



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:17 AM BST

PDB ID : 6C0M
Title : The synthesis, biological evaluation and structural insights of unsaturated 3-N-substituted sialic acids as probes of human parainfluenza virus-3 haemagglutinin-neuraminidase
Authors : Dirr, L.; Ve, T.; von Itzstein, M.
Deposited on : 2018-01-01
Resolution : 1.83 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

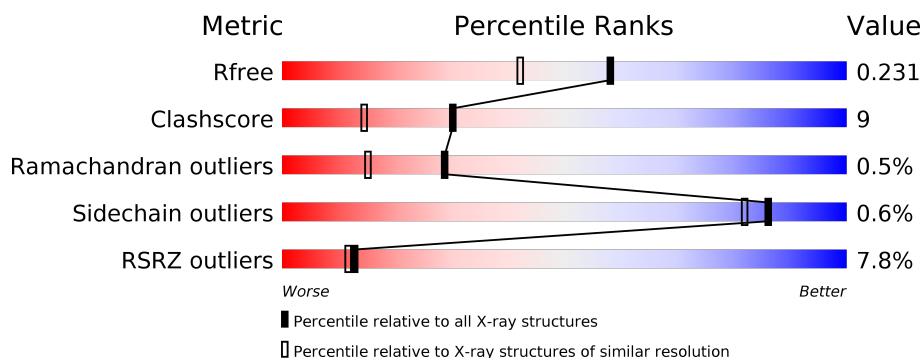
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 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	431	<div> <div>9%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>
1	B	431	<div> <div>6%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>
2	C	4	<div> <div>50%</div> <div>50%</div> </div>
3	D	3	<div> <div>100%</div> </div>

2 Entry composition [i](#)

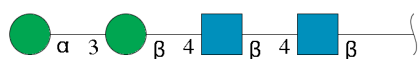
There are 10 unique types of molecules in this entry. The entry contains 7500 atoms, of which 17 are hydrogens and 0 are deuteriums.

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 Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	2	0
			3392	2145	583	644	20			
1	B	428	Total	C	N	O	S	0	2	0
			3361	2126	579	636	20			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

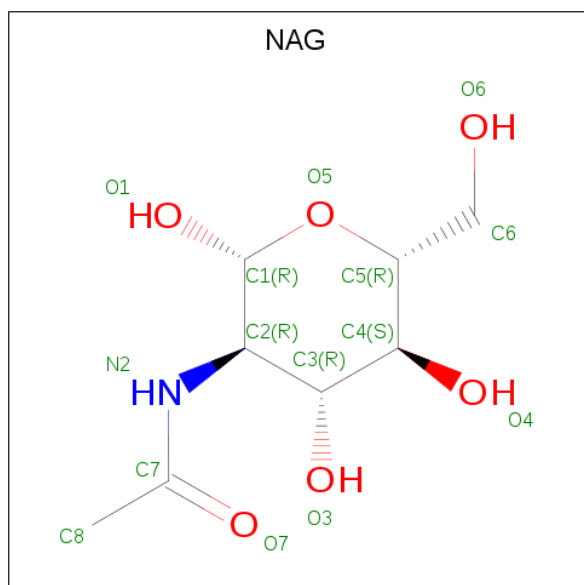


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	3	Total	C	H	N	O	0	0	0
			50	22	11	2	15			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	H	O	0
			10	2	6	2	0

- Molecule 7 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



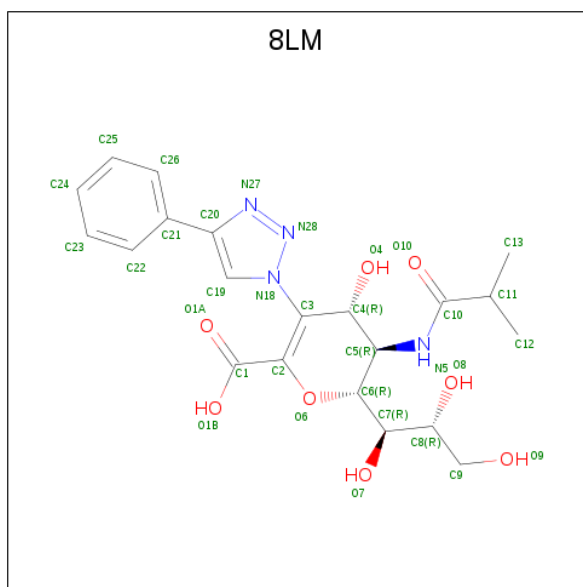
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 8 is 2,6-anhydro-3,5-dideoxy-5-[(2-methylpropanoyl)amino]-3-(4-phenyl-1H-1,2,3-triazol-1-yl)-D-glycero-D-galacto-non-2-enoni c acid (three-letter code: 8LM) (formula: $C_{21}H_{26}N_4O_8$).





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

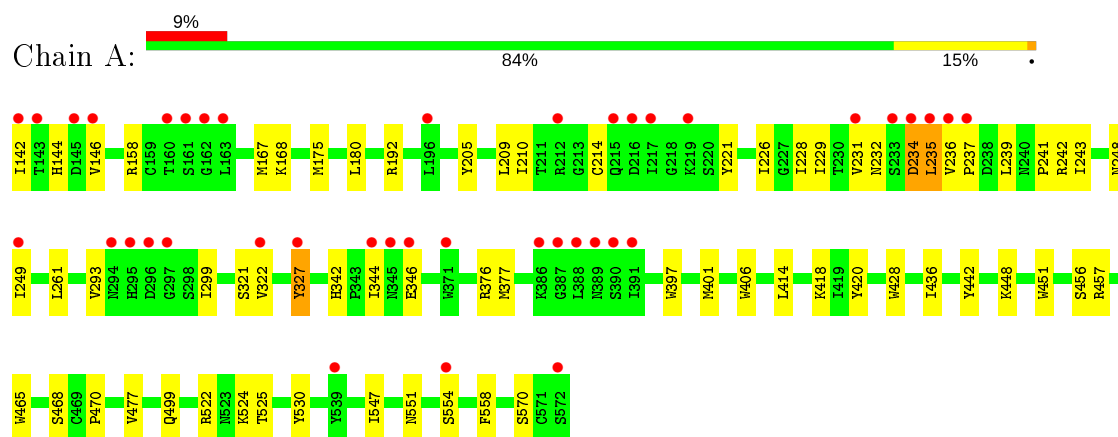
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	254	Total	O	0	0
			254	254		
10	B	225	Total	O	0	0
			225	225		

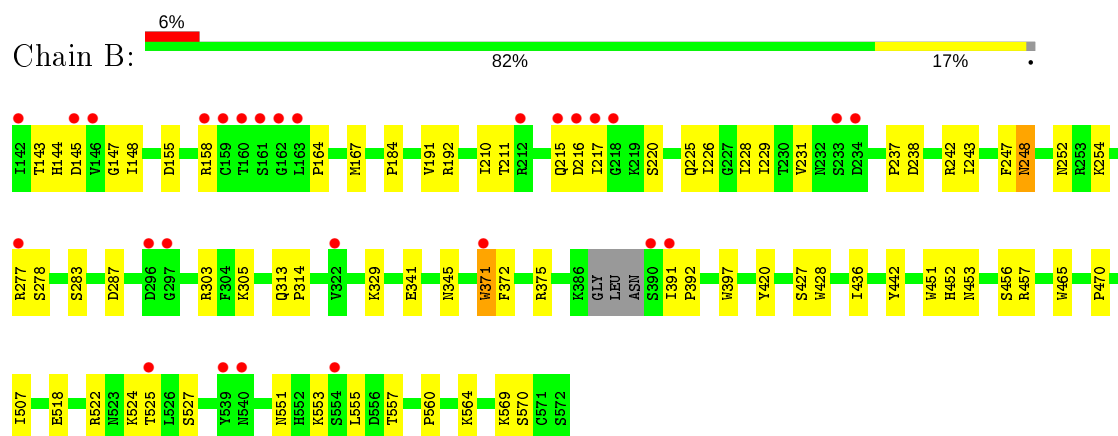
3 Residue-property plots

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: Hemagglutinin-neuraminidase



• Molecule 1: Hemagglutinin-neuraminidase



• Molecule 2: alpha-D-mannopyranose-(1-3)-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

Chain D:

100%

RMS1
RMS2
RMS3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.90Å 95.99Å 105.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 1.83 29.90 – 1.83	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.90-1.83) 91.5 (29.90-1.83)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.181 , 0.228 0.182 , 0.231	Depositor DCC
R_{free} test set	3411 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	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	7500	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: GOL, 8LM, BMA, NAG, CA, EDO, SO4, 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	0.42	0/3474	0.61	2/4735 (0.0%)
1	B	0.41	0/3445	0.59	0/4694
All	All	0.42	0/6919	0.60	2/9429 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	TYR	N-CA-C	-5.90	95.06	111.00
1	A	234	ASP	N-CA-C	-5.31	96.66	111.00

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	3392	0	3346	65	0
1	B	3361	0	3319	59	0
2	C	50	0	43	1	0
3	D	39	11	34	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	14	0	13	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	13	0	0
6	A	8	0	12	3	0
6	B	4	6	6	2	0
7	A	5	0	0	0	0
7	B	10	0	0	0	0
8	A	66	0	0	4	0
8	B	33	0	0	1	0
9	B	6	0	8	1	0
10	A	254	0	0	7	0
10	B	225	0	0	8	0
All	All	7483	17	6794	128	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 9.

All (128) 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:234:ASP:OD1	1:A:234:ASP:O	1.85	0.95
1:A:221[A]:TYR:CE2	1:A:249:ILE:HD12	2.13	0.83
1:A:231:VAL:HG12	1:A:235:LEU:HA	1.59	0.83
1:B:277:ARG:HD3	1:B:371:TRP:CH2	2.14	0.82
1:A:499:GLN:H	6:A:607:EDO:H12	1.45	0.81
1:A:144:HIS:CE1	1:A:229:ILE:H	1.99	0.80
1:A:192:ARG:HD2	8:A:610:8LM:C26	2.11	0.80
1:A:448:LYS:HE3	10:A:725:HOH:O	1.84	0.77
5:A:606:NAG:H3	5:A:606:NAG:H83	1.67	0.75
8:A:610:8LM:O8	10:A:701:HOH:O	2.08	0.72
1:A:192:ARG:NH2	8:A:610:8LM:O4	2.22	0.70
1:B:144:HIS:CD2	1:B:229:ILE:H	2.10	0.69
1:A:221[A]:TYR:CE1	1:A:249:ILE:HB	2.27	0.69
1:A:192:ARG:NH1	1:A:214:CYS:O	2.26	0.69
1:B:277:ARG:HD3	1:B:371:TRP:HH2	1.59	0.67
1:B:527:SER:HB3	1:B:551:ASN:HB3	1.77	0.66
1:A:234:ASP:O	1:A:236:VAL:N	2.28	0.65
1:B:371:TRP:HA	1:B:371:TRP:CE3	2.33	0.63
1:B:155:ASP:HA	1:B:158:ARG:HE	1.62	0.63
1:B:371:TRP:HA	1:B:371:TRP:HE3	1.64	0.63
1:A:175:MET:HE1	1:A:237:PRO:HD2	1.79	0.62
1:B:228:ILE:HD11	1:B:242:ARG:NH2	2.15	0.62
1:A:180:LEU:HB3	1:A:241:PRO:HG2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:HG2	1:A:401:MET:HE3	1.84	0.59
1:A:344:ILE:O	1:A:346:GLU:OE1	2.18	0.59
1:B:220:SER:HB2	1:B:252:ASN:OD1	2.03	0.59
1:A:524:LYS:HE2	10:A:910:HOH:O	2.02	0.58
1:B:283:SER:HB3	1:B:341[A]:GLU:OE2	2.04	0.58
1:A:342:HIS:ND1	1:A:342:HIS:O	2.34	0.58
1:A:168:LYS:H	6:A:608:EDO:H12	1.67	0.58
1:B:217:ILE:O	1:B:217:ILE:HG13	2.04	0.58
1:A:144:HIS:CE1	1:A:229:ILE:N	2.72	0.58
1:B:569:LYS:HG2	1:B:570:SER:N	2.18	0.57
1:B:452:HIS:HB2	10:B:752:HOH:O	2.04	0.57
1:B:184:PRO:HB3	6:B:607:EDO:H12	1.87	0.57
1:B:238:ASP:OD1	1:B:564:LYS:NZ	2.26	0.57
1:A:420:TYR:CE2	1:A:436:ILE:HD11	2.39	0.57
1:B:247:PHE:O	1:B:248:ASN:HB2	2.05	0.57
1:A:231:VAL:HG12	1:A:235:LEU:CA	2.34	0.56
1:A:142:ILE:HG12	1:A:142:ILE:O	2.06	0.56
1:A:180:LEU:HD23	1:A:241:PRO:HG2	1.86	0.56
1:A:232:ASN:HB2	1:A:234:ASP:O	2.06	0.56
1:A:144:HIS:HE1	1:A:228:ILE:HA	1.70	0.55
1:A:477:VAL:HG23	10:A:825:HOH:O	2.06	0.55
1:B:524:LYS:NZ	10:B:710:HOH:O	2.40	0.54
1:A:346:GLU:OE2	1:A:401:MET:HE2	2.07	0.54
1:A:232:ASN:HB2	1:A:234:ASP:OD1	2.08	0.54
1:B:215:GLN:OE1	1:B:215:GLN:HA	2.08	0.54
1:B:148:ILE:HD11	1:B:231:VAL:HG13	1.89	0.53
1:A:192:ARG:HG3	1:A:210:ILE:CD1	2.39	0.53
1:A:499:GLN:H	6:A:607:EDO:C1	2.19	0.52
1:A:226:ILE:HD12	1:A:243:ILE:HD11	1.93	0.51
1:A:468:SER:O	10:A:703:HOH:O	2.19	0.51
1:A:239:LEU:O	1:A:241:PRO:HD3	2.09	0.51
1:B:555:LEU:HB2	1:B:557:THR:HG22	1.92	0.51
1:B:522:ARG:NH2	1:B:525:THR:OG1	2.43	0.51
1:A:209:LEU:HB3	1:A:221[B]:TYR:CZ	2.45	0.51
1:A:377:MET:HG3	1:A:406:TRP:CE2	2.46	0.51
1:A:261:LEU:HG	1:A:327:TYR:CE1	2.46	0.50
1:B:329:LYS:O	10:B:701:HOH:O	2.19	0.50
1:B:237:PRO:O	1:B:564:LYS:HE3	2.09	0.50
1:B:155:ASP:O	1:B:158:ARG:HG2	2.11	0.50
5:A:606:NAG:C8	5:A:606:NAG:H3	2.41	0.50
1:B:192:ARG:HG2	8:B:610:8LM:C22	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASP:OD1	1:B:254:LYS:NZ	2.43	0.49
1:B:570:SER:HA	10:B:882:HOH:O	2.12	0.49
1:B:191:VAL:HB	1:B:560:PRO:HD3	1.94	0.49
1:A:146:VAL:O	1:A:146:VAL:HG12	2.13	0.49
1:A:346:GLU:OE2	1:A:401:MET:CE	2.61	0.48
1:B:427:SER:HB3	10:B:810:HOH:O	2.13	0.48
1:B:167:MET:CG	1:B:570:SER:HB2	2.43	0.48
1:A:221[B]:TYR:OH	10:A:702:HOH:O	2.15	0.48
1:A:397:TRP:CD2	1:A:442:TYR:HB3	2.48	0.48
1:B:451:TRP:CH2	1:B:453:ASN:HB2	2.48	0.48
1:B:451:TRP:CZ2	1:B:453:ASN:HB2	2.49	0.48
1:A:321:SER:O	1:A:322:VAL:HB	2.14	0.47
1:A:456:SER:HB3	1:A:465:TRP:CD2	2.49	0.47
1:A:232:ASN:OD1	8:A:611:8LM:C1	2.62	0.47
5:A:606:NAG:H82	5:A:606:NAG:C1	2.45	0.47
1:B:226:ILE:HB	1:B:243:ILE:HG22	1.96	0.46
1:B:277:ARG:HG3	1:B:278:SER:N	2.30	0.46
1:B:247:PHE:O	1:B:248:ASN:CB	2.62	0.46
1:B:372:PHE:O	1:B:375:ARG:HG2	2.16	0.46
1:A:175:MET:CE	1:A:237:PRO:HD2	2.46	0.45
1:B:164:PRO:HA	1:B:570:SER:O	2.16	0.45
1:A:180:LEU:HD23	1:A:241:PRO:CB	2.47	0.45
1:A:249:ILE:O	1:A:249:ILE:HG12	2.16	0.45
1:A:451:TRP:CZ2	2:C:2:NAG:H5	2.51	0.45
1:B:345:ASN:HB2	10:B:811:HOH:O	2.16	0.45
1:A:428:TRP:CG	1:A:470:PRO:HA	2.52	0.45
1:A:525:THR:HG23	5:A:606:NAG:H82	1.98	0.45
1:B:148:ILE:HD13	1:B:229:ILE:HG22	1.99	0.45
1:A:229:ILE:HG12	1:A:239:LEU:HD23	1.99	0.45
1:B:313:GLN:HB2	1:B:314:PRO:HD2	1.99	0.44
1:A:346:GLU:CG	1:A:401:MET:HE3	2.47	0.44
1:A:167:MET:HG2	1:A:570:SER:HB3	1.99	0.44
1:A:327:TYR:O	1:A:414:LEU:CD2	2.66	0.44
1:A:530:TYR:C	1:A:530:TYR:CD2	2.91	0.44
5:A:606:NAG:C3	5:A:606:NAG:H83	2.43	0.44
1:A:293:VAL:HG22	1:A:299:ILE:HG12	2.00	0.44
1:B:167:MET:HG2	1:B:570:SER:HB2	2.00	0.43
1:B:192:ARG:HD3	1:B:210:ILE:HD12	2.00	0.43
1:B:287:ASP:OD2	1:B:305:LYS:NZ	2.51	0.43
1:A:180:LEU:HD23	1:A:241:PRO:CG	2.48	0.43
1:A:205:TYR:CE1	1:A:547:ILE:HD13	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASN:CB	1:A:234:ASP:OD1	2.67	0.43
1:B:397:TRP:CD2	1:B:442:TYR:HB3	2.54	0.43
1:B:428:TRP:CG	1:B:470:PRO:HA	2.53	0.43
1:A:221[A]:TYR:CD1	1:A:249:ILE:HB	2.53	0.42
1:A:551:ASN:HB2	1:A:558:PHE:CE1	2.54	0.42
1:B:143:THR:HG23	1:B:145:ASP:OD1	2.19	0.42
1:B:428:TRP:CD2	1:B:470:PRO:HA	2.54	0.42
1:B:553:LYS:NZ	10:B:719:HOH:O	2.52	0.42
1:A:242:ARG:HD3	1:A:242:ARG:HA	1.76	0.42
1:B:451:TRP:CD2	3:D:2:NAG:H5	2.55	0.42
1:B:456:SER:HB3	1:B:465:TRP:CD2	2.54	0.42
1:B:242:ARG:CB	9:B:608:GOL:H2	2.49	0.42
1:B:391:ILE:HG13	1:B:392:PRO:HD2	2.02	0.42
1:B:225:GLN:HG2	10:B:713:HOH:O	2.20	0.42
1:A:376:ARG:HG3	1:A:401:MET:CE	2.49	0.41
1:A:554:SER:O	1:B:522:ARG:NH1	2.54	0.41
1:A:418:LYS:HE2	10:A:788:HOH:O	2.19	0.41
1:B:456:SER:HB3	1:B:465:TRP:CE2	2.55	0.41
1:B:507:ILE:O	1:B:518:GLU:HB2	2.21	0.41
1:A:221[A]:TYR:CZ	1:A:249:ILE:HB	2.54	0.41
1:B:145:ASP:C	1:B:147:GLY:H	2.24	0.41
1:B:420:TYR:CE2	1:B:436:ILE:HD11	2.56	0.40
1:B:211:THR:HA	6:B:607:EDO:H11	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	431/431 (100%)	407 (94%)	21 (5%)	3 (1%)	22 9
1	B	425/431 (99%)	399 (94%)	25 (6%)	1 (0%)	47 33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	856/862 (99%)	806 (94%)	46 (5%)	4 (0%)	29	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	B	248	ASN
1	A	248	ASN
1	A	522	ARG

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	391/389 (100%)	389 (100%)	2 (0%)	88	85
1	B	388/389 (100%)	385 (99%)	3 (1%)	81	75
All	All	779/778 (100%)	774 (99%)	5 (1%)	86	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	457	ARG
1	B	303	ARG
1	B	371	TRP
1	B	457	ARG

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

Mol	Chain	Res	Type
1	A	144	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 ⓘ

7 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	0.37	0	17,19,21	0.67	0
2	NAG	C	2	2	14,14,15	0.21	0	17,19,21	0.60	0
2	BMA	C	3	2	11,11,12	0.80	0	15,15,17	0.97	0
2	MAN	C	4	2	11,11,12	1.25	1 (9%)	15,15,17	1.25	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.57	1 (7%)	17,19,21	0.49	0
3	NAG	D	2	3	14,14,15	0.17	0	17,19,21	0.46	0
3	BMA	D	3	3	11,11,12	0.88	0	15,15,17	1.09	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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	MAN	C2-C3	2.36	1.56	1.52
3	D	1	NAG	O5-C1	-2.05	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	2.58	115.68	112.19
2	C	4	MAN	C2-C3-C4	2.21	114.72	110.89
3	D	3	BMA	O5-C5-C4	-2.07	105.79	110.83
2	C	4	MAN	O2-C2-C1	2.06	113.36	109.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

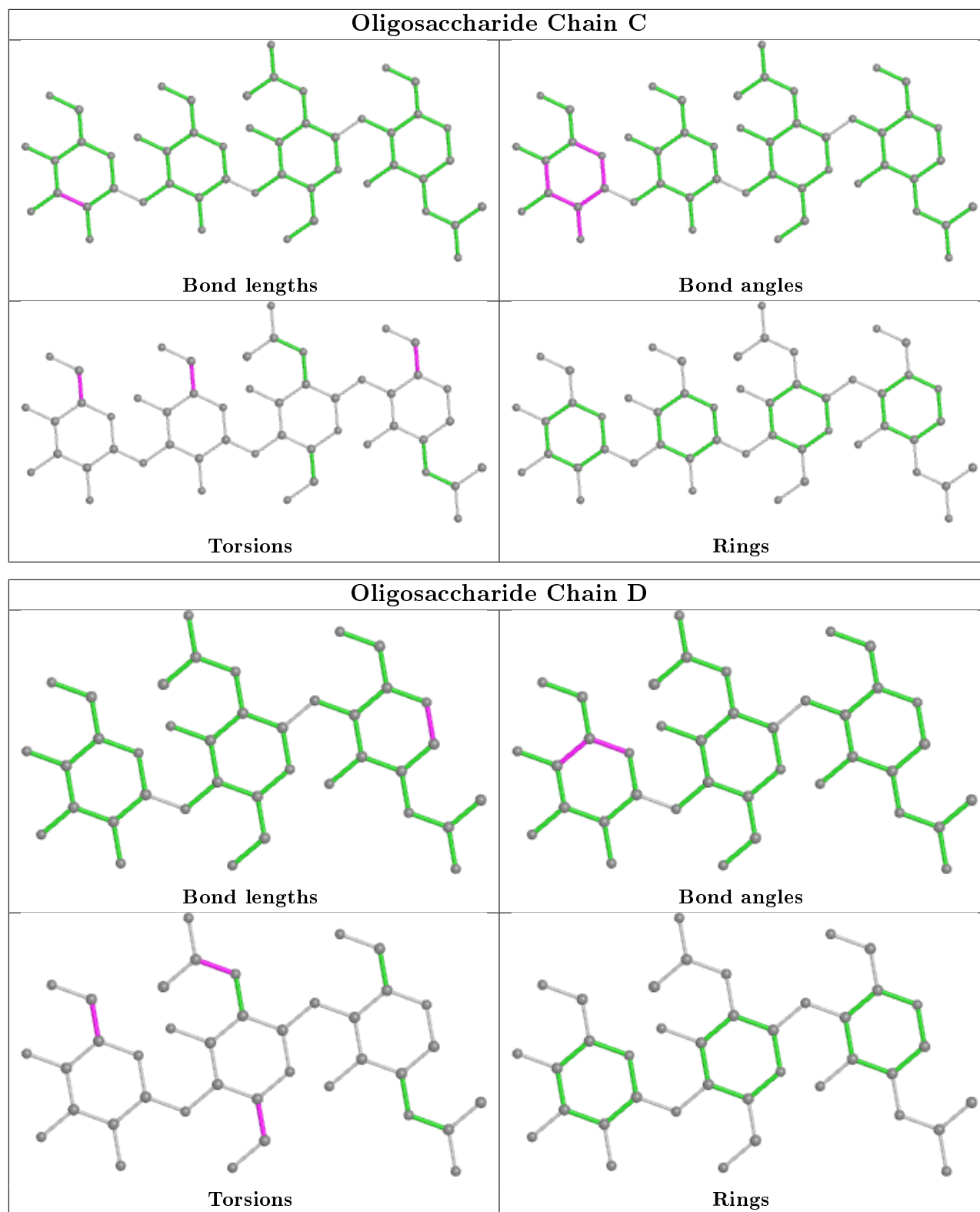
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
2	C	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 ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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
8	8LM	B	610	-	30,35,35	2.13	8 (26%)	29,50,50	2.29	7 (24%)
8	8LM	A	610	-	30,35,35	2.26	9 (30%)	29,50,50	2.50	7 (24%)
6	EDO	A	608	-	3,3,3	0.52	0	2,2,2	0.30	0
8	8LM	A	611	-	30,35,35	2.31	8 (26%)	29,50,50	1.72	4 (13%)
7	SO4	B	609	-	4,4,4	0.10	0	6,6,6	0.12	0
6	EDO	B	607	-	3,3,3	0.55	0	2,2,2	0.69	0
9	GOL	B	608	-	5,5,5	0.37	0	5,5,5	0.18	0
5	NAG	B	605	1	14,14,15	0.20	0	17,19,21	0.67	0
6	EDO	A	607	-	3,3,3	0.52	0	2,2,2	0.26	0
7	SO4	A	609	-	4,4,4	0.21	0	6,6,6	0.32	0
5	NAG	A	606	1	14,14,15	0.36	0	17,19,21	0.97	0
7	SO4	B	606	-	4,4,4	0.13	0	6,6,6	0.11	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
8	8LM	B	610	-	-	2/22/50/50	0/3/3/3
8	8LM	A	610	-	-	2/22/50/50	0/3/3/3
6	EDO	A	608	-	-	0/1/1/1	-
8	8LM	A	611	-	-	6/22/50/50	0/3/3/3
6	EDO	B	607	-	-	1/1/1/1	-
9	GOL	B	608	-	-	0/4/4/4	-
5	NAG	B	605	1	-	0/6/23/26	0/1/1/1
6	EDO	A	607	-	-	1/1/1/1	-
5	NAG	A	606	1	-	3/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	611	8LM	O6-C6	7.45	1.58	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	610	8LM	O6-C6	7.27	1.58	1.46
8	B	610	8LM	O6-C6	6.46	1.57	1.46
8	A	611	8LM	C10-N5	5.61	1.46	1.34
8	A	610	8LM	C10-N5	5.55	1.46	1.34
8	B	610	8LM	C10-N5	4.77	1.44	1.34
8	A	611	8LM	C5-N5	4.26	1.52	1.45
8	B	610	8LM	C5-N5	4.16	1.52	1.45
8	A	610	8LM	C5-N5	3.82	1.51	1.45
8	A	611	8LM	C7-C6	3.76	1.57	1.53
8	A	610	8LM	N28-N18	-3.36	1.32	1.37
8	B	610	8LM	C7-C6	3.22	1.57	1.53
8	B	610	8LM	N28-N18	-3.00	1.32	1.37
8	A	611	8LM	N28-N18	-2.89	1.32	1.37
8	A	611	8LM	C21-C20	2.73	1.53	1.48
8	A	610	8LM	C7-C6	2.72	1.56	1.53
8	A	611	8LM	O6-C2	2.57	1.40	1.36
8	A	610	8LM	C19-N18	-2.55	1.33	1.36
8	B	610	8LM	C19-N18	-2.41	1.33	1.36
8	B	610	8LM	O4-C4	2.41	1.47	1.42
8	B	610	8LM	O10-C10	-2.28	1.18	1.23
8	A	610	8LM	O10-C10	-2.25	1.18	1.23
8	A	610	8LM	O6-C2	2.23	1.40	1.36
8	A	610	8LM	O4-C4	2.18	1.46	1.42
8	A	611	8LM	O4-C4	2.06	1.46	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	610	8LM	C5-N5-C10	-7.86	111.36	123.21
8	A	610	8LM	C11-C10-N5	7.24	123.07	115.95
8	A	610	8LM	C5-N5-C10	-5.68	114.65	123.21
8	B	610	8LM	C11-C10-N5	5.27	121.13	115.95
8	A	610	8LM	O6-C2-C3	-4.96	117.44	123.76
8	A	611	8LM	C11-C10-N5	4.52	120.39	115.95
8	A	610	8LM	C8-C7-C6	-4.39	104.70	113.03
8	A	611	8LM	C21-C20-N27	4.28	127.80	120.96
8	A	610	8LM	C21-C20-N27	4.28	127.79	120.96
8	B	610	8LM	C8-C7-C6	-3.99	105.47	113.03
8	A	611	8LM	C6-C5-N5	3.58	116.85	110.91
8	B	610	8LM	C21-C20-N27	3.35	126.30	120.96
8	A	611	8LM	C5-N5-C10	-2.90	118.83	123.21
8	A	610	8LM	O10-C10-N5	-2.74	117.86	122.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	610	8LM	O10-C10-N5	-2.63	118.06	122.93
8	B	610	8LM	O6-C2-C3	-2.18	120.97	123.76
8	B	610	8LM	C6-C5-N5	-2.04	107.53	110.91
8	A	610	8LM	O10-C10-C11	-2.00	119.07	122.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	611	8LM	O8-C8-C9-O9
8	A	611	8LM	C6-C7-C8-C9
8	A	611	8LM	O7-C7-C8-O8
8	A	611	8LM	C6-C7-C8-O8
8	A	611	8LM	C7-C8-C9-O9
5	A	606	NAG	C8-C7-N2-C2
5	A	606	NAG	O7-C7-N2-C2
8	A	611	8LM	O7-C7-C8-C9
8	A	610	8LM	N5-C10-C11-C13
8	A	610	8LM	O10-C10-C11-C13
6	B	607	EDO	O1-C1-C2-O2
8	B	610	8LM	O10-C10-C11-C12
5	A	606	NAG	C3-C2-N2-C7
8	B	610	8LM	N5-C10-C11-C12
6	A	607	EDO	O1-C1-C2-O2

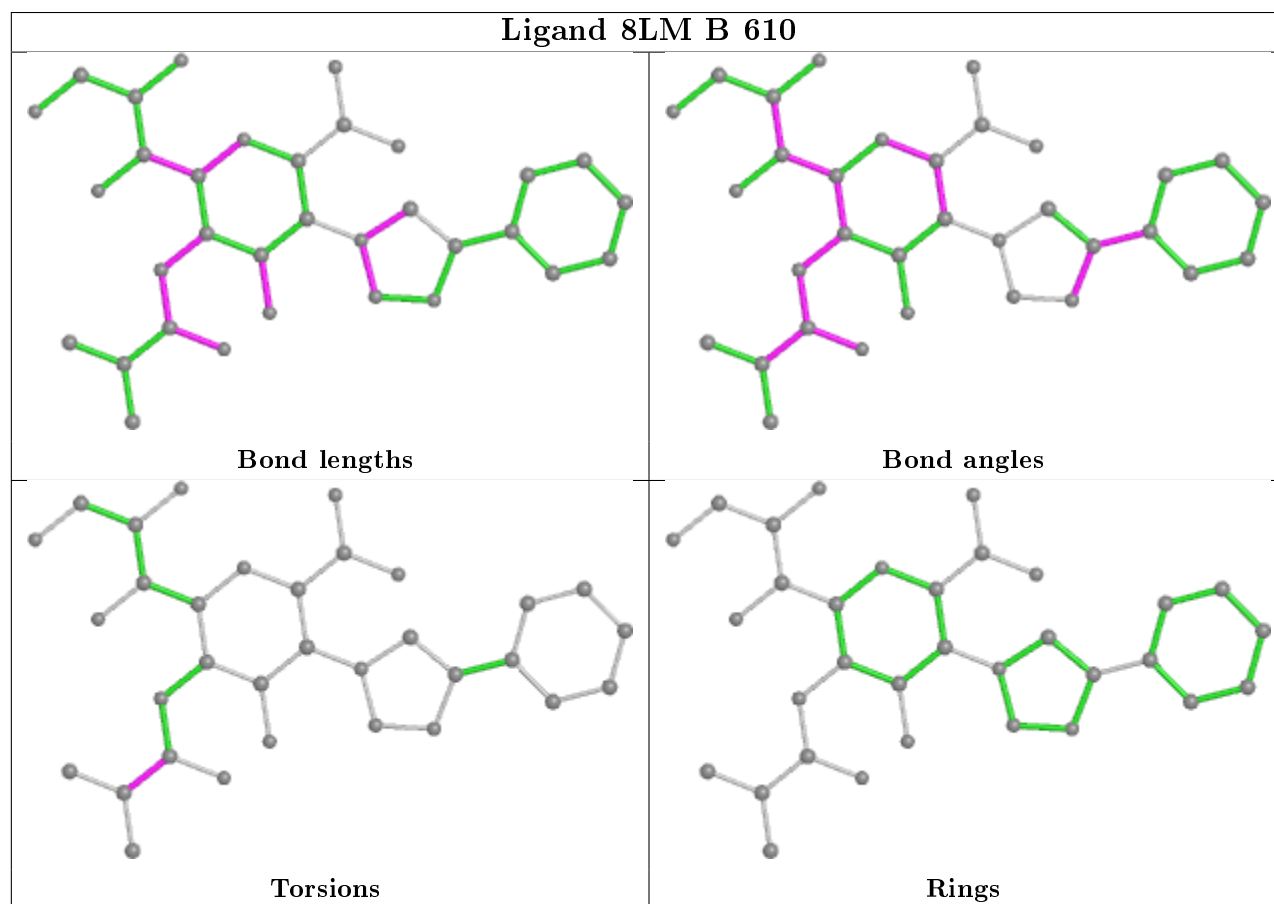
There are no ring outliers.

8 monomers are involved in 16 short contacts:

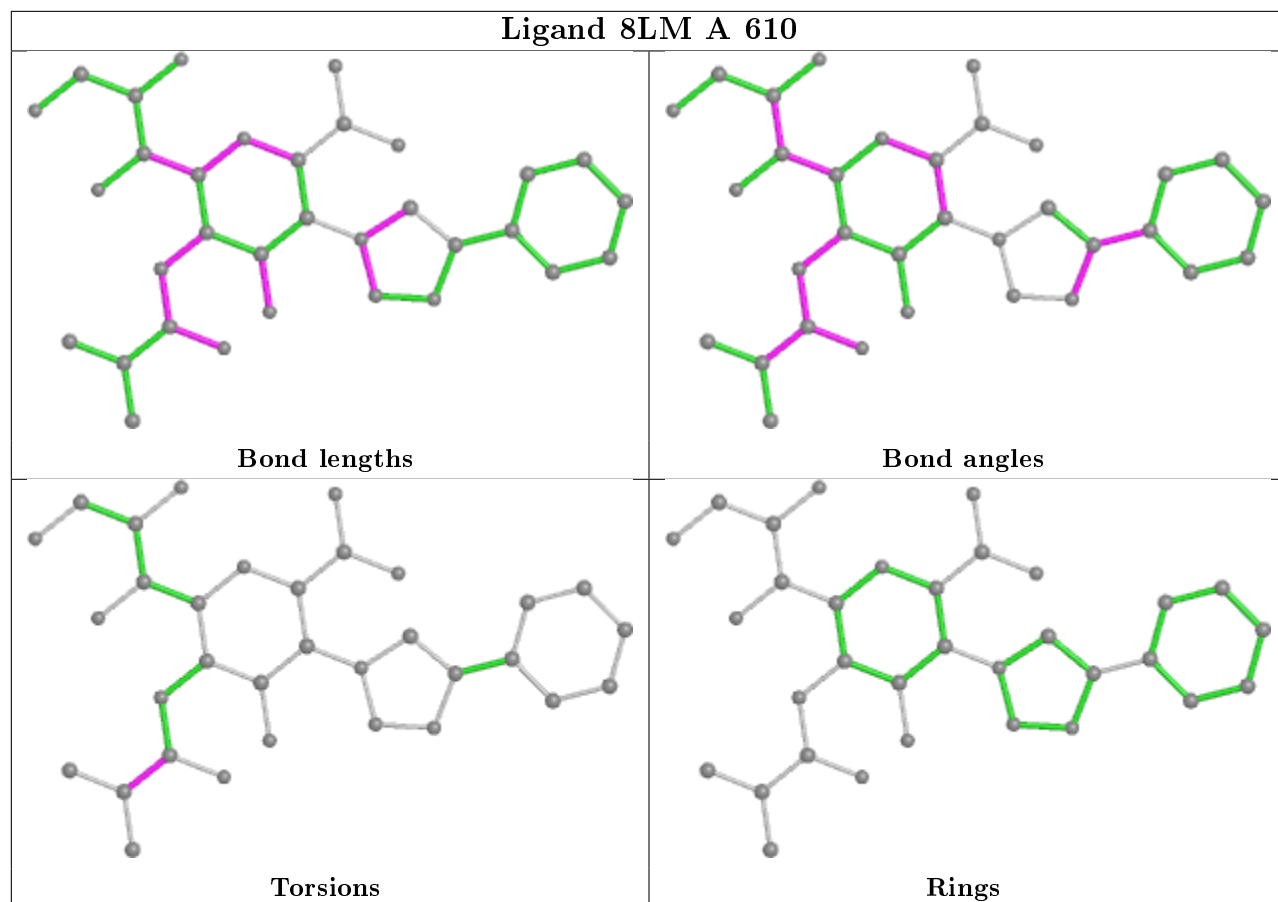
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	610	8LM	1	0
8	A	610	8LM	3	0
6	A	608	EDO	1	0
8	A	611	8LM	1	0
6	B	607	EDO	2	0
9	B	608	GOL	1	0
6	A	607	EDO	2	0
5	A	606	NAG	5	0

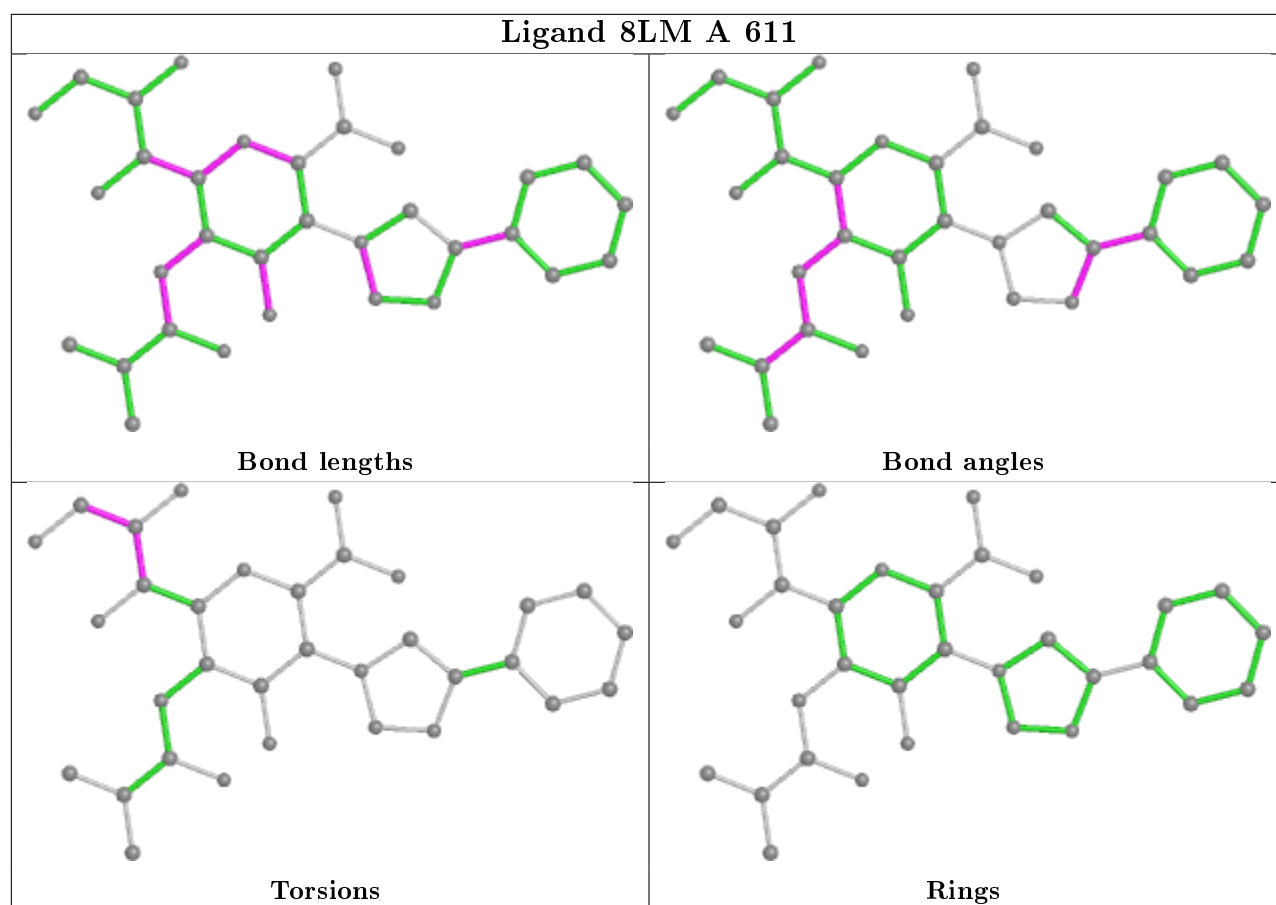
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.



Ligand 8LM A 610





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	431/431 (100%)	0.30	40 (9%) 8 7	16, 28, 69, 92	0
1	B	428/431 (99%)	0.23	27 (6%) 20 17	18, 30, 61, 110	0
All	All	859/862 (99%)	0.26	67 (7%) 13 12	16, 29, 66, 110	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	VAL	10.4
1	B	145	ASP	9.0
1	A	388	LEU	8.8
1	A	146	VAL	8.4
1	B	217	ILE	8.4
1	A	234	ASP	6.5
1	B	539	TYR	5.7
1	A	235	LEU	5.7
1	A	145	ASP	5.7
1	A	539	TYR	5.5
1	A	217	ILE	5.4
1	A	142	ILE	4.8
1	A	143	THR	4.8
1	B	163	LEU	4.6
1	B	160	THR	4.3
1	A	163	LEU	4.1
1	A	391	ILE	4.1
1	B	161	SER	4.0
1	A	162	GLY	3.9
1	B	234	ASP	3.8
1	A	387	GLY	3.8
1	A	389	ASN	3.7
1	B	297	GLY	3.7
1	B	371	TRP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	391	ILE	3.7
1	B	216	ASP	3.6
1	B	218	GLY	3.5
1	A	215	GLN	3.5
1	B	215	GLN	3.5
1	A	231	VAL	3.5
1	A	346	GLU	3.4
1	A	344	ILE	3.4
1	B	233	SER	3.2
1	A	237	PRO	3.0
1	A	386	LYS	3.0
1	A	572	SER	2.9
1	A	390	SER	2.9
1	A	249	ILE	2.9
1	B	162	GLY	2.8
1	A	345	ASN	2.7
1	B	296	ASP	2.7
1	B	390	SER	2.7
1	A	236	VAL	2.6
1	B	159	CYS	2.6
1	A	161	SER	2.6
1	A	295	HIS	2.5
1	A	233	SER	2.5
1	A	160	THR	2.5
1	B	142	ILE	2.5
1	A	554	SER	2.5
1	A	327	TYR	2.4
1	A	219	LYS	2.4
1	A	322	VAL	2.3
1	B	212	ARG	2.3
1	B	277	ARG	2.3
1	B	540	ASN	2.3
1	A	212	ARG	2.2
1	A	216	ASP	2.2
1	A	196	LEU	2.2
1	A	294	ASN	2.1
1	B	554	SER	2.1
1	B	158	ARG	2.1
1	B	322	VAL	2.1
1	A	297	GLY	2.1
1	B	525	THR	2.1
1	A	296	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	371	TRP	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](#)

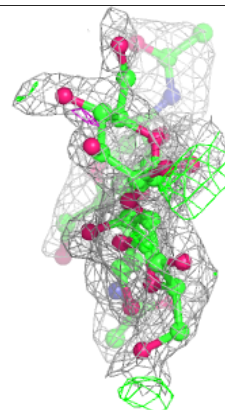
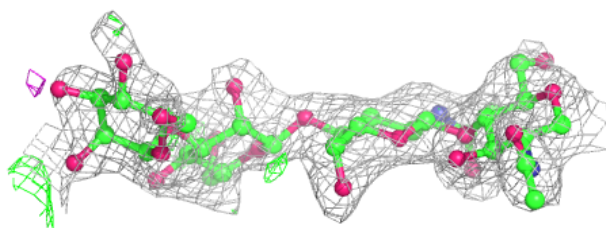
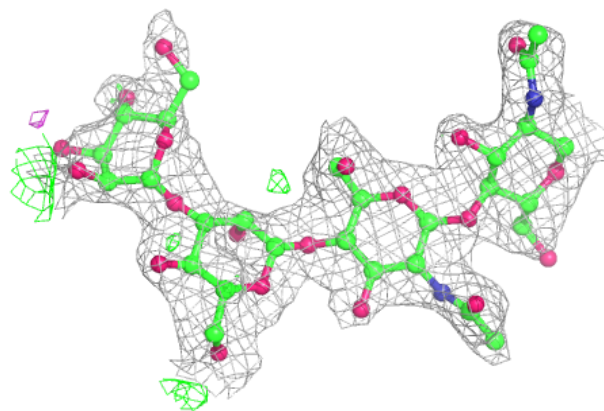
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	D	3	11/12	0.57	0.27	82,99,115,123	0
2	MAN	C	4	11/12	0.76	0.24	58,67,72,78	0
2	BMA	C	3	11/12	0.76	0.18	54,65,73,76	0
3	NAG	D	2	14/15	0.87	0.20	53,59,67,74	0
3	NAG	D	1	14/15	0.90	0.17	51,58,77,80	0
2	NAG	C	2	14/15	0.90	0.10	47,52,57,61	0
2	NAG	C	1	14/15	0.92	0.12	37,47,58,64	0

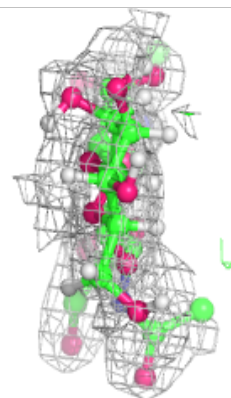
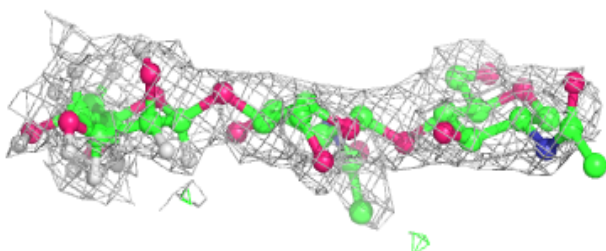
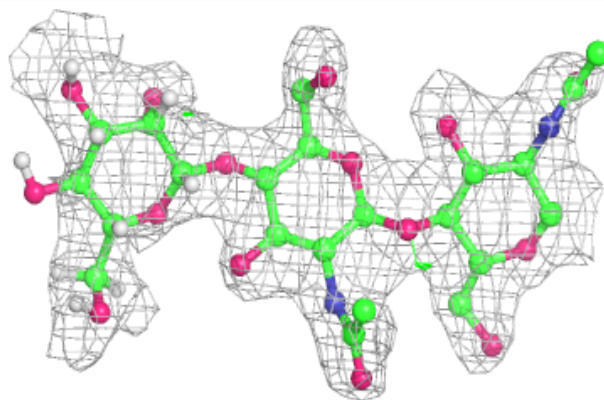
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 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 ⓘ

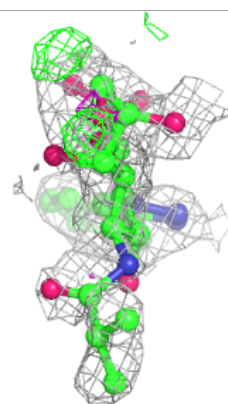
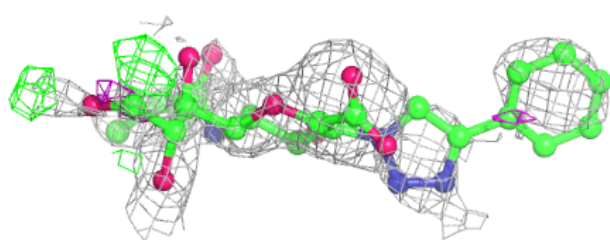
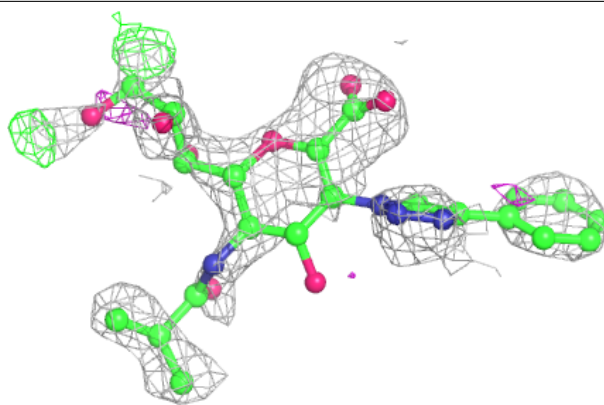
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	605	14/15	0.66	0.27	63,75,86,91	0
8	8LM	A	610	33/33	0.69	0.29	43,74,87,87	0
9	GOL	B	608	6/6	0.74	0.27	43,54,56,59	0
8	8LM	A	611	33/33	0.74	0.25	48,62,71,75	0
6	EDO	A	608	4/4	0.78	0.14	53,57,57,61	0
5	NAG	A	606	14/15	0.80	0.27	41,53,60,64	0
6	EDO	A	607	4/4	0.83	0.12	36,40,42,52	0
6	EDO	B	607	4/4	0.84	0.14	27,36,44,44	0
8	8LM	B	610	33/33	0.92	0.11	24,40,58,59	0
7	SO4	B	609	5/5	0.95	0.10	43,49,56,57	0
7	SO4	B	606	5/5	0.98	0.07	50,50,52,56	0
7	SO4	A	609	5/5	0.99	0.11	28,31,36,40	0
4	CA	A	601	1/1	0.99	0.05	29,29,29,29	0
4	CA	B	601	1/1	0.99	0.04	32,32,32,32	0

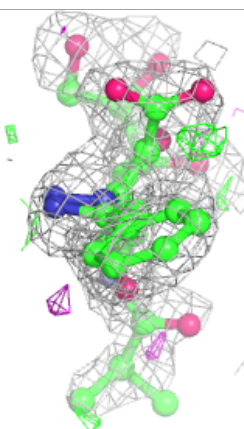
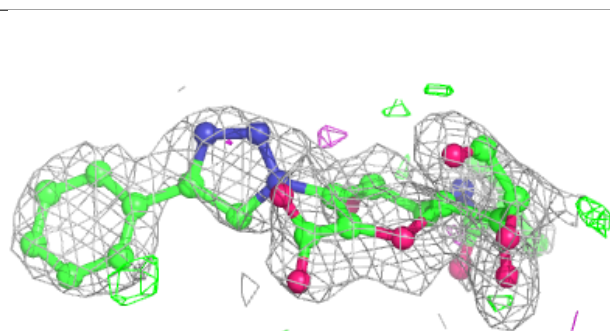
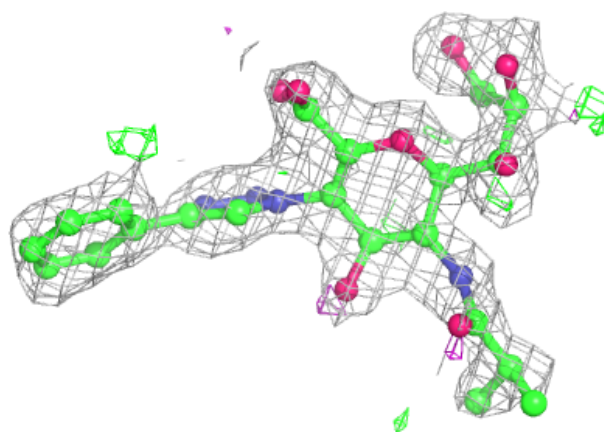
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

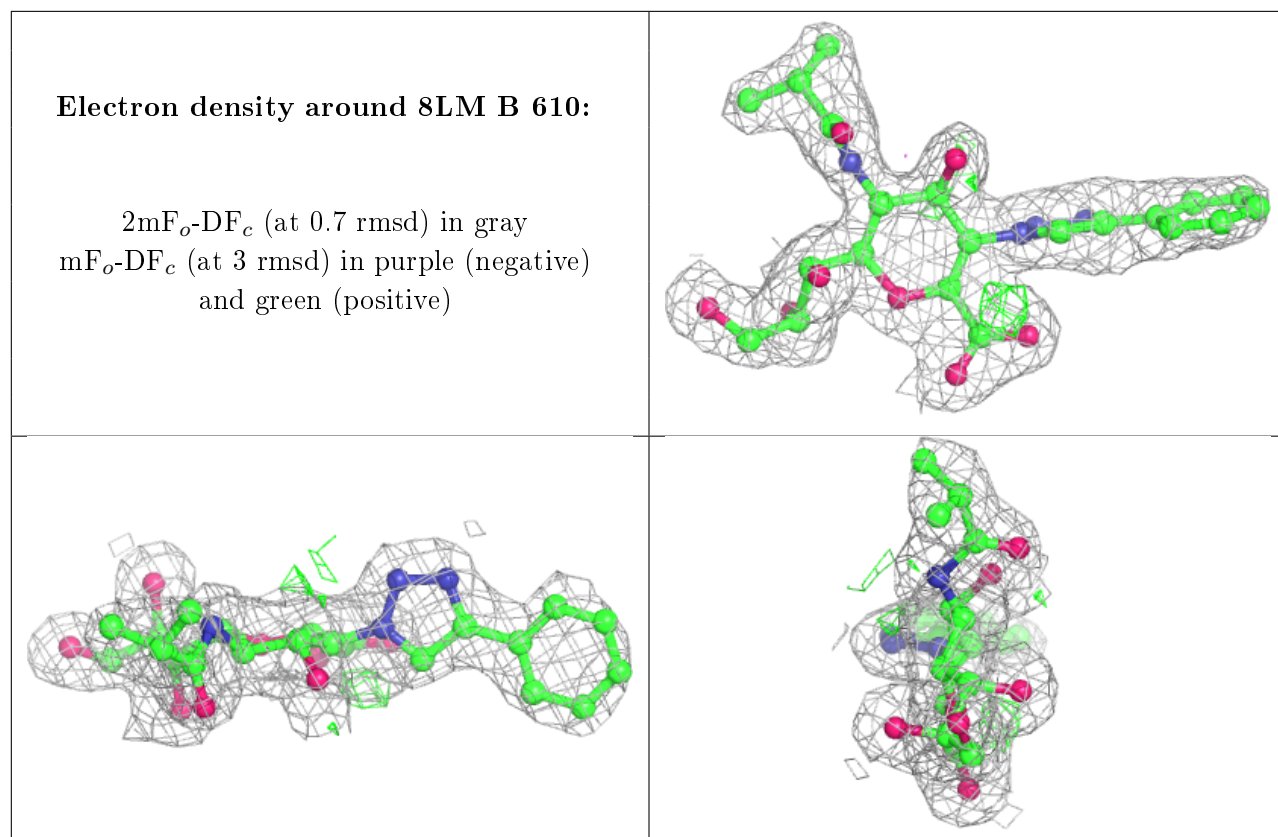
Electron density around 8LM A 610:

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

**Electron density around 8LM A 611:**

$2mF_o-DF_c$ (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.