



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:15 PM BST

PDB ID : 3W3N
Title : Crystal structure of human TLR8 in complex with Resiquimod (R848) crystal form 3
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2012-12-22
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

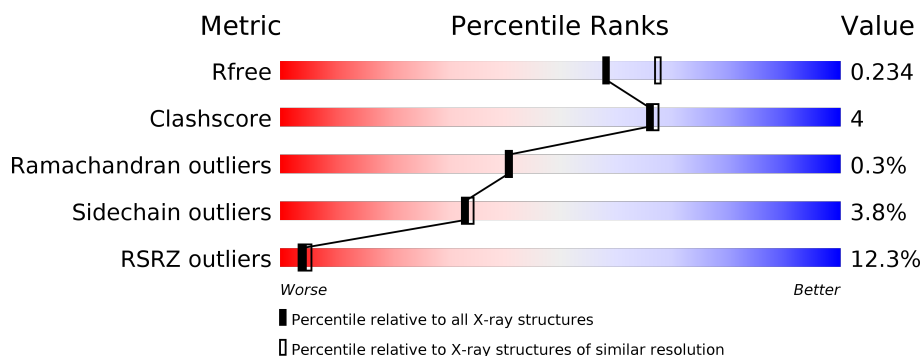
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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 $\leq 5\%$. 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	
1	B	811	
2	C	5	
2	E	5	
2	F	5	
2	H	5	

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Mol	Chain	Length	Quality of chain
3	D	3	 100%
3	G	3	 67%33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13256 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.

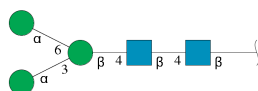
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			6039	3861	1025	1134	19			
1	B	749	Total	C	N	O	S	0	0	0
			5994	3836	1019	1120	19			

There are 20 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



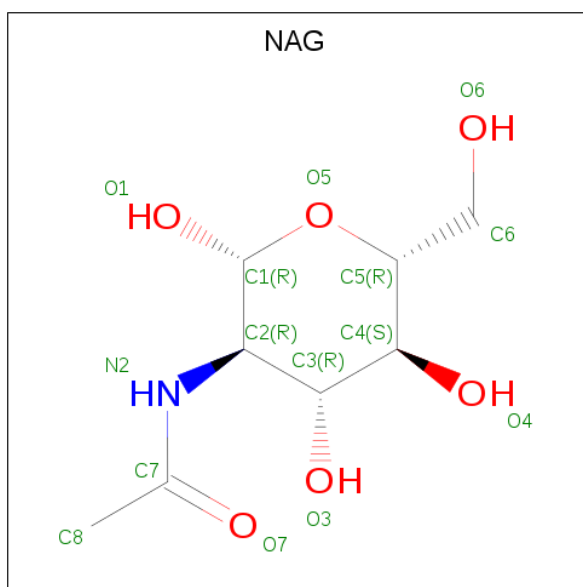
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

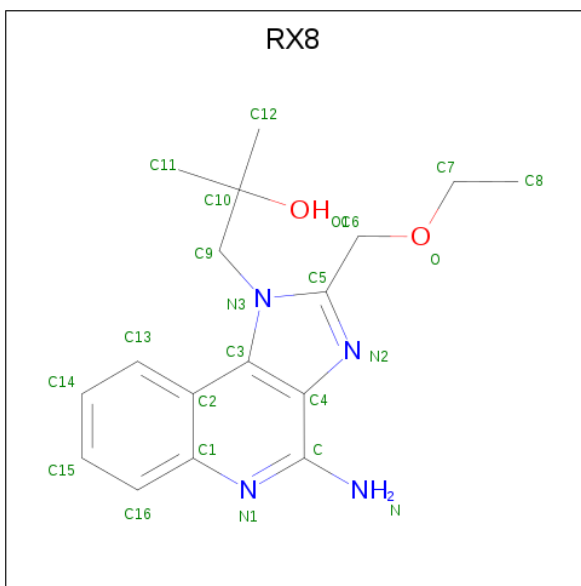
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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	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	B	1	Total	C	N	O	0	0
			14	8	1	5		

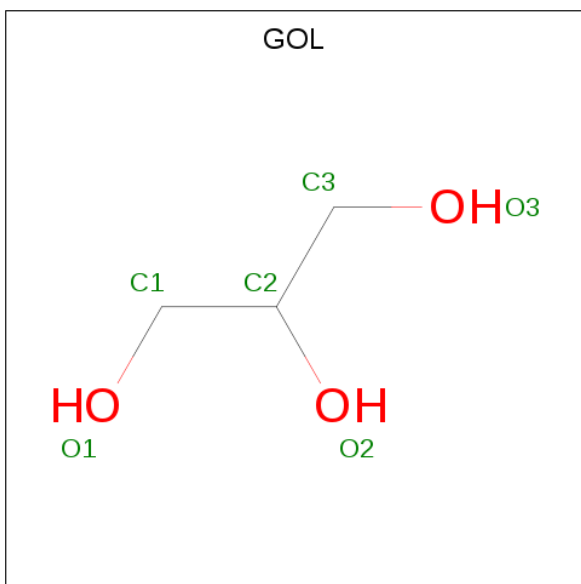
- Molecule 5 is 1-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-2-methylpropan-

2-ol (three-letter code: RX8) (formula: C₁₇H₂₂N₄O₂).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

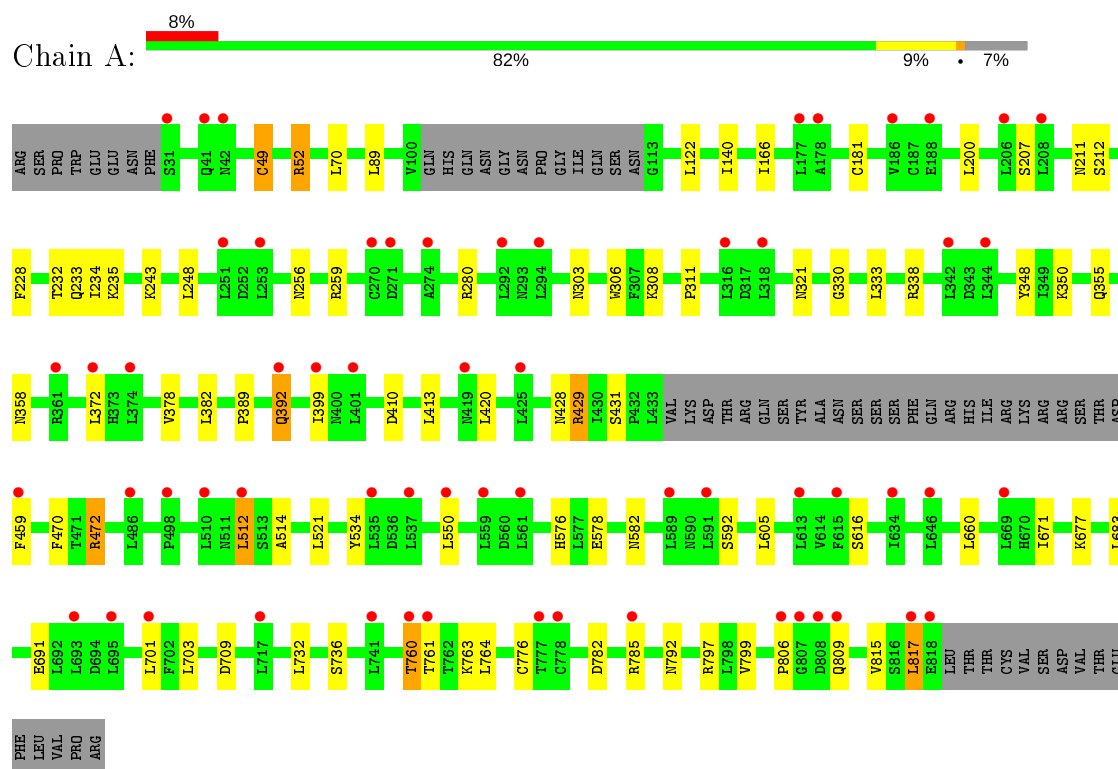
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	419	Total 419	O 419	0	0
7	B	248	Total 248	O 248	0	0

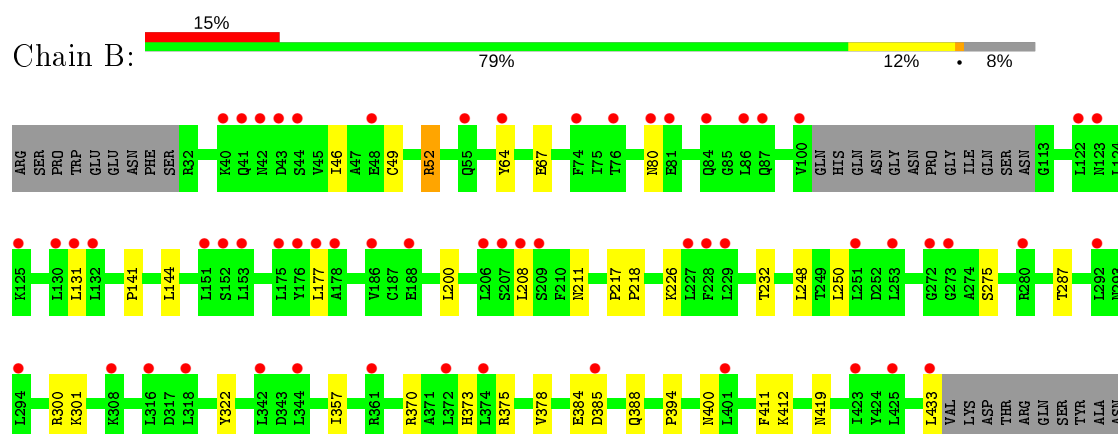
3 Residue-property plots [i](#)

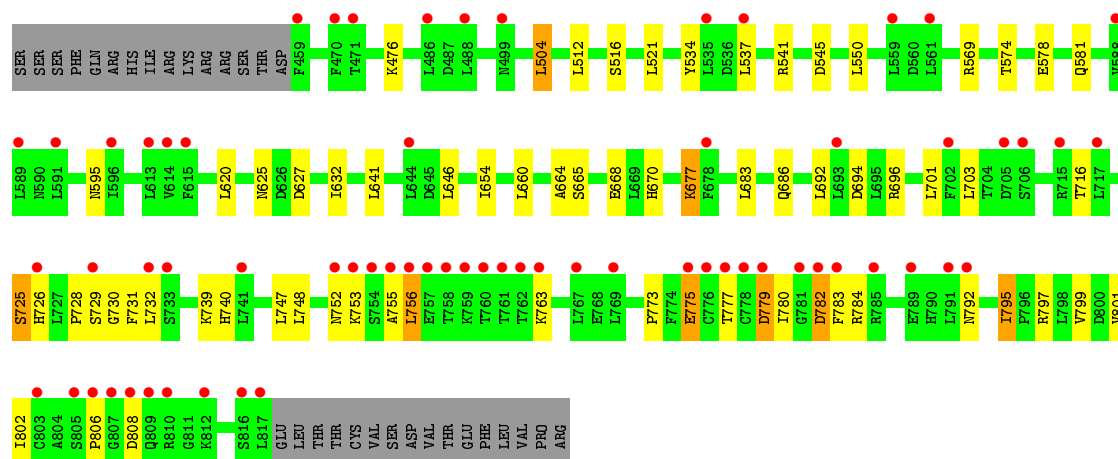
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



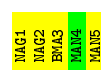
• Molecule 1: Toll-like receptor 8





- 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 C: 20% 80%



- 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: 20% 80%



- 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 F: 60% 40%



- 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: 20% 80%



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

Chain D:  100%

HA01
HA02
BO03

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

Chain G:  67% 33%

HA01
HA02
BO03

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.22Å 100.78Å 265.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.39 – 2.10 28.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (28.39-2.10) 95.7 (28.39-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.200 , 0.233 0.201 , 0.234	Depositor DCC
R_{free} test set	6498 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13256	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 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MAN, GOL, BMA, NAG, RX8

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	0.27	0/6164	0.47	0/8361
1	B	0.27	0/6119	0.46	0/8302
All	All	0.27	0/12283	0.46	0/16663

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6039	0	6005	41	0
1	B	5994	0	5937	57	0
2	C	61	0	52	0	0
2	E	61	0	52	0	0
2	F	61	0	52	0	0
2	H	61	0	52	0	0
3	D	39	0	34	0	0
3	G	39	0	34	1	0
4	A	84	0	78	1	0
4	B	98	0	91	0	0
5	A	23	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	23	0	22	3	0
6	A	6	0	8	0	0
7	A	419	0	0	10	0
7	B	248	0	0	9	0
All	All	13256	0	12439	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ALA:O	7:B:1025:HOH:O	1.89	0.91
1:B:625:ASN:OD1	7:B:1187:HOH:O	1.95	0.83
1:A:333:LEU:O	7:A:1220:HOH:O	2.05	0.74
1:B:775:GLU:O	1:B:780:ILE:HD11	1.91	0.71
1:A:691:GLU:OE2	7:A:1158:HOH:O	2.09	0.70
1:A:389:PRO:O	1:A:392:GLN:NE2	2.25	0.69
1:A:358:ASN:ND2	7:A:1436:HOH:O	2.26	0.69
1:B:779:ASP:N	1:B:779:ASP:OD1	2.25	0.69
1:B:384:GLU:OE2	7:B:1199:HOH:O	2.12	0.68
1:A:760:THR:OG1	1:A:761:THR:N	2.27	0.68
1:A:459:PHE:HB2	7:A:1160:HOH:O	1.94	0.66
1:B:370:ARG:NH1	7:B:1094:HOH:O	2.17	0.65
1:A:350:LYS:NZ	7:A:1454:HOH:O	2.30	0.64
1:A:732:LEU:HD21	1:A:764:LEU:HD22	1.81	0.63
1:B:52:ARG:HG2	1:B:799:VAL:HG11	1.82	0.62
1:B:660:LEU:HD22	1:B:686:GLN:HG3	1.83	0.61
1:B:46:ILE:HG12	1:B:67:GLU:HB2	1.82	0.61
1:A:677:LYS:O	7:A:1410:HOH:O	2.16	0.61
5:B:901:RX8:H19	5:B:901:RX8:H9	1.82	0.60
1:B:795:ILE:HD11	1:B:801:VAL:HG21	1.83	0.60
1:B:748:LEU:H	1:B:773:PRO:HD2	1.66	0.60
1:B:753:LYS:HA	1:B:756:LEU:HD22	1.82	0.60
1:A:776:CYS:HB3	1:A:817:LEU:HD11	1.84	0.60
4:A:1018:NAG:O7	7:A:1384:HOH:O	2.17	0.59
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.83	0.59
1:B:654:ILE:O	7:B:1210:HOH:O	2.16	0.58
1:B:300:ARG:HG2	1:B:322:TYR:HB2	1.84	0.58
1:A:782:ASP:OD1	1:A:785:ARG:NH1	2.37	0.58
1:B:677:LYS:HD3	7:B:1204:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:ILE:O	1:B:783:PHE:N	2.37	0.57
5:A:1020:RX8:H9	5:A:1020:RX8:H19	1.87	0.56
1:A:355:GLN:NE2	7:A:1476:HOH:O	2.16	0.56
1:B:574:THR:HG23	5:B:901:RX8:H10	1.88	0.56
1:A:399:ILE:HG12	1:A:420:LEU:HD21	1.86	0.55
1:B:394:PRO:O	1:B:419:ASN:ND2	2.40	0.55
1:B:782:ASP:N	1:B:782:ASP:OD1	2.37	0.55
1:B:357:ILE:HG22	7:B:1031:HOH:O	2.06	0.55
1:A:514:ALA:C	1:B:541:ARG:HH22	2.11	0.54
1:A:392:GLN:NE2	1:A:392:GLN:H	2.08	0.52
1:B:375:ARG:HD2	1:B:400:ASN:HD21	1.74	0.52
1:B:739:LYS:HG2	1:B:763:LYS:NZ	2.24	0.52
1:A:212:SER:OG	1:A:233:GLN:NE2	2.42	0.52
1:A:52:ARG:HG2	1:A:799:VAL:HG21	1.91	0.52
1:B:660:LEU:HD21	1:B:683:LEU:HD22	1.92	0.51
1:A:521:LEU:HD13	1:A:550:LEU:HD21	1.93	0.51
1:B:694:ASP:OD2	1:B:696:ARG:NH2	2.42	0.50
1:A:470:PHE:CD1	1:A:472:ARG:HG3	2.47	0.50
1:B:739:LYS:HG2	1:B:763:LYS:HZ3	1.77	0.50
1:A:207:SER:HA	1:A:228:PHE:HB2	1.93	0.49
1:B:64:TYR:H	1:B:64:TYR:HD1	1.61	0.49
1:B:627:ASP:HB2	7:B:1187:HOH:O	2.12	0.48
1:B:730:GLY:H	1:B:755:ALA:HA	1.78	0.48
1:B:476:LYS:HD2	3:G:1:NAG:H83	1.94	0.48
1:B:668:GLU:HG3	1:B:692:LEU:HB3	1.96	0.48
1:A:806:PRO:HD2	1:A:809:GLN:HB2	1.95	0.48
1:B:725:SER:HA	1:B:747:LEU:O	2.13	0.48
1:B:792:ASN:N	1:B:792:ASN:OD1	2.47	0.47
1:B:777:THR:H	1:B:780:ILE:CD1	2.27	0.47
1:A:311:PRO:O	1:A:338:ARG:HG3	2.15	0.47
1:A:49:CYS:HB3	1:A:70:LEU:HD23	1.97	0.47
1:B:732:LEU:HD12	1:B:756:LEU:HD12	1.96	0.47
1:A:235:LYS:HE3	1:A:235:LYS:HB3	1.61	0.46
1:A:792:ASN:OD1	1:A:792:ASN:N	2.47	0.46
1:B:716:THR:HG23	1:B:740:HIS:HB3	1.98	0.45
1:A:348:TYR:CD2	5:B:901:RX8:H3	2.51	0.45
1:B:512:LEU:HB2	1:B:537:LEU:HD23	1.98	0.45
1:A:140:ILE:HD13	1:A:166:ILE:HD11	1.99	0.45
1:B:545:ASP:OD1	1:B:574:THR:OG1	2.26	0.45
1:B:177:LEU:HB2	1:B:208:LEU:HD23	2.00	0.43
1:B:385:ASP:HA	1:B:388:GLN:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PRO:HB2	1:B:144:LEU:HD21	2.01	0.43
1:B:729:SER:HA	1:B:755:ALA:HA	2.01	0.43
1:B:806:PRO:HG2	1:B:808:ASP:OD1	2.19	0.43
1:B:375:ARG:NE	7:B:1195:HOH:O	2.52	0.43
1:A:259:ARG:NH1	1:A:321:ASN:O	2.48	0.42
1:B:373:HIS:HA	1:B:400:ASN:HB3	2.01	0.42
1:A:280:ARG:HH22	1:A:308:LYS:HE2	1.84	0.42
1:B:728:PRO:HG2	1:B:731:PHE:HD2	1.85	0.42
1:A:211:ASN:O	1:A:232:THR:HA	2.19	0.42
1:B:411:PHE:HB3	1:B:504:LEU:HD13	2.02	0.42
1:B:211:ASN:O	1:B:232:THR:HA	2.19	0.42
1:B:217:PRO:HA	1:B:218:PRO:HD3	1.84	0.41
1:B:226:LYS:HG2	1:B:250:LEU:HB3	2.01	0.41
1:A:234:ILE:O	1:A:256:ASN:HB3	2.21	0.41
1:A:512:LEU:HD12	1:A:512:LEU:HA	1.90	0.41
1:B:780:ILE:HG22	1:B:784:ARG:HG2	2.02	0.41
1:A:428:ASN:HB3	1:A:429:ARG:H	1.75	0.41
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.20	0.41
1:B:670:HIS:HA	1:B:694:ASP:HB3	2.02	0.41
1:A:736:SER:O	1:A:763:LYS:HG2	2.21	0.41
1:B:521:LEU:HD13	1:B:550:LEU:HD21	2.03	0.41
1:B:677:LYS:HE3	1:B:677:LYS:HB3	1.85	0.41
1:A:181:CYS:HB3	7:A:1506:HOH:O	2.21	0.41
1:A:592:SER:HA	1:A:616:SER:O	2.21	0.40
1:B:620:LEU:HD11	1:B:646:LEU:HD22	2.03	0.40
1:B:641:LEU:O	1:B:665:SER:OG	2.36	0.40
1:A:303:ASN:HB3	1:A:306:TRP:CE2	2.56	0.40
1:A:709:ASP:OD1	7:A:1460:HOH:O	2.21	0.40
1:B:578:GLU:O	1:B:581:GLN:HG2	2.22	0.40
1:A:382:LEU:HG	1:A:413:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	711 (95%)	32 (4%)	2 (0%)	41	41
1	B	743/811 (92%)	710 (96%)	31 (4%)	2 (0%)	41	41
All	All	1488/1622 (92%)	1421 (96%)	63 (4%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	797	ARG
1	A	378	VAL
1	B	378	VAL
1	A	330	GLY

5.3.2 Protein sidechains ⓘ

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%)	670 (96%)	24 (4%)	36	38
1	B	683/755 (90%)	654 (96%)	29 (4%)	30	30
All	All	1377/1510 (91%)	1324 (96%)	53 (4%)	33	34

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	52	ARG
1	A	89	LEU
1	A	122	LEU
1	A	200	LEU
1	A	243	LYS
1	A	248	LEU
1	A	372	LEU
1	A	392	GLN

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Mol	Chain	Res	Type
1	A	410	ASP
1	A	429	ARG
1	A	431	SER
1	A	472	ARG
1	A	512	LEU
1	A	534	TYR
1	A	582	ASN
1	A	605	LEU
1	A	671	ILE
1	A	701	LEU
1	A	703	LEU
1	A	760	THR
1	A	797	ARG
1	A	815	VAL
1	A	817	LEU
1	B	49	CYS
1	B	52	ARG
1	B	80	ASN
1	B	131	LEU
1	B	200	LEU
1	B	248	LEU
1	B	275	SER
1	B	287	THR
1	B	301	LYS
1	B	412	LYS
1	B	433	LEU
1	B	504	LEU
1	B	516	SER
1	B	534	TYR
1	B	569	ARG
1	B	595	ASN
1	B	632	ILE
1	B	677	LYS
1	B	701	LEU
1	B	703	LEU
1	B	725	SER
1	B	726	HIS
1	B	752	ASN
1	B	756	LEU
1	B	775	GLU
1	B	779	ASP
1	B	782	ASP

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Mol	Chain	Res	Type
1	B	795	ILE
1	B	802	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	233	GLN
1	A	392	GLN
1	A	790	HIS
1	B	309	ASN
1	B	499	ASN
1	B	809	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

26 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	0.78	1 (5%)
2	NAG	C	2	2	14,14,15	0.67	0	17,19,21	0.77	1 (5%)
2	BMA	C	3	2	11,11,12	0.82	1 (9%)	15,15,17	0.89	0
2	MAN	C	4	2	11,11,12	0.63	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	C	5	2	11,11,12	0.64	0	15,15,17	0.85	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.56	0	17,19,21	0.84	0
3	NAG	D	2	3	14,14,15	0.61	0	17,19,21	0.80	0
3	BMA	D	3	3	11,11,12	0.59	0	15,15,17	0.80	0
2	NAG	E	1	1,2	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
2	NAG	E	2	2	14,14,15	0.60	0	17,19,21	0.74	0
2	BMA	E	3	2	11,11,12	1.33	2 (18%)	15,15,17	1.94	3 (20%)
2	MAN	E	4	2	11,11,12	0.56	0	15,15,17	1.18	2 (13%)
2	MAN	E	5	2	11,11,12	0.79	0	15,15,17	1.27	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.51	0	17,19,21	0.81	0
2	NAG	F	2	2	14,14,15	0.67	0	17,19,21	0.94	2 (11%)
2	BMA	F	3	2	11,11,12	0.84	1 (9%)	15,15,17	1.03	2 (13%)
2	MAN	F	4	2	11,11,12	0.68	0	15,15,17	0.74	0
2	MAN	F	5	2	11,11,12	0.67	0	15,15,17	0.84	0
3	NAG	G	1	1,3	14,14,15	0.52	0	17,19,21	0.91	1 (5%)
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	0.79	0
3	BMA	G	3	3	11,11,12	0.68	0	15,15,17	0.72	0
2	NAG	H	1	1,2	14,14,15	0.51	0	17,19,21	0.83	0
2	NAG	H	2	2	14,14,15	0.62	0	17,19,21	0.93	1 (5%)
2	BMA	H	3	2	11,11,12	0.85	1 (9%)	15,15,17	0.77	0
2	MAN	H	4	2	11,11,12	0.61	0	15,15,17	0.99	1 (6%)
2	MAN	H	5	2	11,11,12	0.68	0	15,15,17	0.74	1 (6%)

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

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	BMA	O5-C1	-3.13	1.38	1.43
2	E	3	BMA	C4-C5	2.46	1.58	1.53
2	C	3	BMA	O5-C1	-2.27	1.40	1.43
2	F	3	BMA	O5-C1	-2.26	1.40	1.43
2	H	3	BMA	O5-C1	-2.19	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	5.88	120.15	112.19
2	E	5	MAN	O5-C1-C2	-2.99	106.15	110.77
2	E	4	MAN	O5-C1-C2	-2.91	106.28	110.77
2	E	3	BMA	O5-C5-C6	-2.87	102.70	107.20
2	E	1	NAG	O5-C1-C2	-2.77	106.92	111.29
2	E	5	MAN	C1-O5-C5	-2.71	108.53	112.19
3	G	1	NAG	C1-O5-C5	2.44	115.50	112.19
2	H	4	MAN	O5-C1-C2	-2.34	107.16	110.77
2	F	3	BMA	O2-C2-C3	-2.33	105.47	110.14
2	H	2	NAG	C2-N2-C7	-2.19	119.78	122.90
2	F	2	NAG	O5-C1-C2	-2.16	107.87	111.29
2	C	2	NAG	O5-C1-C2	-2.15	107.90	111.29
2	C	1	NAG	O5-C1-C2	-2.13	107.92	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	BMA	C1-C2-C3	2.12	112.27	109.67
2	E	3	BMA	C3-C4-C5	2.09	113.97	110.24
2	F	2	NAG	O5-C5-C6	2.07	110.45	107.20
2	E	4	MAN	C1-O5-C5	2.03	114.94	112.19
2	C	5	MAN	O5-C1-C2	-2.02	107.66	110.77
2	H	5	MAN	O5-C1-C2	-2.00	107.68	110.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

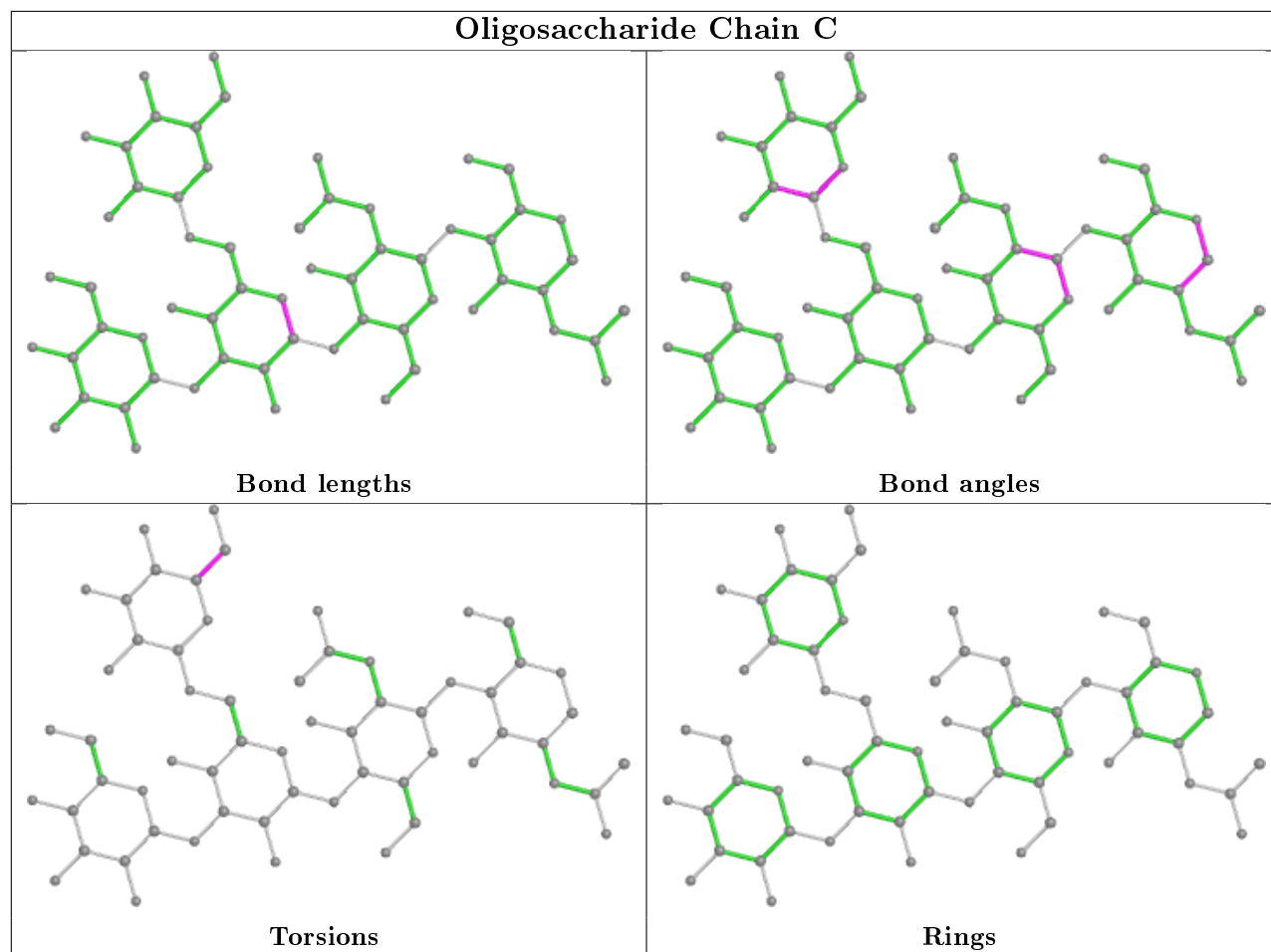
Mol	Chain	Res	Type	Atoms
2	C	5	MAN	O5-C5-C6-O6
2	H	5	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
2	H	5	MAN	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	F	5	MAN	C4-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6

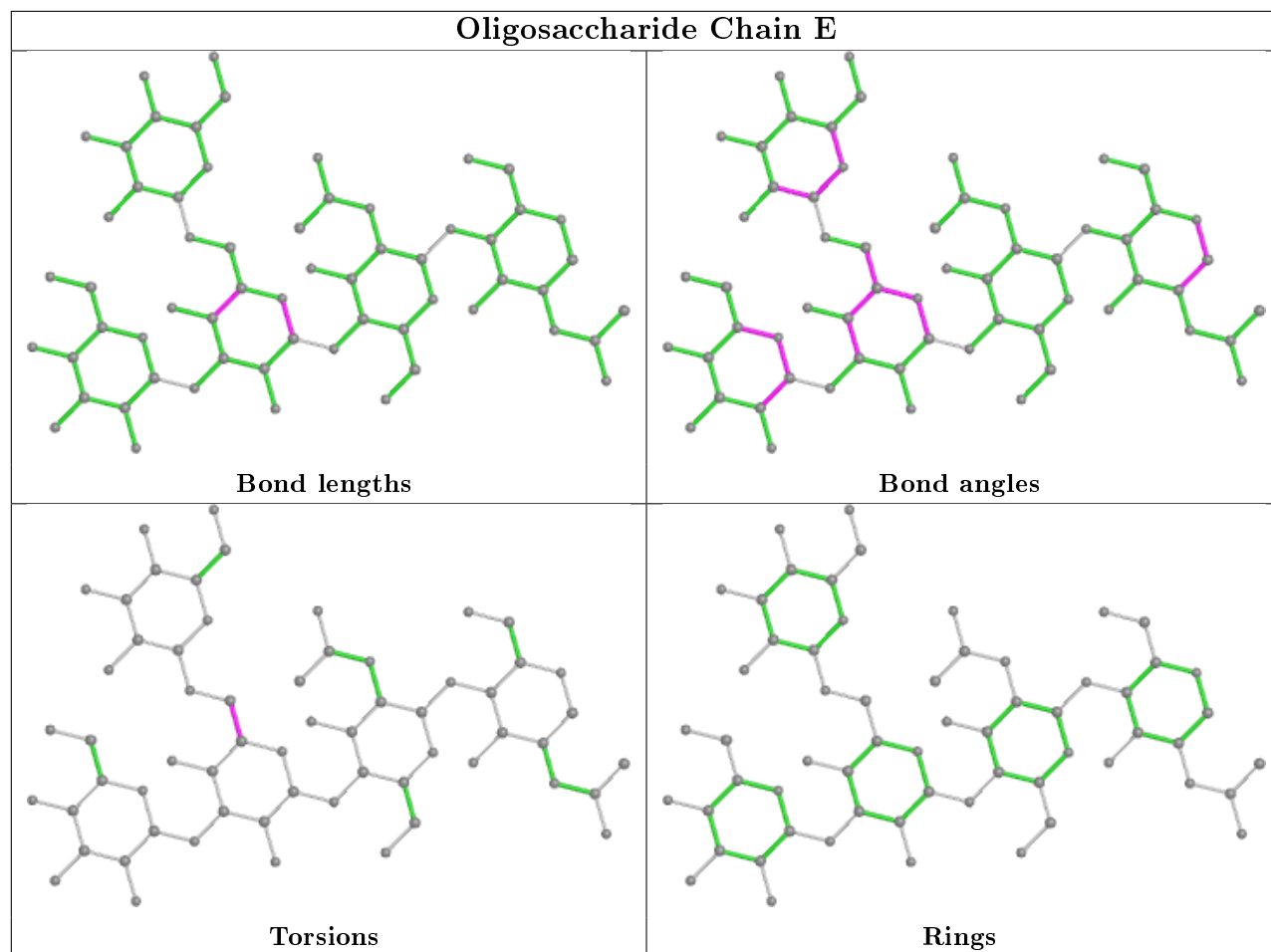
There are no ring outliers.

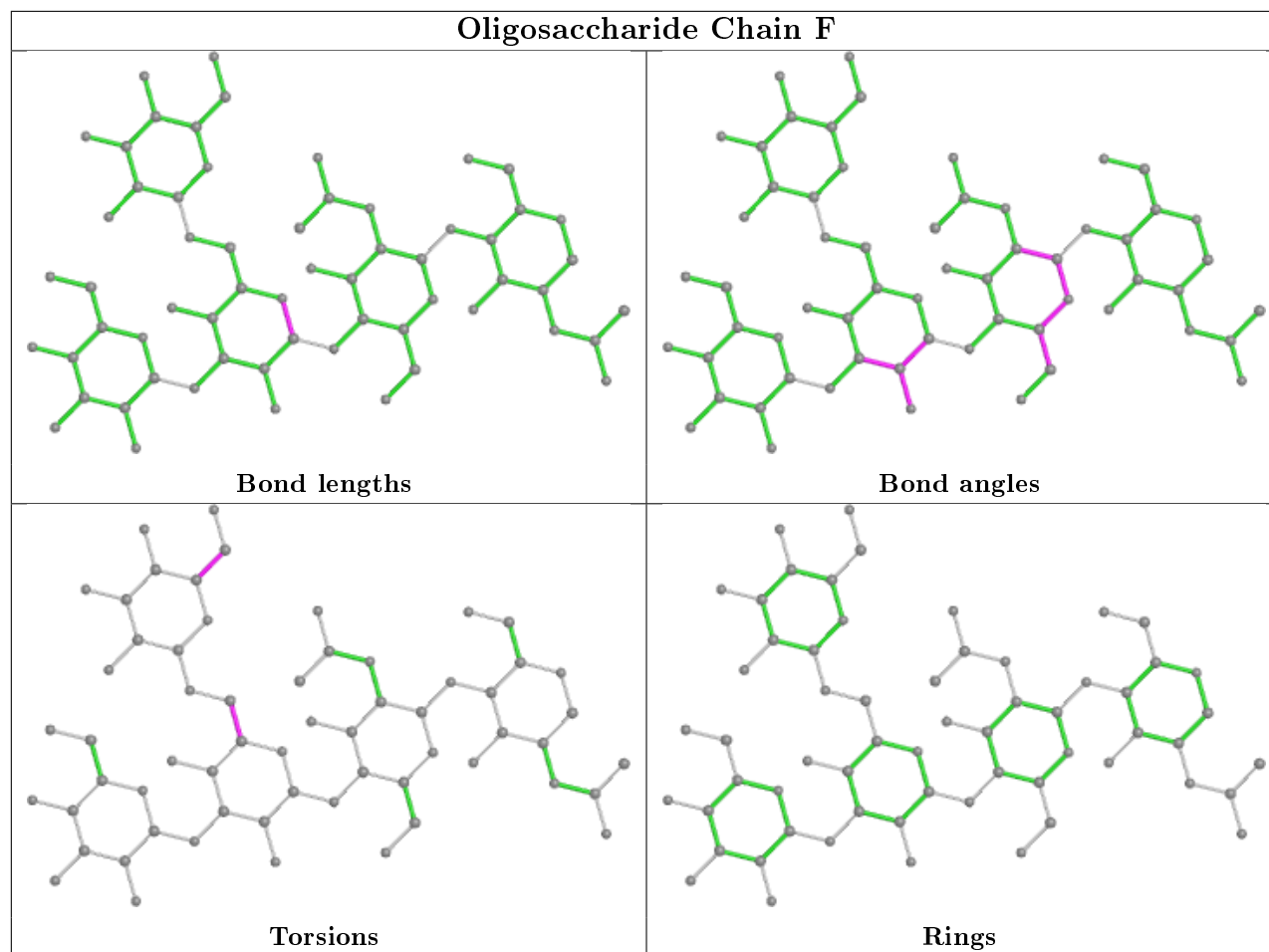
1 monomer is involved in 1 short contact:

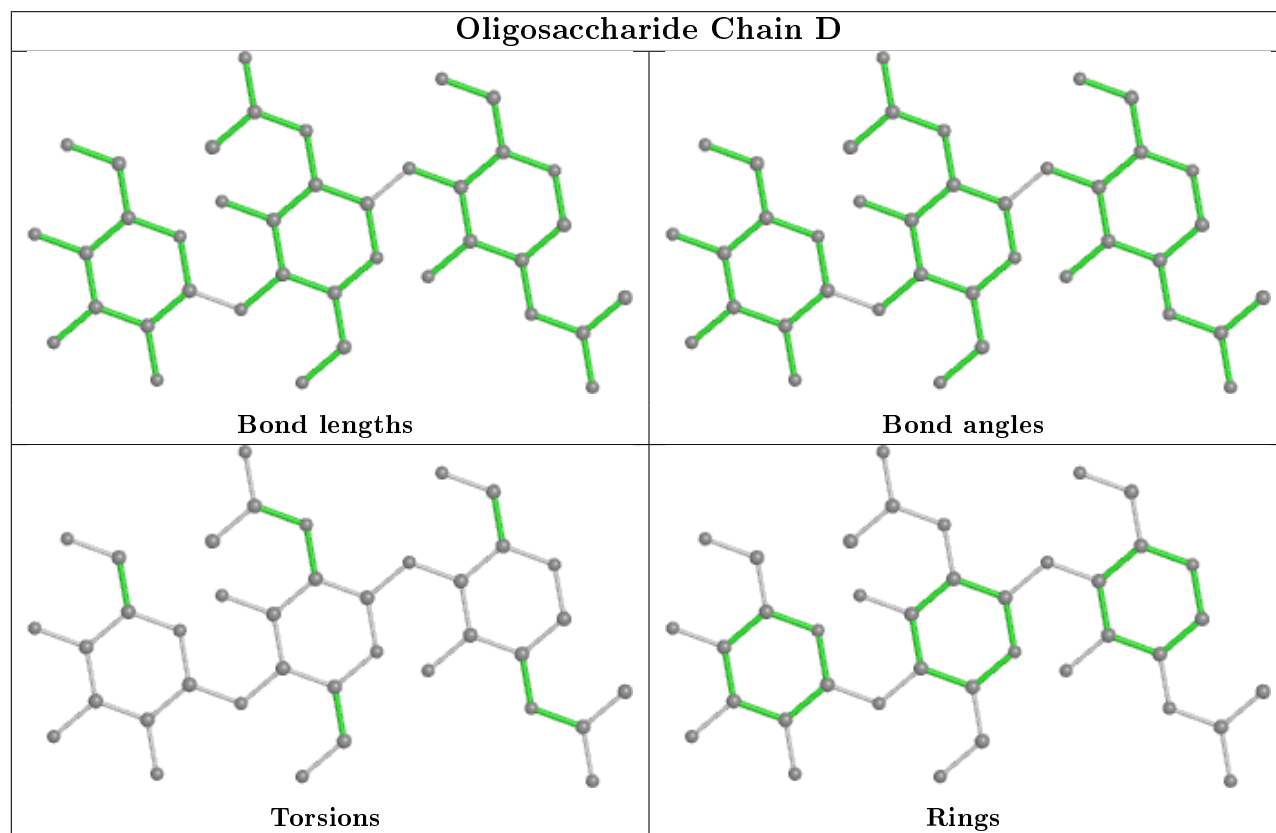
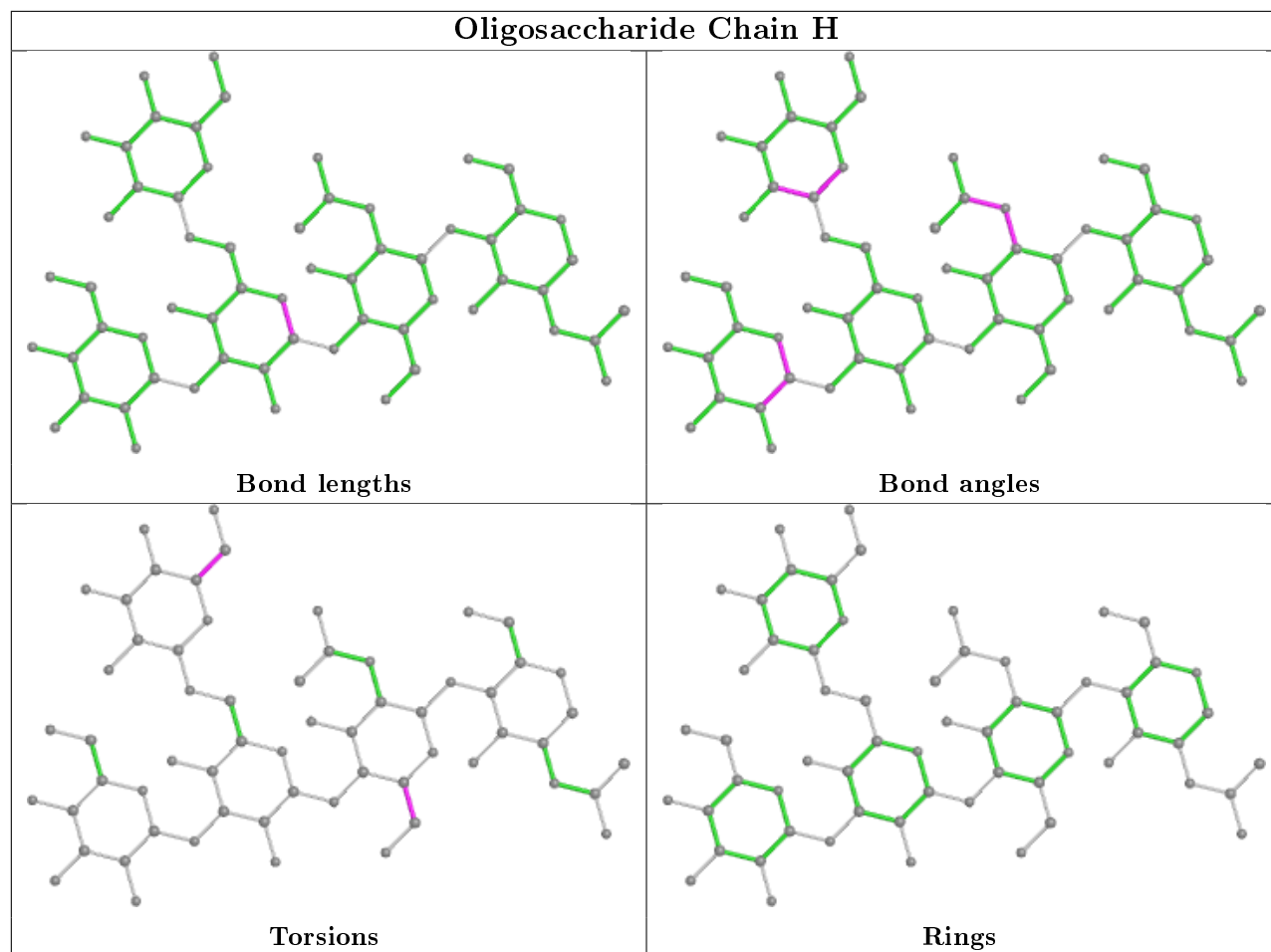
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0

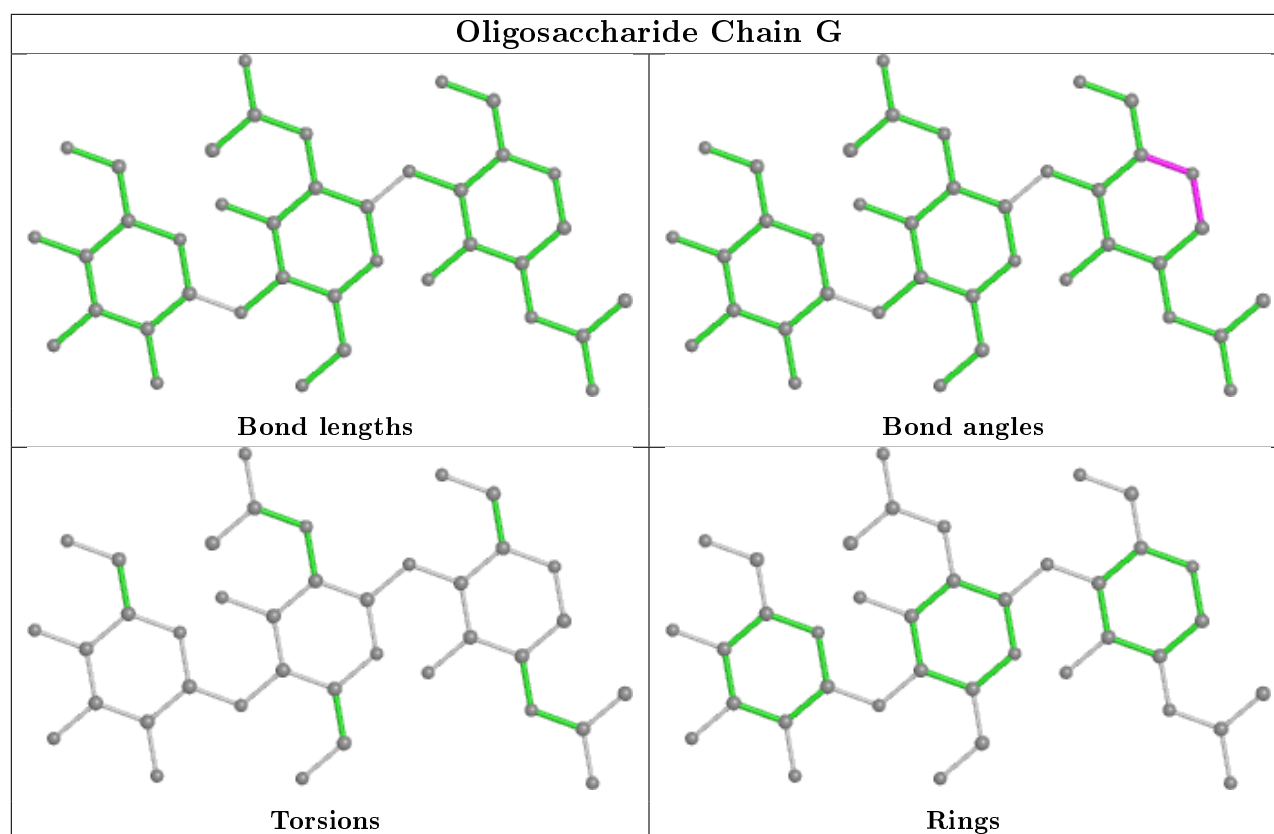
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	NAG	A	1018	1	14,14,15	0.59	0	17,19,21	0.87	1 (5%)
4	NAG	B	920	1	14,14,15	0.49	0	17,19,21	0.82	0
4	NAG	B	917	1	14,14,15	0.53	0	17,19,21	0.82	0
5	RX8	B	901	-	21,25,25	1.58	4 (19%)	26,37,37	1.10	3 (11%)
4	NAG	A	1017	1	14,14,15	0.47	0	17,19,21	1.92	1 (5%)
4	NAG	A	1019	1	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
6	GOL	A	1021	-	5,5,5	0.38	0	5,5,5	0.24	0
4	NAG	B	921	1	14,14,15	0.45	0	17,19,21	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1015	1	14,14,15	0.50	0	17,19,21	1.22	2 (11%)
4	NAG	A	1009	1	14,14,15	0.53	0	17,19,21	0.71	0
5	RX8	A	1020	-	21,25,25	1.62	3 (14%)	26,37,37	1.14	4 (15%)
4	NAG	A	1016	1	14,14,15	0.52	0	17,19,21	0.76	0
4	NAG	B	910	1	14,14,15	0.51	0	17,19,21	1.05	1 (5%)
4	NAG	B	918	1	14,14,15	0.59	0	17,19,21	0.65	0
4	NAG	B	916	1	14,14,15	0.47	0	17,19,21	0.97	1 (5%)
4	NAG	B	919	1	14,14,15	0.44	0	17,19,21	1.66	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1018	1	-	0/6/23/26	0/1/1/1
4	NAG	B	920	1	-	1/6/23/26	0/1/1/1
4	NAG	B	917	1	-	1/6/23/26	0/1/1/1
5	RX8	B	901	-	-	4/5/9/9	0/3/3/3
4	NAG	A	1017	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1019	1	-	0/6/23/26	0/1/1/1
6	GOL	A	1021	-	-	1/4/4/4	-
4	NAG	B	921	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1015	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
5	RX8	A	1020	-	-	4/5/9/9	0/3/3/3
4	NAG	A	1016	1	-	1/6/23/26	0/1/1/1
4	NAG	B	910	1	-	2/6/23/26	0/1/1/1
4	NAG	B	918	1	-	0/6/23/26	0/1/1/1
4	NAG	B	916	1	-	2/6/23/26	0/1/1/1
4	NAG	B	919	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1020	RX8	C2-C3	5.08	1.49	1.40
5	B	901	RX8	C2-C3	4.84	1.48	1.40
5	A	1020	RX8	O1-C10	-2.68	1.37	1.44
5	B	901	RX8	O1-C10	-2.64	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1020	RX8	C-N	2.60	1.43	1.34
5	B	901	RX8	C-N	2.55	1.43	1.34
5	B	901	RX8	C2-C1	-2.05	1.37	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1017	NAG	C1-O5-C5	6.86	121.49	112.19
4	B	919	NAG	C1-O5-C5	4.27	117.98	112.19
4	B	921	NAG	C1-O5-C5	3.71	117.22	112.19
4	B	910	NAG	C1-O5-C5	3.17	116.49	112.19
4	A	1015	NAG	C1-O5-C5	3.11	116.41	112.19
5	A	1020	RX8	C6-O-C7	2.74	120.07	112.92
4	B	919	NAG	C6-C5-C4	-2.72	106.63	113.00
4	A	1015	NAG	C2-N2-C7	-2.60	119.19	122.90
5	A	1020	RX8	C2-C1-N1	-2.31	120.78	123.01
4	A	1019	NAG	C1-O5-C5	2.31	115.32	112.19
5	B	901	RX8	C6-O-C7	2.29	118.91	112.92
5	B	901	RX8	C3-C2-C1	-2.27	117.92	119.65
4	A	1018	NAG	C1-O5-C5	2.27	115.27	112.19
5	B	901	RX8	C2-C1-N1	-2.25	120.85	123.01
4	B	916	NAG	C2-N2-C7	-2.22	119.74	122.90
5	A	1020	RX8	C2-C3-N3	2.22	135.11	130.42
4	B	919	NAG	C3-C4-C5	2.18	114.12	110.24
5	A	1020	RX8	C3-C2-C1	-2.10	118.05	119.65
4	B	919	NAG	C2-N2-C7	-2.05	119.98	122.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	RX8	O1-C10-C9-N3
5	B	901	RX8	C11-C10-C9-N3
5	B	901	RX8	C12-C10-C9-N3
5	B	901	RX8	C5-C6-O-C7
4	A	1017	NAG	C8-C7-N2-C2
4	A	1017	NAG	O7-C7-N2-C2
4	A	1009	NAG	C8-C7-N2-C2
4	A	1009	NAG	O7-C7-N2-C2
5	A	1020	RX8	O1-C10-C9-N3
5	A	1020	RX8	C5-C6-O-C7
4	B	916	NAG	C4-C5-C6-O6

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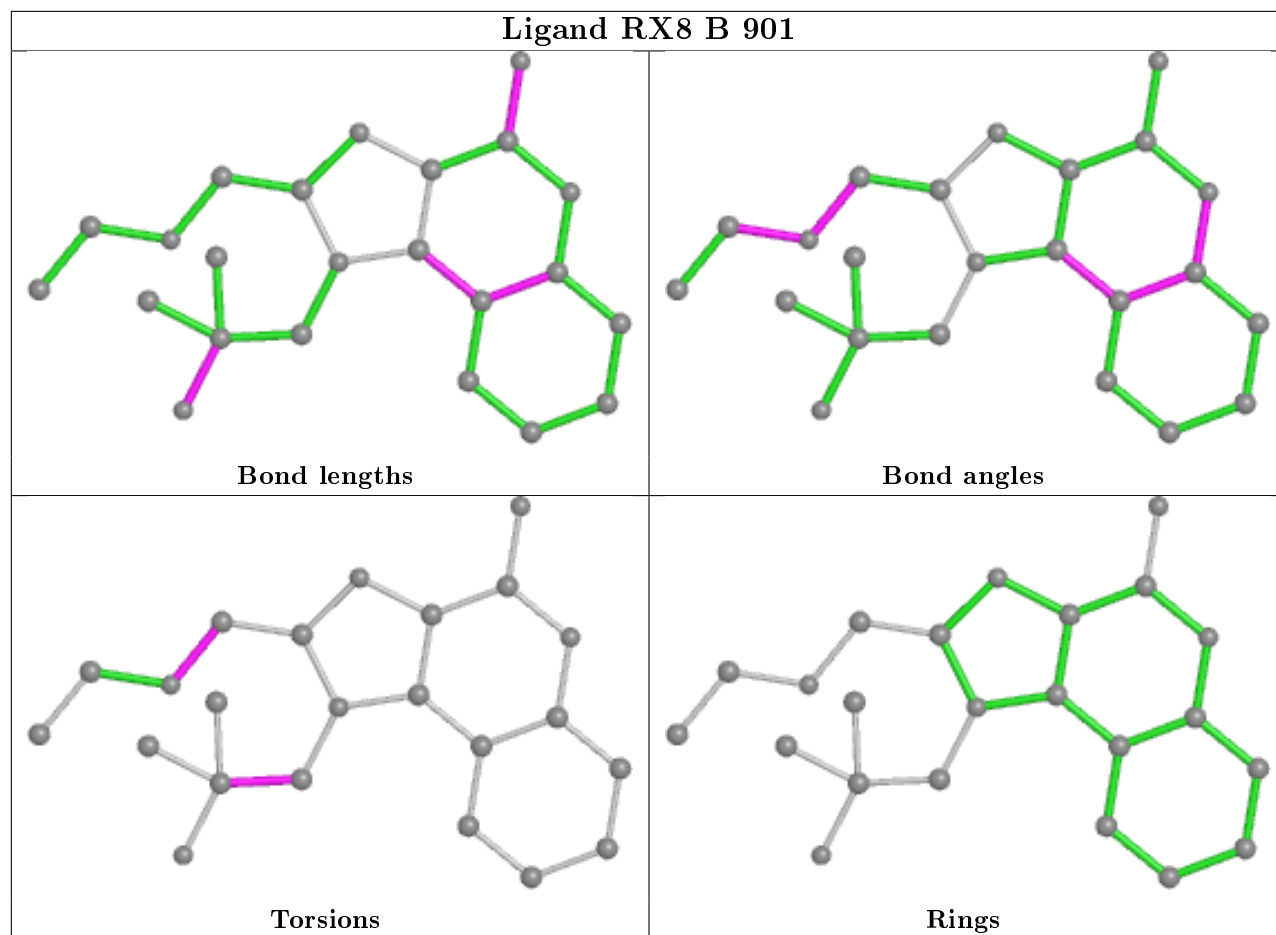
Mol	Chain	Res	Type	Atoms
4	B	910	NAG	C8-C7-N2-C2
4	B	910	NAG	O7-C7-N2-C2
4	B	916	NAG	O5-C5-C6-O6
4	A	1015	NAG	C4-C5-C6-O6
5	A	1020	RX8	C12-C10-C9-N3
4	A	1015	NAG	C8-C7-N2-C2
4	B	917	NAG	C4-C5-C6-O6
5	A	1020	RX8	C11-C10-C9-N3
4	A	1015	NAG	O5-C5-C6-O6
4	B	920	NAG	C4-C5-C6-O6
4	B	921	NAG	C8-C7-N2-C2
4	A	1015	NAG	O7-C7-N2-C2
4	B	921	NAG	O7-C7-N2-C2
6	A	1021	GOL	O1-C1-C2-C3
4	A	1016	NAG	O5-C5-C6-O6

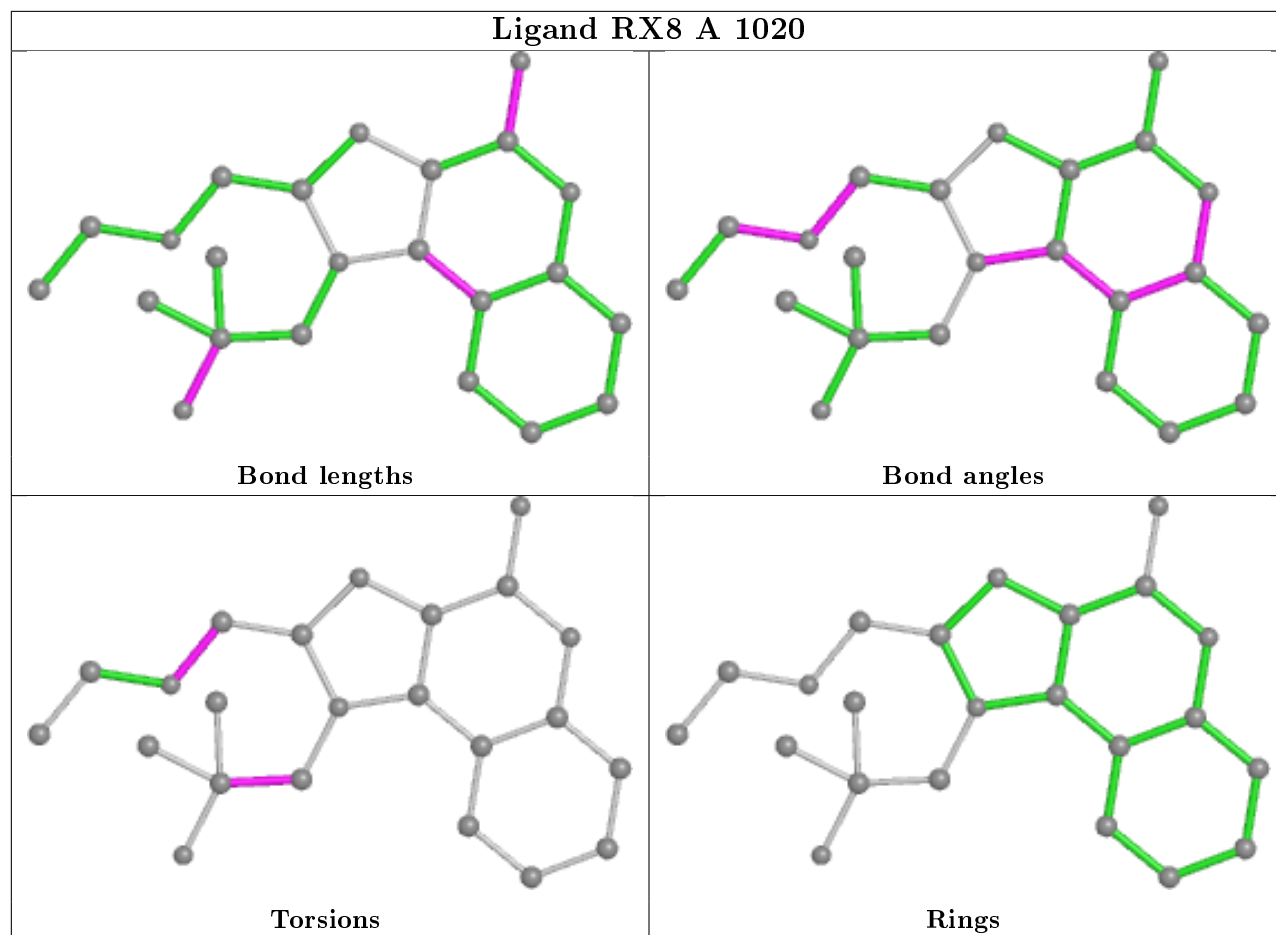
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1018	NAG	1	0
5	B	901	RX8	3	0
5	A	1020	RX8	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/811 (92%)	0.29	61 (8%) 12 15	19, 35, 62, 92	0
1	B	749/811 (92%)	0.71	124 (16%) 1 2	21, 46, 87, 107	0
All	All	1500/1622 (92%)	0.50	185 (12%) 4 5	19, 40, 78, 107	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	THR	9.8
1	B	759	LYS	8.0
1	B	64	TYR	6.9
1	B	754	SER	6.4
1	B	778	CYS	6.3
1	A	761	THR	6.2
1	B	808	ASP	6.0
1	B	758	THR	5.6
1	B	753	LYS	5.5
1	A	392	GLN	5.3
1	B	806	PRO	5.1
1	B	757	GLU	5.0
1	B	782	ASP	4.8
1	B	229	LEU	4.8
1	B	84	GLN	4.8
1	A	760	THR	4.7
1	B	805	SER	4.5
1	B	42	ASN	4.5
1	B	294	LEU	4.4
1	B	591	LEU	4.4
1	B	785	ARG	4.4
1	B	589	LEU	4.3
1	B	762	THR	4.3
1	B	810	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	760	THR	4.3
1	B	272	GLY	4.1
1	B	776	CYS	4.1
1	B	186	VAL	4.0
1	B	43	ASP	4.0
1	B	779	ASP	3.9
1	B	470	PHE	3.9
1	B	733	SER	3.9
1	B	678	PHE	3.9
1	B	535	LEU	3.9
1	A	374	LEU	3.8
1	B	177	LEU	3.8
1	B	206	LEU	3.7
1	B	561	LEU	3.7
1	B	817	LEU	3.6
1	A	591	LEU	3.6
1	A	778	CYS	3.6
1	B	227	LEU	3.6
1	B	807	GLY	3.5
1	B	74	PHE	3.5
1	B	702	PHE	3.5
1	B	613	LEU	3.5
1	A	807	GLY	3.5
1	B	471	THR	3.5
1	B	153	LEU	3.4
1	A	818	GLU	3.4
1	A	372	LEU	3.4
1	A	559	LEU	3.4
1	B	208	LEU	3.4
1	A	510	LEU	3.4
1	B	559	LEU	3.4
1	A	401	LEU	3.3
1	A	535	LEU	3.3
1	B	87	GLN	3.3
1	B	81	GLU	3.3
1	B	318	LEU	3.3
1	B	41	GLN	3.3
1	B	792	ASN	3.2
1	A	777	THR	3.2
1	B	775	GLU	3.2
1	B	809	GLN	3.2
1	A	251	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	344	LEU	3.1
1	B	717	LEU	3.1
1	B	152	SER	3.1
1	A	717	LEU	3.1
1	B	80	ASN	3.1
1	B	131	LEU	3.1
1	B	756	LEU	3.1
1	B	791	LEU	3.1
1	A	177	LEU	3.0
1	B	100	VAL	3.0
1	B	209	SER	3.0
1	A	561	LEU	3.0
1	B	615	PHE	3.0
1	B	372	LEU	3.0
1	A	701	LEU	3.0
1	B	175	LEU	3.0
1	B	816	SER	2.9
1	A	208	LEU	2.9
1	A	316	LEU	2.9
1	A	693	LEU	2.9
1	B	789	GLU	2.9
1	B	741	LEU	2.9
1	A	292	LEU	2.9
1	B	763	LYS	2.9
1	A	271	ASP	2.9
1	B	374	LEU	2.9
1	A	809	GLN	2.9
1	B	486	LEU	2.9
1	B	178	ALA	2.8
1	B	644	LEU	2.8
1	A	741	LEU	2.8
1	A	537	LEU	2.8
1	A	31	SER	2.8
1	A	186	VAL	2.7
1	A	615	PHE	2.7
1	B	44	SER	2.7
1	B	86	LEU	2.7
1	B	151	LEU	2.7
1	A	419	ASN	2.7
1	A	178	ALA	2.7
1	A	808	ASP	2.7
1	B	344	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	806	PRO	2.7
1	A	669	LEU	2.7
1	B	732	LEU	2.7
1	B	188	GLU	2.6
1	A	318	LEU	2.6
1	A	342	LEU	2.6
1	B	292	LEU	2.6
1	B	122	LEU	2.6
1	B	385	ASP	2.6
1	B	537	LEU	2.6
1	B	769	LEU	2.6
1	B	273	GLY	2.6
1	B	715	ARG	2.6
1	B	752	ASN	2.6
1	A	294	LEU	2.6
1	A	817	LEU	2.6
1	A	42	ASN	2.6
1	B	251	LEU	2.6
1	A	361	ARG	2.6
1	A	613	LEU	2.6
1	B	614	VAL	2.5
1	B	125	LYS	2.5
1	B	207	SER	2.5
1	A	589	LEU	2.5
1	B	316	LEU	2.5
1	A	486	LEU	2.5
1	A	646	LEU	2.5
1	B	308	LYS	2.5
1	B	596	ILE	2.5
1	B	40	LYS	2.4
1	B	76	THR	2.4
1	B	253	LEU	2.4
1	B	401	LEU	2.4
1	A	274	ALA	2.4
1	B	777	THR	2.4
1	B	781	GLY	2.4
1	B	425	LEU	2.4
1	A	41	GLN	2.3
1	B	729	SER	2.3
1	A	206	LEU	2.3
1	B	767	LEU	2.3
1	A	498	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	812	LYS	2.3
1	B	726	HIS	2.3
1	A	785	ARG	2.3
1	A	425	LEU	2.3
1	B	132	LEU	2.3
1	B	693	LEU	2.3
1	B	755	ALA	2.3
1	A	270	CYS	2.3
1	A	253	LEU	2.3
1	B	228	PHE	2.3
1	B	48	GLU	2.3
1	B	433	LEU	2.2
1	A	459	PHE	2.2
1	B	488	LEU	2.2
1	A	399	ILE	2.2
1	B	423	ILE	2.2
1	B	783	PHE	2.2
1	B	706	SER	2.2
1	B	361	ARG	2.2
1	A	634	ILE	2.1
1	B	499	ASN	2.1
1	B	55	GLN	2.1
1	B	130	LEU	2.1
1	B	459	PHE	2.1
1	A	188	GLU	2.1
1	B	342	LEU	2.1
1	B	123	ASN	2.1
1	B	705	ASP	2.1
1	B	803	CYS	2.1
1	A	550	LEU	2.0
1	B	588	VAL	2.0
1	B	280	ARG	2.0
1	A	512	LEU	2.0
1	B	176	TYR	2.0
1	A	695	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

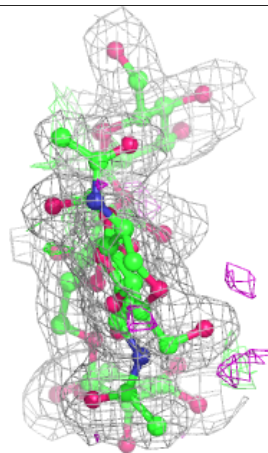
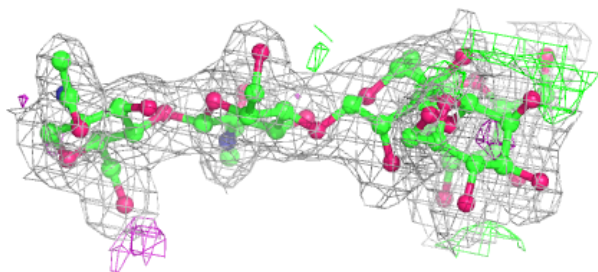
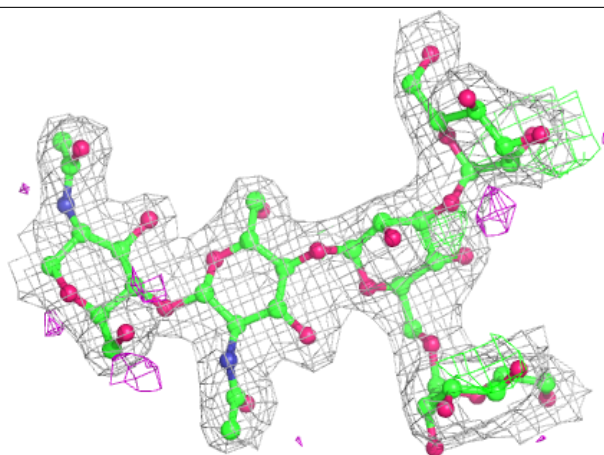
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	E	5	11/12	0.65	0.38	67,73,81,82	0
2	MAN	H	5	11/12	0.68	0.37	73,79,84,86	0
2	MAN	C	4	11/12	0.79	0.22	33,39,47,55	0
2	MAN	F	4	11/12	0.81	0.24	45,60,66,67	0
2	MAN	C	5	11/12	0.84	0.29	56,66,71,76	0
3	BMA	G	3	11/12	0.85	0.33	69,72,73,74	0
2	MAN	E	4	11/12	0.85	0.35	69,73,76,76	0
2	MAN	H	4	11/12	0.86	0.41	72,78,86,87	0
3	NAG	G	2	14/15	0.86	0.19	44,57,67,72	0
2	BMA	H	3	11/12	0.87	0.24	49,63,71,74	0
2	NAG	H	2	14/15	0.88	0.12	30,34,43,43	0
3	BMA	D	3	11/12	0.88	0.32	63,67,69,69	0
2	MAN	F	5	11/12	0.89	0.31	70,73,76,77	0
3	NAG	D	2	14/15	0.91	0.16	36,49,53,56	0
2	NAG	H	1	14/15	0.91	0.12	23,31,34,41	0
2	BMA	C	3	11/12	0.92	0.13	32,43,54,56	0
2	BMA	F	3	11/12	0.93	0.20	39,56,63,64	0
2	BMA	E	3	11/12	0.93	0.23	40,55,67,75	0
2	NAG	E	2	14/15	0.94	0.09	21,26,36,47	0
2	NAG	F	2	14/15	0.95	0.10	30,33,37,38	0
2	NAG	F	1	14/15	0.95	0.14	27,29,35,37	0
3	NAG	G	1	14/15	0.96	0.08	22,28,36,37	0
2	NAG	C	2	14/15	0.96	0.10	19,23,32,35	0
3	NAG	D	1	14/15	0.96	0.08	20,23,28,34	0
2	NAG	E	1	14/15	0.97	0.08	18,21,27,28	0
2	NAG	C	1	14/15	0.97	0.09	17,21,29,31	0

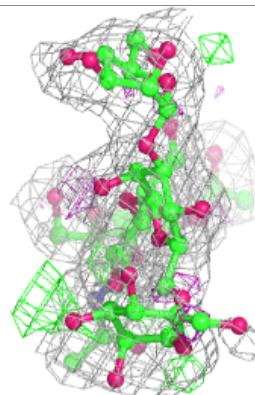
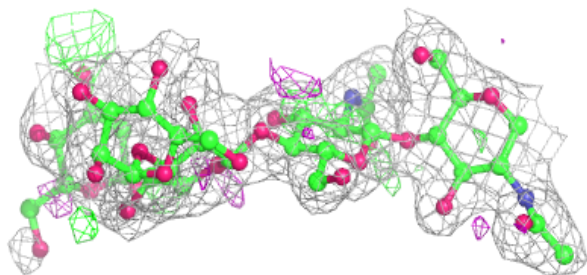
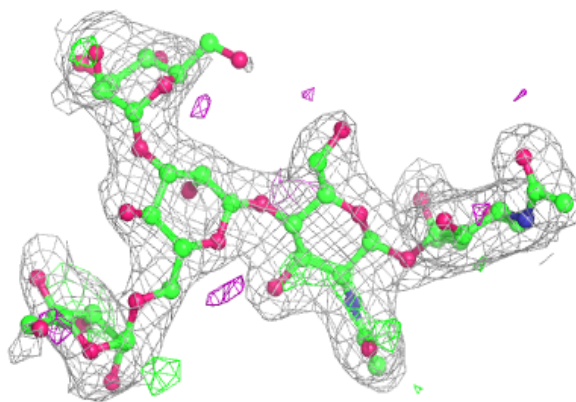
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

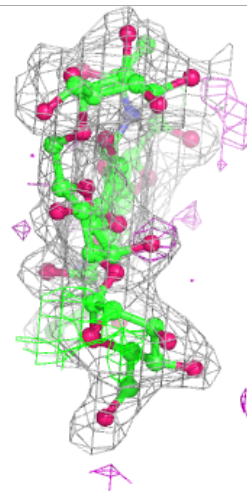
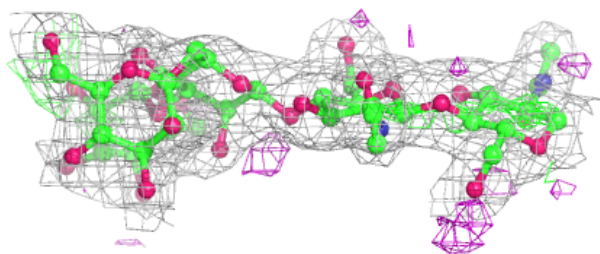
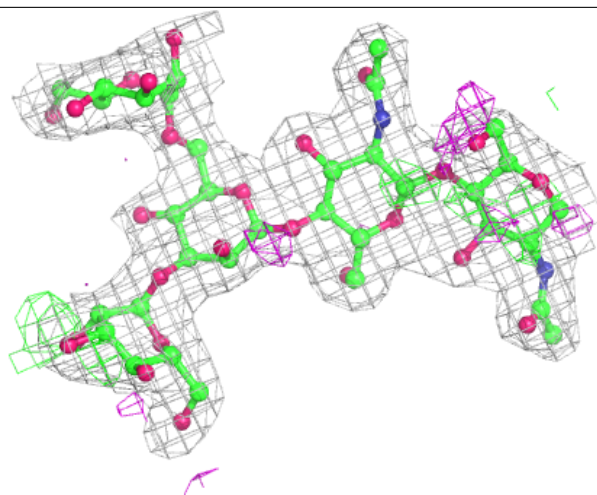
**Electron density around Chain E:**

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



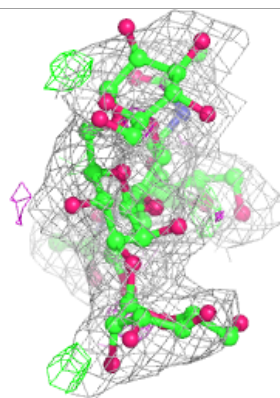
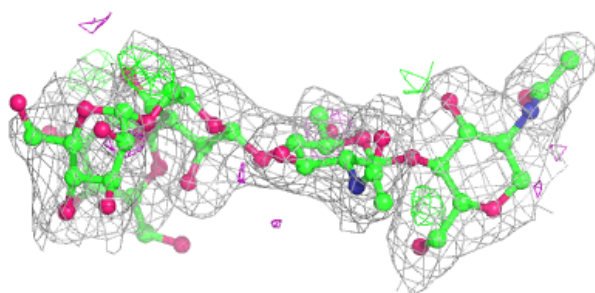
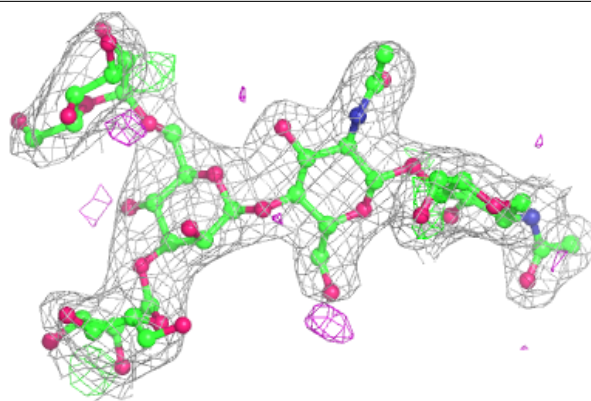
Electron density around Chain F:

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

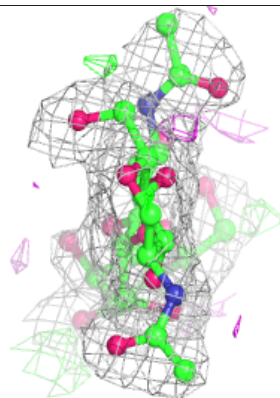
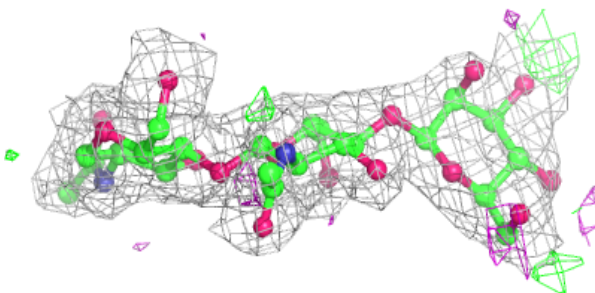
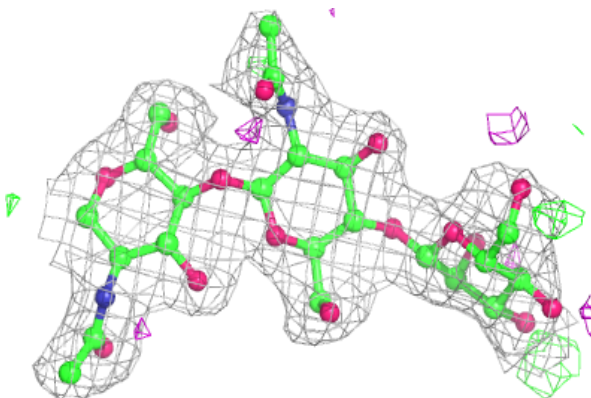


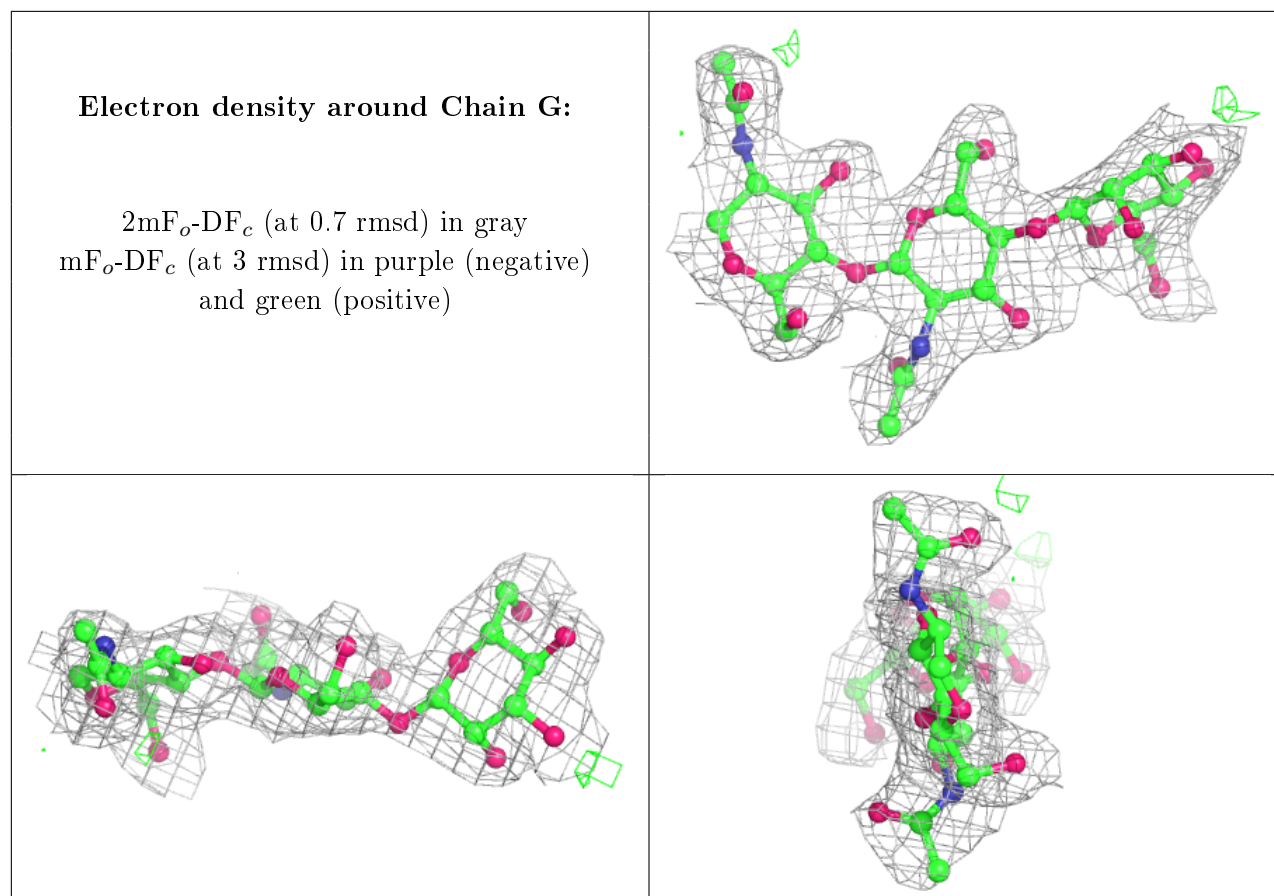
Electron density around Chain H:

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

**Electron density around Chain D:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	1021	6/6	0.76	0.14	66,71,73,74	0
4	NAG	B	921	14/15	0.77	0.30	68,72,74,77	0
4	NAG	A	1017	14/15	0.87	0.37	62,68,75,78	0
4	NAG	A	1016	14/15	0.87	0.34	62,65,67,69	0
4	NAG	A	1015	14/15	0.89	0.29	52,64,74,75	0
4	NAG	B	920	14/15	0.89	0.33	77,82,86,87	0
4	NAG	A	1009	14/15	0.91	0.20	48,56,68,73	0
4	NAG	B	910	14/15	0.91	0.12	44,60,67,75	0
4	NAG	B	916	14/15	0.91	0.27	64,75,83,83	0
4	NAG	B	919	14/15	0.91	0.22	52,57,63,69	0
4	NAG	B	918	14/15	0.92	0.14	44,52,56,57	0
4	NAG	B	917	14/15	0.93	0.31	50,60,73,76	0
4	NAG	A	1019	14/15	0.94	0.10	29,31,34,34	0

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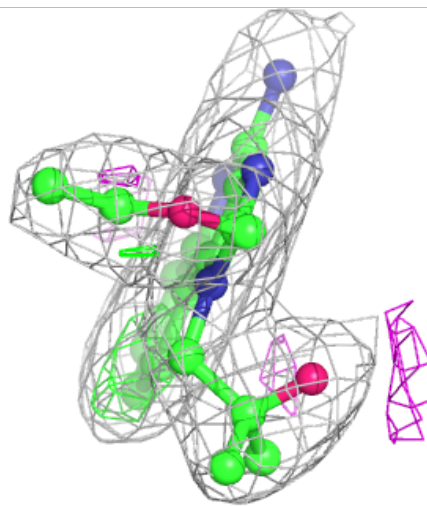
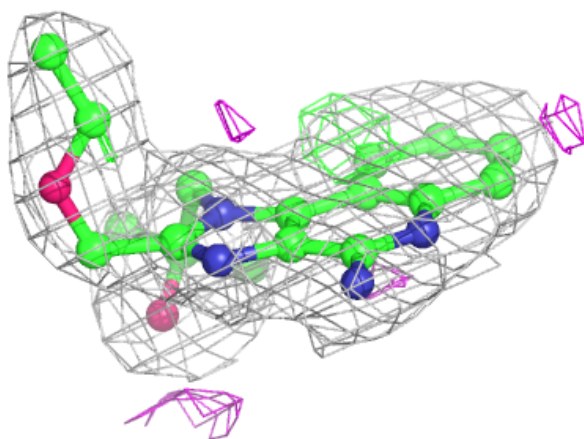
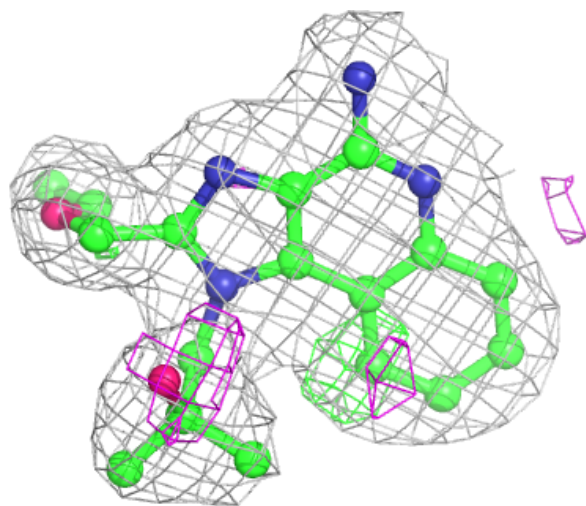
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	RX8	B	901	23/23	0.94	0.12	22,29,41,45	0
5	RX8	A	1020	23/23	0.96	0.10	22,32,41,42	0
4	NAG	A	1018	14/15	0.97	0.12	36,42,50,51	0

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.

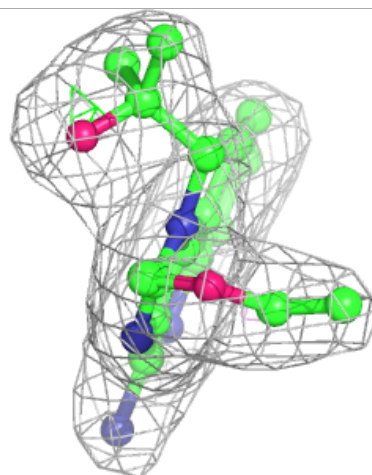
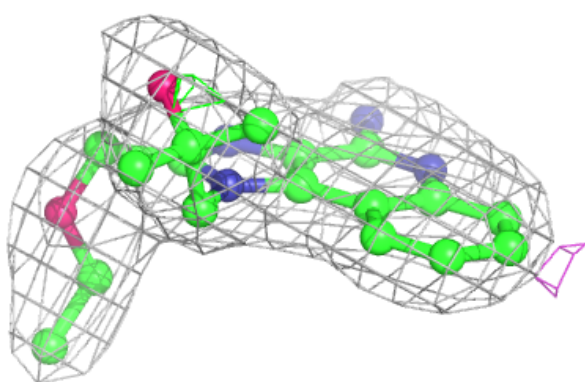
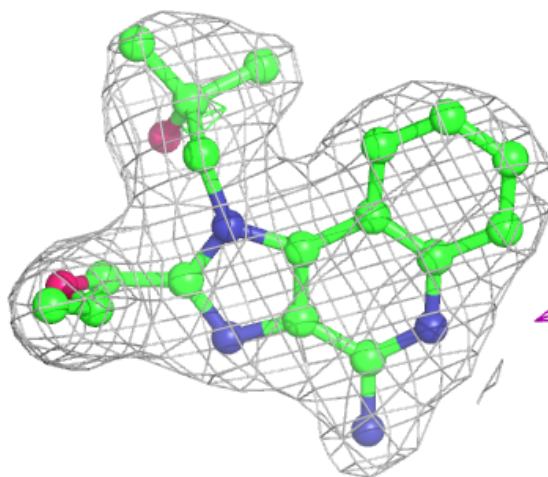
Electron density around RX8 B 901:

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 A 1020:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.