



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:33 PM BST

PDB ID : 5GMH
Title : Crystal structure of monkey TLR7 in complex with R848
Authors : Zhang, Z.; Ohto, U.; Shimizu, T.
Deposited on : 2016-07-14
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

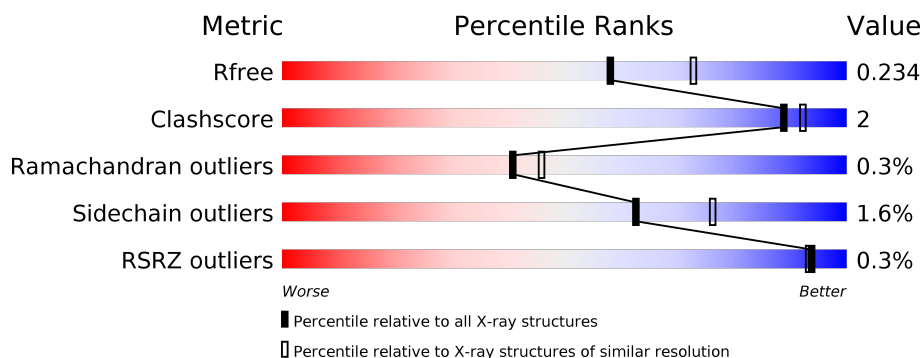
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	817	<div> <div>88%</div> <div>7%</div> <div>6%</div> </div>
1	B	817	<div> <div>%</div> <div>87%</div> <div>8%</div> <div>6%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13621 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

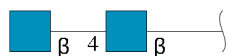
- Molecule 1 is a protein called Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	1	0
			6258	4010	1066	1152	30			
1	B	772	Total	C	N	O	S	0	3	0
			6272	4017	1068	1157	30			

There are 16 discrepancies between the modelled and reference sequences:

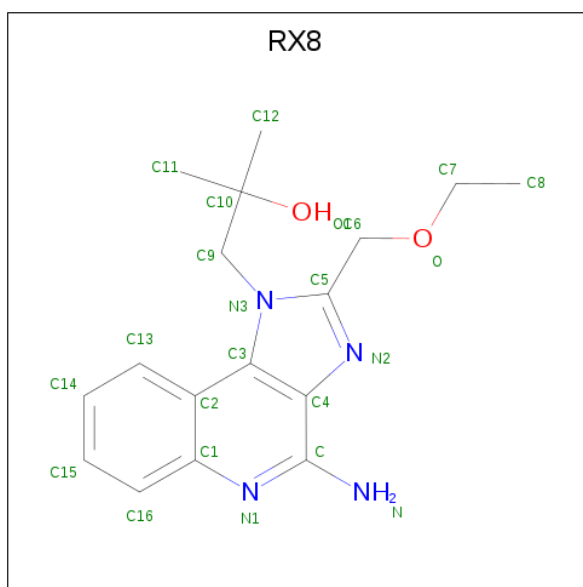
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653

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



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

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			23	17	4	2		
3	B	1	Total	C	N	O	0	0
			23	17	4	2		

- 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	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		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	397	Total	O	0	0
			397	397		
6	B	256	Total	O	0	0
			256	256		

Chain D:  50% 50%

 MAG1
MAG2

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

Chain E:  50% 50%

 MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.10Å 140.09Å 151.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.20 47.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.01-2.20) 98.7 (47.08-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.185 , 0.225 0.192 , 0.234	Depositor DCC
R_{free} test set	5212 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13621	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RX8, 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	0.85	0/6389	0.94	19/8657 (0.2%)
1	B	0.81	0/6403	0.92	21/8676 (0.2%)
All	All	0.83	0/12792	0.93	40/17333 (0.2%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	B	378	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	A	622	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	115	ARG	NE-CZ-NH2	9.24	124.92	120.30
1	A	115	ARG	NE-CZ-NH2	9.22	124.91	120.30

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	6258	0	6301	21	0
1	B	6272	0	6309	23	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	25	1	0
3	A	23	0	22	4	0
3	B	23	0	22	2	0
4	A	98	0	91	1	0
4	B	70	0	65	1	0
5	A	85	0	0	1	0
5	B	55	0	0	0	0
6	A	397	0	0	4	1
6	B	256	0	0	4	0
All	All	13621	0	12885	49	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 49 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:279:LEU:HA	6:A:1198:HOH:O	1.62	0.99
5:A:920:SO4:O2	6:A:1001:HOH:O	1.87	0.93
1:A:431:ASN:HB2	1:A:503:ASN:HD21	1.58	0.69
1:B:431:ASN:HB2	1:B:503:ASN:HD21	1.58	0.68
1:B:206:LEU:O	1:B:226:THR:HG23	1.97	0.65

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1362:HOH:O	6:A:1380:HOH:O[2_555]	2.15	0.05

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	767/817 (94%)	721 (94%)	44 (6%)	2 (0%)	41	46
1	B	769/817 (94%)	724 (94%)	42 (6%)	3 (0%)	34	37
All	All	1536/1634 (94%)	1445 (94%)	86 (6%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLY
1	B	818	GLY
1	A	381	VAL
1	B	381	VAL
1	B	430	VAL

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	726/768 (94%)	714 (98%)	12 (2%)	60	74
1	B	728/768 (95%)	717 (98%)	11 (2%)	65	78
All	All	1454/1536 (95%)	1431 (98%)	23 (2%)	62	76

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	810	THR
1	B	43	SER
1	B	810	THR
1	A	813	THR
1	B	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	734	GLN

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Mol	Chain	Res	Type
1	A	748	GLN
1	B	503	ASN
1	A	708	HIS
1	B	173	ASN

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 ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	1,2	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
2	NAG	C	2	2	14,14,15	0.64	0	17,19,21	1.43	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.70	0	17,19,21	1.10	0
2	NAG	D	2	2	14,14,15	0.96	1 (7%)	17,19,21	1.84	4 (23%)
2	NAG	E	1	1,2	14,14,15	0.73	0	17,19,21	2.32	7 (41%)
2	NAG	E	2	2	14,14,15	1.10	1 (7%)	17,19,21	2.46	6 (35%)

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	-	1/6/23/26	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C5	2.28	1.48	1.43
2	E	2	NAG	C1-C2	2.05	1.55	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	7.52	122.38	112.19
2	E	1	NAG	C8-C7-N2	6.17	126.55	116.10
2	D	2	NAG	C1-O5-C5	3.83	117.38	112.19
2	D	2	NAG	C3-C4-C5	-3.66	103.71	110.24
2	D	2	NAG	O4-C4-C5	3.53	118.07	109.30

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

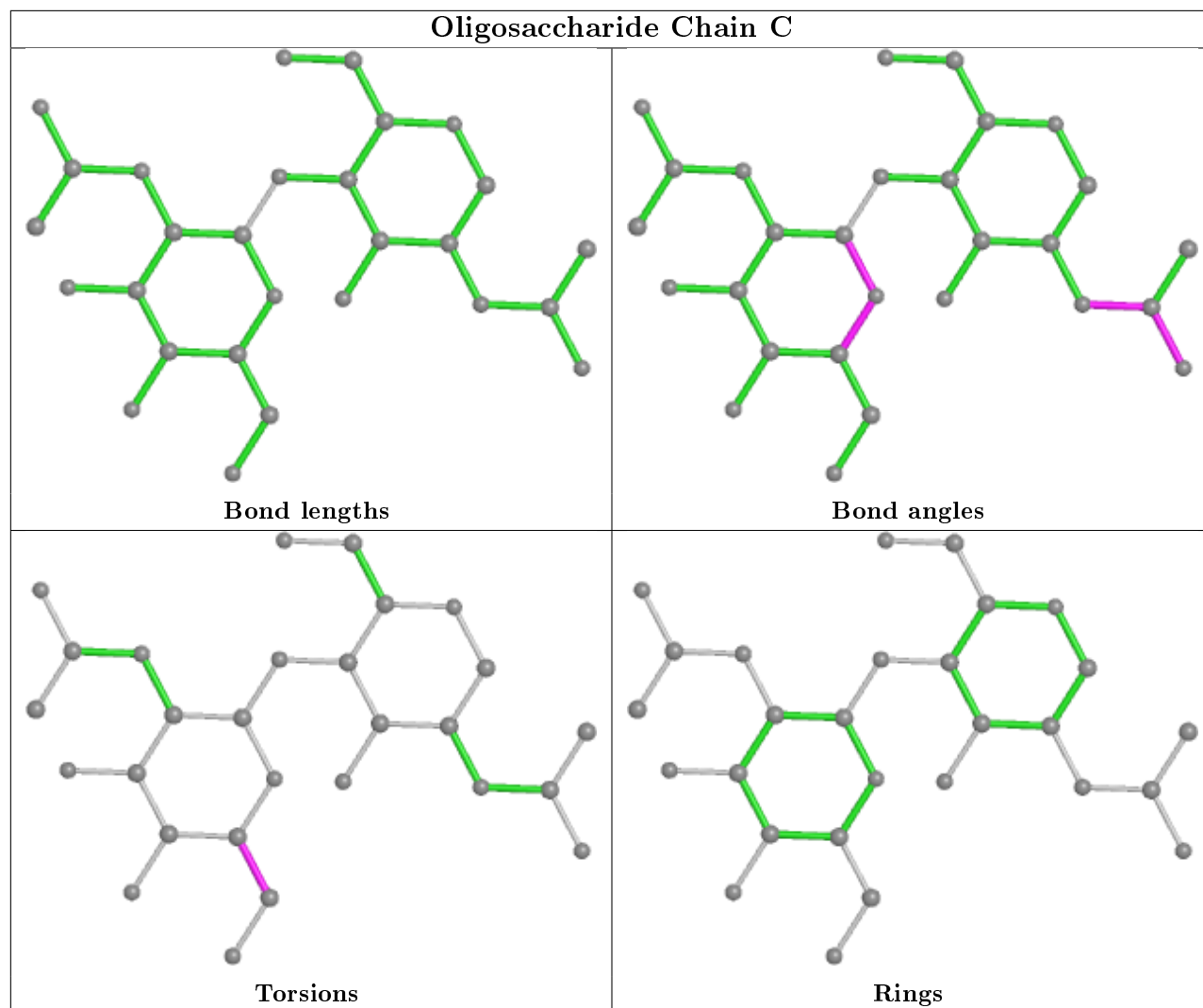
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6

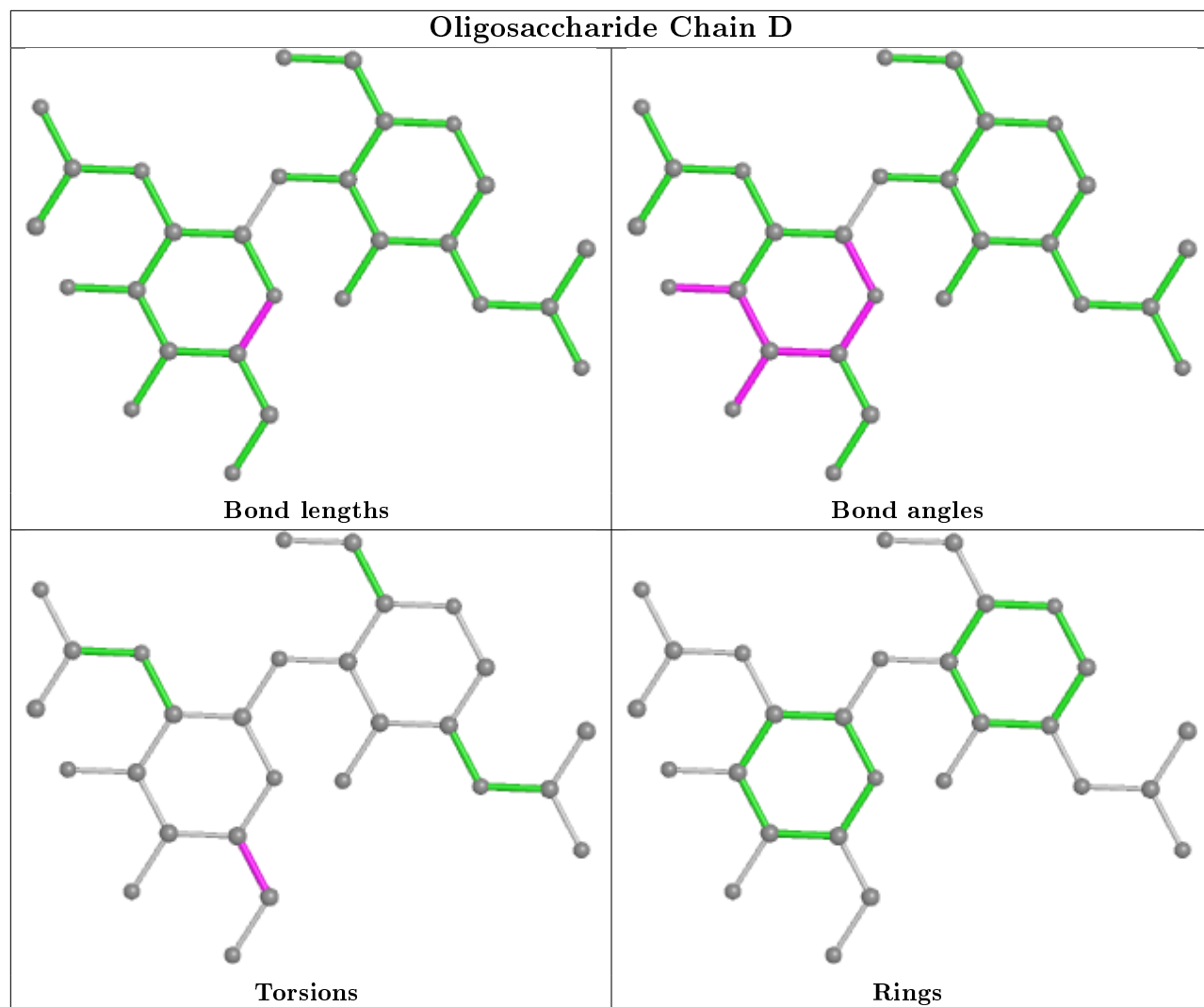
There are no ring outliers.

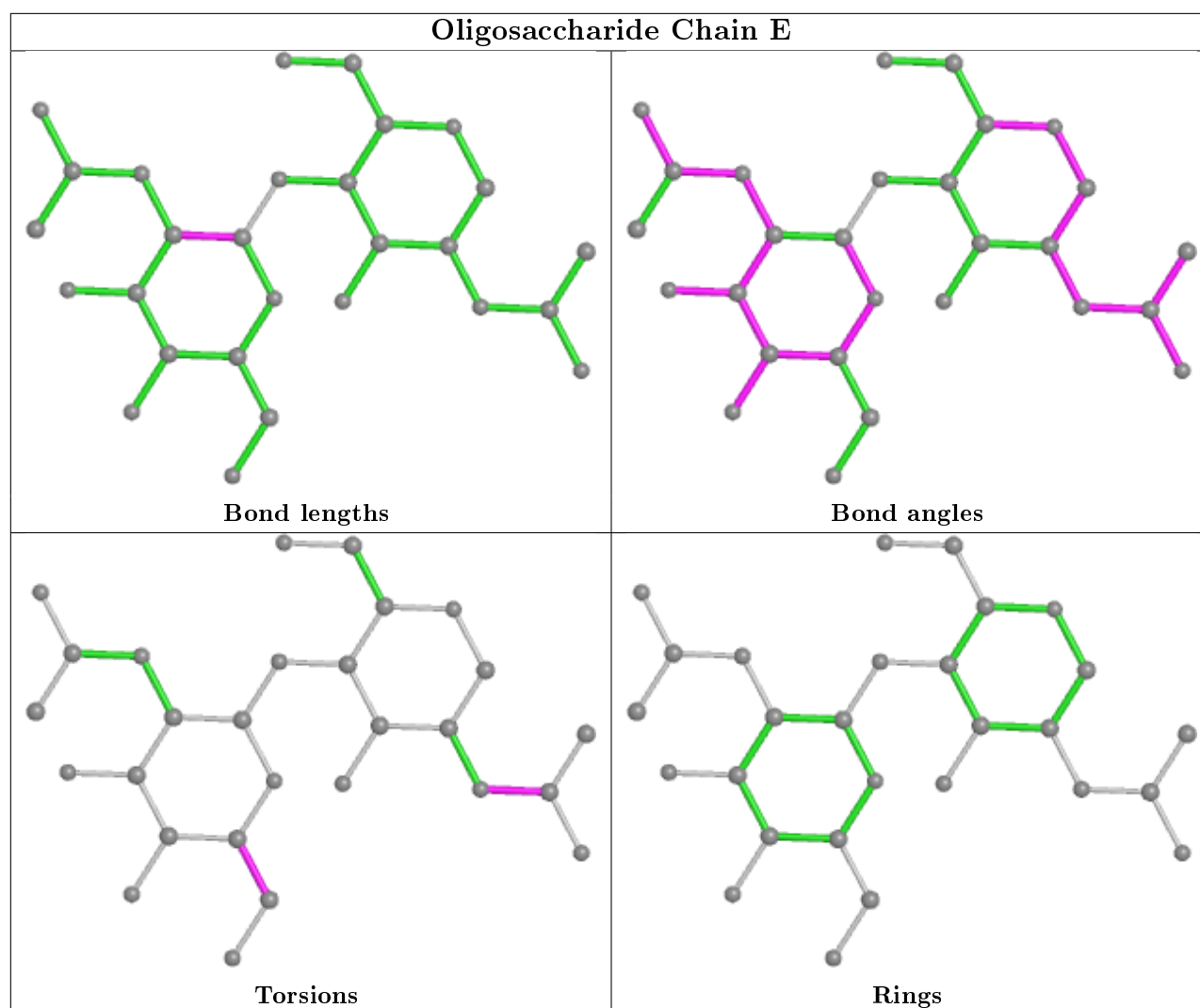
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	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](#)

42 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	B	920	-	4,4,4	0.52	0	6,6,6	0.68	0
5	SO4	A	926	-	4,4,4	0.54	0	6,6,6	0.73	0
5	SO4	A	914	-	4,4,4	0.54	0	6,6,6	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	910	1	14,14,15	0.59	0	17,19,21	3.34	3 (17%)
5	SO4	B	913	-	4,4,4	0.41	0	6,6,6	0.51	0
5	SO4	B	918	-	4,4,4	0.51	0	6,6,6	0.31	0
5	SO4	B	921	-	4,4,4	0.50	0	6,6,6	0.78	0
4	NAG	A	906	1	14,14,15	0.78	0	17,19,21	2.35	4 (23%)
5	SO4	A	917	-	4,4,4	0.63	0	6,6,6	0.66	0
4	NAG	A	907	1	14,14,15	0.98	1 (7%)	17,19,21	1.52	3 (17%)
5	SO4	B	917	-	4,4,4	0.45	0	6,6,6	0.27	0
5	SO4	A	916	-	4,4,4	0.48	0	6,6,6	0.58	0
5	SO4	A	927	-	4,4,4	0.38	0	6,6,6	0.20	0
5	SO4	A	915	-	4,4,4	0.59	0	6,6,6	0.32	0
5	SO4	A	911	-	4,4,4	0.60	0	6,6,6	0.60	0
4	NAG	A	905	1	14,14,15	1.02	1 (7%)	17,19,21	1.70	4 (23%)
5	SO4	B	915	-	4,4,4	0.66	0	6,6,6	0.42	0
5	SO4	A	913	-	4,4,4	0.40	0	6,6,6	0.44	0
5	SO4	A	921	-	4,4,4	0.56	0	6,6,6	0.97	1 (16%)
3	RX8	A	901	-	21,25,25	1.52	5 (23%)	26,37,37	2.17	6 (23%)
4	NAG	A	909	1	14,14,15	0.50	0	17,19,21	1.41	3 (17%)
4	NAG	B	910	1	14,14,15	0.52	0	17,19,21	1.62	1 (5%)
5	SO4	A	919	-	4,4,4	0.73	0	6,6,6	1.33	1 (16%)
3	RX8	B	901	-	21,25,25	1.64	4 (19%)	26,37,37	2.11	8 (30%)
5	SO4	B	914	-	4,4,4	0.49	0	6,6,6	0.93	0
5	SO4	A	925	-	4,4,4	0.56	0	6,6,6	0.41	0
4	NAG	A	902	1	14,14,15	1.38	2 (14%)	17,19,21	2.13	7 (41%)
4	NAG	B	902	1	14,14,15	1.21	1 (7%)	17,19,21	1.78	5 (29%)
4	NAG	B	908	1	14,14,15	0.56	0	17,19,21	1.74	5 (29%)
5	SO4	A	922	-	4,4,4	0.70	0	6,6,6	0.58	0
5	SO4	B	911	-	4,4,4	0.41	0	6,6,6	0.74	0
4	NAG	B	909	1	14,14,15	0.38	0	17,19,21	1.48	4 (23%)
5	SO4	A	923	-	4,4,4	0.48	0	6,6,6	0.48	0
4	NAG	A	908	1	14,14,15	0.55	0	17,19,21	1.50	3 (17%)
5	SO4	B	912	-	4,4,4	0.68	0	6,6,6	0.47	0
4	NAG	B	907	1	14,14,15	0.52	0	17,19,21	2.45	6 (35%)
5	SO4	A	920	-	4,4,4	0.52	0	6,6,6	0.65	0
5	SO4	B	916	-	4,4,4	0.49	0	6,6,6	0.58	0
5	SO4	A	912	-	4,4,4	0.53	0	6,6,6	0.76	0
5	SO4	A	924	-	4,4,4	0.37	0	6,6,6	0.39	0
5	SO4	B	919	-	4,4,4	0.44	0	6,6,6	0.34	0
5	SO4	A	918	-	4,4,4	0.44	0	6,6,6	0.41	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
3	RX8	A	901	-	-	1/5/9/9	0/3/3/3
4	NAG	A	910	1	-	2/6/23/26	0/1/1/1
4	NAG	B	909	1	-	0/6/23/26	0/1/1/1
4	NAG	A	909	1	-	2/6/23/26	0/1/1/1
4	NAG	B	910	1	-	2/6/23/26	0/1/1/1
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
3	RX8	B	901	-	-	3/5/9/9	0/3/3/3
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	B	902	1	-	2/6/23/26	0/1/1/1
4	NAG	B	908	1	-	0/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	908	1	-	0/6/23/26	0/1/1/1
4	NAG	A	907	1	-	0/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	RX8	C9-C10	4.89	1.60	1.54
3	A	901	RX8	C2-C3	3.42	1.46	1.40
3	A	901	RX8	C9-C10	3.29	1.58	1.54
3	B	901	RX8	O1-C10	-2.69	1.37	1.44
4	A	902	NAG	O7-C7	-2.69	1.17	1.23

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	910	NAG	C1-O5-C5	12.77	129.50	112.19
4	B	907	NAG	C1-O5-C5	7.32	122.11	112.19
4	A	906	NAG	C1-O5-C5	6.81	121.42	112.19
3	B	901	RX8	C6-O-C7	5.73	127.87	112.92
4	B	910	NAG	C1-O5-C5	5.49	119.63	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

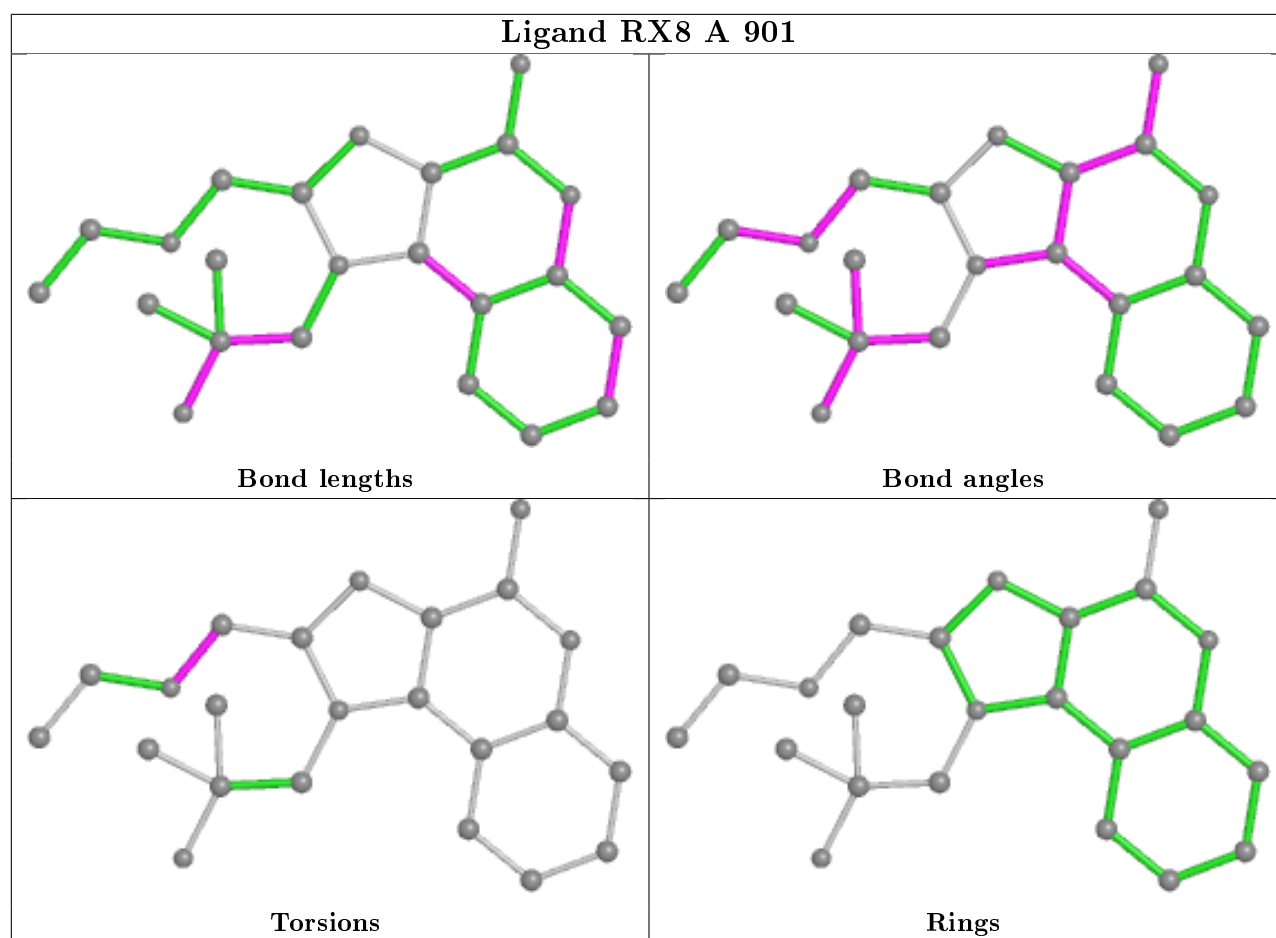
Mol	Chain	Res	Type	Atoms
3	A	901	RX8	C5-C6-O-C7
3	B	901	RX8	C5-C6-O-C7
4	B	910	NAG	O5-C5-C6-O6
4	A	910	NAG	C4-C5-C6-O6
4	A	909	NAG	O5-C5-C6-O6

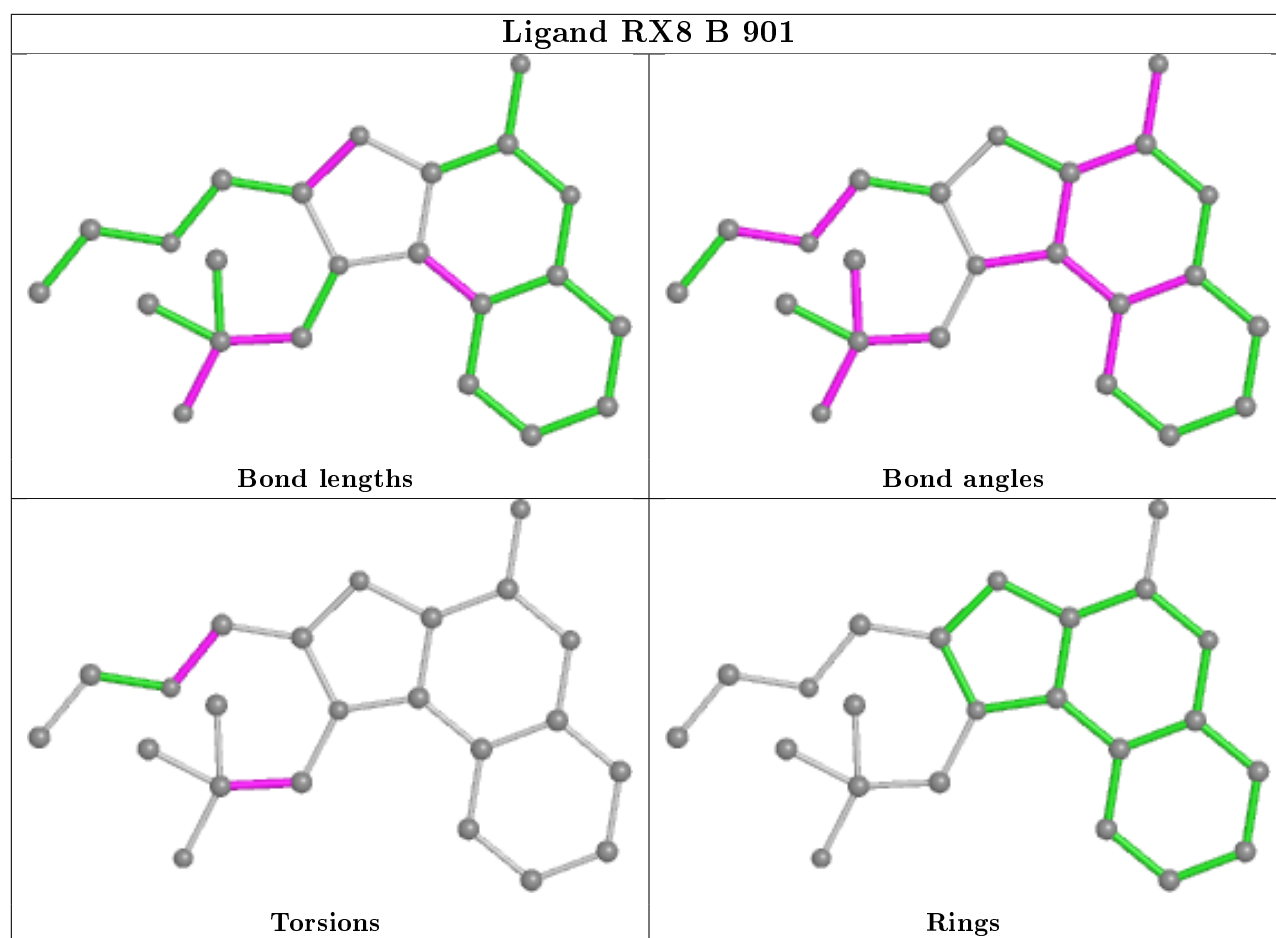
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	906	NAG	1	0
3	A	901	RX8	4	0
3	B	901	RX8	2	0
4	B	902	NAG	1	0
5	A	920	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	772/817 (94%)	-0.42	0 100 100	20, 35, 58, 98	0
1	B	772/817 (94%)	-0.28	5 (0%) 89 88	26, 44, 69, 99	0
All	All	1544/1634 (94%)	-0.35	5 (0%) 94 93	20, 40, 66, 99	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	PHE	3.5
1	B	723	ARG	3.0
1	B	463	LEU	2.9
1	B	42	VAL	2.7
1	B	776	LYS	2.1

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.

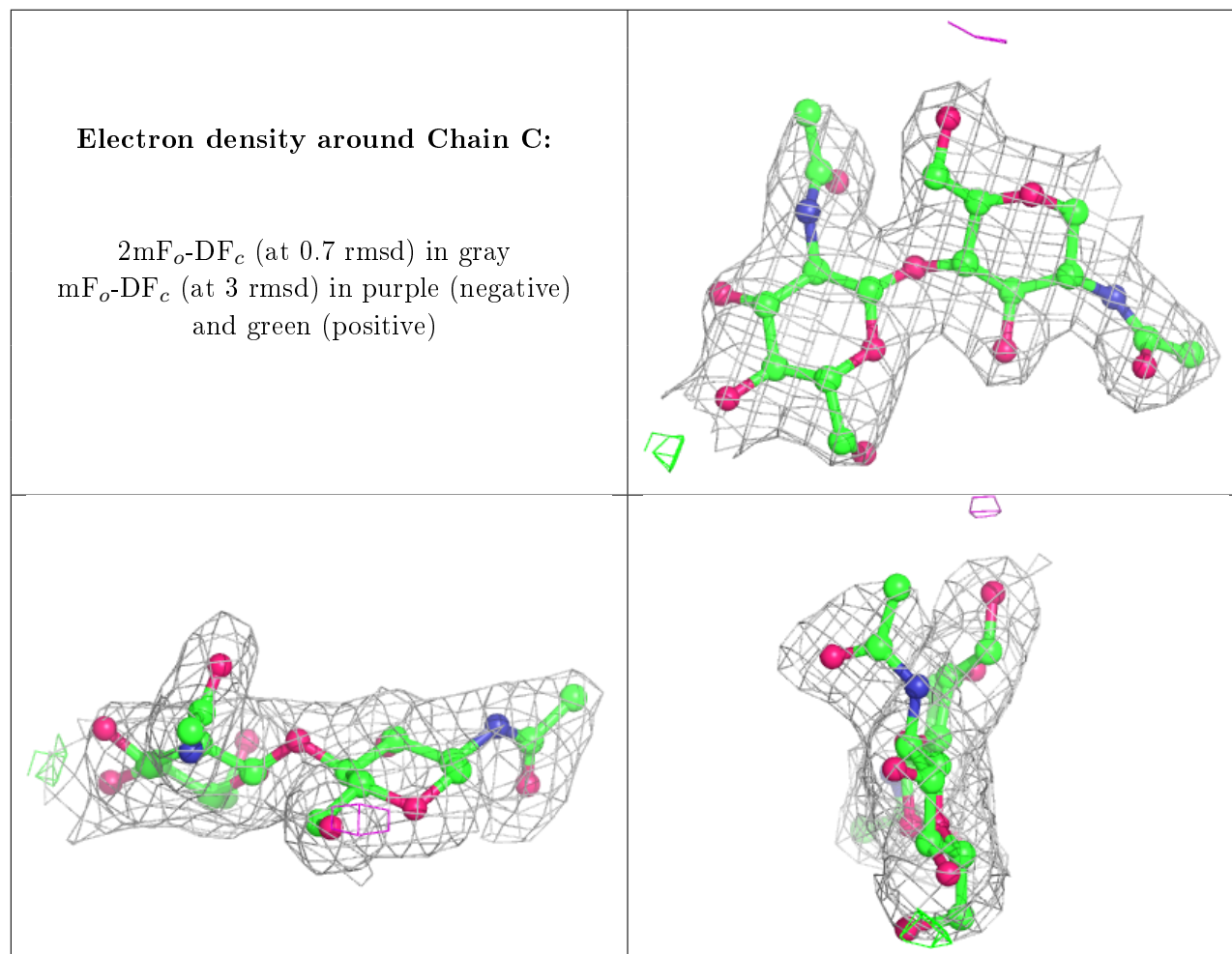
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.83	0.22	69,87,102,104	0
2	NAG	D	2	14/15	0.90	0.10	57,66,72,75	0
2	NAG	C	2	14/15	0.92	0.13	58,63,68,71	0
2	NAG	E	1	14/15	0.96	0.08	45,51,60,64	0

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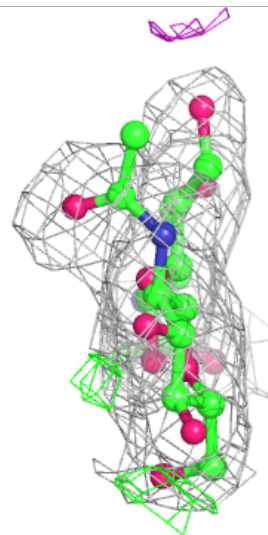
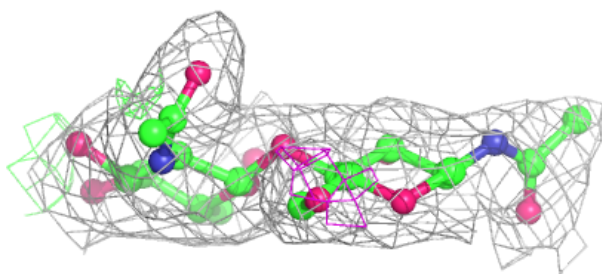
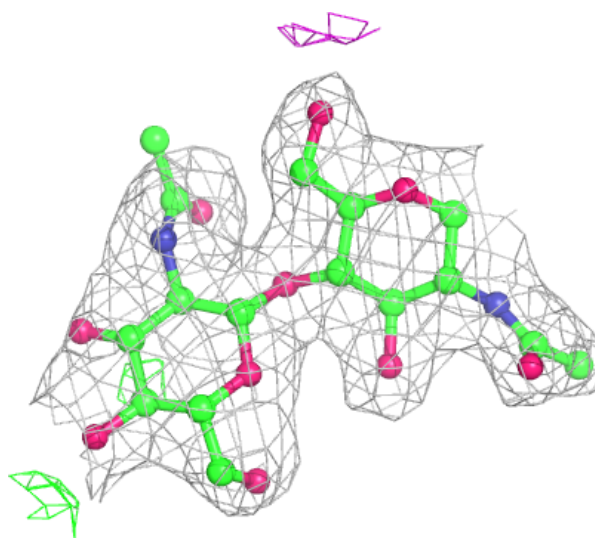
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	1	14/15	0.97	0.09	41,44,49,52	0
2	NAG	C	1	14/15	0.97	0.07	36,42,45,51	0

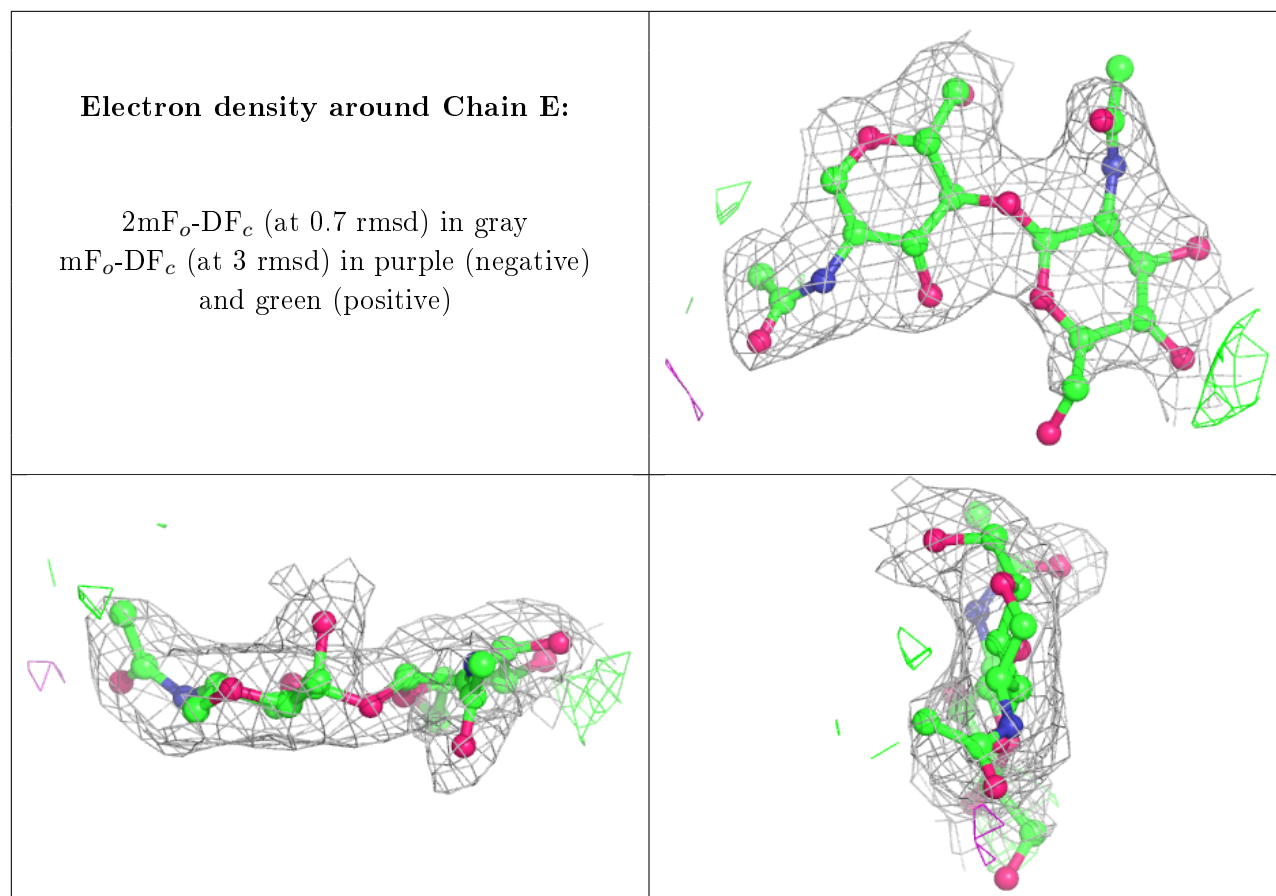
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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
5	SO4	B	915	5/5	0.56	0.29	69,92,102,124	0
5	SO4	A	925	5/5	0.71	0.36	83,106,114,121	0
5	SO4	A	922	5/5	0.75	0.40	68,75,112,112	0
5	SO4	A	926	5/5	0.76	0.27	88,91,96,104	0
5	SO4	B	912	5/5	0.77	0.24	65,83,97,98	0
5	SO4	A	927	5/5	0.81	0.48	117,121,136,153	0
5	SO4	B	911	5/5	0.81	0.24	92,96,101,110	0
5	SO4	A	911	5/5	0.81	0.28	74,83,108,126	0
5	SO4	B	918	5/5	0.82	0.38	91,98,113,117	0
5	SO4	B	920	5/5	0.83	0.23	81,86,100,102	0
5	SO4	B	916	5/5	0.84	0.29	99,102,109,111	0
5	SO4	A	912	5/5	0.86	0.14	67,82,98,103	0
5	SO4	B	921	5/5	0.86	0.16	79,86,103,114	0

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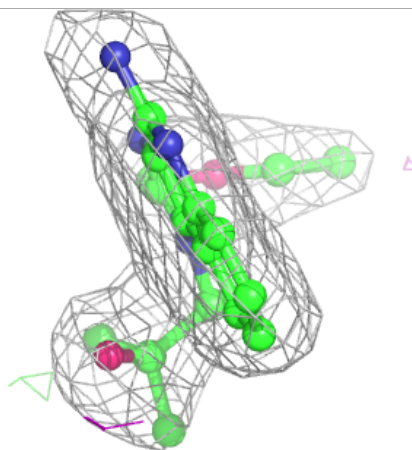
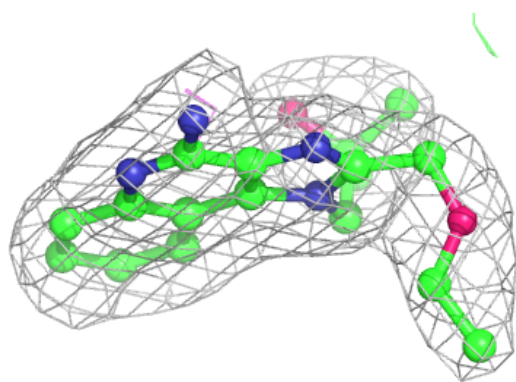
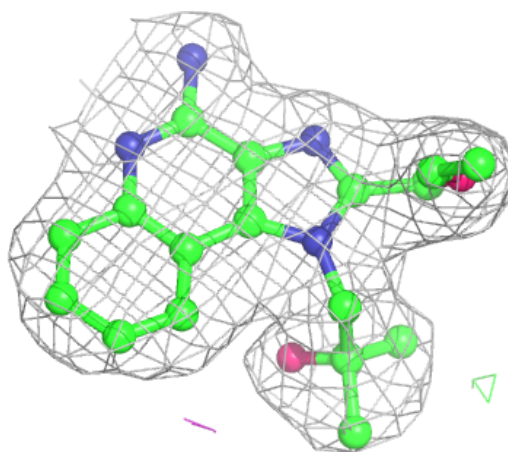
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	913	5/5	0.87	0.17	77,85,97,108	0
5	SO4	B	919	5/5	0.87	0.31	102,104,115,117	0
5	SO4	A	921	5/5	0.88	0.22	79,84,98,109	0
5	SO4	A	923	5/5	0.88	0.12	86,87,93,107	0
4	NAG	B	908	14/15	0.89	0.13	71,81,91,98	0
5	SO4	B	917	5/5	0.89	0.28	81,93,101,109	0
5	SO4	A	920	5/5	0.89	0.24	58,62,89,95	0
5	SO4	A	916	5/5	0.89	0.29	77,101,114,134	0
4	NAG	A	910	14/15	0.89	0.12	54,68,79,81	0
5	SO4	A	918	5/5	0.89	0.19	94,95,107,116	0
4	NAG	B	910	14/15	0.90	0.24	68,83,93,108	0
4	NAG	B	907	14/15	0.90	0.12	58,68,80,83	0
5	SO4	A	919	5/5	0.91	0.12	47,54,78,95	0
5	SO4	A	915	5/5	0.92	0.15	68,83,88,96	0
5	SO4	B	913	5/5	0.92	0.10	64,83,93,97	0
4	NAG	A	909	14/15	0.92	0.10	60,67,72,80	0
5	SO4	A	914	5/5	0.92	0.14	47,69,80,80	0
4	NAG	B	909	14/15	0.92	0.16	55,66,71,72	0
5	SO4	A	917	5/5	0.92	0.14	49,68,84,92	0
4	NAG	A	908	14/15	0.93	0.14	48,57,59,67	0
4	NAG	B	902	14/15	0.94	0.11	34,41,45,46	0
4	NAG	A	906	14/15	0.94	0.11	45,54,71,71	0
4	NAG	A	907	14/15	0.95	0.10	39,41,45,49	0
5	SO4	A	924	5/5	0.95	0.23	88,93,105,120	0
4	NAG	A	905	14/15	0.96	0.10	35,43,46,52	0
5	SO4	B	914	5/5	0.96	0.14	54,56,77,78	0
3	RX8	B	901	23/23	0.97	0.16	29,33,48,52	0
4	NAG	A	902	14/15	0.97	0.12	27,31,37,44	0
3	RX8	A	901	23/23	0.97	0.14	31,36,45,51	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.

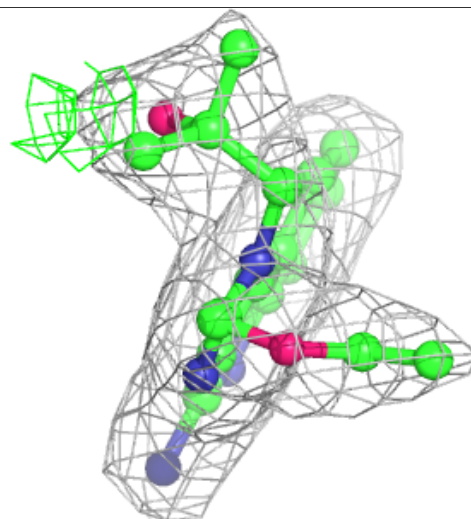
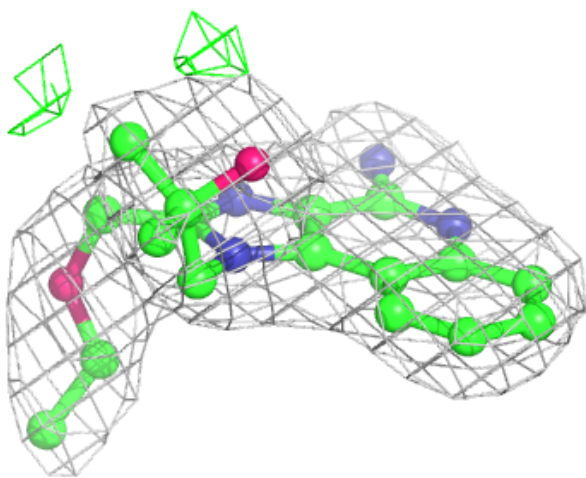
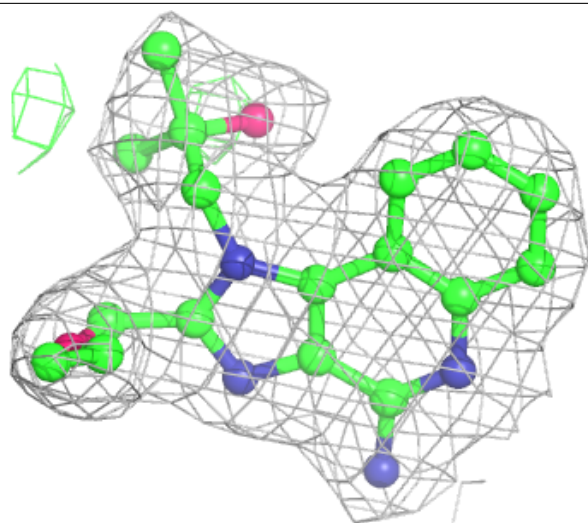
Electron density around RX8 B 901:

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



Electron density around RX8 A 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.