



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2022 – 03:09 pm GMT

PDB ID : 7R54
Title : Crystal structure of human TLR8 in complex with Compound 4
Authors : Faller, M.; Zink, F.
Deposited on : 2022-02-10
Resolution : 2.84 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

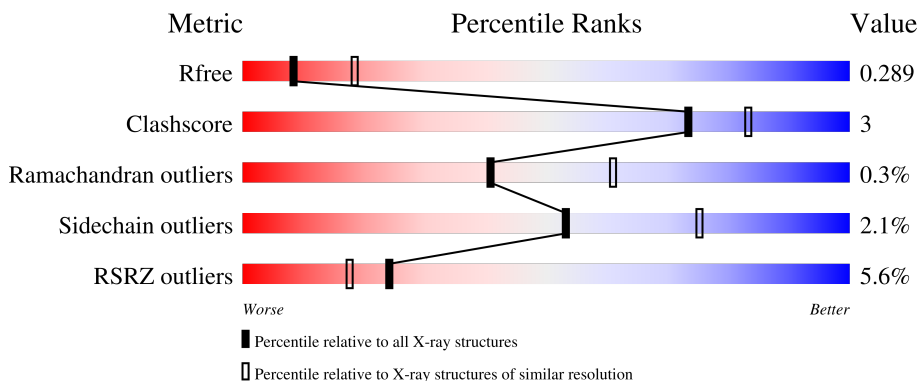
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	807	
1	B	807	
2	C	5	
2	E	5	
2	F	5	

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Mol	Chain	Length	Quality of chain
2	H	5	 60% 40%
3	D	3	 67% 33%
3	G	3	 67% 33%

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
4	NAG	A	906	-	-	-	X
4	NAG	B	1107	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 12042 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.

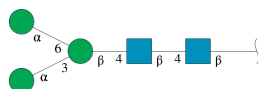
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	740	5657	3608	958	1072	19	0	0	0
1	B	734	5766	3683	976	1088	19	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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.



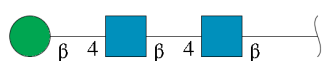
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	61	34	2	25	0	0	0

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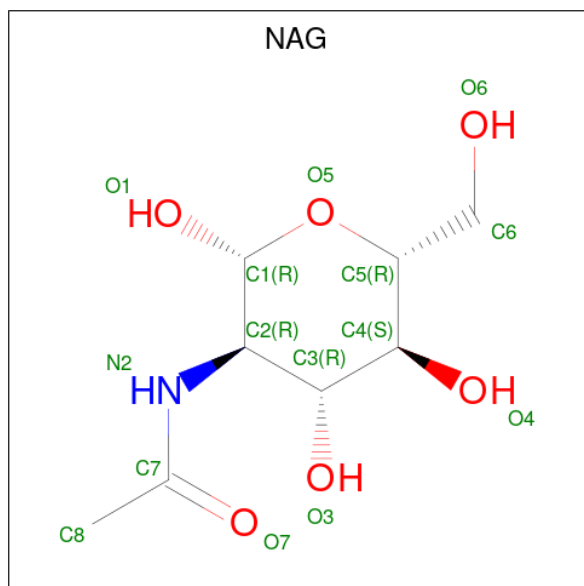
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	5	61	34	2	25	0	0	0
2	F	5	61	34	2	25	0	0	0
2	H	5	61	34	2	25	0	0	0

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



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

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



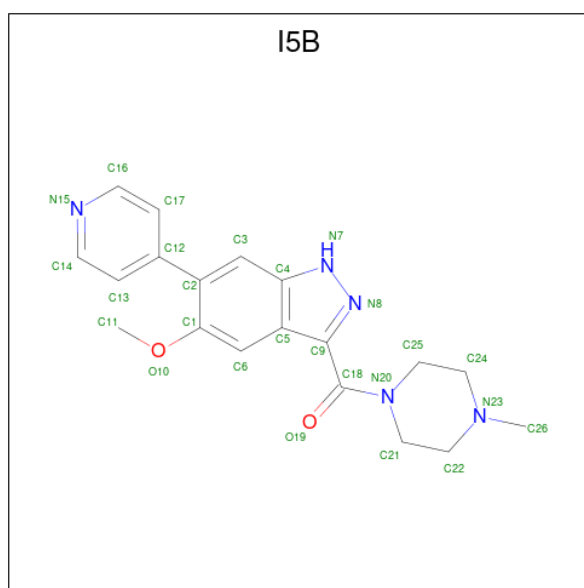
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

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

- Molecule 5 is (5-methoxy-6-pyridin-4-yl-1 {H}-indazol-3-yl)-(4-methylpiperazin-1-yl)met hanone (three-letter code: I5B) (formula: C₁₉H₂₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			26	19	5	2		
5	B	1	Total	C	N	O	0	0
			26	19	5	2		

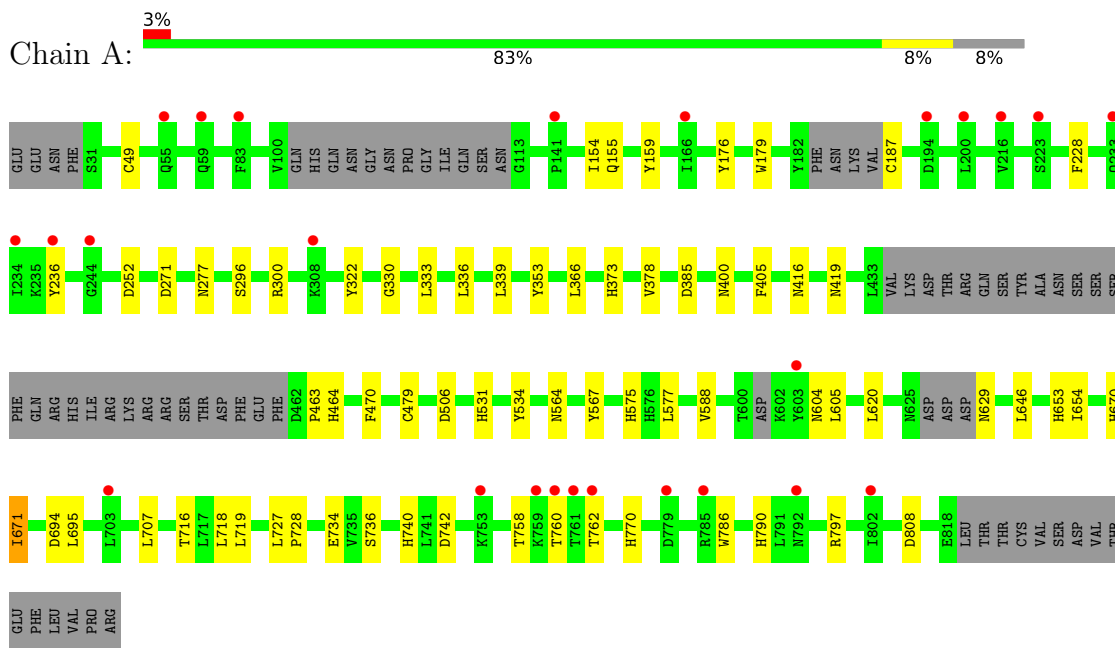
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	33	Total	O	0	0
			33	33		

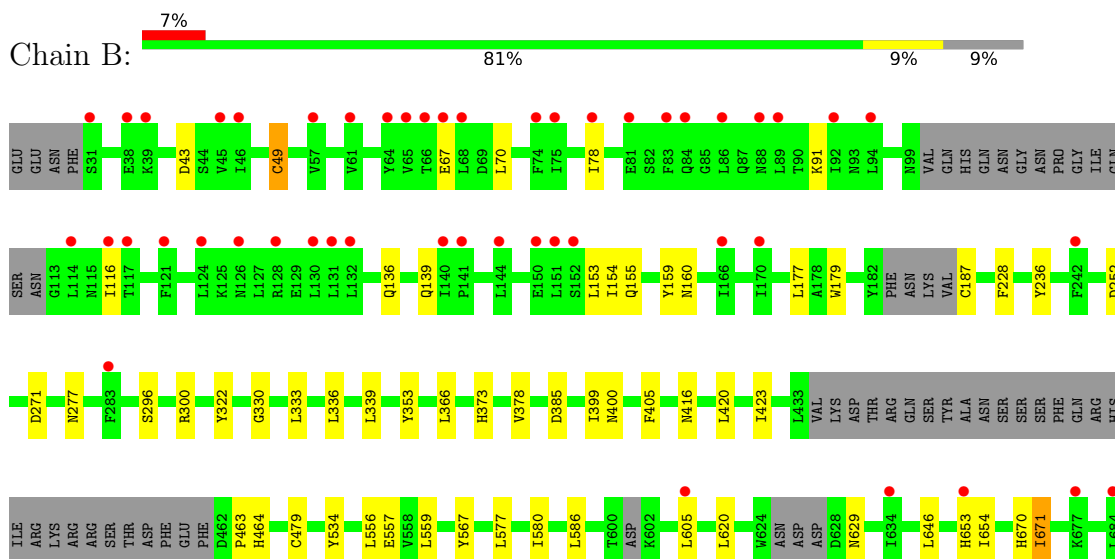
3 Residue-property plots [i](#)

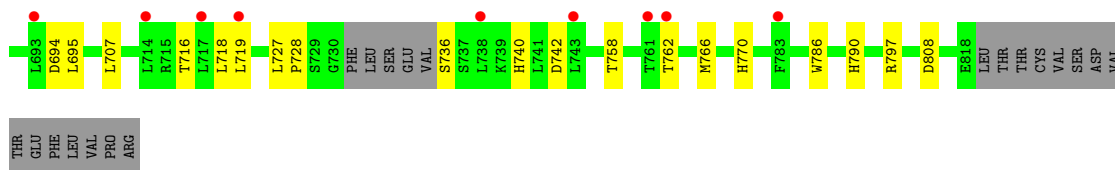
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Toll-like receptor 8



- Molecule 1: Toll-like receptor 8





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



- 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-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-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.37Å 86.97Å 152.35Å 90.00° 119.52° 90.00°	Depositor
Resolution (Å)	67.81 – 2.84 74.07 – 2.84	Depositor EDS
% Data completeness (in resolution range)	90.9 (67.81-2.84) 90.9 (74.07-2.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.82Å)	Xtrriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.258 , 0.295 0.251 , 0.289	Depositor DCC
R_{free} test set	1895 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtrriage
Anisotropy	0.521	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12042	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: I5B, BMA, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/5771	0.44	0/7867
1	B	0.23	0/5879	0.44	0/7990
All	All	0.23	0/11650	0.44	0/15857

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	5657	0	5353	35	0
1	B	5766	0	5651	41	0
2	C	61	0	52	0	0
2	E	61	0	52	1	0
2	F	61	0	52	0	0
2	H	61	0	52	0	0
3	D	39	0	34	0	0
3	G	39	0	34	0	0
4	A	84	0	78	0	0
4	B	84	0	78	0	0
5	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	26	0	0	0	0
6	A	44	0	0	1	0
6	B	33	0	0	0	0
All	All	12042	0	11436	76	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 3.

All (76) 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:373:HIS:HA	1:A:400:ASN:HB3	1.69	0.72
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.69	0.72
1:B:670:HIS:HA	1:B:694:ASP:HB3	1.84	0.60
1:B:139:GLN:HE22	1:B:160:ASN:HD22	1.50	0.58
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.85	0.57
1:B:49:CYS:HB3	1:B:70:LEU:HD23	1.89	0.54
1:B:736:SER:HA	1:B:762:THR:HA	1.89	0.53
1:B:228:PHE:HA	1:B:252:ASP:HB3	1.90	0.53
1:B:159:TYR:CD1	1:B:187:CYS:SG	3.02	0.53
1:A:228:PHE:HA	1:A:252:ASP:HB3	1.90	0.52
1:A:736:SER:HA	1:A:762:THR:HA	1.90	0.52
1:B:139:GLN:NE2	1:B:160:ASN:HD22	2.07	0.52
1:B:336:LEU:HD13	1:B:339:LEU:HD22	1.92	0.52
1:B:577:LEU:HD12	1:B:605:LEU:HD11	1.92	0.51
1:B:716:THR:HG23	1:B:740:HIS:ND1	2.26	0.51
1:A:620:LEU:HD11	1:A:646:LEU:HD22	1.94	0.50
1:A:336:LEU:HD13	1:A:339:LEU:HD22	1.93	0.50
1:A:734:GLU:H	1:A:760:THR:HG21	1.77	0.50
1:B:620:LEU:HD11	1:B:646:LEU:HD22	1.94	0.50
1:B:78:ILE:HB	1:B:116:ILE:HG12	1.93	0.50
1:B:154:ILE:HG22	1:B:155:GLN:HG3	1.94	0.50
1:A:159:TYR:CD1	1:A:187:CYS:SG	3.05	0.49
1:A:716:THR:HG23	1:A:740:HIS:ND1	2.27	0.49
1:B:420:LEU:HD13	1:B:423:ILE:HG12	1.93	0.49
1:B:770:HIS:CD2	1:B:797:ARG:NH2	2.80	0.49
1:A:770:HIS:CD2	1:A:797:ARG:NH2	2.80	0.49
1:A:154:ILE:HG22	1:A:155:GLN:HG3	1.93	0.49
1:B:718:LEU:HA	1:B:742:ASP:HB3	1.94	0.49
1:B:399:ILE:HD12	1:B:420:LEU:HD11	1.94	0.48
1:A:479:CYS:SG	1:A:534:TYR:CD1	3.06	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:LEU:HB3	1:B:580:ILE:HD12	1.96	0.48
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.95	0.47
1:B:758:THR:CG2	1:B:790:HIS:CE1	2.97	0.47
1:A:506:ASP:OD1	1:A:531:HIS:HD2	1.98	0.46
1:A:758:THR:CG2	1:A:790:HIS:CE1	2.97	0.46
1:B:654:ILE:HD11	1:B:671:ILE:HG21	1.97	0.46
1:A:654:ILE:HD11	1:A:671:ILE:HG21	1.96	0.46
1:A:758:THR:HG21	1:A:790:HIS:NE2	2.31	0.46
1:B:333:LEU:HD22	1:B:366:LEU:HD11	1.96	0.46
1:B:758:THR:HG21	1:B:790:HIS:NE2	2.31	0.45
1:A:758:THR:CG2	1:A:790:HIS:NE2	2.79	0.45
1:A:333:LEU:HD22	1:A:366:LEU:HD11	1.97	0.45
1:A:236:TYR:HD1	1:A:277:ASN:HB3	1.82	0.45
1:B:758:THR:CG2	1:B:790:HIS:NE2	2.79	0.45
1:B:300:ARG:HG2	1:B:322:TYR:HB2	1.98	0.44
1:B:479:CYS:SG	1:B:534:TYR:CD1	3.10	0.44
1:A:300:ARG:HG2	1:A:322:TYR:HB2	1.98	0.44
1:B:330:GLY:HA3	1:B:333:LEU:HD12	2.00	0.44
1:B:154:ILE:HD12	1:B:464:HIS:CE1	2.53	0.44
1:B:557:GLU:HA	1:B:586:LEU:HA	1.98	0.44
1:A:577:LEU:HD12	1:A:605:LEU:HD11	2.00	0.44
1:A:727:LEU:HD12	1:A:728:PRO:HD2	2.00	0.43
1:B:154:ILE:CD1	1:B:464:HIS:CE1	3.02	0.43
1:A:758:THR:HG21	1:A:790:HIS:CE1	2.54	0.43
1:B:727:LEU:HD12	1:B:728:PRO:HD2	2.01	0.43
1:B:758:THR:HG21	1:B:790:HIS:CE1	2.54	0.43
1:B:236:TYR:HD1	1:B:277:ASN:HB3	1.83	0.43
1:A:575:HIS:HD2	6:A:1019:HOH:O	2.00	0.43
1:B:67:GLU:HG2	1:B:91:LYS:HB3	2.00	0.43
1:B:353:TYR:OH	1:B:405:PHE:O	2.33	0.43
1:A:154:ILE:CD1	1:A:464:HIS:CE1	3.02	0.43
1:A:353:TYR:OH	1:A:405:PHE:O	2.33	0.43
1:B:758:THR:CG2	1:B:786:TRP:HE1	2.32	0.43
1:A:154:ILE:HD12	1:A:464:HIS:CE1	2.53	0.42
1:A:179:TRP:NE1	1:A:463:PRO:HB3	2.35	0.42
1:A:758:THR:CG2	1:A:786:TRP:HE1	2.32	0.42
1:B:695:LEU:HB2	1:B:719:LEU:HD23	2.02	0.42
1:A:330:GLY:HA3	1:A:333:LEU:HD12	2.01	0.41
1:A:758:THR:HG23	1:A:790:HIS:CE1	2.55	0.41
1:A:588:VAL:HG11	2:E:2:NAG:H82	2.03	0.41
1:B:758:THR:HG23	1:B:790:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:HB2	1:A:719:LEU:HD23	2.02	0.40
1:A:154:ILE:HD11	1:A:176:TYR:HB3	2.04	0.40
1:B:179:TRP:NE1	1:B:463:PRO:HB3	2.36	0.40
1:B:556:LEU:HD21	1:B:559:LEU:HB2	2.02	0.40
1:B:153:LEU:HB2	1:B:177:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

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	728/807 (90%)	670 (92%)	56 (8%)	2 (0%)	41 61
1	B	720/807 (89%)	666 (92%)	52 (7%)	2 (0%)	41 61
All	All	1448/1614 (90%)	1336 (92%)	108 (8%)	4 (0%)	41 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	ASP
1	B	271	ASP
1	A	378	VAL
1	B	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	608/751 (81%)	594 (98%)	14 (2%)	50	73
1	B	649/751 (86%)	636 (98%)	13 (2%)	55	76
All	All	1257/1502 (84%)	1230 (98%)	27 (2%)	53	75

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	296	SER
1	A	385	ASP
1	A	416	ASN
1	A	419	ASN
1	A	470	PHE
1	A	564	ASN
1	A	567	TYR
1	A	604	ASN
1	A	629	ASN
1	A	653	HIS
1	A	671	ILE
1	A	707	LEU
1	A	808	ASP
1	B	43	ASP
1	B	49	CYS
1	B	136	GLN
1	B	296	SER
1	B	385	ASP
1	B	416	ASN
1	B	567	TYR
1	B	629	ASN
1	B	653	HIS
1	B	671	ILE
1	B	707	LEU
1	B	766	MET
1	B	808	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	469	HIS
1	A	531	HIS

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Mol	Chain	Res	Type
1	A	566	HIS
1	A	594	ASN
1	B	136	GLN
1	B	139	GLN
1	B	233	GLN
1	B	469	HIS
1	B	566	HIS
1	B	594	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

26 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.45	0
2	BMA	C	3	2	11,11,12	0.23	0	15,15,17	0.79	1 (6%)
2	MAN	C	4	2	11,11,12	0.32	0	15,15,17	0.73	1 (6%)
2	MAN	C	5	2	11,11,12	0.36	0	15,15,17	0.81	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.26	0	17,19,21	0.62	1 (5%)
3	NAG	D	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	BMA	D	3	3	11,11,12	0.35	0	15,15,17	0.51	0
2	NAG	E	1	2,1	14,14,15	0.27	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	BMA	E	3	2	11,11,12	0.27	0	15,15,17	0.59	0
2	MAN	E	4	2	11,11,12	0.28	0	15,15,17	0.83	1 (6%)
2	MAN	E	5	2	11,11,12	0.33	0	15,15,17	0.75	1 (6%)
2	NAG	F	1	2,1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.45	0
2	BMA	F	3	2	11,11,12	0.24	0	15,15,17	0.66	1 (6%)
2	MAN	F	4	2	11,11,12	0.32	0	15,15,17	0.72	1 (6%)
2	MAN	F	5	2	11,11,12	0.33	0	15,15,17	0.78	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	G	3	3	11,11,12	0.34	0	15,15,17	0.53	0
2	NAG	H	1	2,1	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.41	0
2	BMA	H	3	2	11,11,12	0.22	0	15,15,17	0.42	0
2	MAN	H	4	2	11,11,12	0.29	0	15,15,17	0.83	1 (6%)
2	MAN	H	5	2	11,11,12	0.32	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	2,1	-	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	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	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	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	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

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	MAN	C1-O5-C5	3.03	116.30	112.19
2	E	4	MAN	C1-O5-C5	3.03	116.29	112.19
2	C	5	MAN	C1-O5-C5	2.97	116.22	112.19
2	F	5	MAN	C1-O5-C5	2.91	116.14	112.19
2	H	5	MAN	C1-O5-C5	2.78	115.96	112.19
2	C	3	BMA	C1-O5-C5	2.75	115.91	112.19
2	E	5	MAN	C1-O5-C5	2.74	115.90	112.19
2	C	4	MAN	C1-O5-C5	2.53	115.62	112.19
2	F	4	MAN	C1-O5-C5	2.53	115.62	112.19
3	G	1	NAG	C1-O5-C5	2.21	115.19	112.19
2	F	3	BMA	C1-O5-C5	2.17	115.14	112.19
3	D	1	NAG	C1-O5-C5	2.04	114.96	112.19
2	E	1	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

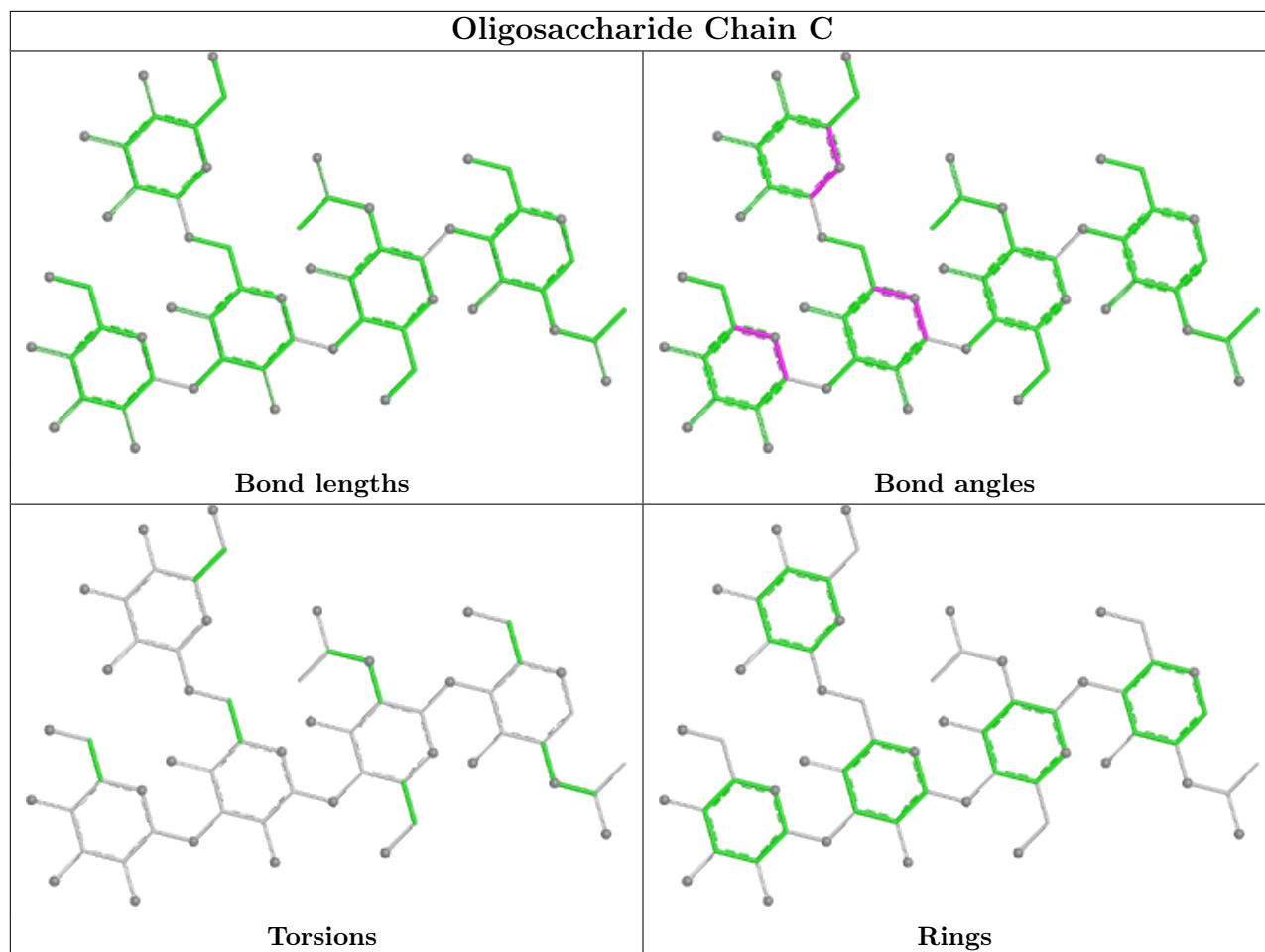
There are no torsion outliers.

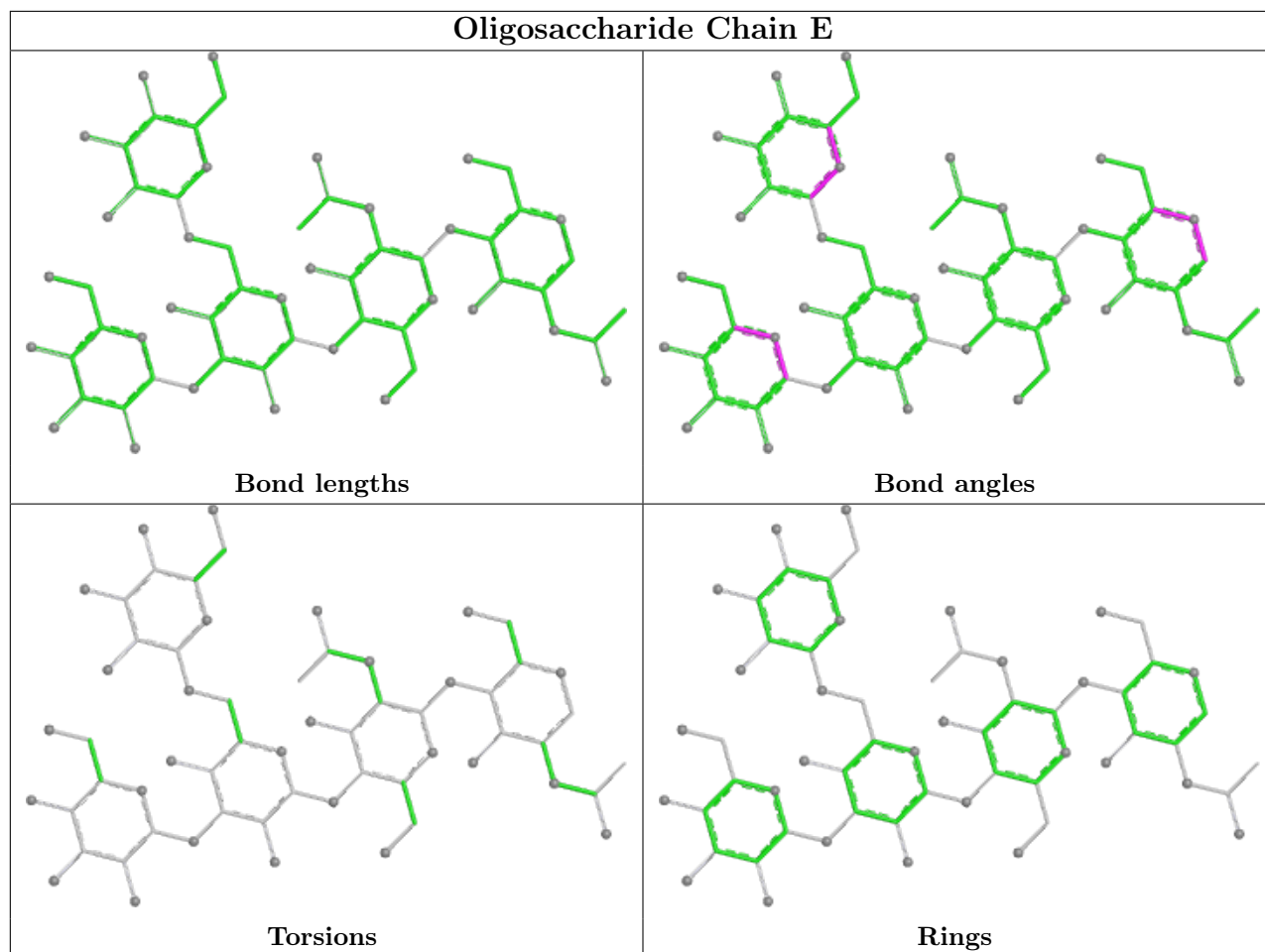
There are no ring outliers.

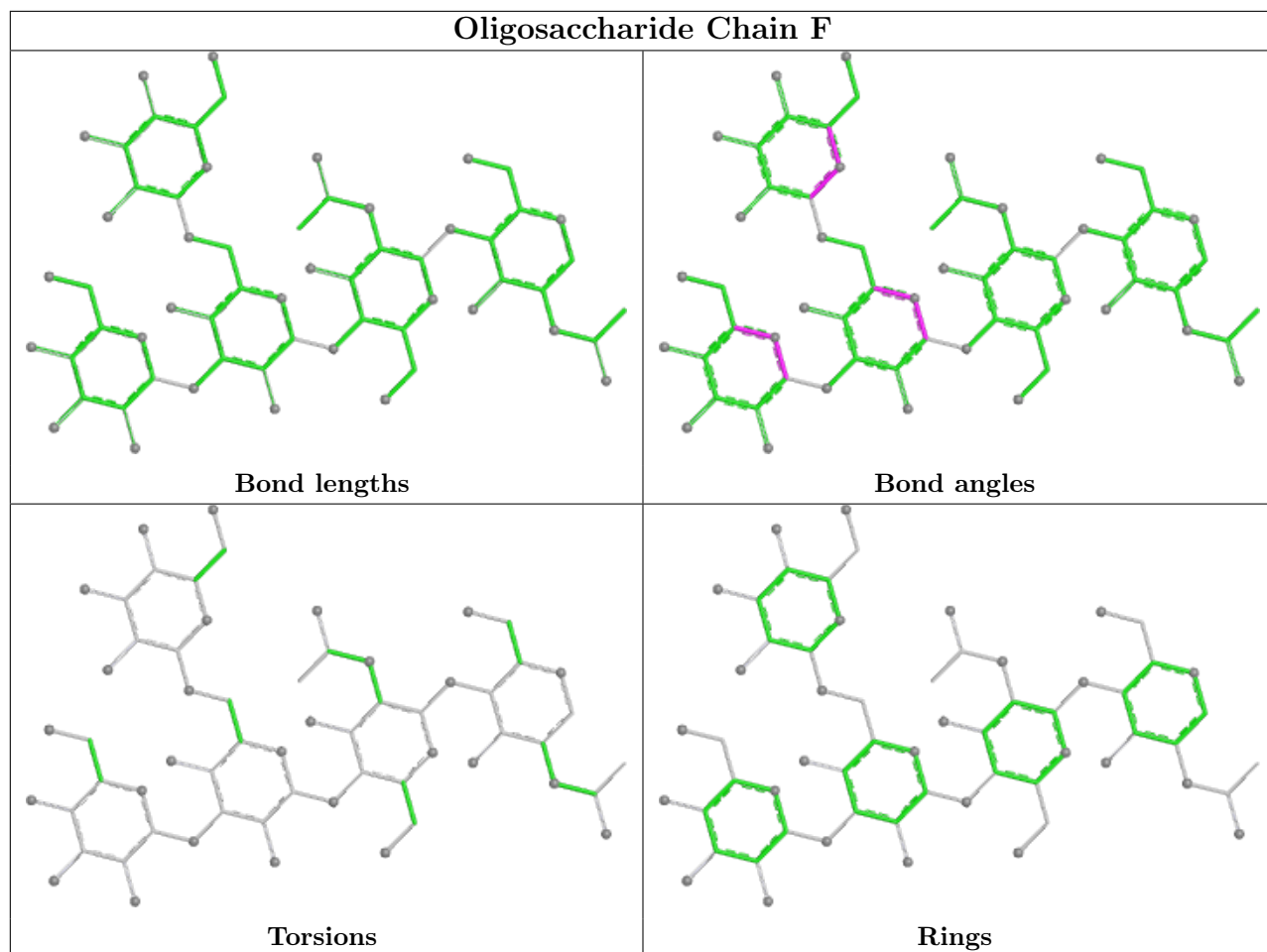
1 monomer is involved in 1 short contact:

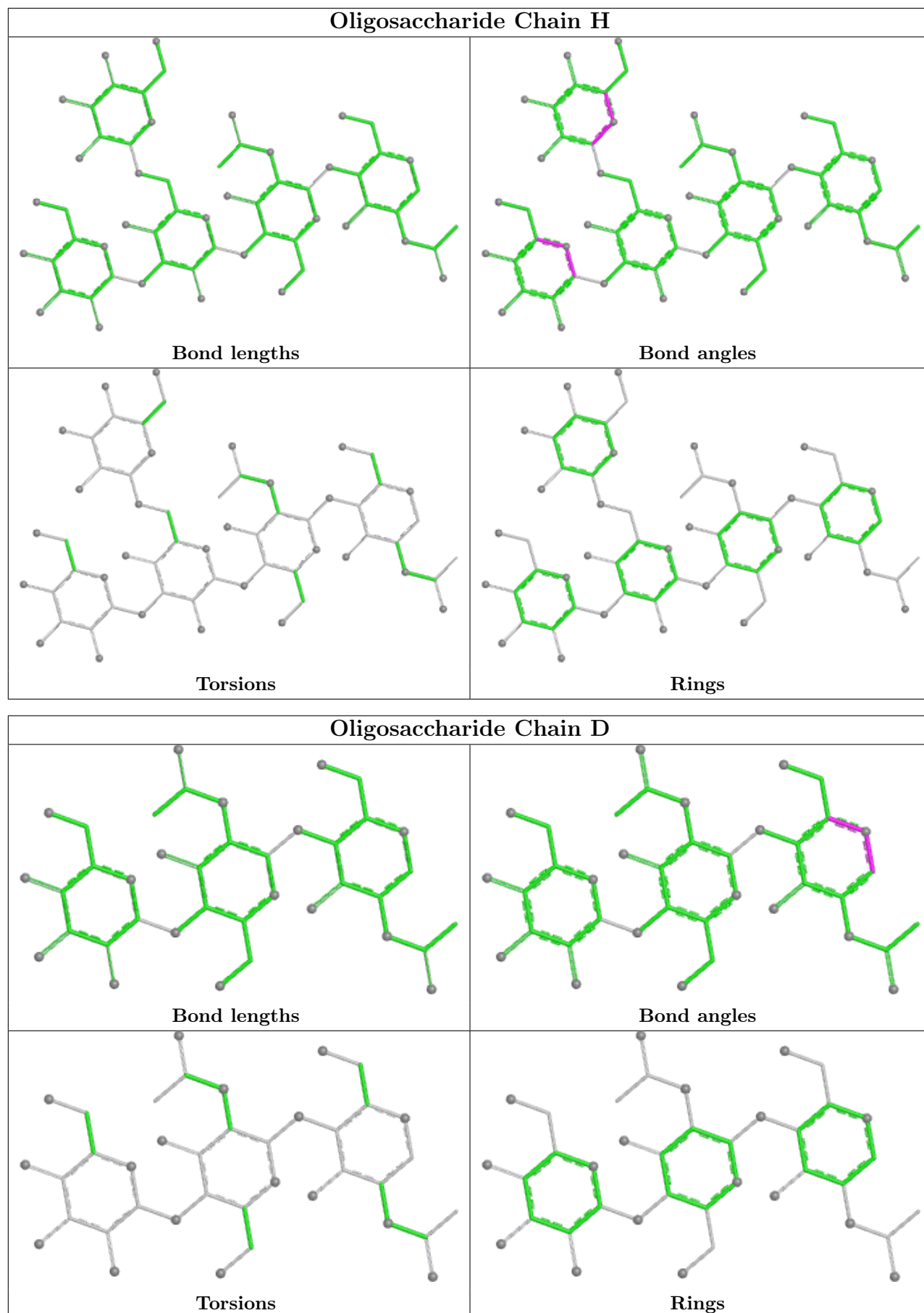
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0

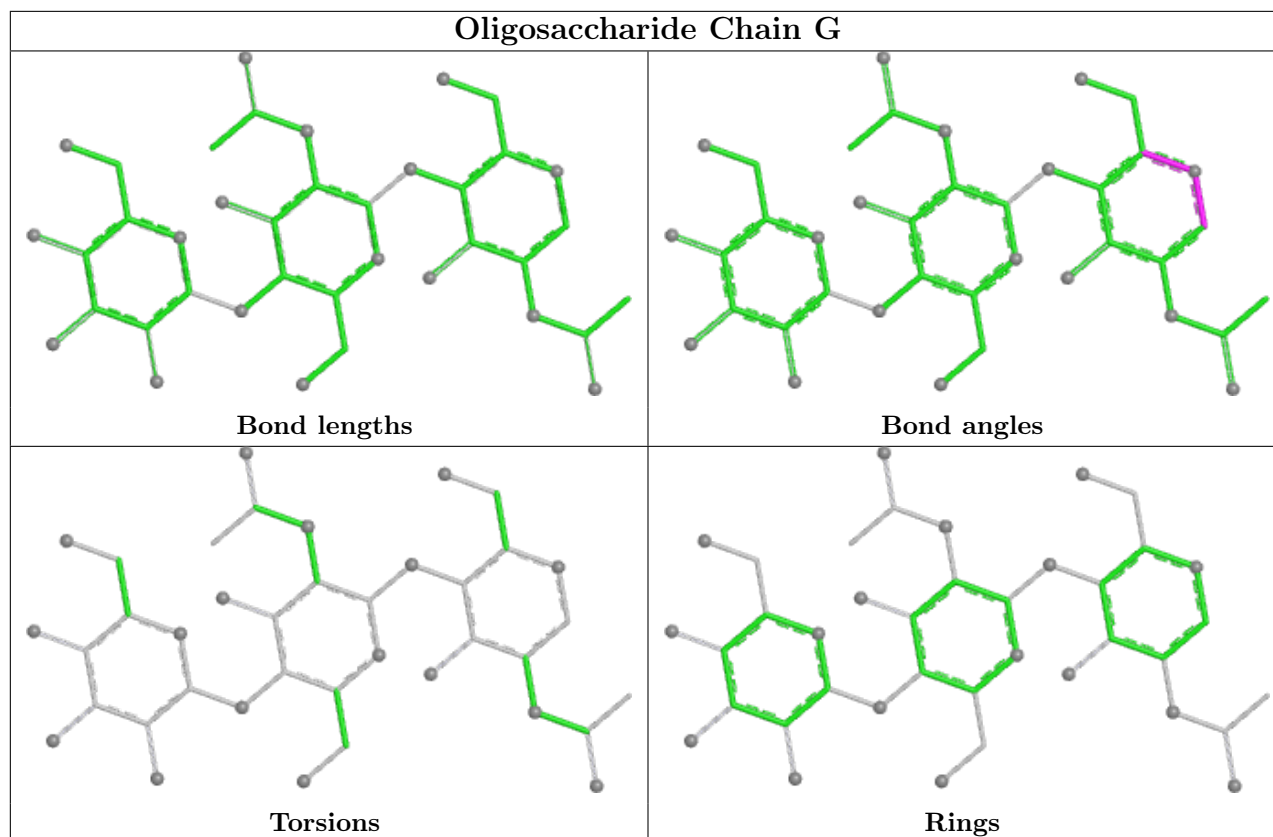
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	906	1	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	B	1103	1	14,14,15	0.28	0	17,19,21	0.56	1 (5%)
4	NAG	B	1102	1	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	A	901	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	B	1104	1	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
4	NAG	B	1105	1	14,14,15	0.32	0	17,19,21	0.67	0
4	NAG	B	1106	1	14,14,15	0.31	0	17,19,21	0.61	1 (5%)
4	NAG	B	1107	1	14,14,15	0.29	0	17,19,21	0.55	0
4	NAG	A	904	1	14,14,15	0.30	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	902	1	14,14,15	0.28	0	17,19,21	0.56	1 (5%)
4	NAG	A	905	1	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
5	I5B	B	1101	-	27,29,29	1.31	3 (11%)	32,41,41	1.79	9 (28%)
5	I5B	A	907	-	27,29,29	1.31	3 (11%)	32,41,41	1.87	10 (31%)
4	NAG	A	903	1	14,14,15	0.30	0	17,19,21	0.74	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1103	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1102	1	-	0/6/23/26	0/1/1/1
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1104	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1105	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1106	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1107	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	0/6/23/26	0/1/1/1
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
5	I5B	B	1101	-	-	0/10/24/24	0/4/4/4
5	I5B	A	907	-	-	0/10/24/24	0/4/4/4
4	NAG	A	903	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1101	I5B	C9-N8	-3.74	1.27	1.35
5	A	907	I5B	C9-N8	-3.69	1.28	1.35
5	A	907	I5B	C6-C1	2.60	1.41	1.36
5	B	1101	I5B	C6-C1	2.42	1.40	1.36
5	A	907	I5B	O10-C1	2.34	1.40	1.37
5	B	1101	I5B	O10-C1	2.25	1.40	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	I5B	O10-C1-C6	-4.25	119.74	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	907	I5B	O10-C1-C6	-3.50	120.71	125.24
5	B	1101	I5B	C25-N20-C21	3.35	119.08	112.62
5	A	907	I5B	C25-N20-C21	3.27	118.92	112.62
5	A	907	I5B	C6-C5-C4	3.15	122.56	118.26
5	A	907	I5B	C26-N23-C22	3.10	115.30	110.66
5	A	907	I5B	C11-O10-C1	3.06	122.14	117.53
5	B	1101	I5B	C6-C5-C4	3.00	122.36	118.26
4	A	905	NAG	C1-O5-C5	2.69	115.84	112.19
5	B	1101	I5B	O10-C1-C2	2.65	120.20	116.26
5	B	1101	I5B	C18-C9-N8	2.55	127.19	120.55
5	B	1101	I5B	O19-C18-C9	-2.53	113.57	118.58
4	B	1106	NAG	C1-O5-C5	2.33	115.35	112.19
5	A	907	I5B	C18-C9-N8	2.31	126.56	120.55
4	A	903	NAG	C1-O5-C5	2.22	115.20	112.19
5	B	1101	I5B	C24-N23-C22	2.21	112.61	109.52
4	B	1104	NAG	C1-O5-C5	2.20	115.18	112.19
5	A	907	I5B	C25-C24-N23	-2.17	108.35	110.80
4	B	1103	NAG	C1-O5-C5	2.12	115.07	112.19
4	A	902	NAG	C1-O5-C5	2.09	115.02	112.19
5	B	1101	I5B	C17-C16-N15	-2.08	119.99	123.62
5	A	907	I5B	O10-C1-C2	2.07	119.35	116.26
5	B	1101	I5B	C16-N15-C14	2.05	121.67	116.85
5	A	907	I5B	C16-N15-C14	2.02	121.60	116.85
5	A	907	I5B	C22-C21-N20	-2.02	106.11	110.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

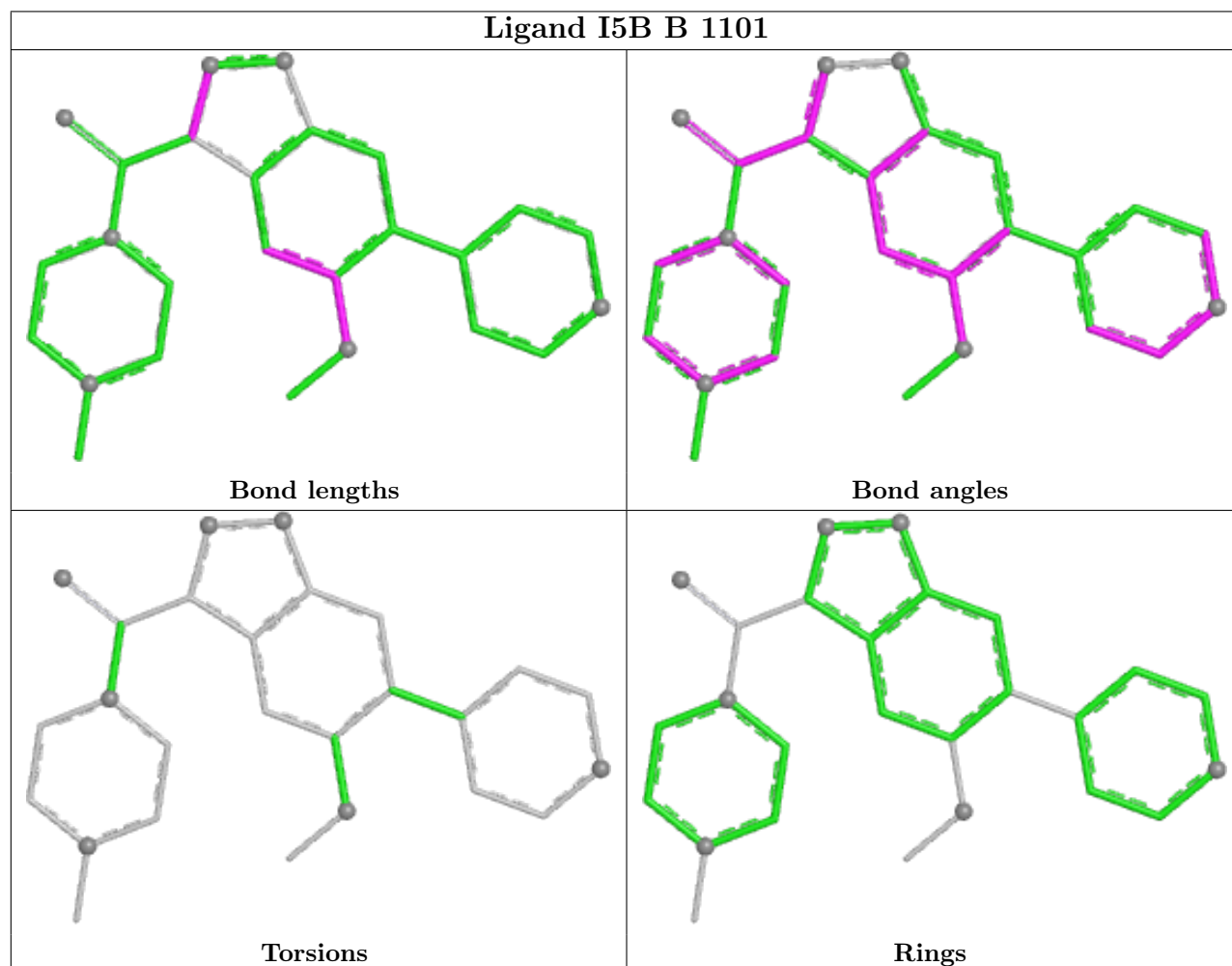
Mol	Chain	Res	Type	Atoms
4	B	1105	NAG	C1-C2-N2-C7

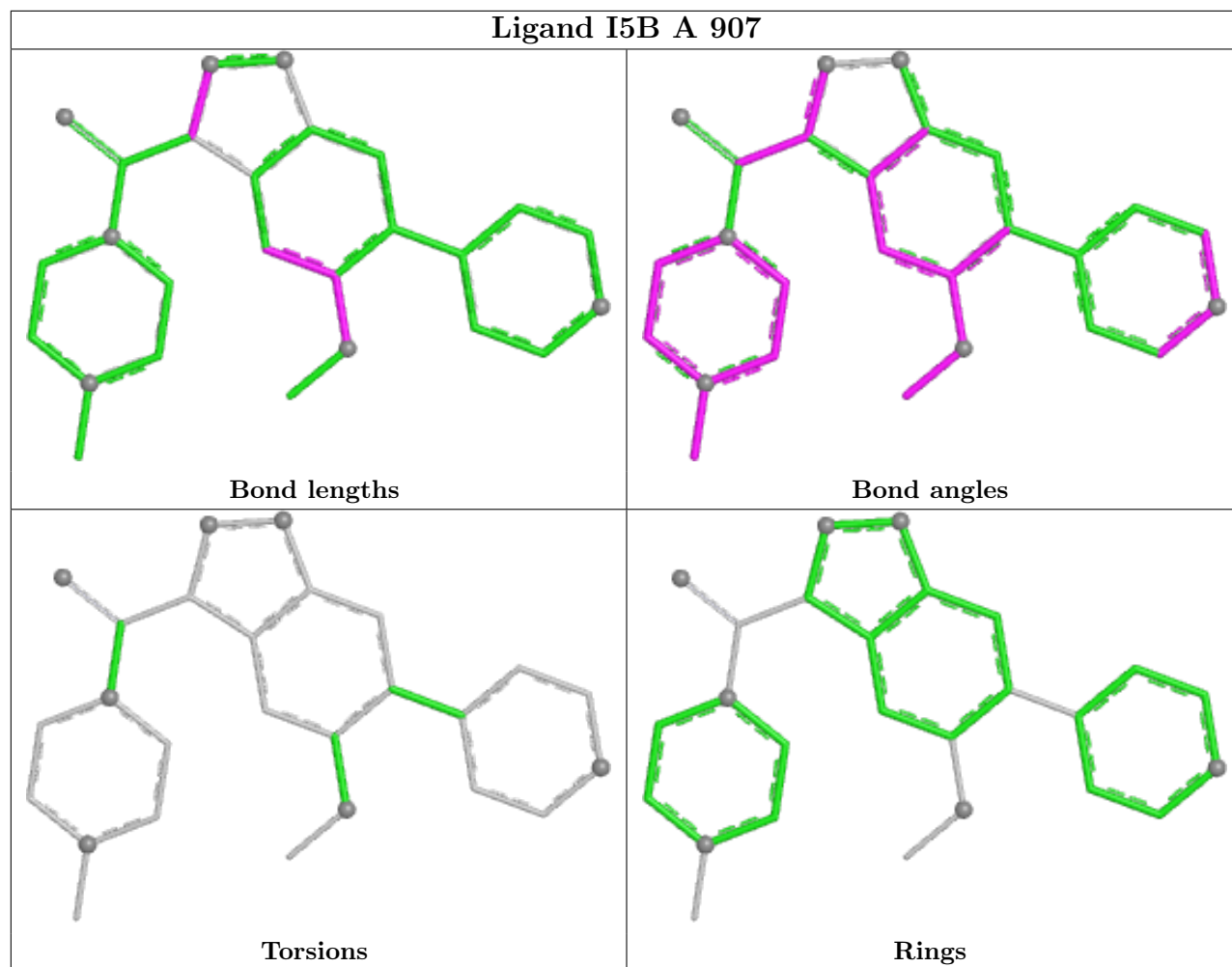
There are no ring outliers.

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	740/807 (91%)	0.09	25 (3%) 45 37	44, 89, 120, 140	0
1	B	734/807 (90%)	0.33	57 (7%) 13 8	52, 102, 143, 176	0
All	All	1474/1614 (91%)	0.21	82 (5%) 24 17	44, 94, 138, 176	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PHE	10.0
1	B	121	PHE	7.9
1	B	761	THR	6.9
1	B	78	ILE	5.1
1	B	130	LEU	5.1
1	B	116	ILE	5.0
1	A	761	THR	4.7
1	B	144	LEU	4.3
1	B	65	VAL	4.0
1	B	92	ILE	3.9
1	B	132	LEU	3.8
1	B	719	LEU	3.7
1	A	166	ILE	3.6
1	A	603	TYR	3.4
1	B	45	VAL	3.4
1	A	233	GLN	3.4
1	B	283	PHE	3.3
1	B	124	LEU	3.3
1	A	83	PHE	3.3
1	B	68	LEU	3.2
1	A	760	THR	3.1
1	A	55	GLN	3.1
1	B	39	LYS	3.1
1	A	762	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	242	PHE	3.0
1	B	714	LEU	3.0
1	B	152	SER	3.0
1	B	141	PRO	2.9
1	A	234	ILE	2.9
1	B	64	TYR	2.9
1	A	703	LEU	2.9
1	B	67	GLU	2.9
1	B	31	SER	2.8
1	B	634	ILE	2.8
1	B	81	GLU	2.8
1	B	74	PHE	2.8
1	B	114	LEU	2.8
1	A	792	ASN	2.8
1	B	717	LEU	2.8
1	B	94	LEU	2.7
1	A	59	GLN	2.7
1	B	86	LEU	2.7
1	B	117	THR	2.7
1	B	150	GLU	2.7
1	A	141	PRO	2.7
1	B	66	THR	2.6
1	B	677	LYS	2.6
1	B	605	LEU	2.6
1	A	223	SER	2.6
1	B	88	ASN	2.6
1	B	762	THR	2.6
1	B	84	GLN	2.6
1	B	738	LEU	2.6
1	B	46	ILE	2.5
1	A	753	LYS	2.5
1	B	38	GLU	2.5
1	B	89	LEU	2.5
1	A	194	ASP	2.5
1	A	244	GLY	2.5
1	B	743	LEU	2.5
1	A	785	ARG	2.4
1	A	216	VAL	2.4
1	A	308	LYS	2.3
1	B	693	LEU	2.3
1	B	75	ILE	2.3
1	B	653	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	170	ILE	2.3
1	B	140	ILE	2.2
1	B	57	VAL	2.2
1	B	126	ASN	2.2
1	B	166	ILE	2.2
1	B	783	PHE	2.2
1	A	236	TYR	2.2
1	B	128	ARG	2.1
1	A	779	ASP	2.1
1	B	151	LEU	2.1
1	B	131	LEU	2.1
1	B	61	VAL	2.1
1	B	684	LEU	2.1
1	A	802	ILE	2.1
1	A	200	LEU	2.0
1	A	759	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

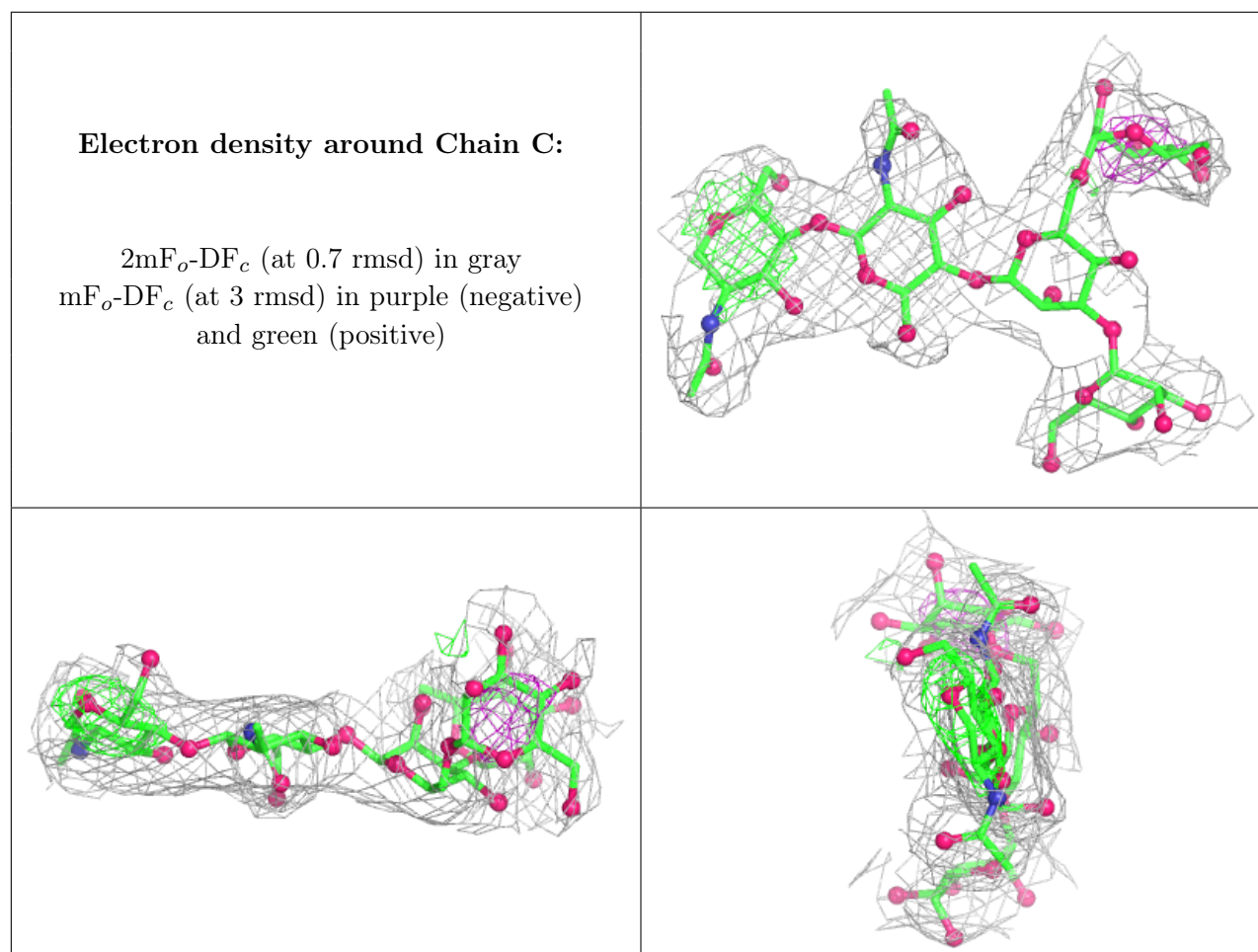
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	5	11/12	0.54	0.30	106,106,106,106	0
2	MAN	F	5	11/12	0.69	0.23	116,116,116,116	0
2	MAN	F	4	11/12	0.71	0.20	114,115,115,115	0
2	MAN	E	5	11/12	0.76	0.16	87,88,89,89	0
2	BMA	F	3	11/12	0.77	0.22	111,113,114,115	0
2	MAN	H	5	11/12	0.78	0.17	104,105,105,105	0
2	MAN	C	4	11/12	0.82	0.15	105,105,105,105	0
2	BMA	C	3	11/12	0.84	0.13	101,103,104,105	0
3	BMA	D	3	11/12	0.85	0.16	75,76,76,76	0
2	MAN	H	4	11/12	0.86	0.15	102,103,103,103	0
3	BMA	G	3	11/12	0.86	0.13	84,84,85,85	0
2	MAN	E	4	11/12	0.90	0.10	87,87,88,88	0

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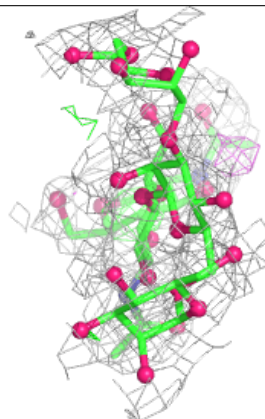
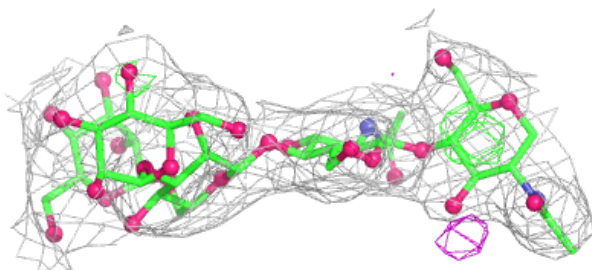
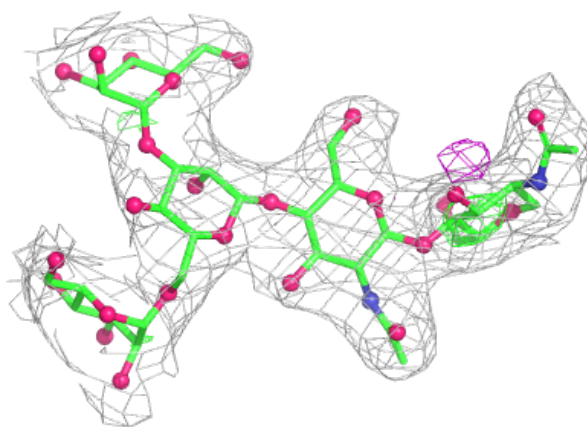
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	F	2	14/15	0.91	0.20	106,107,108,110	0
2	NAG	H	2	14/15	0.91	0.22	91,92,94,96	0
3	NAG	D	2	14/15	0.92	0.16	69,71,72,74	0
2	BMA	E	3	11/12	0.92	0.14	81,84,85,86	0
3	NAG	G	2	14/15	0.92	0.13	80,81,82,83	0
2	BMA	H	3	11/12	0.92	0.14	99,101,102,103	0
2	NAG	C	2	14/15	0.93	0.15	94,95,97,99	0
2	NAG	E	2	14/15	0.94	0.14	70,71,74,77	0
2	NAG	C	1	14/15	0.95	0.25	89,89,91,92	0
2	NAG	H	1	14/15	0.95	0.18	85,86,87,89	0
3	NAG	G	1	14/15	0.96	0.15	74,75,76,78	0
2	NAG	F	1	14/15	0.96	0.17	102,102,104,105	0
2	NAG	E	1	14/15	0.96	0.21	63,64,66,68	0
3	NAG	D	1	14/15	0.97	0.18	61,63,65,67	0

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



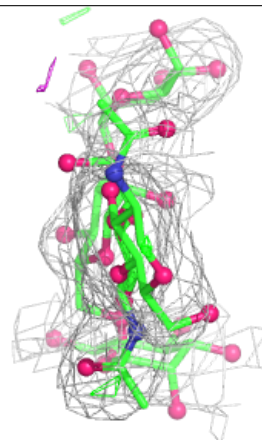
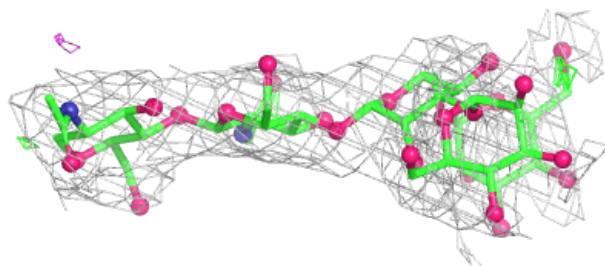
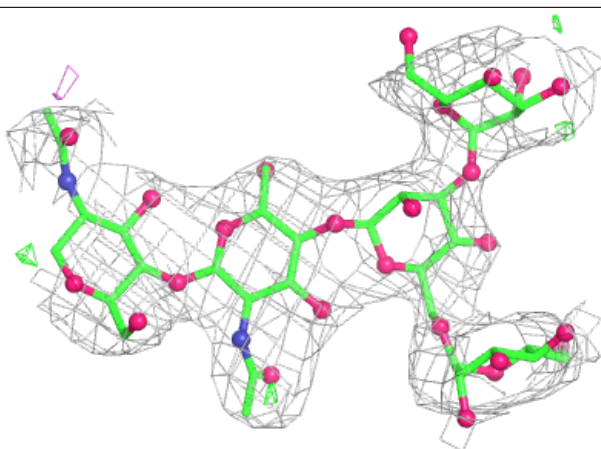
Electron density around Chain E:

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

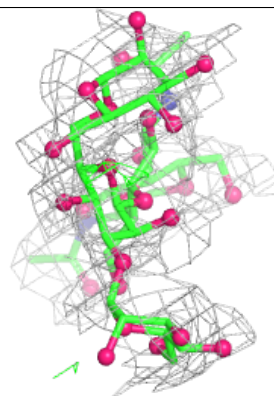
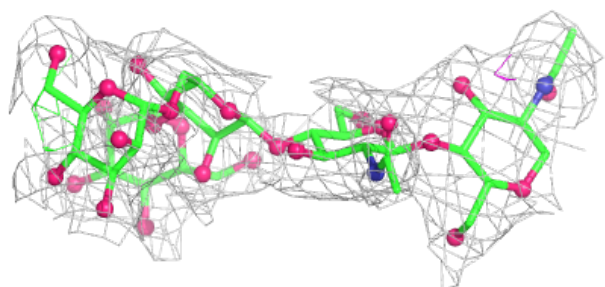
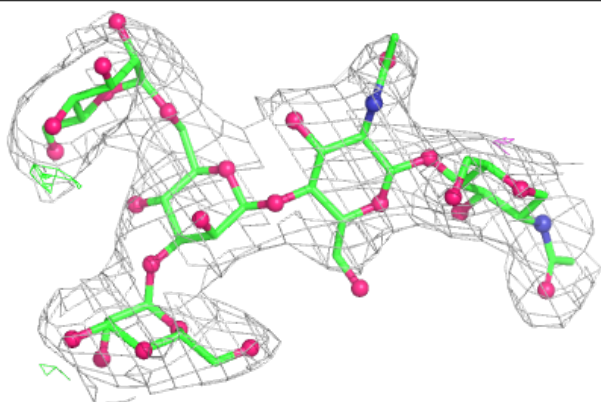


Electron density around Chain F:

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

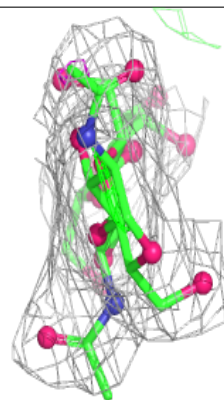
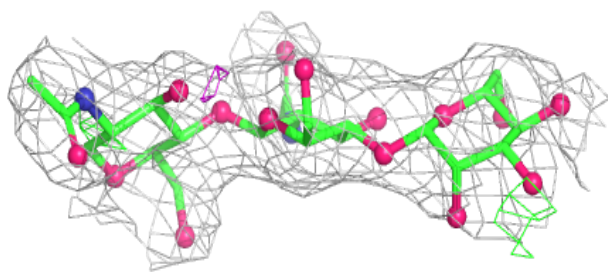
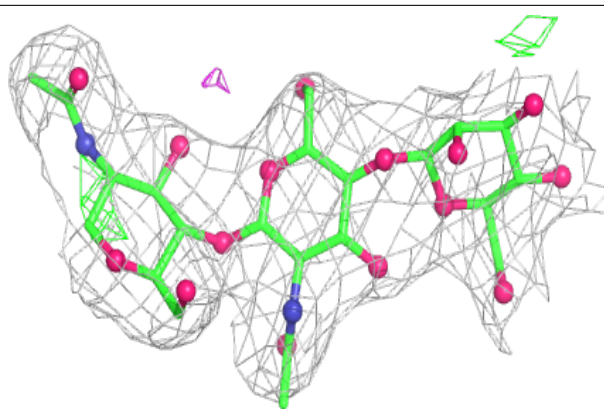
**Electron density around Chain H:**

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

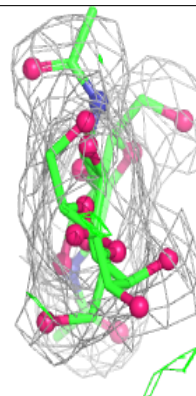
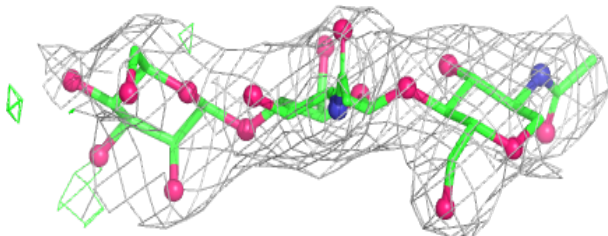
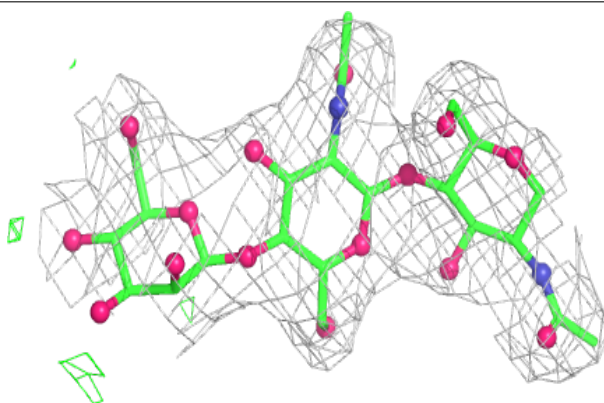


Electron density around Chain D:

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

**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

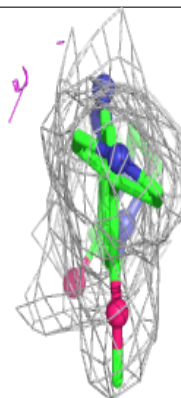
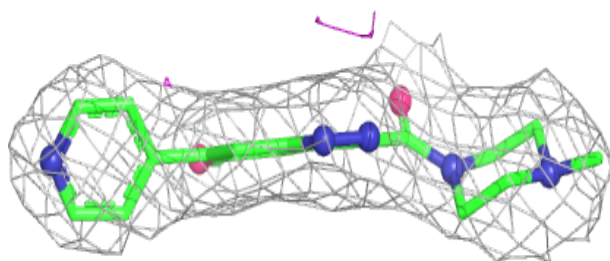
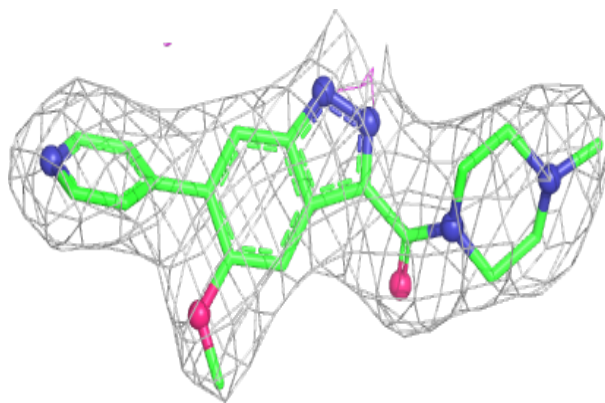
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1107	14/15	0.41	0.54	165,166,167,168	0
4	NAG	A	905	14/15	0.74	0.31	101,101,102,102	0
4	NAG	A	904	14/15	0.75	0.28	102,104,105,105	0
4	NAG	B	1106	14/15	0.79	0.20	112,113,113,113	0
4	NAG	A	906	14/15	0.79	0.47	130,130,130,130	0
4	NAG	B	1104	14/15	0.84	0.41	102,104,104,105	0
4	NAG	A	903	14/15	0.85	0.34	95,96,96,96	0
4	NAG	B	1103	14/15	0.87	0.20	116,116,117,117	0
4	NAG	A	902	14/15	0.90	0.13	103,104,104,104	0
4	NAG	B	1102	14/15	0.91	0.16	86,87,87,87	0
4	NAG	B	1105	14/15	0.93	0.16	87,87,88,88	0
4	NAG	A	901	14/15	0.95	0.18	76,76,77,77	0
5	I5B	A	907	26/26	0.97	0.18	54,55,56,56	0
5	I5B	B	1101	26/26	0.97	0.19	49,51,52,52	0

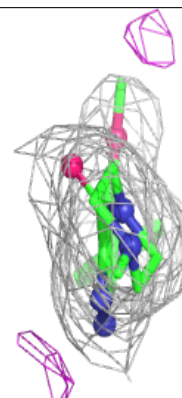
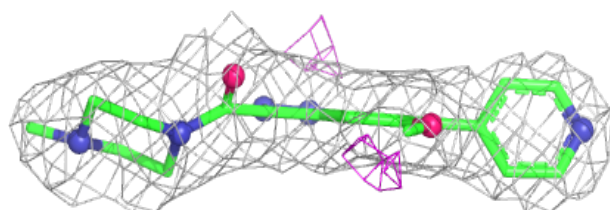
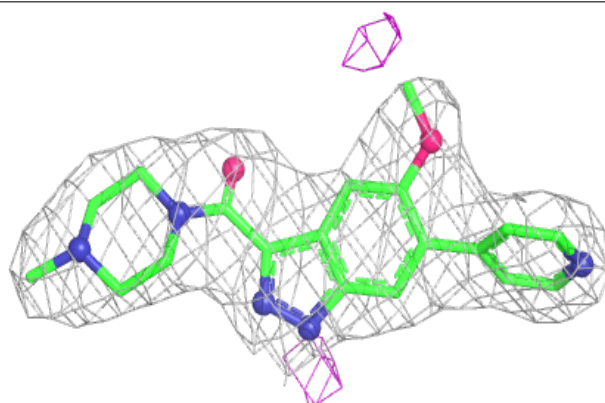
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around I5B A 907:

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

**Electron density around I5B B 1101:**

$2mF_o-DF_c$ (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.