



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:33 PM BST

PDB ID : 6V9U
Title : Crystal structure of human TLR8 ectodomain bound to small molecule antagonist 14c
Authors : Critton, D.A.
Deposited on : 2019-12-16
Resolution : 2.65 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

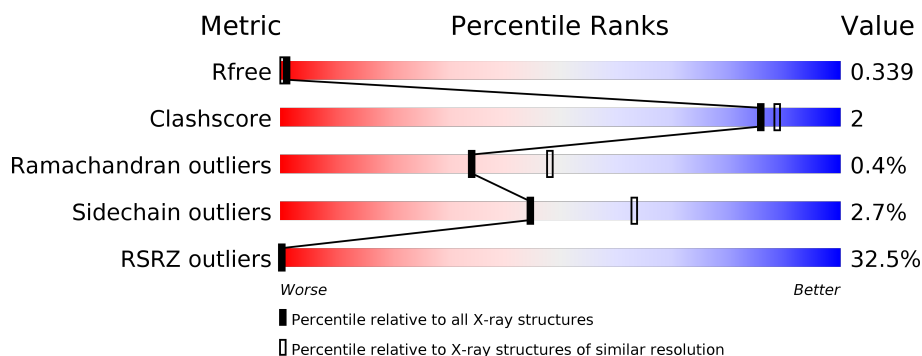
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	<div> <div>33%</div> <div>83%</div> <div>8%</div> <div>9%</div> </div>
1	B	811	<div> <div>26%</div> <div>82%</div> <div>8%</div> <div>9%</div> </div>
2	C	5	<div> <div>20%</div> <div>80%</div> </div>
2	E	5	<div> <div>60%</div> <div>40%</div> </div>
2	F	5	<div> <div>40%</div> <div>60%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	3	 <div>67%33%</div>
5	H	5	 <div>60%40%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	918	-	-	-	X
6	NAG	A	921	-	-	-	X
6	NAG	B	901	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12082 atoms, of which 60 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.

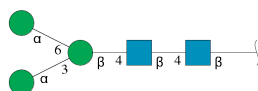
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	2	0
			5731	3689	952	1071	19			
1	B	735	Total	C	N	O	S	0	1	0
			5646	3637	927	1063	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.



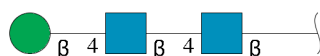
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

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



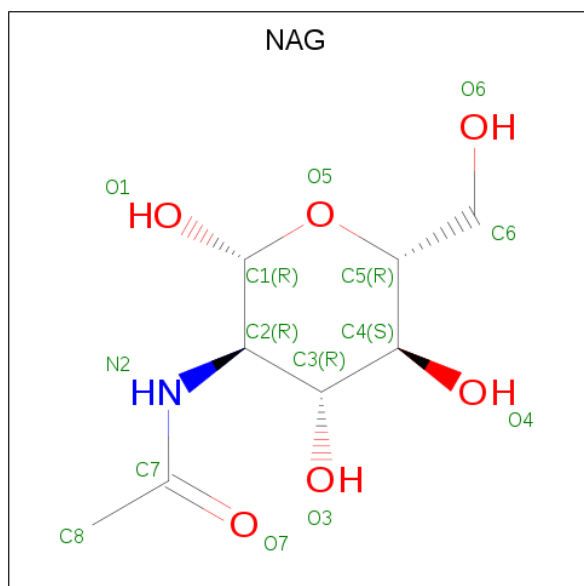
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



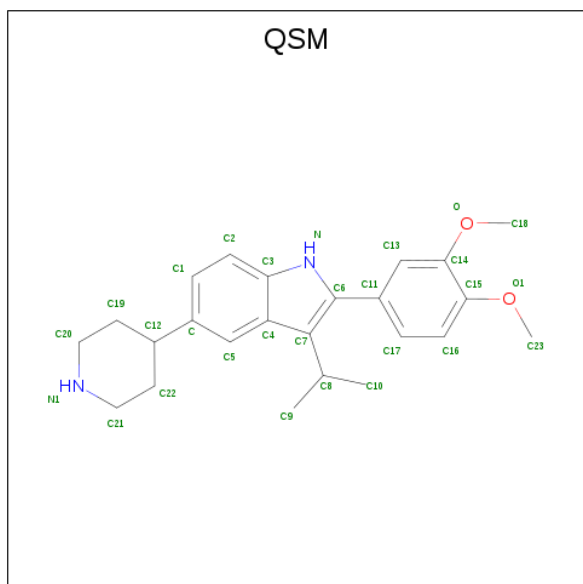
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1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

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

- Molecule 7 is 2-(3,4-dimethoxyphenyl)-5-(piperidin-4-yl)-3-(propan-2-yl)-1H-indole (three-letter code: QSM) (formula: C₂₄H₃₀N₂O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	30	0
			58	24	30	2	2		
7	B	1	Total	C	H	N	O	30	0
			58	24	30	2	2		

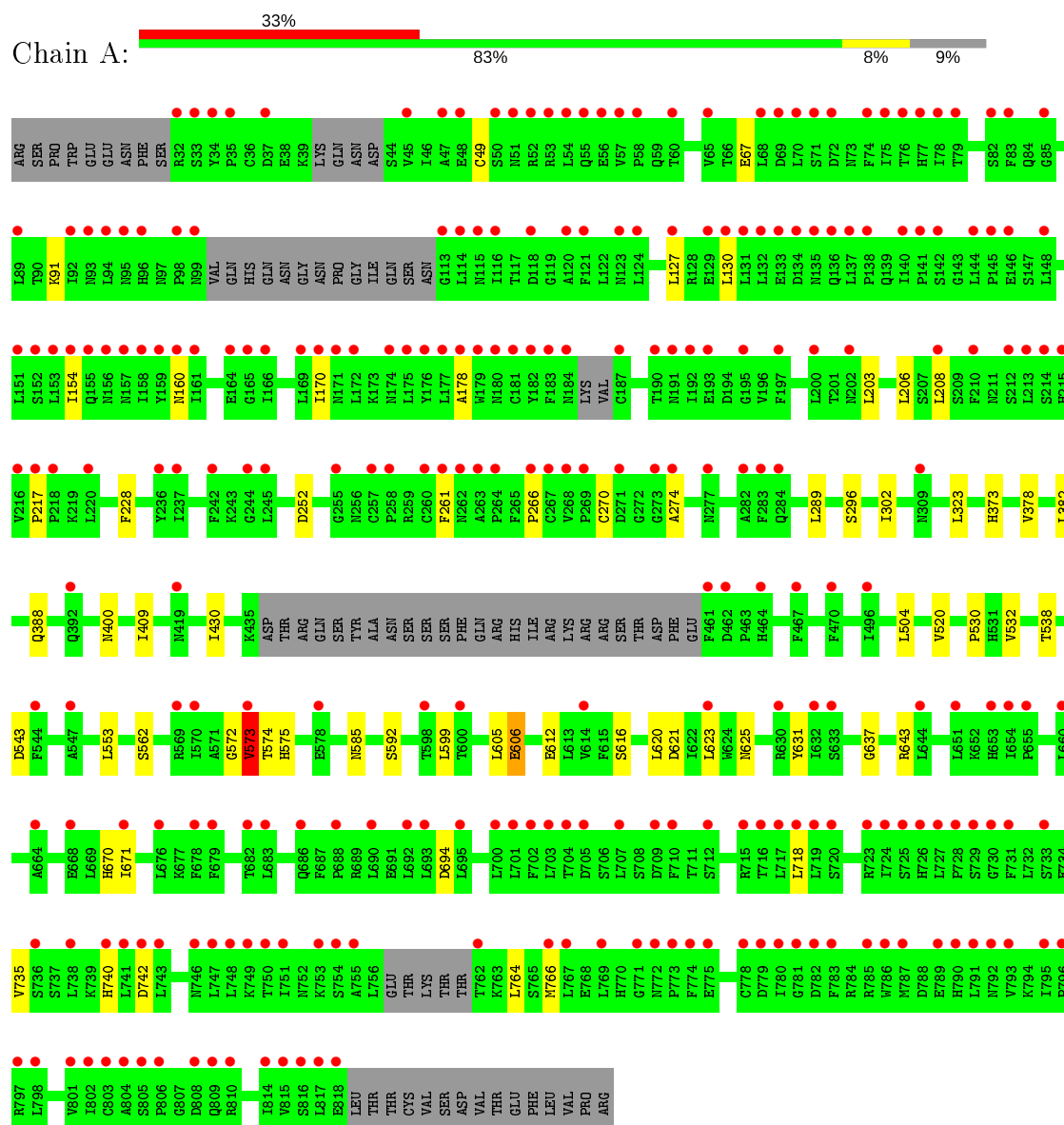
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	23	Total 23	O 23	0	0
8	B	17	Total 17	O 17	0	0

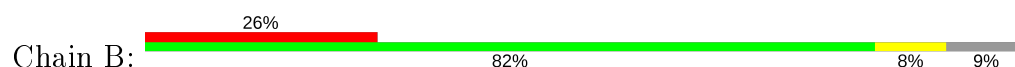
3 Residue-property plots

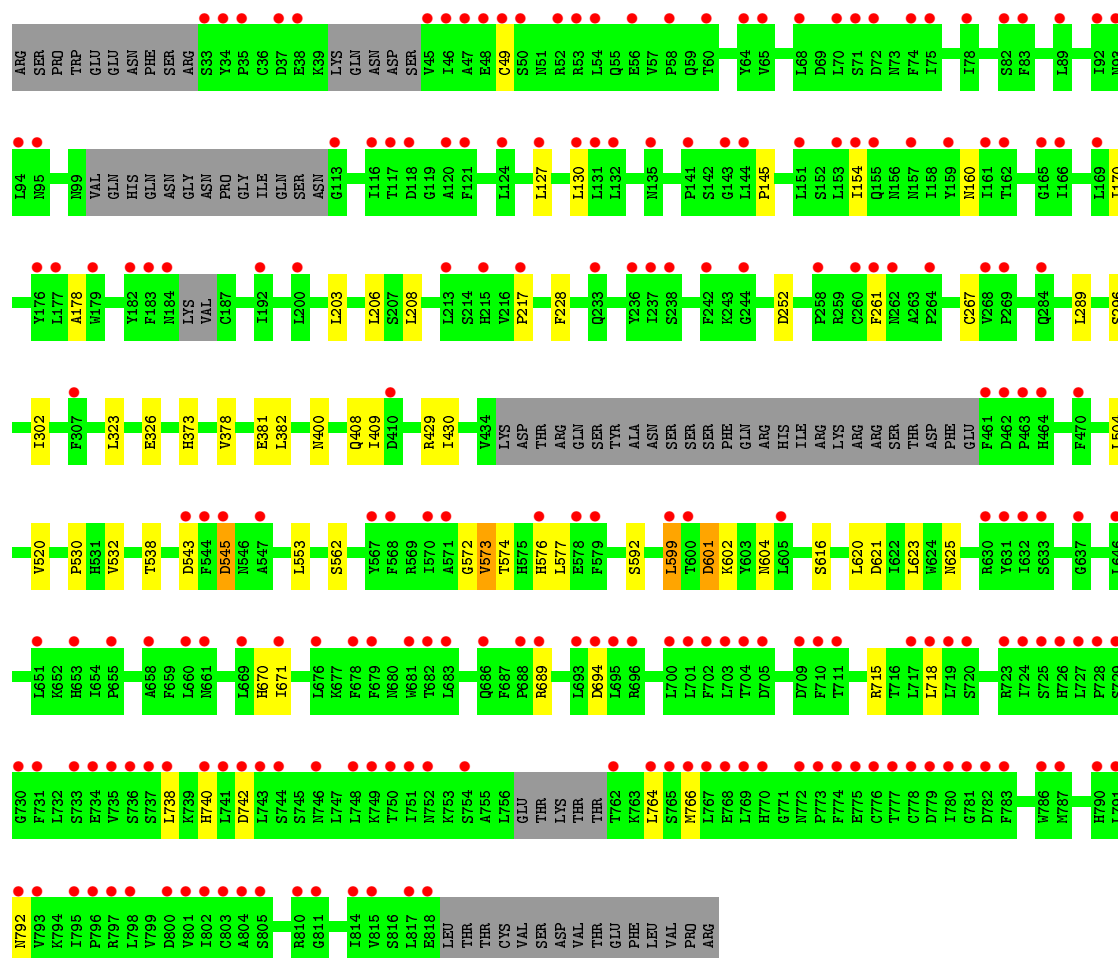
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1: Toll-like receptor 8





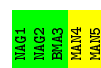
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 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 F: 40% 60%



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

Chain D:



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

Chain G:



- Molecule 5: 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:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.59 Å 86.75 Å 151.40 Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	131.37 – 2.65 81.69 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (131.37-2.65) 99.3 (81.69-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.65 Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.296 , 0.306 0.324 , 0.339	Depositor DCC
R_{free} test set	2652 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: BMA, NAG, QSM, MAN

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	0.40	0/5861	0.58	0/7992
1	B	0.40	0/5768	0.59	1/7877 (0.0%)
All	All	0.40	0/11629	0.58	1/15869 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	601	ASP	C-N-CA	6.70	138.45	121.70

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	5731	0	5492	27	0
1	B	5646	0	5370	27	0
2	C	61	0	52	0	0
2	E	61	0	52	0	0
2	F	61	0	52	0	0
3	D	28	0	25	0	0
4	G	39	0	34	0	0
5	H	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	126	0	117	0	0
6	B	112	0	104	0	0
7	A	28	30	0	0	0
7	B	28	30	0	0	0
8	A	23	0	0	0	0
8	B	17	0	0	0	0
All	All	12022	60	11350	52	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 2.

All (52) 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:670:HIS:HA	1:B:694:ASP:HB3	1.89	0.55
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.89	0.54
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.90	0.54
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.89	0.54
1:A:538:THR:HG22	1:A:562:SER:HB2	1.89	0.53
1:B:409:ILE:HD12	1:B:430:ILE:HD11	1.90	0.53
1:A:409:ILE:HD12	1:A:430:ILE:HD11	1.91	0.52
1:A:606:GLU:HB3	1:A:637:GLY:HA3	1.91	0.52
1:A:572:GLY:HA2	1:B:267:CYS:H	1.76	0.51
1:A:620:LEU:HA	1:A:623:LEU:HD12	1.93	0.51
1:B:381:GLU:HG3	1:B:408:GLN:HB3	1.92	0.50
1:B:592:SER:HA	1:B:616:SER:O	2.12	0.50
1:A:382:LEU:HB3	1:A:409:ILE:HG12	1.93	0.50
1:B:382:LEU:HB3	1:B:409:ILE:HG12	1.92	0.50
1:B:532:VAL:HB	1:B:553:LEU:HD22	1.95	0.49
1:B:127:LEU:HD21	1:B:130:LEU:HD13	1.95	0.48
1:A:532:VAL:HB	1:A:553:LEU:HD22	1.94	0.48
1:A:266:PRO:HA	1:B:572:GLY:HA3	1.95	0.48
1:A:127:LEU:HD21	1:A:130:LEU:HD13	1.95	0.47
1:A:599:LEU:HB2	1:A:631:TYR:HE1	1.80	0.46
1:B:302:ILE:HD11	1:B:323:LEU:HD13	1.98	0.46
1:B:154:ILE:HG12	1:B:178:ALA:HB3	1.98	0.46
1:A:302:ILE:HD11	1:A:323:LEU:HD13	1.98	0.45
1:B:577:LEU:HD12	1:B:599:LEU:HD21	1.98	0.45
1:B:620:LEU:HA	1:B:623:LEU:HD12	1.98	0.45
1:B:718:LEU:HA	1:B:742:ASP:HB3	1.99	0.45
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HG12	1:A:178:ALA:HB3	1.99	0.44
1:A:592:SER:HA	1:A:616:SER:O	2.17	0.44
1:A:67:GLU:HG2	1:A:91:LYS:HB3	2.00	0.44
1:B:228:PHE:HA	1:B:252:ASP:HB3	2.01	0.42
1:A:740:HIS:HD2	1:A:766:MET:HB3	1.84	0.42
1:B:323:LEU:HB3	1:B:326:GLU:HB2	2.02	0.42
1:B:740:HIS:HD2	1:B:766:MET:HB3	1.84	0.42
1:A:228:PHE:HA	1:A:252:ASP:HB3	2.00	0.42
1:A:573:VAL:HB	1:A:574:THR:H	1.74	0.41
1:B:530:PRO:HA	1:B:553:LEU:HD23	2.01	0.41
1:B:545:ASP:HA	1:B:576:HIS:HB2	2.01	0.41
1:B:127:LEU:HD23	1:B:145:PRO:HG2	2.03	0.41
1:A:530:PRO:HA	1:A:553:LEU:HD23	2.01	0.41
1:B:520:VAL:HA	1:B:543:ASP:HB3	2.02	0.41
1:B:208:LEU:HD13	1:B:217:PRO:HG2	2.02	0.41
1:A:612:GLU:HG3	1:A:643:ARG:HB3	2.03	0.41
1:A:208:LEU:HD13	1:A:217:PRO:HG2	2.02	0.41
1:B:203:LEU:HD21	1:B:206:LEU:HB2	2.03	0.41
1:B:715:ARG:HA	1:B:738:LEU:HA	2.01	0.41
1:A:520:VAL:HA	1:A:543:ASP:HB3	2.02	0.40
1:A:270:CYS:HB3	1:A:274:ALA:HB3	2.02	0.40
1:A:621:ASP:O	1:A:625:ASN:HB2	2.22	0.40
1:B:538:THR:HG22	1:B:562:SER:HB2	2.04	0.40
1:A:203:LEU:HD21	1:A:206:LEU:HB2	2.03	0.40
1:B:621:ASP:O	1:B:625:ASN:HB2	2.22	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	728/811 (90%)	667 (92%)	58 (8%)	3 (0%)	34 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	724/811 (89%)	661 (91%)	60 (8%)	3 (0%)	34	48
All	All	1452/1622 (90%)	1328 (92%)	118 (8%)	6 (0%)	34	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	602	LYS
1	B	573	VAL
1	A	575	HIS
1	A	378	VAL
1	B	378	VAL
1	A	573	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	625/755 (83%)	610 (98%)	15 (2%)	49	67
1	B	612/755 (81%)	594 (97%)	18 (3%)	42	60
All	All	1237/1510 (82%)	1204 (97%)	33 (3%)	44	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	160	ASN
1	A	170	ILE
1	A	261	PHE
1	A	289	LEU
1	A	296	SER
1	A	388	GLN
1	A	504	LEU
1	A	573	VAL
1	A	585	ASN

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Mol	Chain	Res	Type
1	A	605	LEU
1	A	606	GLU
1	A	671	ILE
1	A	735	VAL
1	A	764	LEU
1	B	49	CYS
1	B	160	ASN
1	B	170	ILE
1	B	261	PHE
1	B	289	LEU
1	B	296	SER
1	B	429	ARG
1	B	504	LEU
1	B	545	ASP
1	B	573	VAL
1	B	574	THR
1	B	599	LEU
1	B	601	ASP
1	B	604	ASN
1	B	671	ILE
1	B	689	ARG
1	B	764	LEU
1	B	792	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	284	GLN
1	B	97	ASN
1	B	262	ASN
1	B	576	HIS

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 ⓘ

25 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	0.32	0	17,19,21	0.83	1 (5%)
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
2	BMA	C	3	2	11,11,12	0.35	0	15,15,17	0.66	0
2	MAN	C	4	2	11,11,12	0.39	0	15,15,17	0.82	1 (6%)
2	MAN	C	5	2	11,11,12	0.39	0	15,15,17	0.85	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.30	0	17,19,21	0.60	0
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.62	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.60	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.52	0
2	BMA	E	3	2	11,11,12	0.32	0	15,15,17	0.48	0
2	MAN	E	4	2	11,11,12	0.37	0	15,15,17	0.80	1 (6%)
2	MAN	E	5	2	11,11,12	0.41	0	15,15,17	0.97	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
2	NAG	F	2	2	14,14,15	0.27	0	17,19,21	0.64	0
2	BMA	F	3	2	11,11,12	0.31	0	15,15,17	0.65	0
2	MAN	F	4	2	11,11,12	0.37	0	15,15,17	0.95	1 (6%)
2	MAN	F	5	2	11,11,12	0.42	0	15,15,17	1.10	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	G	2	4	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
4	BMA	G	3	4	11,11,12	0.35	0	15,15,17	0.53	0
5	NAG	H	1	1,5	14,14,15	0.26	0	17,19,21	0.60	0
5	NAG	H	2	5	14,14,15	0.28	0	17,19,21	0.54	0
5	BMA	H	3	5	11,11,12	0.30	0	15,15,17	0.47	0
5	MAN	H	4	5	11,11,12	0.41	0	15,15,17	0.94	2 (13%)
5	MAN	H	5	5	11,11,12	0.35	0	15,15,17	0.76	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	-	1/2/19/22	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
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	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
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	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	1/2/19/22	1/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	MAN	C1-O5-C5	3.67	117.16	112.19
2	F	4	MAN	C1-O5-C5	3.36	116.75	112.19
2	E	5	MAN	C1-O5-C5	2.92	116.14	112.19
2	C	5	MAN	C1-O5-C5	2.58	115.69	112.19
2	E	4	MAN	C1-O5-C5	2.57	115.68	112.19
2	C	2	NAG	O5-C1-C2	-2.57	107.23	111.29
5	H	5	MAN	C1-O5-C5	2.53	115.62	112.19
2	F	1	NAG	O5-C1-C2	-2.46	107.41	111.29
5	H	4	MAN	C1-O5-C5	2.46	115.52	112.19
2	C	1	NAG	O5-C1-C2	-2.44	107.43	111.29
4	G	2	NAG	C1-O5-C5	2.37	115.41	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	4	MAN	C1-C2-C3	2.36	112.57	109.67
2	C	4	MAN	C1-O5-C5	2.34	115.37	112.19
3	D	2	NAG	C1-O5-C5	2.19	115.17	112.19
2	E	5	MAN	C1-C2-C3	2.01	112.13	109.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

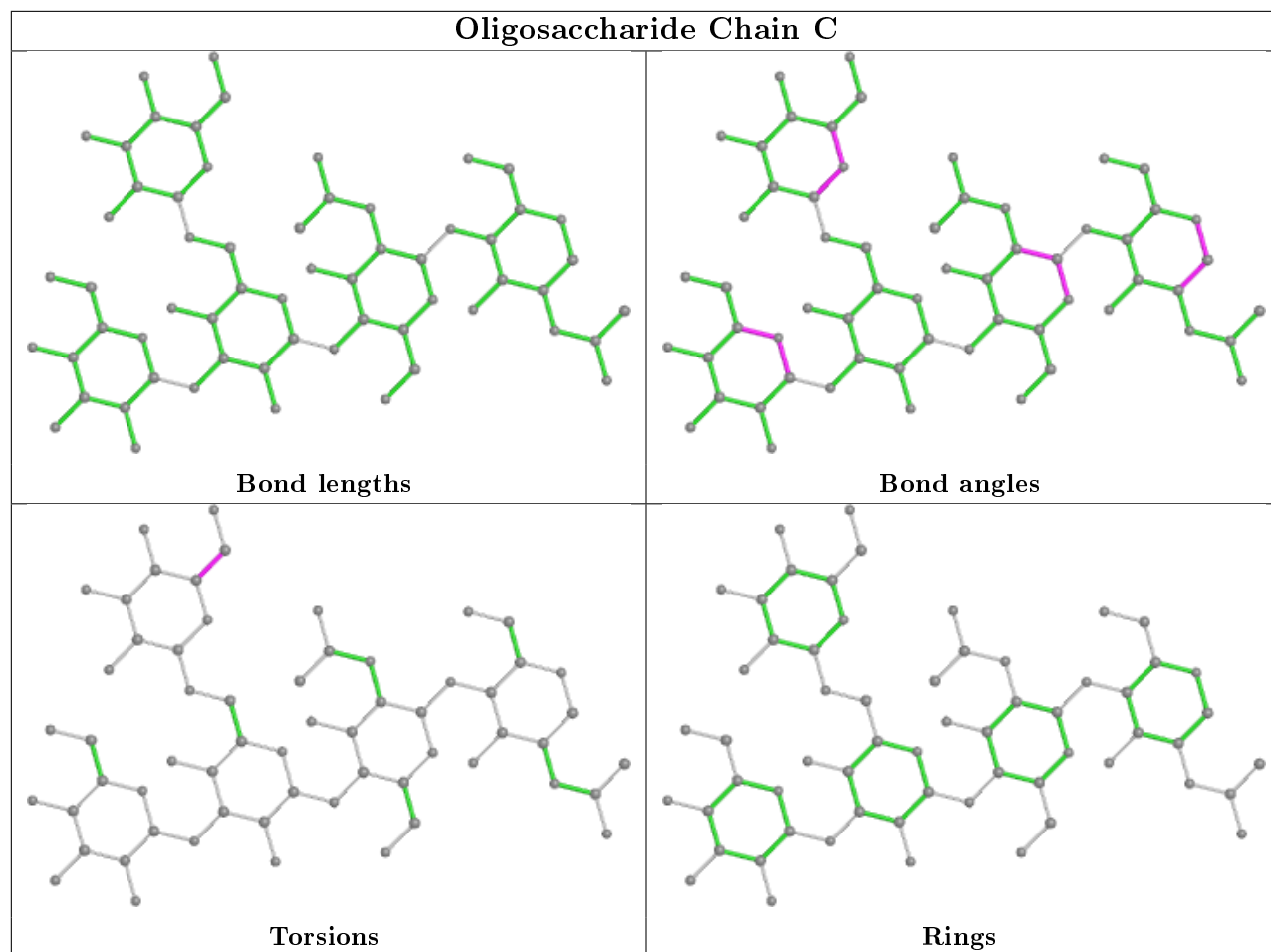
Mol	Chain	Res	Type	Atoms
5	H	4	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6

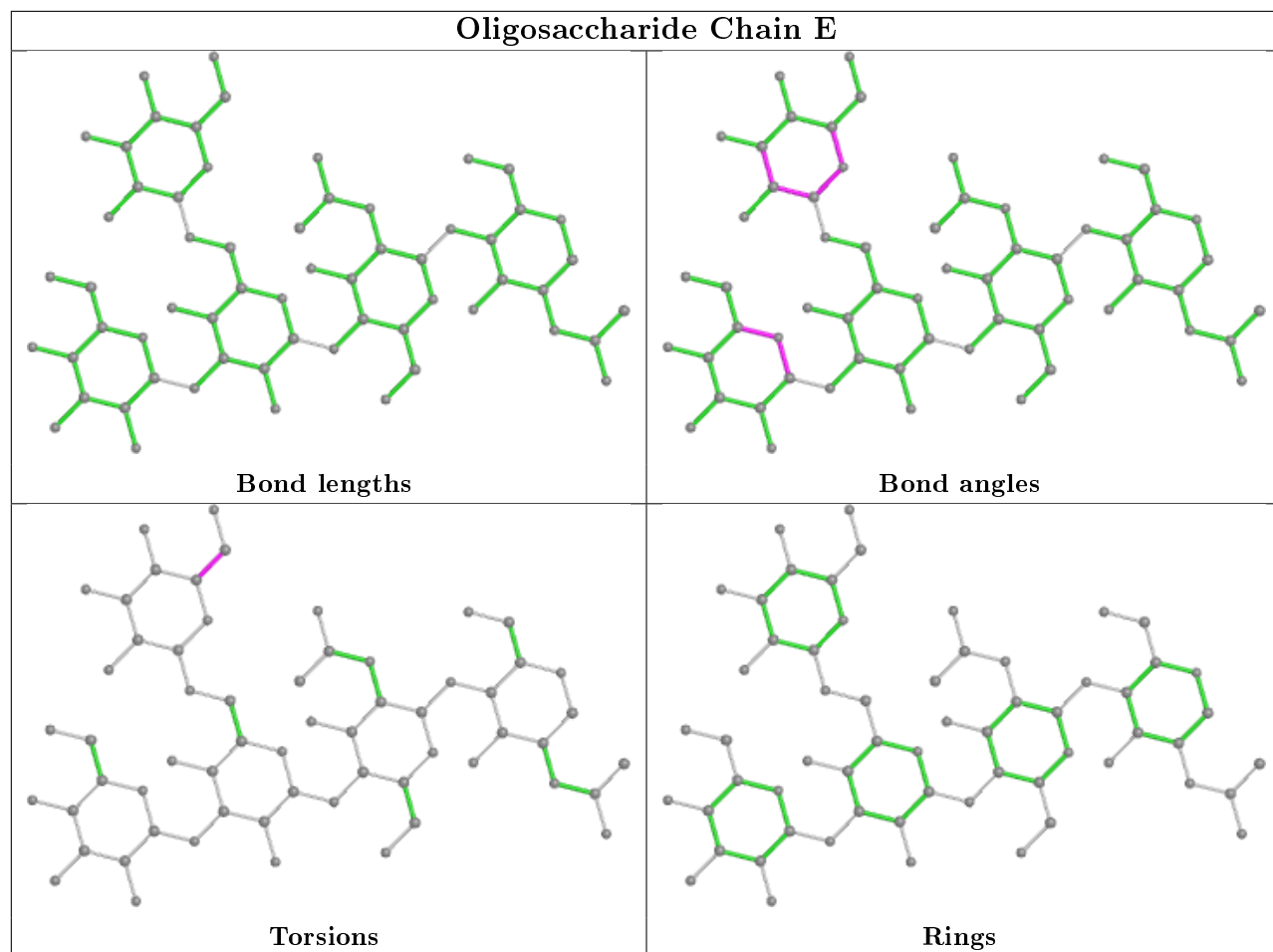
All (1) ring outliers are listed below:

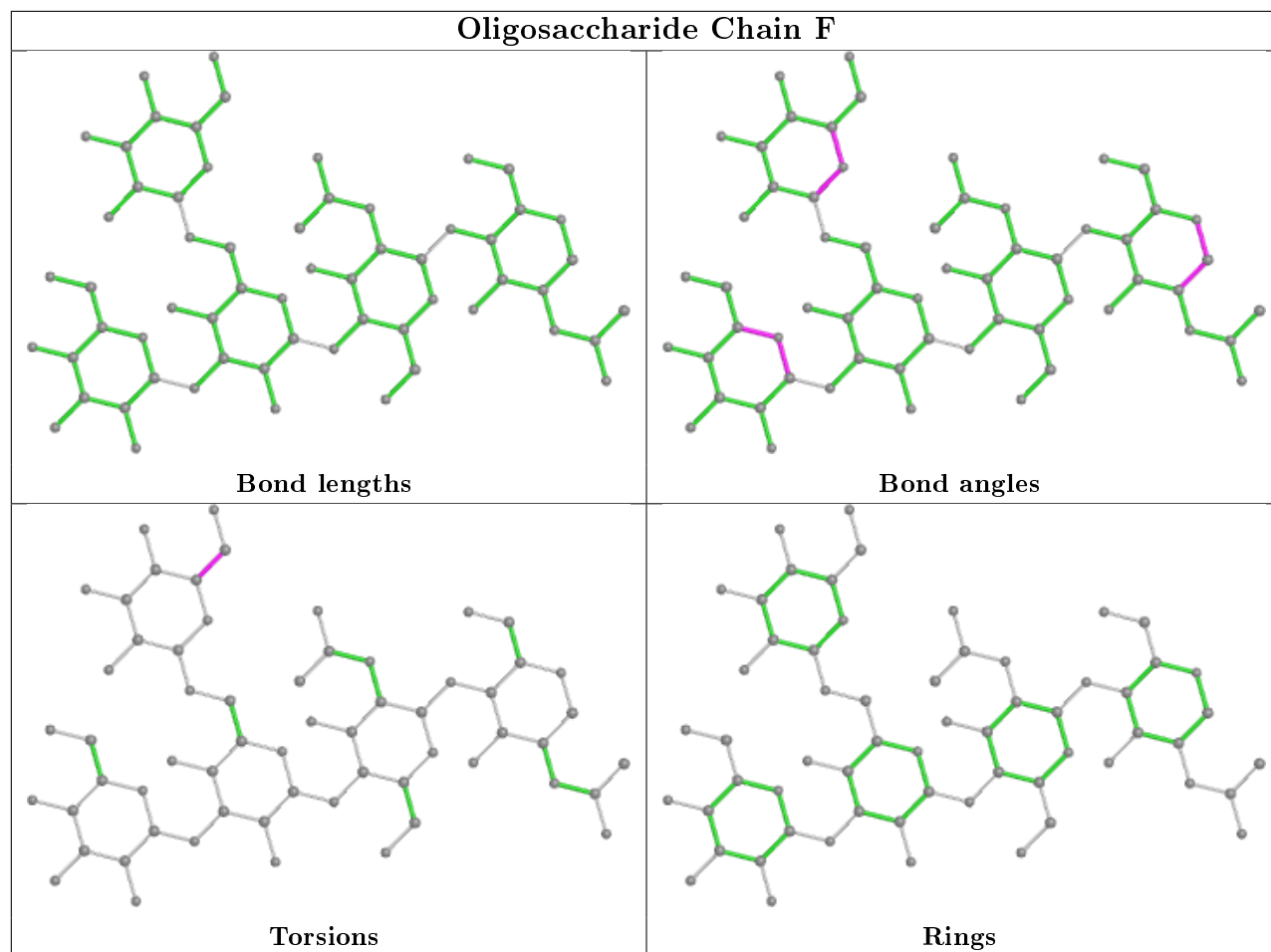
Mol	Chain	Res	Type	Atoms
5	H	5	MAN	C1-C2-C3-C4-C5-O5

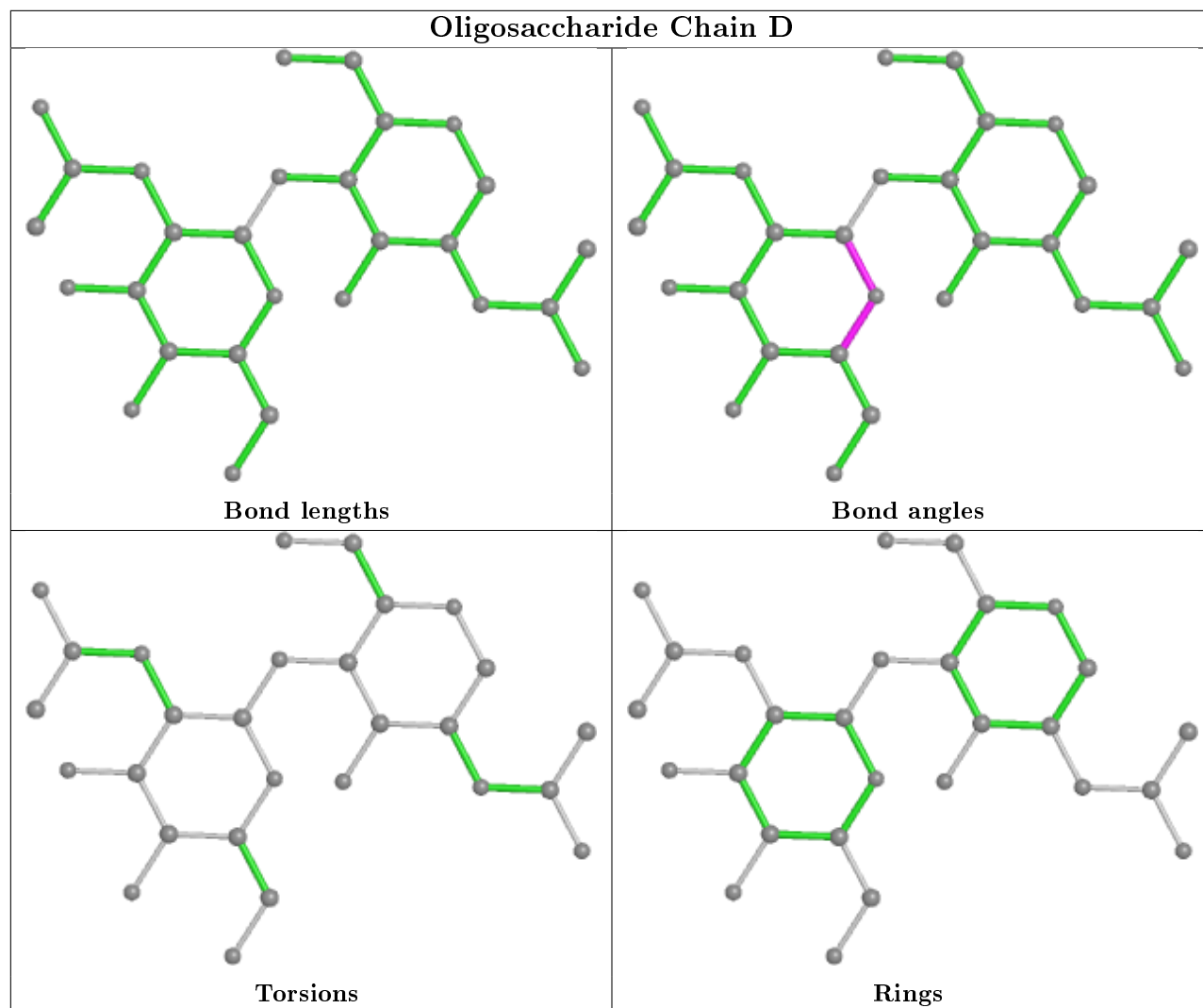
No monomer is involved in short contacts.

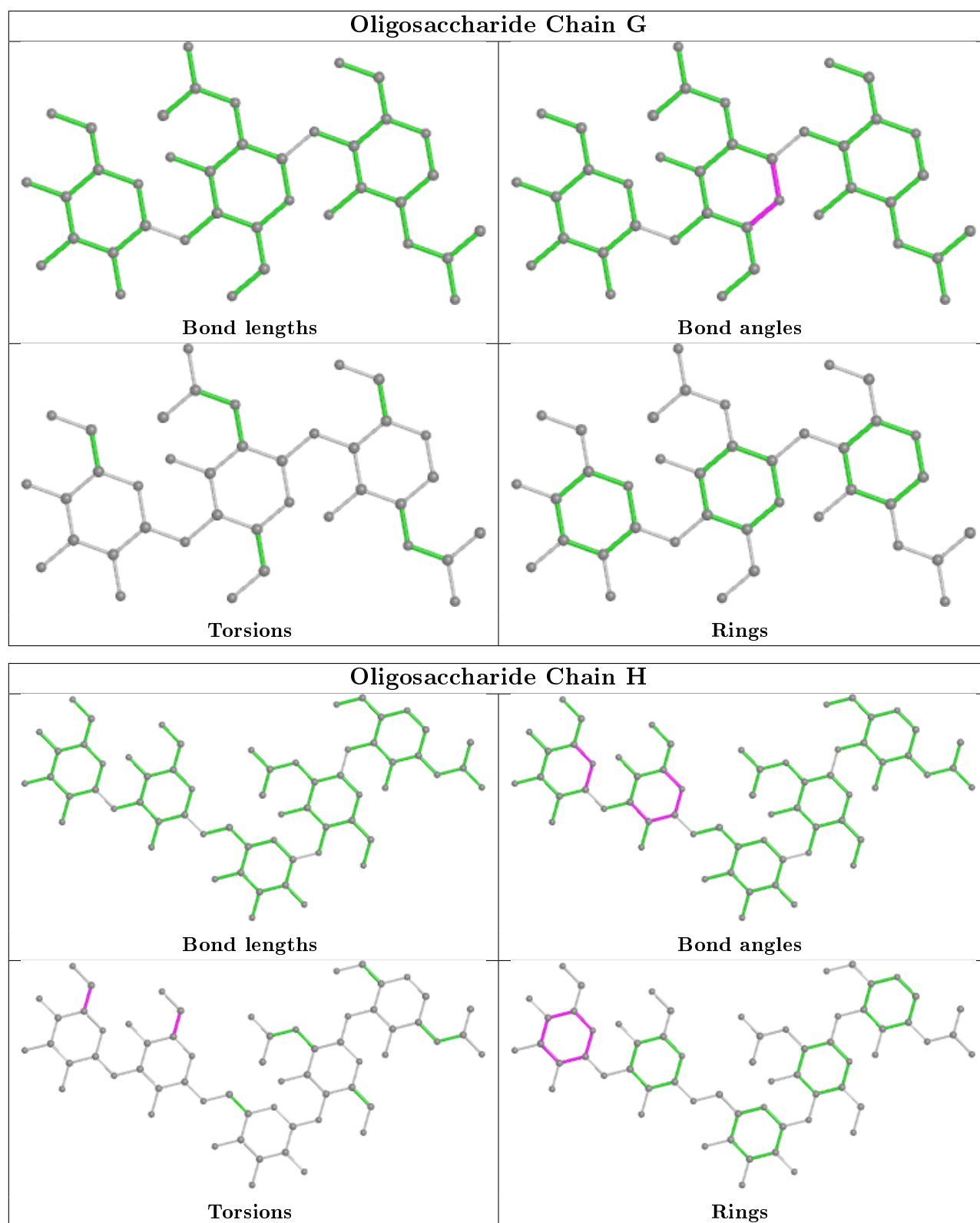
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
6	NAG	A	921	1	14,14,15	0.29	0	17,19,21	0.55	0
6	NAG	B	921	1	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
6	NAG	B	901	1	14,14,15	0.30	0	17,19,21	0.55	0
7	QSM	A	922	-	31,31,31	0.97	1 (3%)	35,44,44	0.91	2 (5%)
6	NAG	A	901	1	14,14,15	0.44	0	17,19,21	1.60	2 (11%)
6	NAG	A	908	1	14,14,15	0.31	0	17,19,21	0.40	0
6	NAG	A	902	1	14,14,15	0.30	0	17,19,21	0.59	0
6	NAG	A	918	1	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	B	919	1	14,14,15	0.30	0	17,19,21	0.50	0
6	NAG	A	919	1	14,14,15	0.30	0	17,19,21	0.66	1 (5%)
6	NAG	A	912	1	14,14,15	0.34	0	17,19,21	0.49	0
6	NAG	A	920	1	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
6	NAG	B	902	1	14,14,15	0.31	0	17,19,21	0.45	0
6	NAG	B	920	1	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
7	QSM	B	922	-	31,31,31	0.96	1 (3%)	35,44,44	0.91	2 (5%)
6	NAG	B	908	1	14,14,15	0.30	0	17,19,21	0.42	0
6	NAG	B	913	1	14,14,15	0.28	0	17,19,21	0.51	0
6	NAG	B	909	1	14,14,15	0.28	0	17,19,21	0.54	0
6	NAG	A	909	1	14,14,15	0.34	0	17,19,21	1.13	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	921	1	-	1/6/23/26	0/1/1/1
6	NAG	B	921	1	-	0/6/23/26	0/1/1/1
6	NAG	B	901	1	-	1/6/23/26	0/1/1/1
7	QSM	A	922	-	-	2/16/24/24	0/4/4/4
6	NAG	A	901	1	-	3/6/23/26	0/1/1/1
6	NAG	A	908	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
6	NAG	A	918	1	-	1/6/23/26	0/1/1/1
6	NAG	B	919	1	-	1/6/23/26	0/1/1/1
6	NAG	A	919	1	-	0/6/23/26	0/1/1/1
6	NAG	A	912	1	-	2/6/23/26	0/1/1/1
6	NAG	A	920	1	-	0/6/23/26	0/1/1/1
6	NAG	B	902	1	-	0/6/23/26	0/1/1/1
6	NAG	B	920	1	-	0/6/23/26	0/1/1/1
7	QSM	B	922	-	-	2/16/24/24	0/4/4/4
6	NAG	B	908	1	-	2/6/23/26	0/1/1/1
6	NAG	B	913	1	-	0/6/23/26	0/1/1/1
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	A	909	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	922	QSM	C7-C4	4.27	1.45	1.40
7	B	922	QSM	C7-C4	4.22	1.45	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	901	NAG	C1-C2-N2	4.91	118.87	110.49
6	A	901	NAG	C2-N2-C7	4.23	128.93	122.90
6	A	909	NAG	C1-O5-C5	3.13	116.43	112.19
7	A	922	QSM	C-C5-C4	-3.09	119.94	122.00
7	B	922	QSM	C-C5-C4	-3.08	119.95	122.00
7	B	922	QSM	C6-N-C3	2.71	109.46	103.90
7	A	922	QSM	C6-N-C3	2.68	109.42	103.90
6	A	909	NAG	C2-N2-C7	2.33	126.22	122.90
6	A	920	NAG	C1-O5-C5	2.33	115.35	112.19
6	B	920	NAG	C1-O5-C5	2.19	115.16	112.19
6	B	921	NAG	C1-O5-C5	2.18	115.15	112.19
6	A	919	NAG	C1-O5-C5	2.16	115.12	112.19
6	A	909	NAG	C1-C2-N2	2.10	114.08	110.49

There are no chirality outliers.

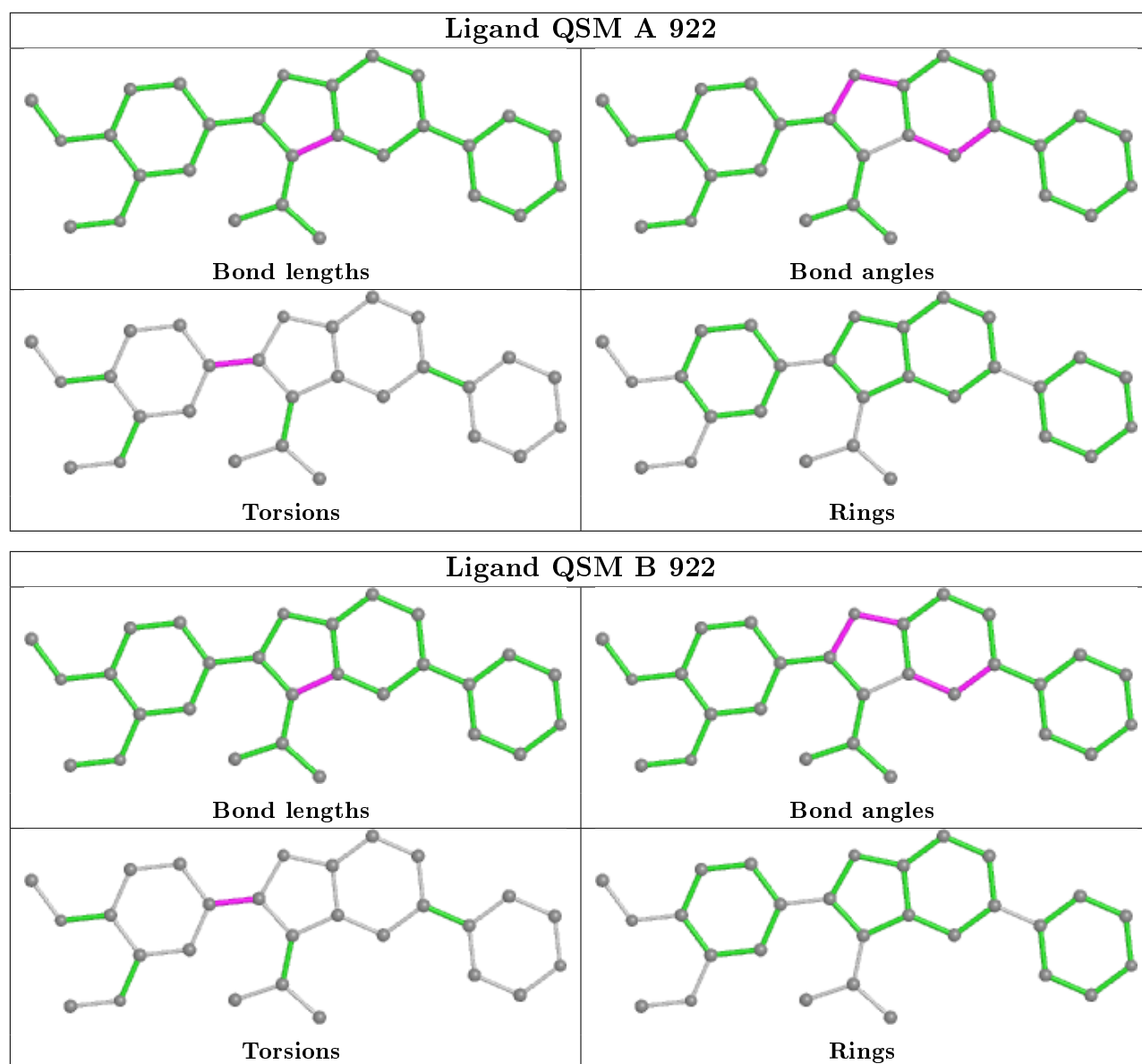
All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	922	QSM	C13-C11-C6-N
7	B	922	QSM	C13-C11-C6-N
7	B	922	QSM	C17-C11-C6-N
6	A	908	NAG	O5-C5-C6-O6
6	B	908	NAG	O5-C5-C6-O6
6	B	908	NAG	C4-C5-C6-O6
6	A	912	NAG	O5-C5-C6-O6
6	A	908	NAG	C4-C5-C6-O6
6	A	901	NAG	O5-C5-C6-O6
6	B	901	NAG	O5-C5-C6-O6
6	A	912	NAG	C4-C5-C6-O6
6	A	918	NAG	O5-C5-C6-O6
6	B	919	NAG	O5-C5-C6-O6
7	A	922	QSM	C17-C11-C6-N
6	A	921	NAG	O5-C5-C6-O6
6	A	909	NAG	C3-C2-N2-C7
6	A	901	NAG	C1-C2-N2-C7
6	A	901	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	738/811 (90%)	1.90	264 (35%) 0 0	34, 105, 188, 224	0
1	B	735/811 (90%)	1.54	214 (29%) 0 0	30, 92, 170, 203	0
All	All	1473/1622 (90%)	1.72	478 (32%) 0 0	30, 96, 181, 224	0

All (478) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	LEU	21.2
1	A	750	THR	21.1
1	B	783	PHE	14.2
1	A	805	SER	14.1
1	A	113	GLY	13.4
1	A	809	GLN	12.1
1	B	728	PRO	11.9
1	B	750	THR	11.8
1	A	814	ILE	11.0
1	B	779	ASP	11.0
1	B	769	LEU	10.7
1	A	804	ALA	10.5
1	B	801	VAL	9.9
1	A	815	VAL	9.8
1	A	165	GLY	9.6
1	A	121	PHE	9.5
1	B	804	ALA	9.3
1	A	783	PHE	9.3
1	B	817	LEU	9.0
1	B	780	ILE	8.8
1	A	729	SER	8.7
1	A	702	PHE	8.5
1	B	58	PRO	8.5
1	B	702	PHE	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	751	ILE	8.2
1	B	46	ILE	7.9
1	A	159	TYR	7.9
1	B	773	PRO	7.9
1	A	780	ILE	7.8
1	A	703	LEU	7.8
1	B	774	PHE	7.7
1	A	724	ILE	7.7
1	B	74	PHE	7.7
1	A	52	ARG	7.7
1	A	141	PRO	7.7
1	A	779	ASP	7.7
1	B	814	ILE	7.6
1	B	678	PHE	7.4
1	A	782	ASP	7.3
1	A	710	PHE	7.3
1	A	728	PRO	7.3
1	A	767	LEU	7.3
1	A	169	LEU	7.3
1	B	52	ARG	7.2
1	A	801	VAL	7.2
1	A	792	ASN	7.2
1	A	731	PHE	7.1
1	A	818	GLU	7.1
1	A	56	GLU	6.9
1	A	774	PHE	6.9
1	B	743	LEU	6.9
1	A	60	THR	6.7
1	A	704	THR	6.6
1	A	695	LEU	6.5
1	A	164	GLU	6.4
1	A	679	PHE	6.3
1	A	78	ILE	6.3
1	A	114	LEU	6.3
1	B	726	HIS	6.1
1	B	802	ILE	6.1
1	B	700	LEU	6.0
1	A	156	ASN	5.9
1	B	731	PHE	5.9
1	B	805	SER	5.9
1	B	733	SER	5.9
1	A	157	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	121	PHE	5.8
1	A	772	ASN	5.6
1	B	676	LEU	5.6
1	B	724	ILE	5.6
1	B	544	PHE	5.5
1	A	741	LEU	5.5
1	A	58	PRO	5.5
1	A	92	ILE	5.5
1	A	183	PHE	5.5
1	B	811	GLY	5.5
1	A	769	LEU	5.5
1	A	793	VAL	5.5
1	A	787	MET	5.5
1	B	710	PHE	5.5
1	B	236	TYR	5.4
1	A	94	LEU	5.4
1	A	131	LEU	5.4
1	A	766	MET	5.4
1	A	142	SER	5.3
1	A	719	LEU	5.3
1	B	741	LEU	5.3
1	A	74	PHE	5.3
1	A	692	LEU	5.3
1	B	701	LEU	5.3
1	A	96	HIS	5.3
1	B	748	LEU	5.3
1	A	118	ASP	5.2
1	A	748	LEU	5.2
1	B	793	VAL	5.2
1	A	82	SER	5.1
1	B	815	VAL	5.1
1	A	693	LEU	5.0
1	A	678	PHE	5.0
1	A	137	LEU	5.0
1	A	470	PHE	5.0
1	A	99	ASN	4.9
1	A	184	ASN	4.9
1	B	729	SER	4.9
1	B	723	ARG	4.9
1	B	144	LEU	4.9
1	B	719	LEU	4.9
1	A	155	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	83	PHE	4.8
1	A	255	GLY	4.8
1	B	183	PHE	4.8
1	A	718	LEU	4.8
1	A	754	SER	4.8
1	B	767	LEU	4.7
1	A	743	LEU	4.7
1	A	161	ILE	4.7
1	B	113	GLY	4.7
1	A	197	PHE	4.7
1	B	179	TRP	4.6
1	B	778	CYS	4.6
1	A	751	ILE	4.6
1	A	717	LEU	4.6
1	A	762	THR	4.6
1	B	718	LEU	4.6
1	A	786	TRP	4.5
1	B	790	HIS	4.5
1	B	796	PRO	4.5
1	B	730	GLY	4.5
1	A	753	LYS	4.5
1	A	138	PRO	4.4
1	A	70	LEU	4.4
1	B	772	ASN	4.4
1	B	165	GLY	4.4
1	A	65	VAL	4.4
1	B	141	PRO	4.4
1	A	217	PRO	4.4
1	A	68	LEU	4.4
1	A	148	LEU	4.4
1	A	686	GLN	4.4
1	A	262	ASN	4.3
1	B	571	ALA	4.3
1	B	679	PHE	4.3
1	A	154	ILE	4.3
1	A	135	ASN	4.3
1	B	787	MET	4.3
1	A	79	THR	4.3
1	A	653	HIS	4.3
1	A	93	ASN	4.3
1	B	72	ASP	4.3
1	A	115	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	786	TRP	4.2
1	B	762	THR	4.2
1	B	94	LEU	4.2
1	B	795	ILE	4.2
1	A	200	LEU	4.2
1	A	785	ARG	4.2
1	A	177	LEU	4.1
1	A	701	LEU	4.1
1	B	64	TYR	4.1
1	B	782	ASP	4.1
1	A	77	HIS	4.1
1	B	695	LEU	4.1
1	B	261	PHE	4.1
1	B	766	MET	4.1
1	A	130	LEU	4.1
1	A	778	CYS	4.1
1	A	144	LEU	4.1
1	B	70	LEU	4.0
1	A	461	PHE	4.0
1	A	467	PHE	4.0
1	A	95	ASN	4.0
1	A	676	LEU	4.0
1	B	631	TYR	4.0
1	A	132	LEU	4.0
1	B	727	LEU	4.0
1	B	75	ILE	4.0
1	A	709	ASP	4.0
1	A	733	SER	3.9
1	A	202	ASN	3.9
1	A	236[A]	TYR	3.9
1	A	775	GLU	3.9
1	B	547	ALA	3.9
1	A	166	ILE	3.9
1	B	749	LYS	3.9
1	A	730	GLY	3.9
1	A	160	ASN	3.9
1	A	740	HIS	3.8
1	A	790	HIS	3.8
1	B	776	CYS	3.8
1	B	661	ASN	3.8
1	A	727	LEU	3.8
1	B	703	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	53	ARG	3.8
1	A	172	LEU	3.8
1	B	803	CYS	3.8
1	A	700	LEU	3.8
1	B	166	ILE	3.8
1	B	671	ILE	3.8
1	A	191	ASN	3.7
1	A	682	THR	3.7
1	A	32	ARG	3.7
1	B	461	PHE	3.7
1	A	176	TYR	3.7
1	A	544	PHE	3.7
1	B	34	TYR	3.7
1	A	98	PRO	3.7
1	B	686	GLN	3.7
1	A	151	LEU	3.7
1	B	116	ILE	3.7
1	A	35	PRO	3.6
1	B	120	ALA	3.6
1	A	72	ASP	3.6
1	B	754	SER	3.6
1	A	192	ILE	3.6
1	A	264	PRO	3.6
1	A	190	THR	3.6
1	B	60	THR	3.6
1	A	175	LEU	3.6
1	A	53	ARG	3.5
1	A	683	LEU	3.5
1	A	116	ILE	3.5
1	A	266	PRO	3.5
1	A	578	GLU	3.5
1	A	749	LYS	3.5
1	B	797	ARG	3.5
1	A	746	ASN	3.5
1	B	78	ILE	3.5
1	B	131	LEU	3.5
1	B	653	HIS	3.5
1	A	795	ILE	3.5
1	B	45	VAL	3.5
1	B	777	THR	3.5
1	A	34	TYR	3.5
1	A	747	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	187	CYS	3.4
1	B	154	ILE	3.4
1	A	123	ASN	3.4
1	B	200	LEU	3.4
1	A	802	ILE	3.4
1	B	237	ILE	3.4
1	A	127	LEU	3.4
1	A	781	GLY	3.4
1	B	215	HIS	3.4
1	A	755	ALA	3.4
1	B	682	THR	3.3
1	A	215	HIS	3.3
1	B	734	GLU	3.3
1	A	464	HIS	3.3
1	B	71	SER	3.3
1	B	705	ASP	3.3
1	A	269	PRO	3.3
1	B	161	ILE	3.3
1	A	632	ILE	3.3
1	B	464	HIS	3.3
1	B	169	LEU	3.3
1	B	95	ASN	3.2
1	A	273	GLY	3.2
1	A	179	TRP	3.2
1	B	184	ASN	3.2
1	A	85	GLY	3.2
1	B	463	PRO	3.2
1	B	764	LEU	3.2
1	A	277	ASN	3.2
1	A	716	THR	3.2
1	A	69	ASP	3.2
1	A	261	PHE	3.2
1	A	244	GLY	3.2
1	B	83	PHE	3.1
1	B	660	LEU	3.1
1	A	789	GLU	3.1
1	A	736	SER	3.1
1	B	92	ILE	3.1
1	A	725	SER	3.1
1	B	54	LEU	3.1
1	A	808	ASP	3.1
1	B	752	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	PRO	3.1
1	A	796	PRO	3.1
1	A	153	LEU	3.0
1	B	683	LEU	3.0
1	B	717	LEU	3.0
1	A	75	ILE	3.0
1	A	33	SER	3.0
1	A	54	LEU	3.0
1	B	264	PRO	3.0
1	A	48	GLU	3.0
1	A	630	ARG	3.0
1	B	93	ASN	3.0
1	B	82	SER	3.0
1	A	644	LEU	3.0
1	A	651	LEU	3.0
1	A	55	GLN	3.0
1	B	658	ALA	3.0
1	A	654	ILE	3.0
1	B	688	PRO	3.0
1	B	162	THR	2.9
1	A	623	LEU	2.9
1	B	177	LEU	2.9
1	B	48	GLU	2.9
1	B	792	ASN	2.9
1	B	810	ARG	2.9
1	B	284	GLN	2.9
1	A	210	PHE	2.9
1	A	798	LEU	2.9
1	B	630	ARG	2.8
1	A	129	GLU	2.8
1	A	547	ALA	2.8
1	A	267	CYS	2.8
1	B	238	SER	2.8
1	A	245	LEU	2.8
1	B	543	ASP	2.8
1	A	707	LEU	2.8
1	A	773	PRO	2.8
1	B	65	VAL	2.8
1	B	268	VAL	2.8
1	A	180	ASN	2.8
1	B	600	THR	2.8
1	B	262	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	56	GLU	2.7
1	B	462	ASP	2.7
1	A	181	CYS	2.7
1	A	214	SER	2.7
1	B	470	PHE	2.7
1	A	726	HIS	2.7
1	B	213	LEU	2.7
1	A	462	ASP	2.7
1	B	768	GLU	2.7
1	B	637	GLY	2.7
1	A	771	GLY	2.7
1	B	669	LEU	2.7
1	A	174	ASN	2.7
1	A	124	LEU	2.7
1	A	208	LEU	2.6
1	A	660	LEU	2.6
1	B	68	LEU	2.6
1	B	38	GLU	2.6
1	B	742	ASP	2.6
1	B	800	ASP	2.6
1	B	155	GLN	2.6
1	A	664	ALA	2.6
1	A	816	SER	2.6
1	B	720	SER	2.6
1	A	309	ASN	2.6
1	B	746	ASN	2.6
1	B	681	TRP	2.6
1	A	218	PRO	2.6
1	B	35	PRO	2.6
1	A	89	LEU	2.6
1	A	237	ILE	2.6
1	A	258	PRO	2.6
1	B	576	HIS	2.6
1	B	646	LEU	2.6
1	B	568	PHE	2.6
1	B	737	SER	2.6
1	B	258	PRO	2.6
1	A	220	LEU	2.6
1	A	271	ASP	2.6
1	A	738	LEU	2.6
1	A	720	SER	2.6
1	B	217	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	212	SER	2.5
1	B	260	CYS	2.5
1	A	182	TYR	2.5
1	A	742	ASP	2.5
1	B	307	PHE	2.5
1	B	818	GLU	2.5
1	B	655	PRO	2.5
1	B	599	LEU	2.5
1	B	242	PHE	2.5
1	A	688	PRO	2.5
1	A	791	LEU	2.5
1	A	171	ASN	2.5
1	A	671	ILE	2.5
1	B	570	ILE	2.5
1	B	770	HIS	2.5
1	B	153	LEU	2.5
1	B	132	LEU	2.5
1	A	50	SER	2.5
1	A	120	ALA	2.4
1	A	283	PHE	2.4
1	A	134	ASP	2.4
1	B	765	SER	2.4
1	B	127	LEU	2.4
1	B	798	LEU	2.4
1	A	71	SER	2.4
1	A	57	VAL	2.4
1	A	614	VAL	2.4
1	A	136	GLN	2.4
1	B	130	LEU	2.4
1	A	712	SER	2.4
1	B	50	SER	2.4
1	B	633	SER	2.4
1	B	744	SER	2.4
1	B	736	SER	2.4
1	A	419	ASN	2.4
1	A	655	PRO	2.4
1	B	49	CYS	2.4
1	B	709	ASP	2.4
1	A	242	PHE	2.4
1	A	633	SER	2.4
1	B	33	SER	2.4
1	A	140	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	158	ILE	2.4
1	B	135	ASN	2.3
1	B	696	ARG	2.3
1	A	178	ALA	2.3
1	B	693	LEU	2.3
1	A	573	VAL	2.3
1	B	143	GLY	2.3
1	B	725	SER	2.3
1	A	45	VAL	2.3
1	A	216	VAL	2.3
1	A	268	VAL	2.3
1	B	735	VAL	2.3
1	A	193	GLU	2.3
1	A	723	ARG	2.3
1	A	152	SER	2.3
1	A	146	GLU	2.3
1	B	694	ASP	2.3
1	A	170	ILE	2.3
1	B	37	ASP	2.3
1	B	410	ASP	2.3
1	B	233	GLN	2.2
1	B	124	LEU	2.2
1	A	263	ALA	2.2
1	A	274	ALA	2.2
1	A	715	ARG	2.2
1	B	192	ILE	2.2
1	B	775	GLU	2.2
1	A	496	ILE	2.2
1	B	740	HIS	2.2
1	A	392	GLN	2.2
1	A	213	LEU	2.2
1	A	803	CYS	2.2
1	A	705	ASP	2.2
1	B	545	ASP	2.2
1	B	781	GLY	2.2
1	A	570	ILE	2.2
1	A	797	ARG	2.2
1	B	118	ASP	2.2
1	A	806	PRO	2.2
1	A	47	ALA	2.2
1	B	689	ARG	2.2
1	B	738	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	578	GLU	2.1
1	B	579	PHE	2.1
1	A	569	ARG	2.1
1	A	76	THR	2.1
1	B	605	LEU	2.1
1	B	791	LEU	2.1
1	B	269	PRO	2.1
1	A	195	GLY	2.1
1	A	810	ARG	2.1
1	B	567	TYR	2.1
1	B	651	LEU	2.1
1	A	668	GLU	2.1
1	B	176	TYR	2.1
1	B	182	TYR	2.1
1	A	284	GLN	2.1
1	A	51	ASN	2.1
1	A	37	ASP	2.1
1	A	598	THR	2.1
1	B	117	THR	2.1
1	B	704	THR	2.1
1	B	159	TYR	2.0
1	A	257	CYS	2.0
1	A	260	CYS	2.0
1	A	282	ALA	2.0
1	B	711	THR	2.0
1	B	632	ILE	2.0
1	A	133	GLU	2.0
1	B	47	ALA	2.0
1	B	157	ASN	2.0
1	A	600	THR	2.0
1	B	151	LEU	2.0
1	B	244	GLY	2.0
1	A	690	LEU	2.0
1	B	89	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 ⓘ

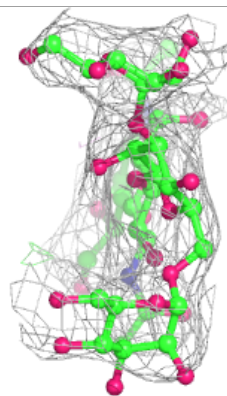
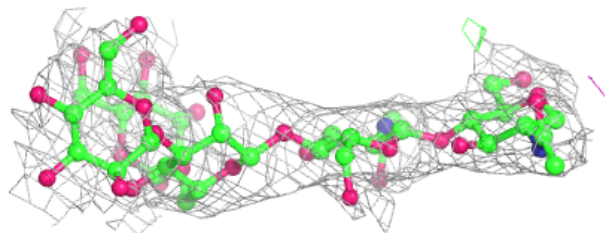
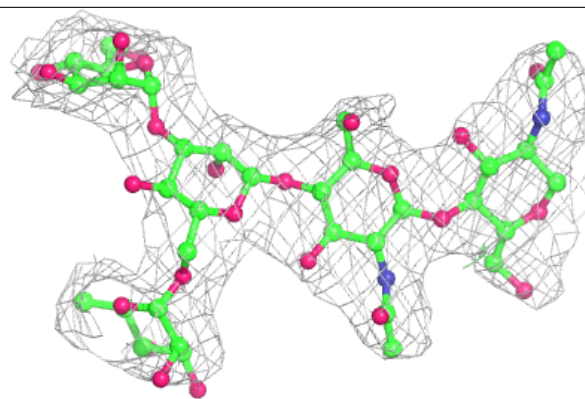
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	4	11/12	0.66	0.28	83,88,90,92	0
5	MAN	H	5	11/12	0.66	0.19	95,98,100,101	0
2	MAN	C	5	11/12	0.69	0.23	99,102,105,107	0
5	MAN	H	4	11/12	0.72	0.18	82,86,88,92	0
4	BMA	G	3	11/12	0.77	0.20	81,85,86,87	0
2	MAN	F	5	11/12	0.81	0.22	92,94,95,96	0
2	MAN	E	5	11/12	0.81	0.15	81,84,89,91	0
2	MAN	F	4	11/12	0.81	0.17	89,89,90,91	0
2	MAN	C	4	11/12	0.84	0.21	97,102,107,109	0
4	NAG	G	2	14/15	0.84	0.19	65,69,73,77	0
2	BMA	C	3	11/12	0.85	0.15	90,97,102,102	0
5	BMA	H	3	11/12	0.85	0.13	63,67,73,78	0
2	BMA	E	3	11/12	0.89	0.13	71,75,79,80	0
3	NAG	D	2	14/15	0.89	0.15	51,55,57,57	0
2	BMA	F	3	11/12	0.89	0.15	79,84,89,90	0
2	NAG	F	2	14/15	0.91	0.20	63,65,68,72	0
2	NAG	E	1	14/15	0.91	0.17	44,51,58,59	0
4	NAG	G	1	14/15	0.93	0.18	50,51,55,60	0
5	NAG	H	2	14/15	0.93	0.14	44,49,53,59	0
2	NAG	F	1	14/15	0.94	0.22	47,55,60,61	0
2	NAG	C	1	14/15	0.94	0.22	60,63,65,69	0
5	NAG	H	1	14/15	0.94	0.14	30,37,42,43	0
2	NAG	C	2	14/15	0.95	0.19	72,76,81,84	0
2	NAG	E	2	14/15	0.96	0.11	54,58,62,68	0
3	NAG	D	1	14/15	0.96	0.17	39,43,45,49	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.

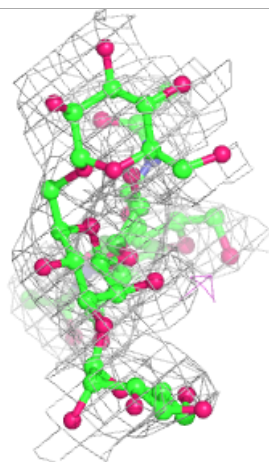
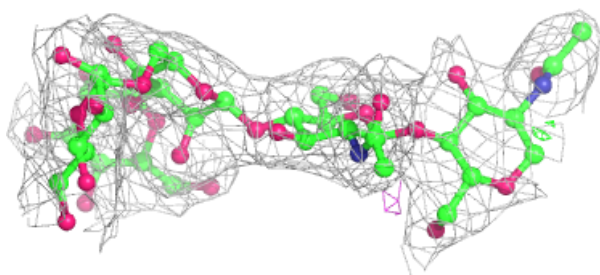
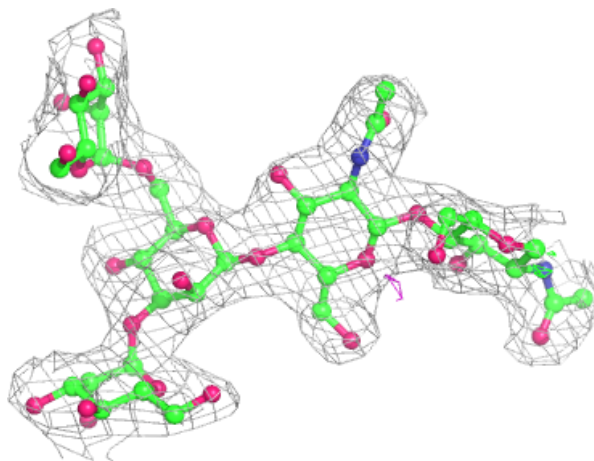
Electron density around Chain C:

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



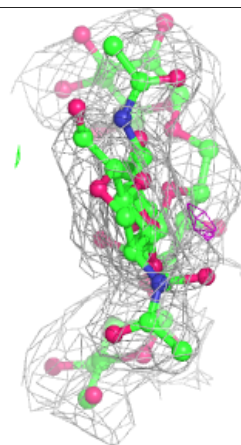
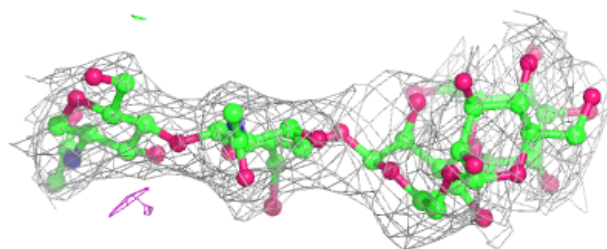
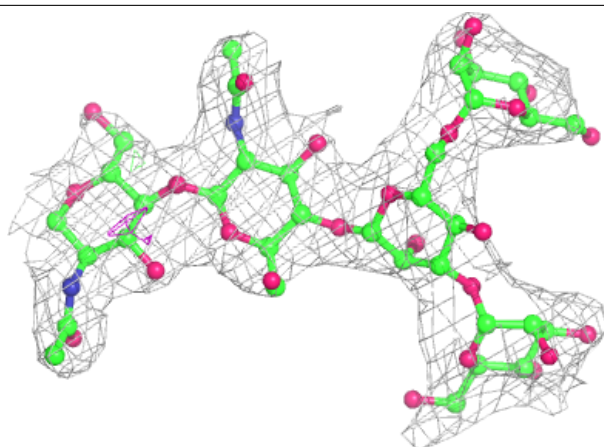
Electron density around Chain E:

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



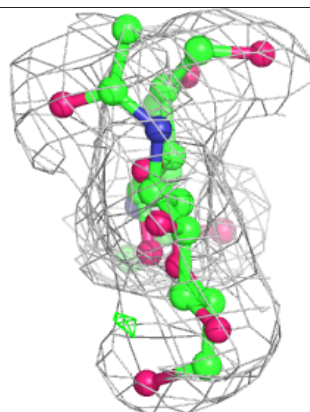
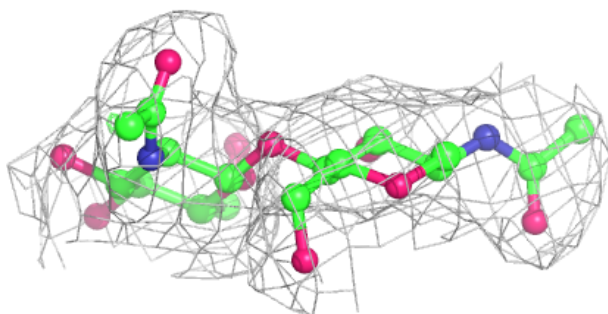
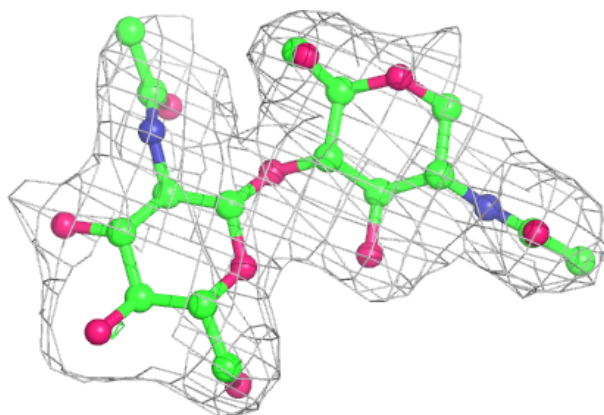
Electron density around Chain F:

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

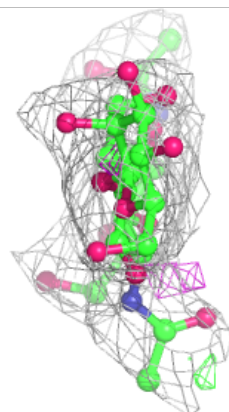
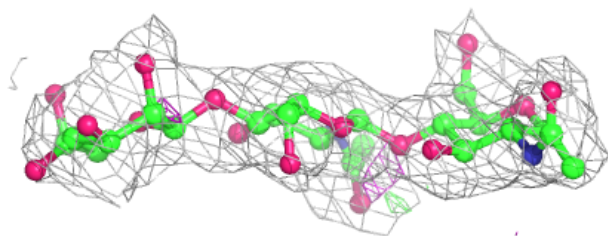
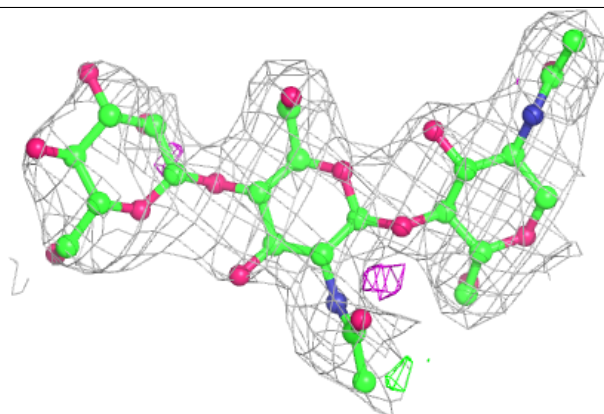


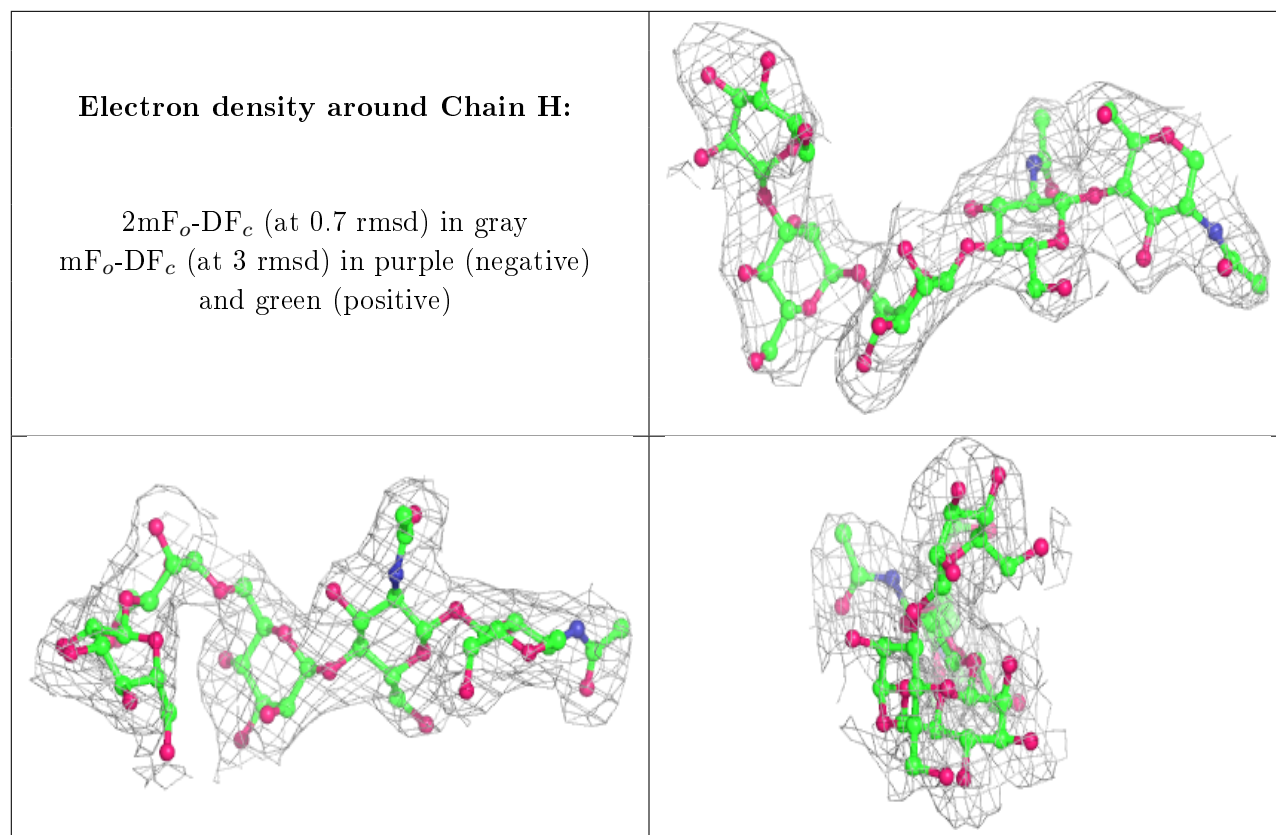
Electron density around Chain D:

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

**Electron density around Chain G:**

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





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.

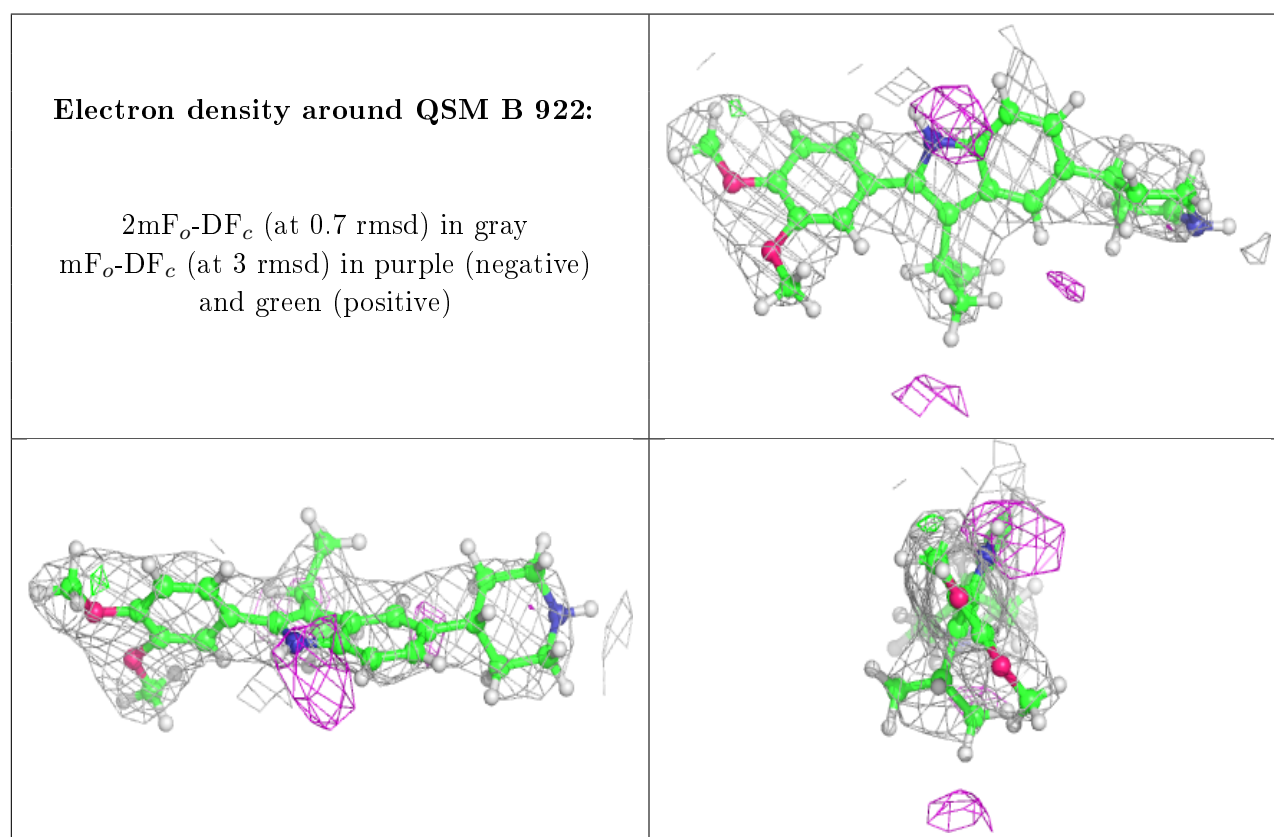
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	B	901	14/15	0.30	0.77	174,174,175,176	0
6	NAG	A	901	14/15	0.45	0.37	195,200,203,204	0
6	NAG	B	908	14/15	0.48	0.40	99,108,115,117	0
6	NAG	A	902	14/15	0.51	0.39	128,138,149,149	0
6	NAG	B	919	14/15	0.55	0.39	115,126,136,140	0
6	NAG	B	909	14/15	0.61	0.26	124,127,134,134	0
6	NAG	A	918	14/15	0.63	0.42	120,134,147,151	0
6	NAG	A	921	14/15	0.67	0.48	110,112,122,122	0
6	NAG	A	920	14/15	0.68	0.36	113,123,129,133	0
6	NAG	A	908	14/15	0.69	0.27	87,89,94,97	0
6	NAG	B	921	14/15	0.70	0.30	137,143,151,151	0
6	NAG	B	902	14/15	0.71	0.30	135,139,147,152	0
6	NAG	A	909	14/15	0.74	0.34	118,124,126,128	0
6	NAG	A	912	14/15	0.76	0.29	124,128,131,134	0

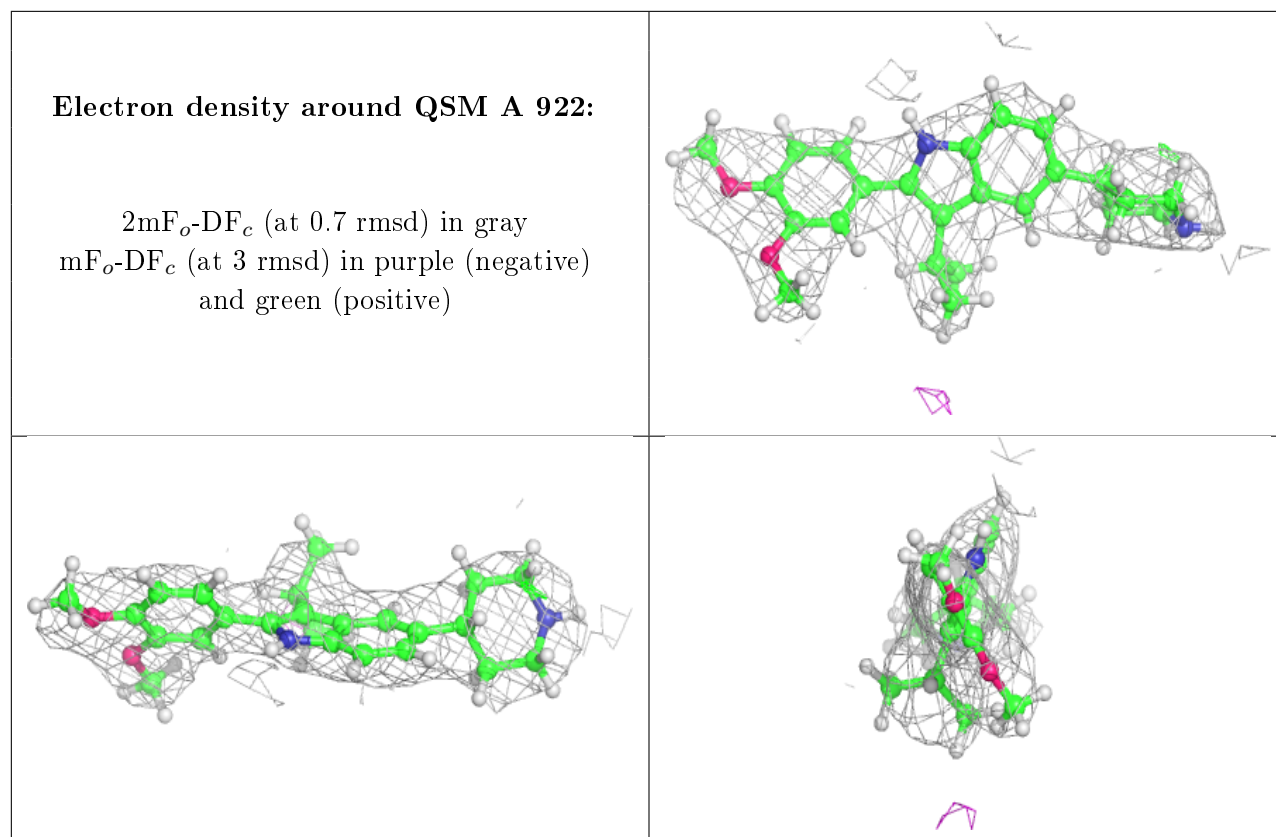
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	B	913	14/15	0.77	0.23	118,122,124,126	0
6	NAG	A	919	14/15	0.79	0.20	150,153,154,154	0
6	NAG	B	920	14/15	0.79	0.19	154,156,158,159	0
7	QSM	B	922	28/28	0.91	0.24	43,50,58,58	30
7	QSM	A	922	28/28	0.95	0.20	38,44,45,45	30

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.