Full wwPDB X-ray Structure Validation Report (i)

Aug 10, 2020 – 04:50 AM BST

PDB ID	:	3W3M
Title	:	Crystal structure of human TLR8 in complex with Resiquimod (R848) crystal form 2
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2012-12-22
Resolution	:	2.70 Å(reported)

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

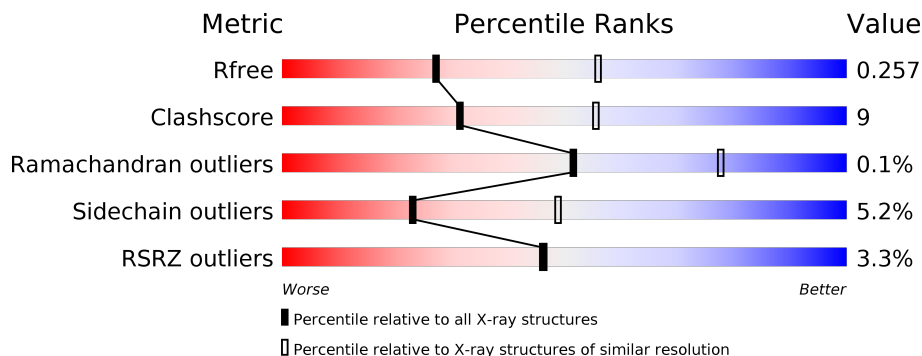|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.70 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		5.2%
RSRZ outliers		3.3%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	3% — 69% / 22% / • / 7%
2	B	5	80% / 20%
2	D	5	20% / 60% / 20%
3	C	3	67% / 33%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6348 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.
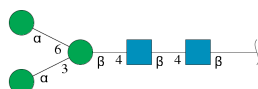
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			

There are 10 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

- 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.

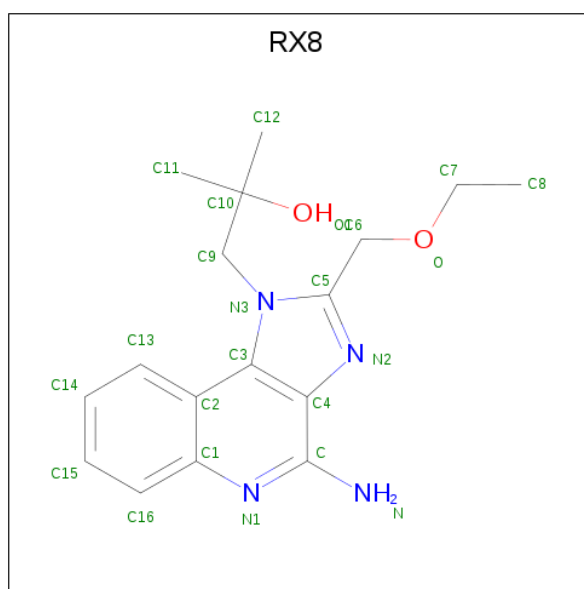| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

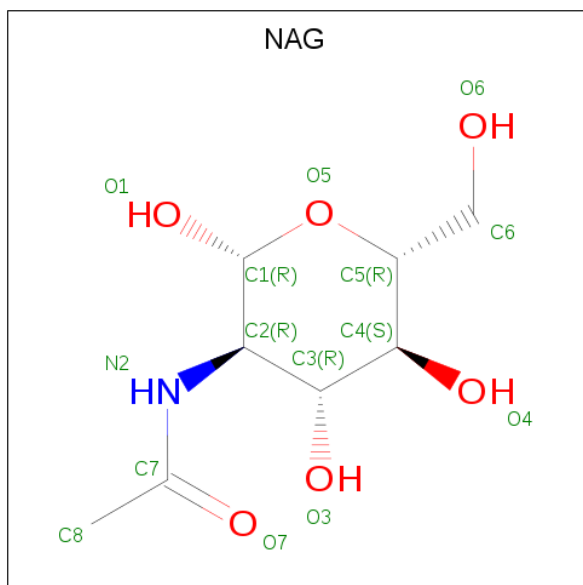eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

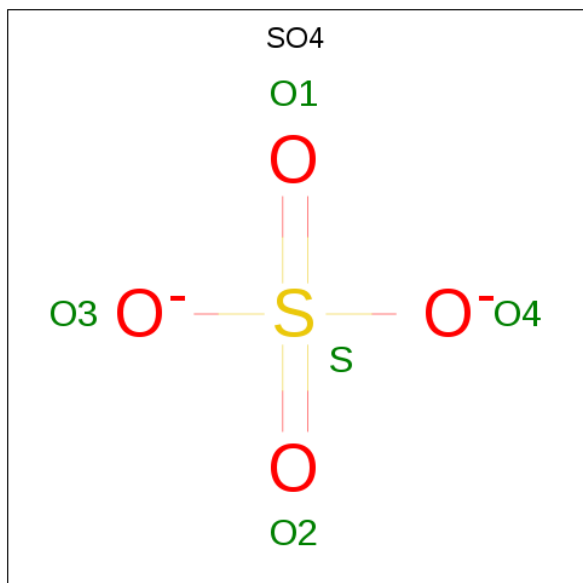| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	17	4	2		

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

NAG

O6
OH

O1
HO

O5
O

C6

C1(R)   C5(R)

C2(R)   C4(S)
C3(R)

N2
HN

OH
O4

C7

OH
O3

C8

O
O7

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

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

SO4

O1

O

O3 O^- — S — O^- O4

S

O

O2

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total	O	0	0
			68	68		

3 Residue-property plots ⓘ

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 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

• 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-glucopyra

nose

Chain D:

| NAG1 | NAG2 | BMA3 | MAN4 | MAN5 |

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

Chain C:

| NAG1 | NAG2 | BMA3 |

4　Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.77Å　　106.00Å　　72.32Å 90.00°　　106.94°　　90.00°	Depositor
Resolution (Å)	41.84　−　2.70 41.84　−　2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.84-2.70) 97.8 (41.84-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$<I/\sigma(I)>$ [1]	2.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.220　,　0.255 0.223　,　0.257	Depositor DCC
R_{free} test set	1339 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.2	EDS
L-test for twinning[2]	$<|L|> = 0.45, <L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6348	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, RX8, BMA, NAG, SO4

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	0.28	0/6160	0.53	0/8356

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6035	0	6002	111	2
2	B	61	0	52	0	0
2	D	61	0	52	1	0
3	C	39	0	34	0	0
4	A	23	0	22	3	0
5	A	56	0	52	0	0
6	A	5	0	0	0	0
7	A	68	0	0	4	1
All	All	6348	0	6214	113	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 9.

All (113) 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:334:THR:HG22	1:A:365:LYS:HG2	1.66	0.77
1:A:344:LEU:O	1:A:347:ASN:ND2	2.23	0.72
1:A:276:ILE:HG22	1:A:299:LEU:HD11	1.75	0.69
1:A:606:GLU:HG2	1:A:637:GLY:HA3	1.75	0.67
1:A:318:LEU:O	1:A:321:ASN:ND2	2.28	0.66
1:A:61:VAL:HG21	1:A:86:LEU:HD11	1.78	0.65
1:A:177:LEU:O	1:A:180:ASN:ND2	2.30	0.65
1:A:72:ASP:OD1	1:A:99:ASN:ND2	2.29	0.64
1:A:199:THR:HG23	1:A:200:LEU:HD13	1.79	0.64
1:A:284:GLN:O	1:A:309:ASN:ND2	2.31	0.64
1:A:760:THR:OG1	1:A:761:THR:N	2.31	0.63
1:A:576:HIS:NE2	7:A:1040:HOH:O	2.31	0.62
1:A:733:SER:OG	1:A:757:GLU:O	2.18	0.60
1:A:197:PHE:HA	1:A:200:LEU:HD22	1.82	0.60
1:A:140:ILE:HD12	1:A:166:ILE:HD11	1.84	0.59
1:A:734:GLU:H	1:A:758:THR:HG23	1.68	0.59
4:A:901:RX8:H9	4:A:901:RX8:H19	1.86	0.58
1:A:782:ASP:OD1	1:A:785:ARG:NH2	2.37	0.58
1:A:45:VAL:HG22	1:A:65:VAL:HA	1.86	0.58
1:A:410:ASP:OD1	1:A:410:ASP:N	2.37	0.57
1:A:44:SER:OG	1:A:45:VAL:N	2.36	0.57
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.87	0.56
1:A:526:PHE:HB2	1:A:553:LEU:HD21	1.88	0.56
1:A:80:ASN:N	1:A:80:ASN:OD1	2.27	0.56
1:A:66:THR:HG22	1:A:67:GLU:HG3	1.87	0.56
1:A:56:GLU:HA	1:A:75:ILE:HG23	1.88	0.55
1:A:493:ILE:O	1:A:515:ASN:HB3	2.07	0.54
2:D:3:BMA:H62	2:D:5:MAN:H3	1.89	0.54
1:A:538:THR:HG22	1:A:562:SER:HB2	1.88	0.54
1:A:518:ALA:HA	1:A:541:ARG:O	2.08	0.54
1:A:769:LEU:HD23	1:A:774:PHE:HZ	1.71	0.54
1:A:378:VAL:HG11	4:A:901:RX8:H2	1.88	0.53
1:A:780:ILE:HD11	1:A:817:LEU:HD13	1.89	0.53
1:A:253:LEU:O	1:A:256:ASN:ND2	2.30	0.53
1:A:226:LYS:HG2	1:A:250:LEU:HB3	1.91	0.53
1:A:259:ARG:NH1	1:A:321:ASN:O	2.42	0.53
1:A:84:GLN:OE1	1:A:123:ASN:ND2	2.42	0.53
1:A:798:LEU:HA	1:A:801:VAL:HG22	1.91	0.52
1:A:385:ASP:HA	1:A:388:GLN:HG2	1.93	0.51
1:A:739:LYS:NZ	7:A:1025:HOH:O	2.44	0.51
1:A:124:LEU:HD23	1:A:126:ASN:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:HE1	1:A:115:ASN:HD22	1.58	0.50
1:A:211:ASN:O	1:A:232:THR:HA	2.11	0.50
1:A:348:TYR:HB3	1:A:376:GLY:O	2.12	0.50
1:A:776:CYS:N	1:A:805:SER:O	2.21	0.49
1:A:668:GLU:HG3	1:A:692:LEU:HD23	1.94	0.49
1:A:808:ASP:N	1:A:808:ASP:OD1	2.41	0.49
1:A:66:THR:O	1:A:89:LEU:HA	2.13	0.49
1:A:258:PRO:HD2	1:A:269:PRO:HA	1.95	0.49
1:A:54:LEU:HD13	1:A:58:PRO:HD3	1.95	0.48
1:A:357:ILE:HG13	1:A:377:TYR:CE1	2.48	0.48
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.95	0.48
1:A:541:ARG:HB3	1:A:566:HIS:CB	2.44	0.48
1:A:70:LEU:O	1:A:73:ASN:ND2	2.46	0.48
1:A:280:ARG:CZ	1:A:305:ALA:HB1	2.44	0.48
1:A:63:LYS:HD2	1:A:85:GLY:O	2.13	0.47
1:A:397:SER:HA	1:A:420:LEU:HA	1.97	0.47
1:A:283:PHE:HD2	1:A:306:TRP:HB3	1.78	0.47
1:A:346:PHE:N	1:A:375:ARG:O	2.27	0.47
1:A:764:LEU:HD21	1:A:767:LEU:HD13	1.96	0.47
1:A:526:PHE:CB	1:A:553:LEU:HD21	2.45	0.47
1:A:769:LEU:HD23	1:A:774:PHE:CZ	2.50	0.46
1:A:89:LEU:CD1	1:A:124:LEU:HD11	2.46	0.46
1:A:378:VAL:HG21	4:A:901:RX8:H9	1.97	0.46
1:A:119:GLY:HA2	1:A:143:GLY:O	2.16	0.46
1:A:521:LEU:HD13	1:A:550:LEU:HD21	1.97	0.46
1:A:357:ILE:HG22	7:A:1016:HOH:O	2.15	0.46
1:A:716:THR:HG23	1:A:740:HIS:HB3	1.98	0.46
1:A:198:GLU:HG3	1:A:219:LYS:HB3	1.97	0.46
1:A:180:ASN:HB2	1:A:211:ASN:OD1	2.16	0.46
1:A:512:LEU:HD12	1:A:512:LEU:HA	1.74	0.46
1:A:61:VAL:HG23	1:A:86:LEU:HD21	1.97	0.46
1:A:86:LEU:HB3	1:A:89:LEU:HD11	1.98	0.45
1:A:122:LEU:HA	1:A:145:PRO:HG3	1.99	0.45
1:A:132:LEU:O	1:A:135:ASN:ND2	2.50	0.45
1:A:39:LYS:HG3	1:A:46:ILE:HG23	2.00	0.44
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.98	0.44
1:A:302:ILE:N	1:A:326:GLU:OE2	2.36	0.44
1:A:81:GLU:N	1:A:81:GLU:OE1	2.50	0.44
1:A:296:SER:HA	1:A:320:PHE:O	2.18	0.44
1:A:167:SER:HB3	1:A:199:THR:HG21	2.00	0.43
1:A:163:LYS:HA	1:A:196:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:CYS:HB3	1:A:47:ALA:HB1	2.00	0.43
1:A:77:HIS:CE1	1:A:115:ASN:HD22	2.35	0.43
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.19	0.43
1:A:725:SER:N	7:A:1023:HOH:O	2.17	0.43
1:A:620:LEU:HD11	1:A:646:LEU:HD22	2.01	0.43
1:A:258:PRO:HA	1:A:296:SER:O	2.18	0.43
1:A:259:ARG:NH2	1:A:348:TYR:O	2.37	0.43
1:A:370:ARG:O	1:A:396:LEU:HD12	2.19	0.43
1:A:608:LYS:O	1:A:640:ASN:HB2	2.19	0.43
1:A:589:LEU:HD23	1:A:613:LEU:HD13	2.01	0.43
1:A:89:LEU:HD13	1:A:124:LEU:HD11	2.02	0.42
1:A:727:LEU:HA	1:A:728:PRO:HD3	1.86	0.42
1:A:95:ASN:OD1	1:A:133:GLU:N	2.52	0.42
1:A:283:PHE:HB3	1:A:310:MET:HE3	2.02	0.41
1:A:128:ARG:HD2	1:A:149:THR:HG23	2.02	0.41
1:A:407:LYS:HE2	1:A:429:ARG:HH11	1.84	0.41
1:A:692:LEU:HD13	1:A:716:THR:HB	2.02	0.41
1:A:302:ILE:HD11	1:A:307:PHE:CZ	2.55	0.41
1:A:153:LEU:O	1:A:156:ASN:ND2	2.34	0.41
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.95	0.41
1:A:560:ASP:OD1	1:A:590:ASN:HB3	2.19	0.41
1:A:798:LEU:H	1:A:798:LEU:HD12	1.84	0.41
1:A:318:LEU:HB2	1:A:344:LEU:HD23	2.03	0.41
1:A:652:LYS:O	1:A:676:LEU:HA	2.21	0.41
1:A:754:SER:HA	1:A:757:GLU:HG2	2.03	0.41
1:A:523:GLY:O	1:A:552:GLU:HB3	2.21	0.41
1:A:309:ASN:OD1	1:A:309:ASN:N	2.54	0.41
1:A:667:THR:HA	1:A:690:LEU:HA	2.03	0.41
1:A:749:LYS:O	1:A:774:PHE:HA	2.21	0.41
1:A:86:LEU:CB	1:A:89:LEU:HD11	2.51	0.40
1:A:261:PHE:CD2	1:A:350:LYS:HE2	2.56	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:280:ARG:NH2	1:A:734:GLU:OE2[3_455]	2.08	0.12
1:A:429:ARG:NH2	7:A:1060:HOH:O[2_555]	2.11	0.09

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%)	714 (96%)	30 (4%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	693/755 (92%)	657 (95%)	36 (5%)	23	49

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	45	VAL
1	A	52	ARG
1	A	80	ASN
1	A	127	LEU
1	A	140	ILE
1	A	147	SER
1	A	170	ILE
1	A	200	LEU
1	A	204	GLU

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Mol	Chain	Res	Type
1	A	248	LEU
1	A	253	LEU
1	A	268	VAL
1	A	287	THR
1	A	317	ASP
1	A	334	THR
1	A	372	LEU
1	A	410	ASP
1	A	421	GLU
1	A	472	ARG
1	A	502	GLU
1	A	512	LEU
1	A	522	SER
1	A	532	VAL
1	A	534	TYR
1	A	541	ARG
1	A	701	LEU
1	A	727	LEU
1	A	735	VAL
1	A	747	LEU
1	A	760	THR
1	A	762	THR
1	A	790	HIS
1	A	793	VAL
1	A	808	ASP
1	A	817	LEU

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

Mol	Chain	Res	Type
1	A	77	HIS

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)

13 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	B	1	1,2	14,14,15	0.53	0	17,19,21	0.75	0
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	0.81	0
2	BMA	B	3	2	11,11,12	0.63	0	15,15,17	0.72	0
2	MAN	B	4	2	11,11,12	0.64	0	15,15,17	0.84	0
2	MAN	B	5	2	11,11,12	0.67	0	15,15,17	0.77	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.50	0	17,19,21	0.82	0
3	NAG	C	2	3	14,14,15	0.59	0	17,19,21	0.97	1 (5%)
3	BMA	C	3	3	11,11,12	0.72	0	15,15,17	0.72	0
2	NAG	D	1	1,2	14,14,15	1.31	1 (7%)	17,19,21	1.86	4 (23%)
2	NAG	D	2	2	14,14,15	1.63	3 (21%)	17,19,21	2.23	7 (41%)
2	BMA	D	3	2	11,11,12	1.49	2 (18%)	15,15,17	2.38	7 (46%)
2	MAN	D	4	2	11,11,12	0.55	0	15,15,17	0.85	0
2	MAN	D	5	2	11,11,12	0.72	0	15,15,17	0.82	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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	O5-C1	-3.20	1.38	1.43
2	D	2	NAG	O5-C1	-2.45	1.39	1.43
2	D	2	NAG	O7-C7	-2.31	1.18	1.23
2	D	2	NAG	C8-C7	-2.29	1.45	1.50
2	D	1	NAG	O7-C7	-2.23	1.18	1.23
2	D	3	BMA	O2-C2	-2.07	1.39	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	4.75	118.63	112.19
2	D	3	BMA	C1-O5-C5	4.71	118.58	112.19
2	D	3	BMA	O5-C1-C2	-4.50	103.82	110.77
2	D	2	NAG	O5-C1-C2	-4.03	104.93	111.29
2	D	3	BMA	O2-C2-C1	-3.99	100.99	109.15
2	D	2	NAG	C1-O5-C5	3.72	117.23	112.19
2	D	2	NAG	O3-C3-C4	-3.71	101.77	110.35
2	D	2	NAG	C6-C5-C4	-3.56	104.66	113.00
2	D	1	NAG	O5-C1-C2	-3.53	105.72	111.29
2	D	1	NAG	C3-C4-C5	-2.92	105.04	110.24
2	D	3	BMA	O2-C2-C3	-2.80	104.53	110.14
2	D	2	NAG	O4-C4-C3	-2.57	104.40	110.35
3	C	2	NAG	C4-C3-C2	2.52	114.72	111.02
2	D	2	NAG	O7-C7-C8	-2.40	117.60	122.06
2	D	2	NAG	C8-C7-N2	2.37	120.11	116.10
2	B	5	MAN	O5-C1-C2	-2.30	107.22	110.77
2	D	3	BMA	C6-C5-C4	-2.19	107.88	113.00
2	D	3	BMA	O4-C4-C5	-2.16	103.94	109.30
2	D	1	NAG	C8-C7-N2	-2.06	112.62	116.10
2	D	3	BMA	C3-C4-C5	2.03	113.86	110.24

There are no chirality outliers.
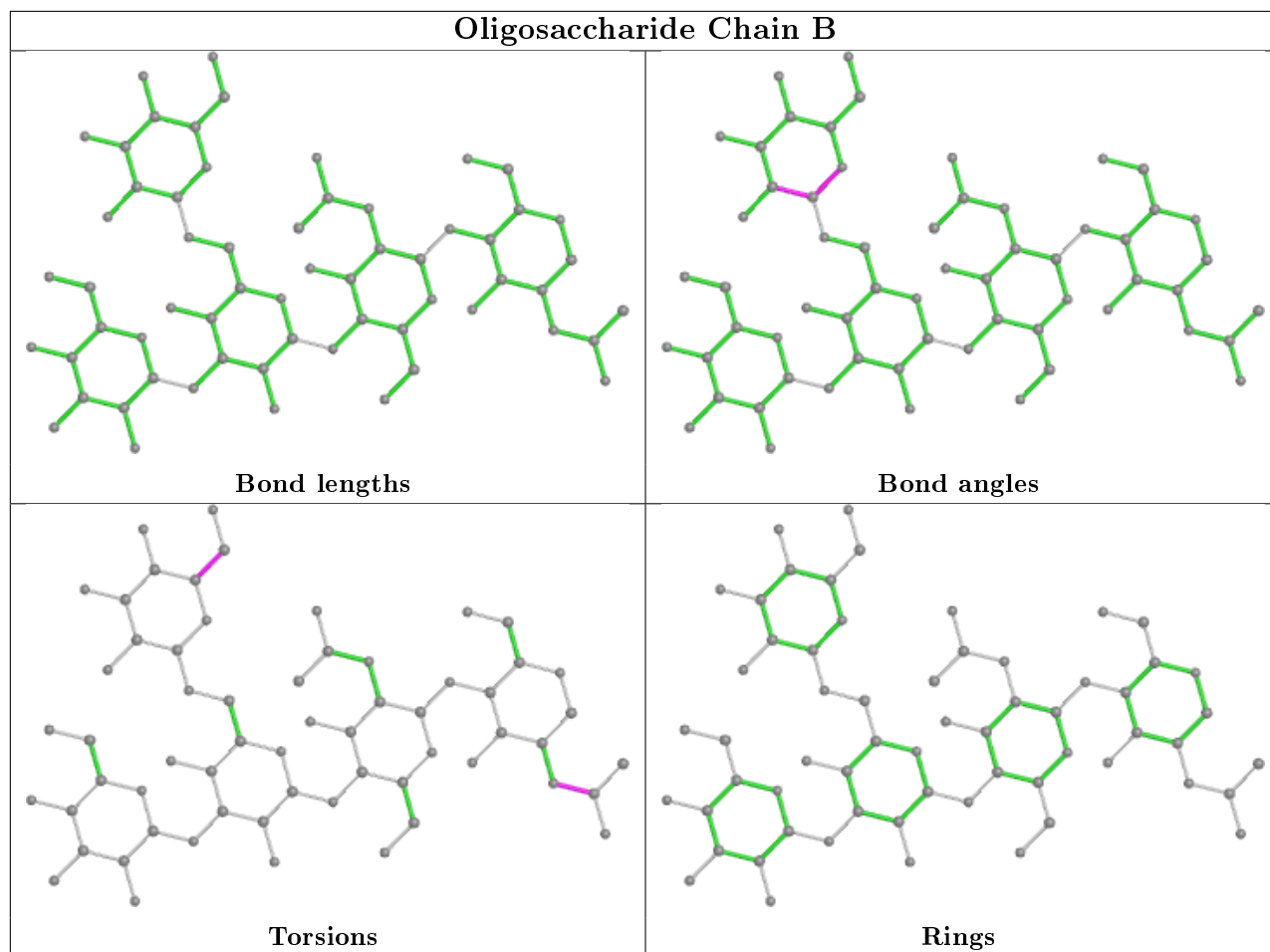
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	D	3	BMA	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
2	B	5	MAN	C4-C5-C6-O6
3	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5	MAN	1	0
2	D	3	BMA	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.

Full wwPDB X-ray Structure Validation Report

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	NAG	A	916	1	14,14,15	0.48	0	17,19,21	0.82	0
5	NAG	A	918	1	14,14,15	0.54	0	17,19,21	0.66	0
6	SO4	A	919	-	4,4,4	0.15	0	6,6,6	0.06	0
5	NAG	A	917	1	14,14,15	0.47	0	17,19,21	0.80	0
5	NAG	A	910	1	14,14,15	0.55	0	17,19,21	0.86	0
4	RX8	A	901	-	21,25,25	1.64	3 (14%)	26,37,37	1.08	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	918	1	-	0/6/23/26	0/1/1/1
5	NAG	A	910	1	-	4/6/23/26	0/1/1/1
5	NAG	A	916	1	-	2/6/23/26	0/1/1/1
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
4	RX8	A	901	-	-	5/5/9/9	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	RX8	C2-C3	5.09	1.49	1.40
4	A	901	RX8	C-N	2.66	1.43	1.34
4	A	901	RX8	O1-C10	-2.56	1.38	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	RX8	C6-O-C7	2.59	119.69	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	RX8	C2-C1-N1	-2.35	120.75	123.01
4	A	901	RX8	O-C6-C5	2.18	117.16	110.95
4	A	901	RX8	C2-C3-N3	2.05	134.76	130.42

There are no chirality outliers.

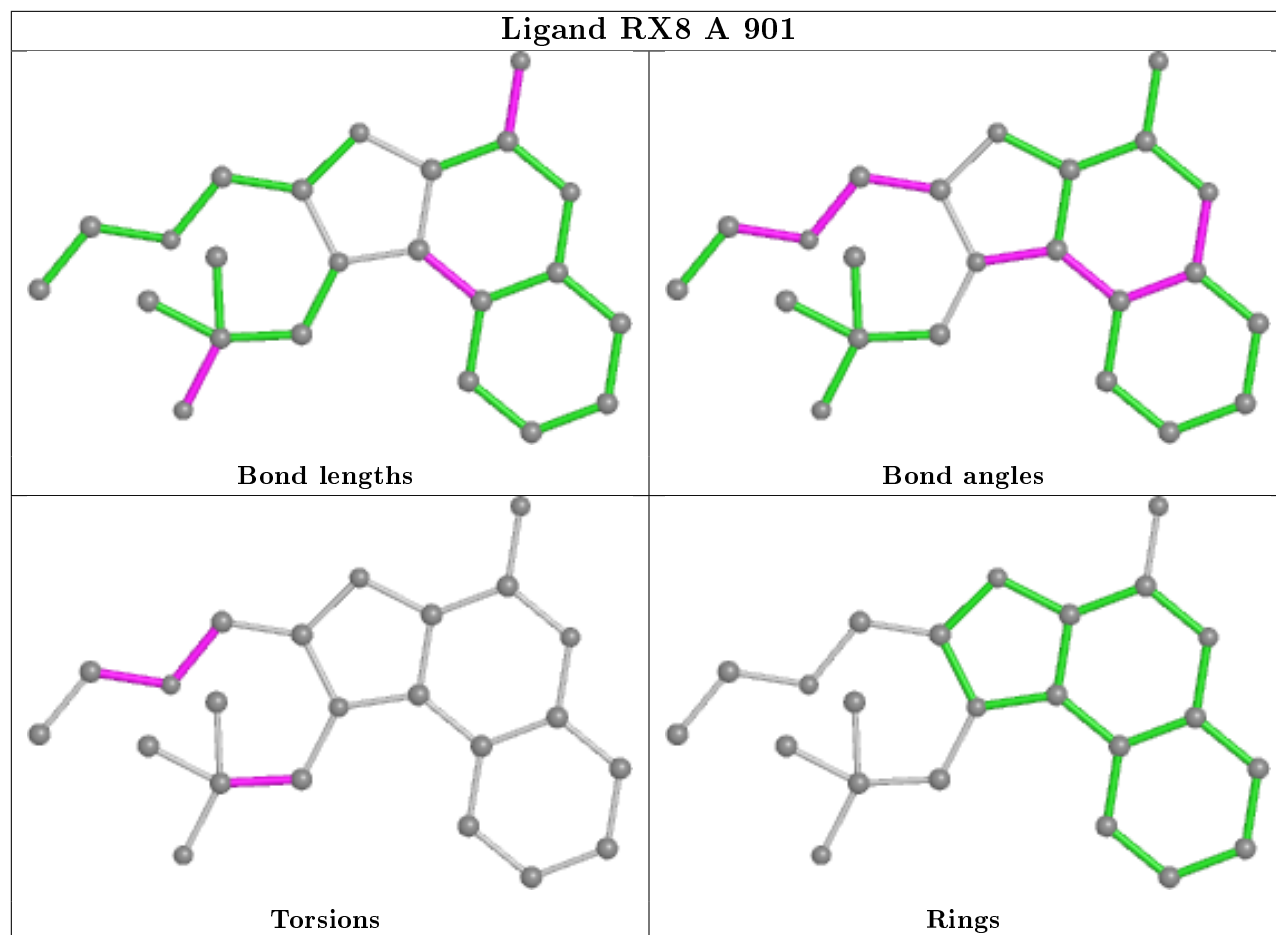All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	RX8	O1-C10-C9-N3
4	A	901	RX8	C11-C10-C9-N3
4	A	901	RX8	C12-C10-C9-N3
4	A	901	RX8	C5-C6-O-C7
5	A	916	NAG	C4-C5-C6-O6
5	A	910	NAG	C8-C7-N2-C2
5	A	910	NAG	O7-C7-N2-C2
5	A	916	NAG	O5-C5-C6-O6
4	A	901	RX8	C8-C7-O-C6
5	A	910	NAG	C4-C5-C6-O6
5	A	910	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	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 A 901

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	751/811 (92%)	0.20	25 (3%)	46	46	21, 54, 99, 122	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	GLY	4.6
1	A	83	PHE	4.6
1	A	166	ILE	4.2
1	A	86	LEU	4.2
1	A	61	VAL	3.7
1	A	202	ASN	3.7
1	A	43	ASP	3.5
1	A	100	VAL	3.2
1	A	82	SER	3.1
1	A	58	PRO	3.0
1	A	197	PHE	3.0
1	A	756	LEU	3.0
1	A	734	GLU	2.9
1	A	769	LEU	2.9
1	A	96	HIS	2.5
1	A	74	PHE	2.4
1	A	817	LEU	2.4
1	A	78	ILE	2.3
1	A	90	THR	2.3
1	A	88	ASN	2.3
1	A	818	GLU	2.3
1	A	94	LEU	2.2
1	A	814	ILE	2.1
1	A	785	ARG	2.1
1	A	161	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.
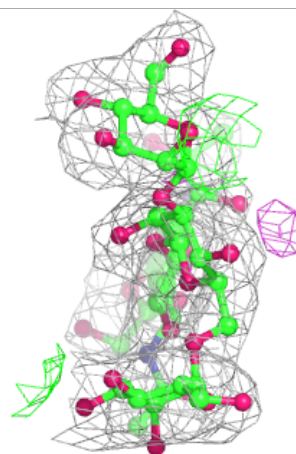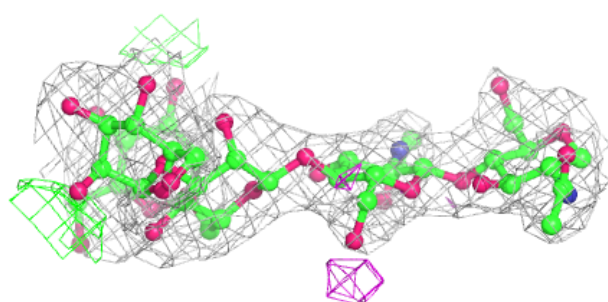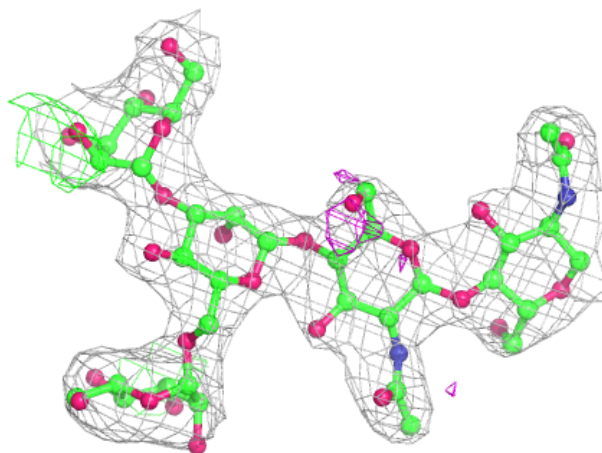
6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	D	5	11/12	0.78	0.16	87,89,92,93	0
2	MAN	B	5	11/12	0.84	0.18	69,72,78,82	0
2	MAN	D	4	11/12	0.84	0.23	81,86,90,91	0
2	MAN	B	4	11/12	0.86	0.14	50,54,56,57	0
3	NAG	C	2	14/15	0.92	0.19	54,64,70,71	0
3	BMA	C	3	11/12	0.93	0.17	68,70,75,77	0
2	NAG	B	1	14/15	0.94	0.19	37,47,50,50	0
2	BMA	D	3	11/12	0.95	0.10	57,67,82,87	0
2	NAG	B	2	14/15	0.96	0.20	34,41,48,50	0
2	BMA	B	3	11/12	0.96	0.12	45,48,55,63	0
2	NAG	D	1	14/15	0.97	0.11	17,30,37,41	0
3	NAG	C	1	14/15	0.97	0.14	28,32,40,43	0
2	NAG	D	2	14/15	0.98	0.13	21,33,44,47	0

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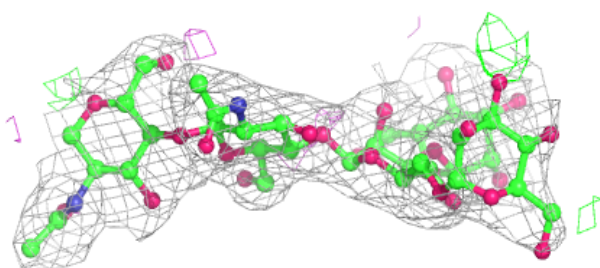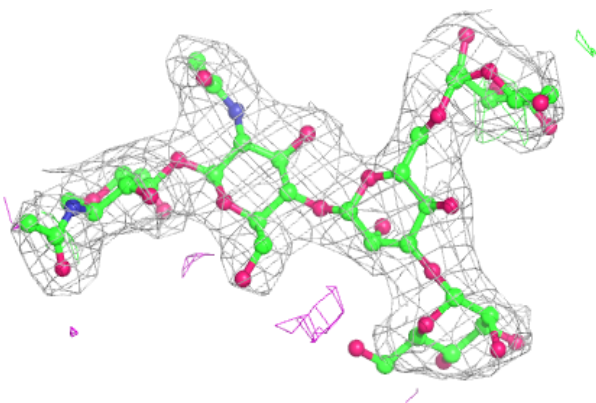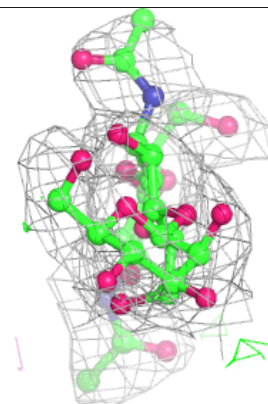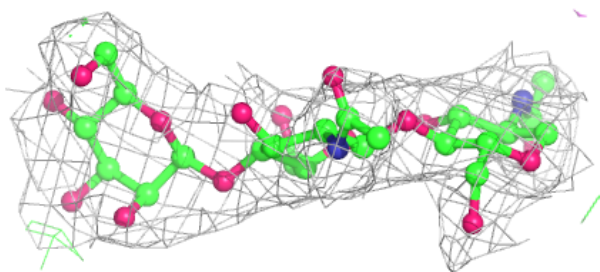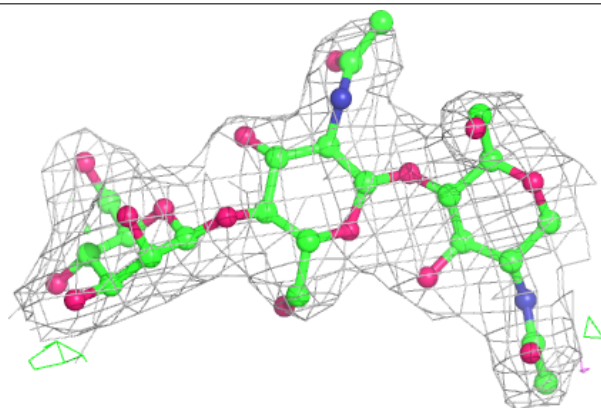
Electron density around Chain B:

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

Electron density around Chain D:

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

Electron density around Chain C:

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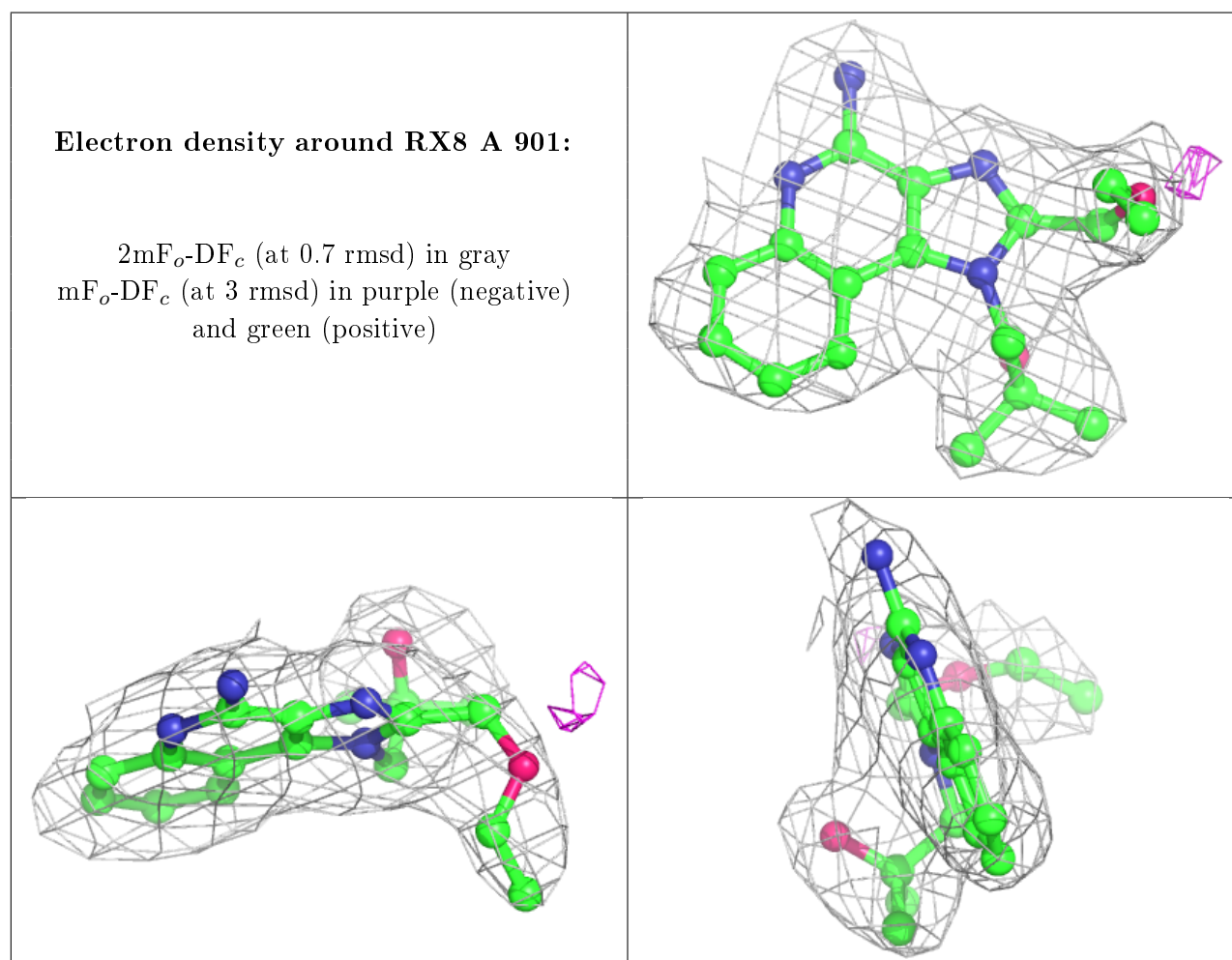mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	919	5/5	0.86	0.26	113,114,115,117	0
5	NAG	A	917	14/15	0.86	0.23	45,60,71,72	0
5	NAG	A	916	14/15	0.87	0.16	60,71,73,76	0
5	NAG	A	910	14/15	0.92	0.13	54,59,75,79	0
5	NAG	A	918	14/15	0.96	0.17	32,47,56,57	0
4	RX8	A	901	23/23	0.98	0.19	28,36,51,52	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 A 901:

$2mF_o$-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.