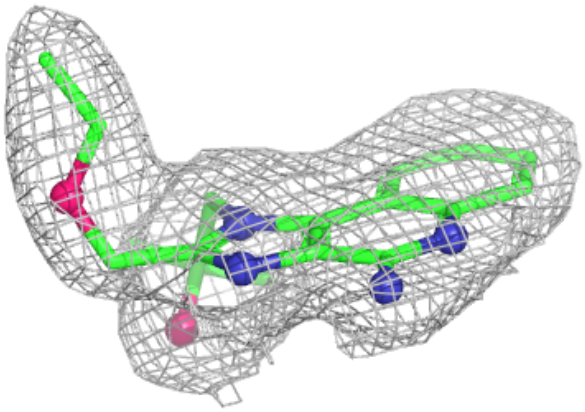
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

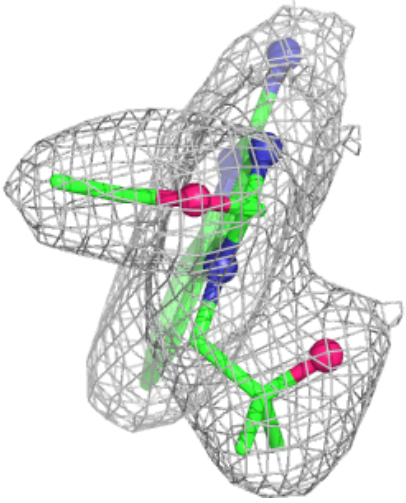


Electron density around RX8 D 902:

$2mF_o$-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

There are no such residues in this entry.