



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:11 AM UTC

PDB ID : 6C0M / pdb_00006c0m
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

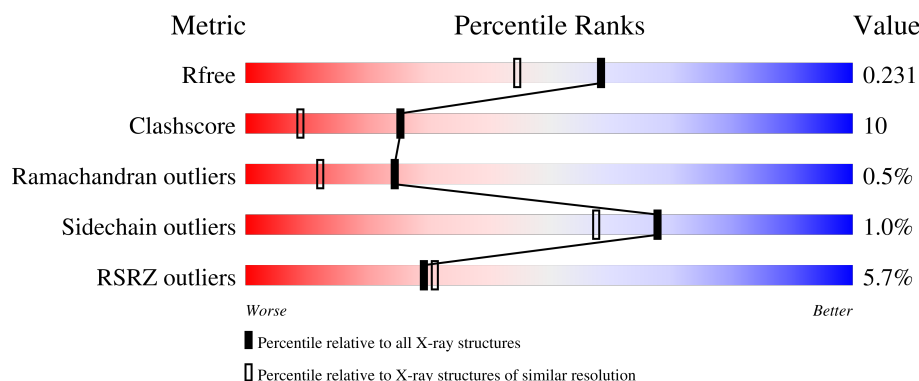
1 Overall quality at a glance

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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	431	7% 84% 15% .
1	B	431	4% 80% 19% .
2	C	4	50% 50%
3	D	3	33% 67%

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.

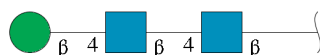
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	2	0
			3392	2145	583	644	20			
1	B	428	Total	C	N	O	S	0	2	0
			3361	2126	579	636	20			

- 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.

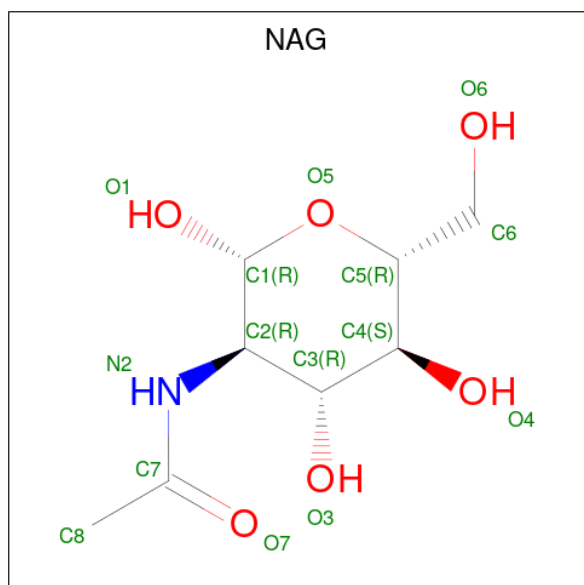


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	3	Total	C	H	N	O	0	0	0
			50	22	11	2	15			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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



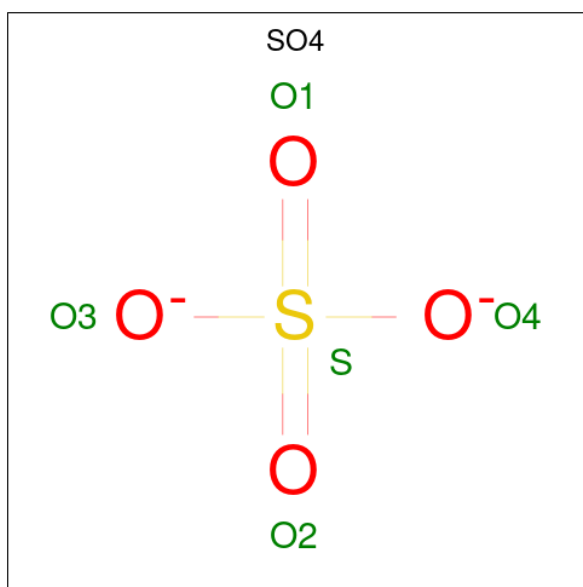
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



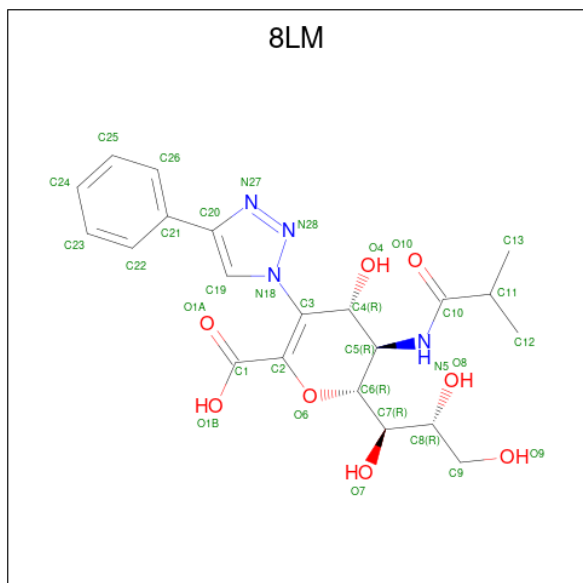
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		

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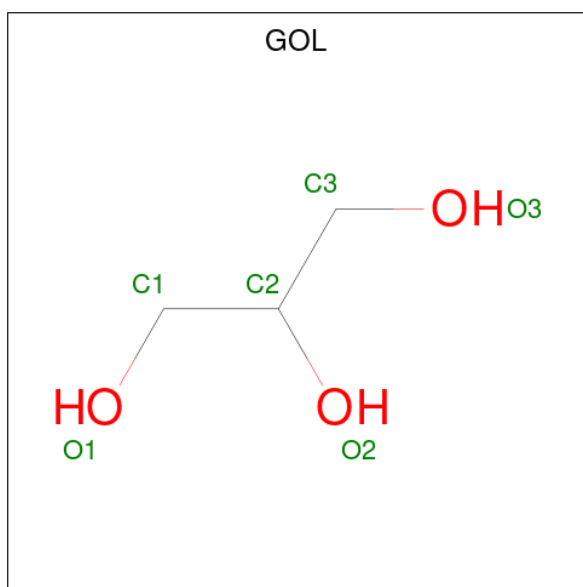
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			33	21	4	8		
8	A	1	Total	C	N	O	0	0
			33	21	4	8		
8	B	1	Total	C	N	O	0	0
			33	21	4	8		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

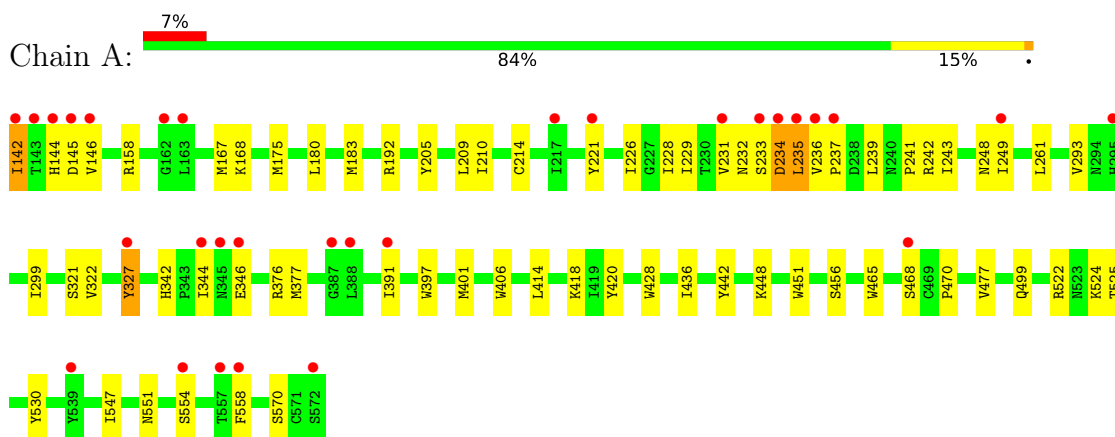
- Molecule 10 is water.

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

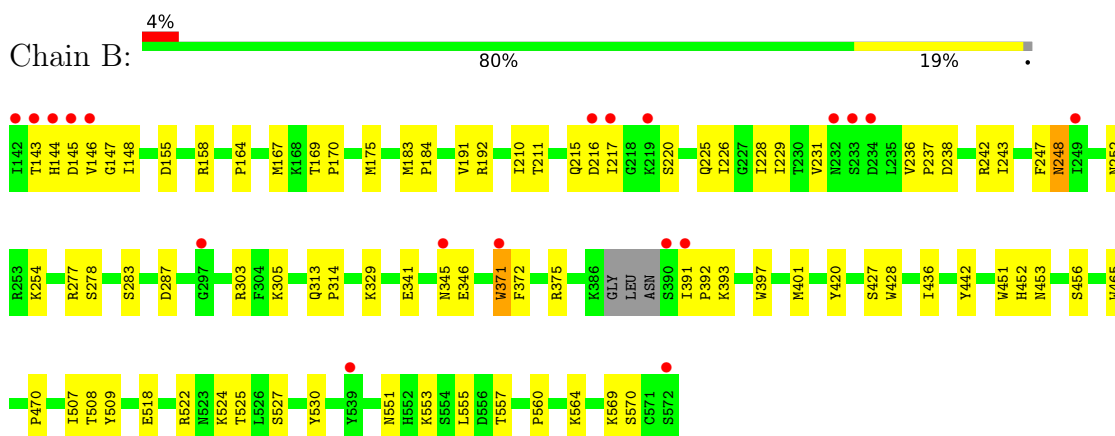
3 Residue-property plots

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



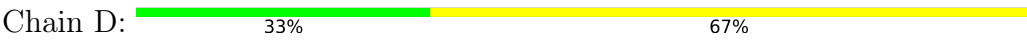
- Molecule 1: Hemagglutinin-neuraminidase



- 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



MAG1
MAG2
BOL3

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 0.183 , 0.231	Depositor DCC
R_{free} test set	3421 reflections (4.51%)	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 , 45.6	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, 8LM, EDO, GOL, SO4, CA, BMA

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	0.37	0/3474	0.63	3/4735 (0.1%)
1	B	0.35	0/3445	0.56	2/4694 (0.0%)
All	All	0.36	0/6919	0.60	5/9429 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	TYR	N-CA-C	-8.70	95.06	109.07
1	A	234	ASP	N-CA-C	-8.23	96.66	109.25
1	A	233	SER	N-CA-C	-6.86	102.65	111.02
1	B	509	TYR	N-CA-C	-5.57	99.44	108.52
1	B	508	THR	N-CA-C	5.04	117.62	109.06

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	64	0
2	C	50	0	43	1	0
3	D	39	11	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	14	0	13	5	0
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	132	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 10.

All (132) 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:O	1:A:234:ASP:OD1	1.85	0.95
1:A:175:MET:HE1	1:A:237:PRO:HD2	1.52	0.89
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:346:GLU:OE2	1:A:401:MET:HE2	1.82	0.80
1:A:448:LYS:HE3	10:A:725:HOH:O	1.84	0.77
5:A:606:NAG:H83	5:A:606:NAG:H3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:O	1:A:342:HIS:ND1	2.34	0.58
1:A:168:LYS:H	6:A:608:EDO:H12	1.67	0.58
1:B:217:ILE:HG13	1:B:217:ILE:O	2.04	0.58
1:B:346:GLU:HG2	1:B:401:MET:HE3	1.86	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:A:376:ARG:HG3	1:A:401:MET:HE1	1.87	0.56
1:A:231:VAL:HG12	1:A:235:LEU:CA	2.34	0.56
1:A:142:ILE:O	1:A:142:ILE:HG12	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:B:247:PHE:O	1:B:248:ASN:HB2	2.05	0.55
1:A:346:GLU:HG2	1:A:401:MET:HE3	1.88	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:232:ASN:HB2	1:A:234:ASP:OD1	2.08	0.54
1:B:215:GLN:HA	1:B:215:GLN:OE1	2.08	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H3	5:A:606:NAG:C8	2.41	0.50
1:B:192:ARG:HG2	8:B:610:8LM:C22	2.42	0.49
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:HG12	1:A:146:VAL:O	2.13	0.49
1:A:183:MET:HE2	1:B:183:MET:HG3	1.95	0.49
1:A:530:TYR:C	1:A:530:TYR:CD2	2.91	0.49
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: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
1:A:321:SER:O	1:A:322:VAL:HB	2.14	0.47
5:A:606:NAG:C1	5:A:606:NAG:H82	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:B:145:ASP:C	1:B:147:GLY:H	2.24	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:346:GLU:OE2	1:A:401:MET:CE	2.61	0.45
1:A:249:ILE:HG12	1:A:249:ILE:O	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: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
5:A:606:NAG:H83	5:A:606:NAG:C3	2.43	0.44
1:A:293:VAL:HG22	1:A:299:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:MET:HE2	1:B:236:VAL:HG22	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
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:530:TYR:CD1	1:B:530:TYR:C	2.97	0.42
1:B:553:LYS:NZ	10:B:719:HOH:O	2.52	0.42
1:A:242:ARG:HA	1:A:242:ARG:HD3	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:B:169:THR:HA	1:B:170:PRO:C	2.46	0.41
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: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 ⓘ

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	431/431 (100%)	407 (94%)	21 (5%)	3 (1%)	18	7
1	B	425/431 (99%)	399 (94%)	25 (6%)	1 (0%)	43	34
All	All	856/862 (99%)	806 (94%)	46 (5%)	4 (0%)	24	12

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%)	387 (99%)	4 (1%)	68	58
1	B	388/389 (100%)	384 (99%)	4 (1%)	68	58
All	All	779/778 (100%)	771 (99%)	8 (1%)	68	58

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ILE
1	A	145	ASP
1	A	158	ARG
1	A	391	ILE
1	B	146	VAL
1	B	303	ARG
1	B	371	TRP
1	B	393	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	250	ASN
1	A	499	GLN
1	A	551	ASN
1	A	559	GLN
1	B	552	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	2,1	14,14,15	0.38	0	17,19,21	0.68	0
2	NAG	C	2	2	14,14,15	0.21	0	17,19,21	0.62	0
2	BMA	C	3	2	11,11,12	0.81	0	15,15,17	0.89	0
2	MAN	C	4	2	11,11,12	1.22	1 (9%)	15,15,17	1.18	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.54	0	17,19,21	0.51	0
3	NAG	D	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	BMA	D	3	3	11,11,12	0.85	0	15,15,17	0.97	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	-	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
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	MAN	C2-C3	2.29	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	2.61	115.68	112.19
2	C	4	MAN	C2-C3-C4	2.20	114.72	110.86
3	D	3	BMA	O5-C5-C4	-2.07	105.79	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

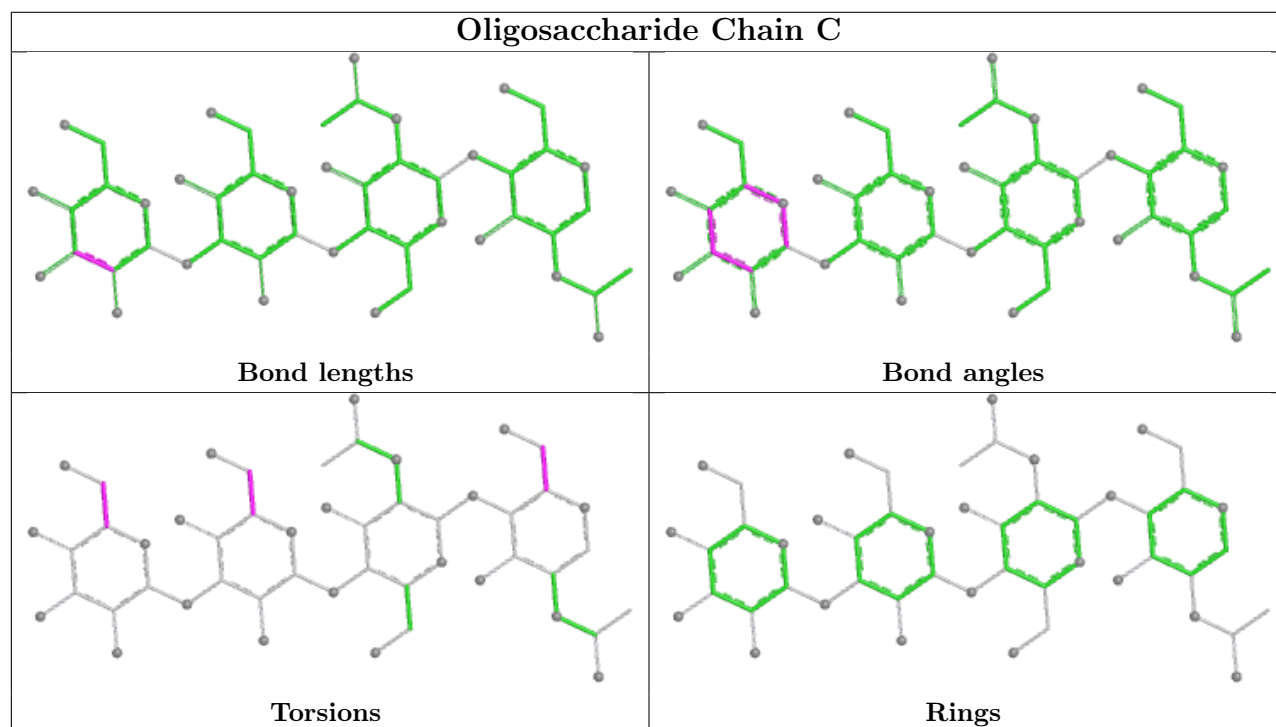
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

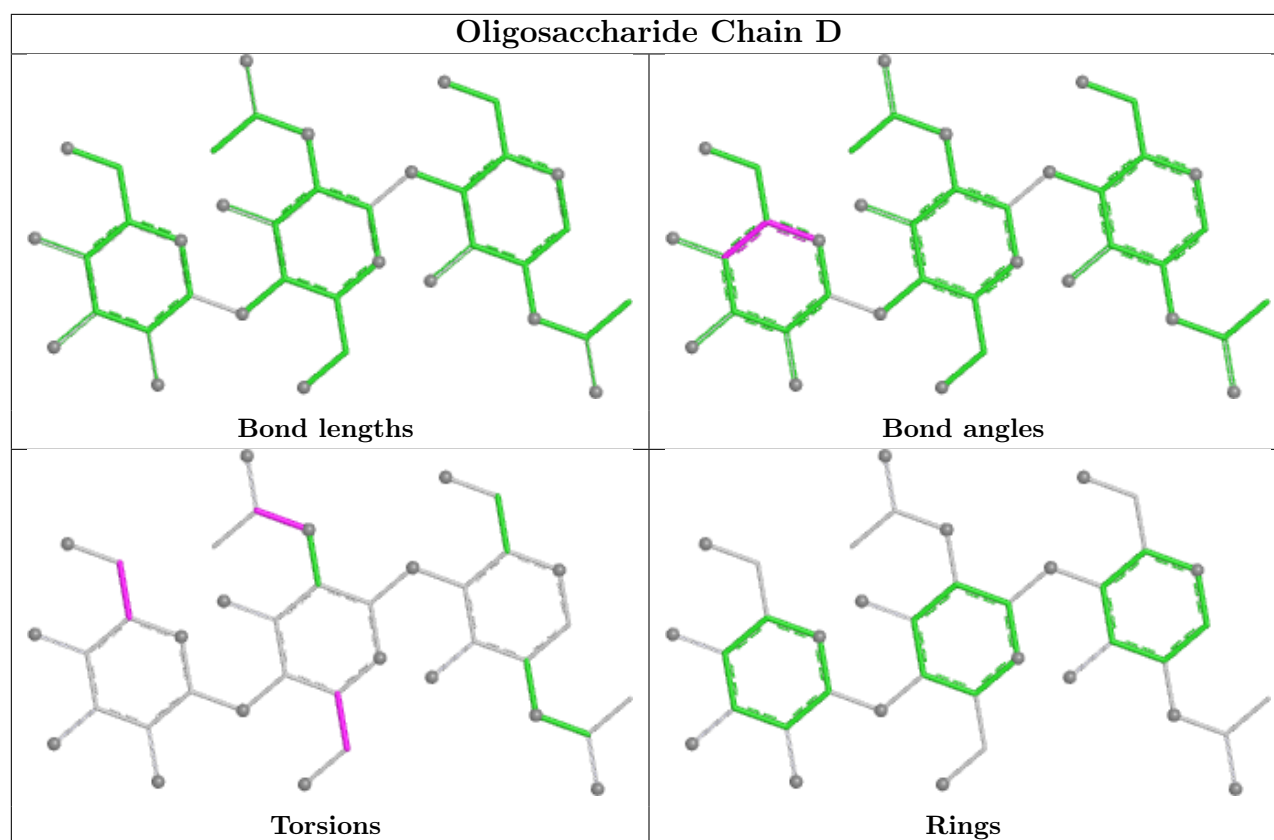
There are no ring outliers.

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 [i](#)

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	A	611	-	33,35,35	2.46	10 (30%)	37,50,50	2.05	10 (27%)
8	8LM	B	610	-	33,35,35	2.26	9 (27%)	37,50,50	2.09	9 (24%)
6	EDO	B	607	-	3,3,3	0.50	0	2,2,2	0.71	0
7	SO4	B	609	-	4,4,4	0.22	0	6,6,6	0.08	0
7	SO4	B	606	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	A	606	1	14,14,15	0.36	0	17,19,21	1.01	0
5	NAG	B	605	1	14,14,15	0.20	0	17,19,21	0.69	0
6	EDO	A	608	-	3,3,3	0.49	0	2,2,2	0.35	0
6	EDO	A	607	-	3,3,3	0.49	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	B	608	-	5,5,5	0.37	0	5,5,5	0.18	0
8	8LM	A	610	-	33,35,35	2.38	11 (33%)	37,50,50	2.13	10 (27%)
7	SO4	A	609	-	4,4,4	0.32	0	6,6,6	0.35	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	A	611	-	-	9/26/50/50	0/3/3/3
8	8LM	B	610	-	-	4/26/50/50	0/3/3/3
6	EDO	B	607	-	-	1/1/1/1	-
5	NAG	A	606	1	-	4/6/23/26	0/1/1/1
5	NAG	B	605	1	-	0/6/23/26	0/1/1/1
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	A	607	-	-	1/1/1/1	-
9	GOL	B	608	-	-	0/4/4/4	-
8	8LM	A	610	-	-	5/26/50/50	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	611	8LM	O6-C6	7.76	1.58	1.46
8	A	610	8LM	O6-C6	7.57	1.58	1.46
8	B	610	8LM	O6-C6	6.73	1.57	1.46
8	A	611	8LM	C10-N5	5.76	1.46	1.34
8	A	610	8LM	C10-N5	5.70	1.46	1.34
8	B	610	8LM	C10-N5	4.90	1.44	1.34
8	A	611	8LM	C5-N5	4.37	1.52	1.45
8	A	610	8LM	N18-N28	-4.27	1.32	1.36
8	B	610	8LM	C5-N5	4.27	1.52	1.45
8	A	611	8LM	C19-C20	4.04	1.44	1.37
8	A	610	8LM	C5-N5	3.91	1.51	1.45
8	A	611	8LM	C7-C6	3.87	1.57	1.52
8	B	610	8LM	C19-C20	3.74	1.43	1.37
8	A	611	8LM	C21-C20	3.74	1.53	1.47
8	B	610	8LM	N18-N28	-3.73	1.32	1.36
8	A	610	8LM	C19-C20	3.69	1.43	1.37
8	A	611	8LM	N18-N28	-3.56	1.32	1.36
8	B	610	8LM	C7-C6	3.31	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	610	8LM	C21-C20	2.91	1.52	1.47
8	A	610	8LM	C21-C20	2.91	1.52	1.47
8	A	610	8LM	C7-C6	2.80	1.56	1.52
8	B	610	8LM	O4-C4	2.49	1.47	1.42
8	B	610	8LM	O10-C10	-2.37	1.18	1.23
8	A	611	8LM	O6-C2	2.35	1.40	1.36
8	A	610	8LM	O10-C10	-2.33	1.18	1.23
8	A	610	8LM	O4-C4	2.25	1.46	1.42
8	A	611	8LM	O4-C4	2.13	1.46	1.42
8	A	610	8LM	C19-N18	-2.08	1.33	1.36
8	A	611	8LM	O10-C10	-2.03	1.19	1.23
8	A	610	8LM	O6-C2	2.03	1.40	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	610	8LM	C5-N5-C10	-7.78	111.36	123.20
8	A	610	8LM	C5-N5-C10	-5.62	114.65	123.20
8	A	610	8LM	C11-C10-N5	5.32	123.07	115.91
8	A	611	8LM	N18-N28-N27	5.25	110.43	106.70
8	A	611	8LM	C4-C5-N5	-4.90	105.45	111.22
8	A	610	8LM	N18-N28-N27	4.62	109.99	106.70
8	A	610	8LM	C8-C7-C6	-4.45	104.70	113.05
8	B	610	8LM	C8-C7-C6	-4.04	105.47	113.05
8	B	610	8LM	C11-C10-N5	3.88	121.13	115.91
8	A	611	8LM	O6-C2-C1	3.76	119.23	112.25
8	A	611	8LM	C6-C5-N5	3.73	116.85	110.91
8	A	611	8LM	C21-C20-N27	3.58	127.80	122.05
8	A	610	8LM	C21-C20-N27	3.57	127.79	122.05
8	B	610	8LM	N18-N28-N27	3.52	109.20	106.70
8	A	611	8LM	C11-C10-N5	3.33	120.39	115.91
8	A	611	8LM	C5-N5-C10	-2.87	118.83	123.20
8	A	610	8LM	C21-C20-C19	-2.85	125.29	129.65
8	A	610	8LM	O10-C10-N5	-2.85	117.86	122.96
8	B	610	8LM	O10-C10-N5	-2.74	118.06	122.96
8	B	610	8LM	C21-C20-N27	2.65	126.30	122.05
8	B	610	8LM	C5-C4-C3	2.38	114.55	108.72
8	A	610	8LM	C22-C21-C20	-2.30	118.29	120.87
8	A	611	8LM	C21-C20-C19	-2.24	126.23	129.65
8	A	610	8LM	C26-C21-C22	2.14	121.29	118.57
8	A	611	8LM	C19-N18-N28	-2.13	108.75	110.55
8	B	610	8LM	C6-C5-N5	-2.12	107.53	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	610	8LM	O6-C2-C1	2.09	116.12	112.25
8	B	610	8LM	C26-C21-C22	2.06	121.19	118.57
8	A	611	8LM	C5-C4-C3	2.02	113.66	108.72

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	610	8LM	O1B-C1-C2-O6
8	A	610	8LM	O1A-C1-C2-O6
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	O1B-C1-C2-O6
8	A	611	8LM	O1A-C1-C2-O6
8	B	610	8LM	C2-C3-N18-C19
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
5	A	606	NAG	C1-C2-N2-C7
5	A	606	NAG	C3-C2-N2-C7
8	B	610	8LM	O10-C10-C11-C12
8	A	610	8LM	O1A-C1-C2-C3
8	A	611	8LM	O1A-C1-C2-C3
6	B	607	EDO	O1-C1-C2-O2
8	B	610	8LM	N5-C10-C11-C12
6	A	607	EDO	O1-C1-C2-O2
8	B	610	8LM	O10-C10-C11-C13

There are no ring outliers.

8 monomers are involved in 16 short contacts:

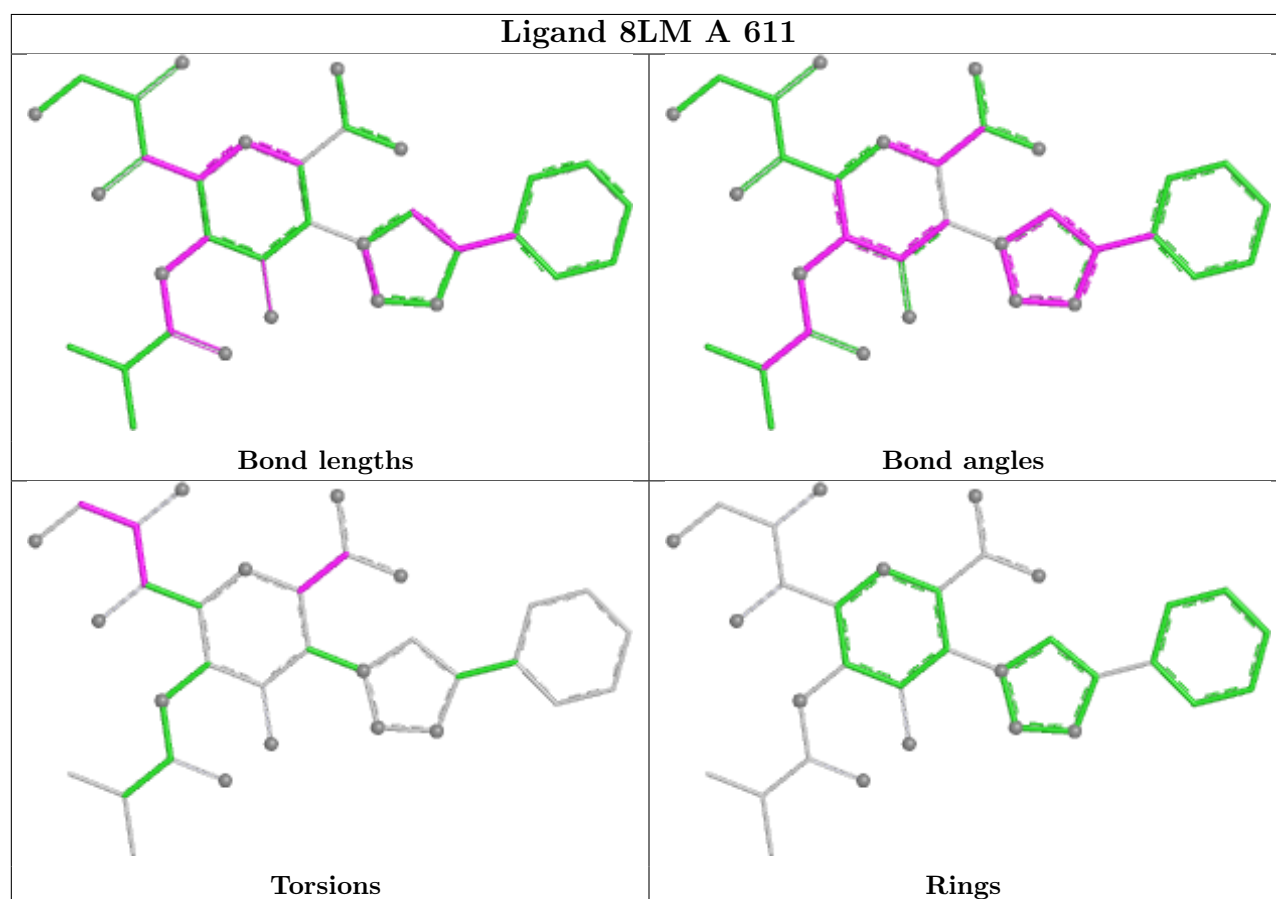
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	611	8LM	1	0
8	B	610	8LM	1	0
6	B	607	EDO	2	0
5	A	606	NAG	5	0

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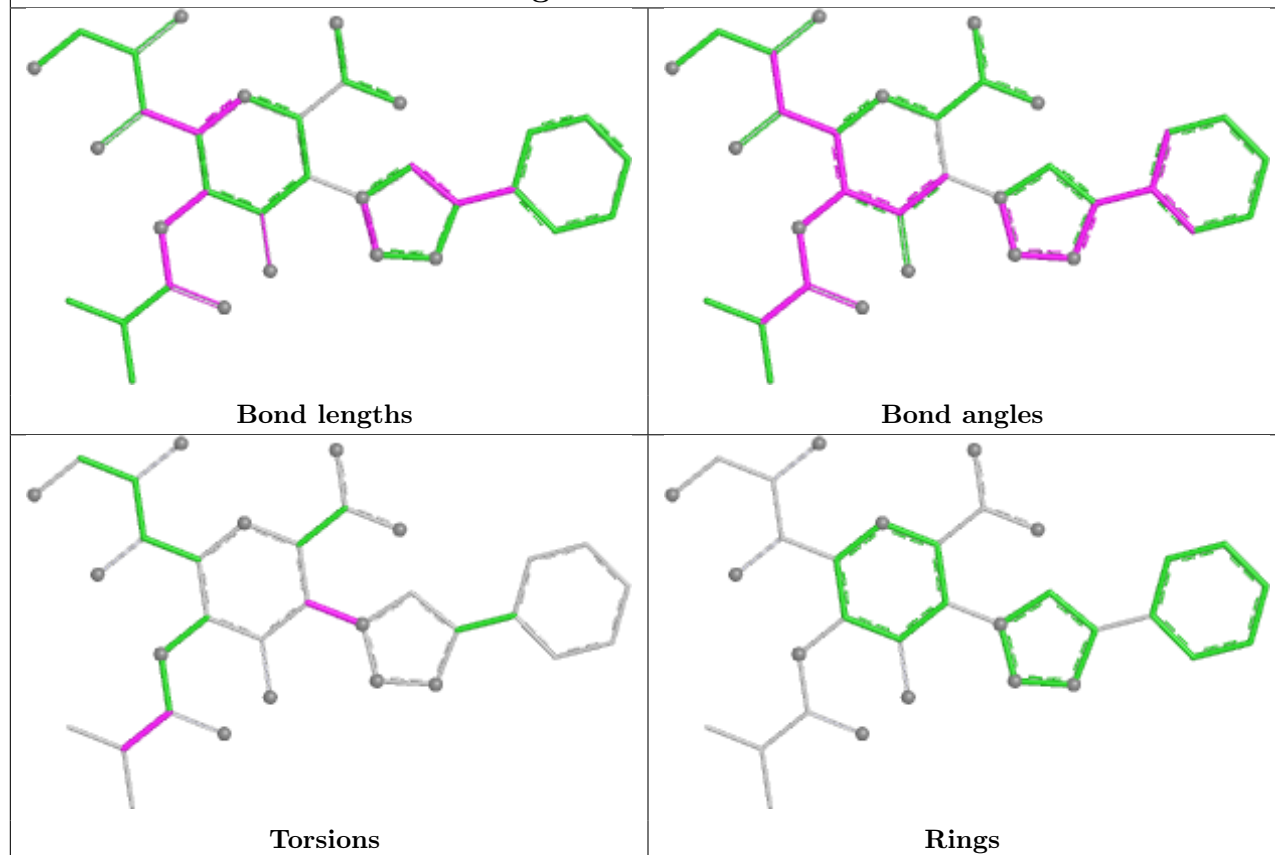
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	608	EDO	1	0
6	A	607	EDO	2	0
9	B	608	GOL	1	0
8	A	610	8LM	3	0

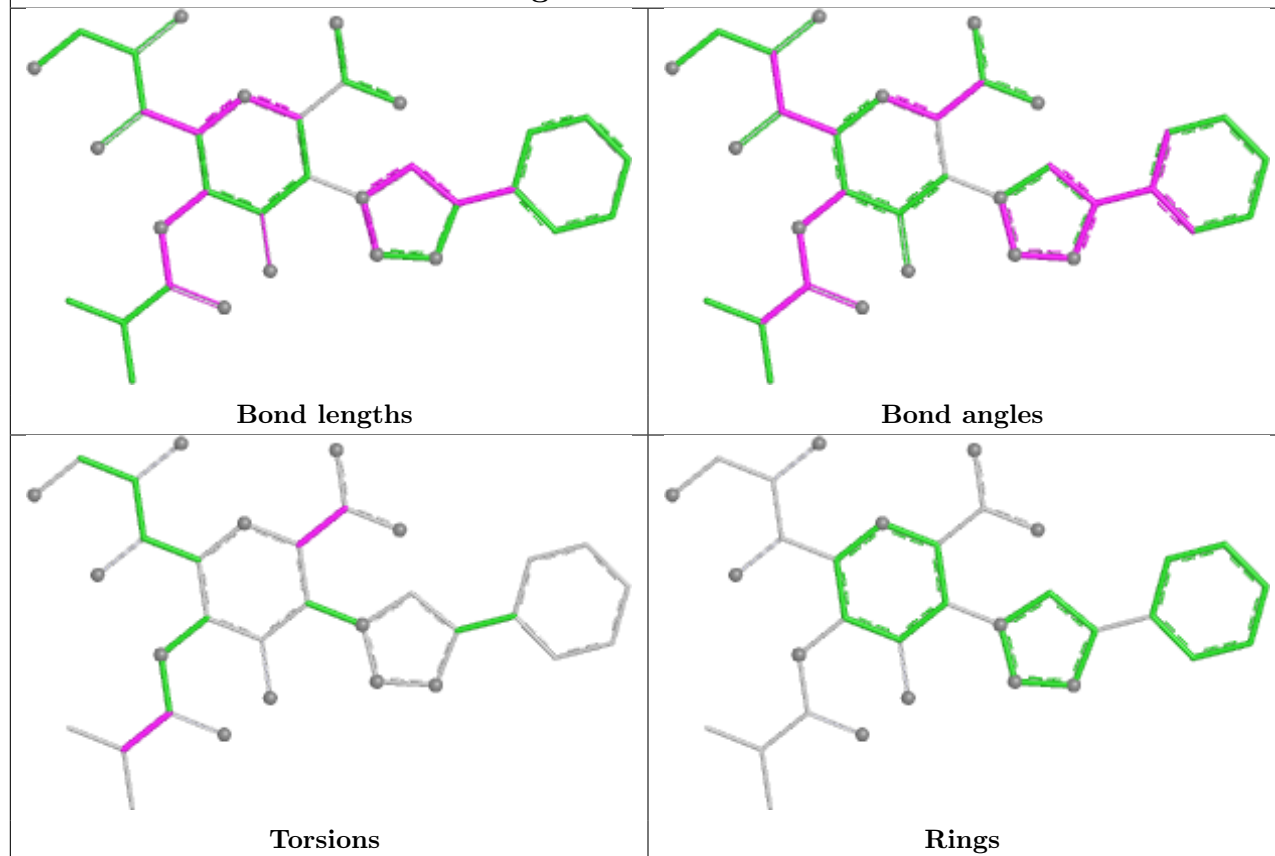
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 B 610



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%)	0.17	30 (6%)	22 23	10, 28, 69, 92	2 (0%)
1	B	428/431 (99%)	0.12	19 (4%)	39 42	17, 30, 61, 110	1 (0%)
All	All	859/862 (99%)	0.14	49 (5%)	29 31	10, 29, 66, 110	3 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	VAL	6.3
1	A	344	ILE	5.9
1	B	145	ASP	5.8
1	A	234	ASP	5.1
1	A	146	VAL	4.6
1	A	237	PRO	4.4
1	B	233	SER	4.3
1	B	234	ASP	4.1
1	A	145	ASP	3.9
1	A	231	VAL	3.8
1	A	235	LEU	3.7
1	B	217	ILE	3.7
1	A	327	TYR	3.6
1	A	539	TYR	3.6
1	A	143	THR	3.6
1	A	346	GLU	3.5
1	B	572	SER	3.5
1	A	391	ILE	3.4
1	A	142	ILE	3.3
1	B	143	THR	3.3
1	B	297	GLY	3.1
1	B	539	TYR	3.0
1	A	217	ILE	3.0
1	A	144	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	558	PHE	2.8
1	A	236	VAL	2.8
1	B	144	HIS	2.7
1	B	142	ILE	2.6
1	B	371	TRP	2.5
1	A	221[A]	TYR	2.5
1	A	572	SER	2.5
1	B	345	ASN	2.4
1	A	345	ASN	2.3
1	B	249	ILE	2.3
1	A	388	LEU	2.3
1	A	162	GLY	2.3
1	A	468	SER	2.3
1	A	249	ILE	2.2
1	B	232	ASN	2.2
1	A	557	THR	2.2
1	B	216	ASP	2.2
1	B	219	LYS	2.2
1	A	163	LEU	2.2
1	B	391	ILE	2.1
1	A	554	SER	2.1
1	A	233	SER	2.1
1	B	390	SER	2.1
1	A	387	GLY	2.1
1	A	295	HIS	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.

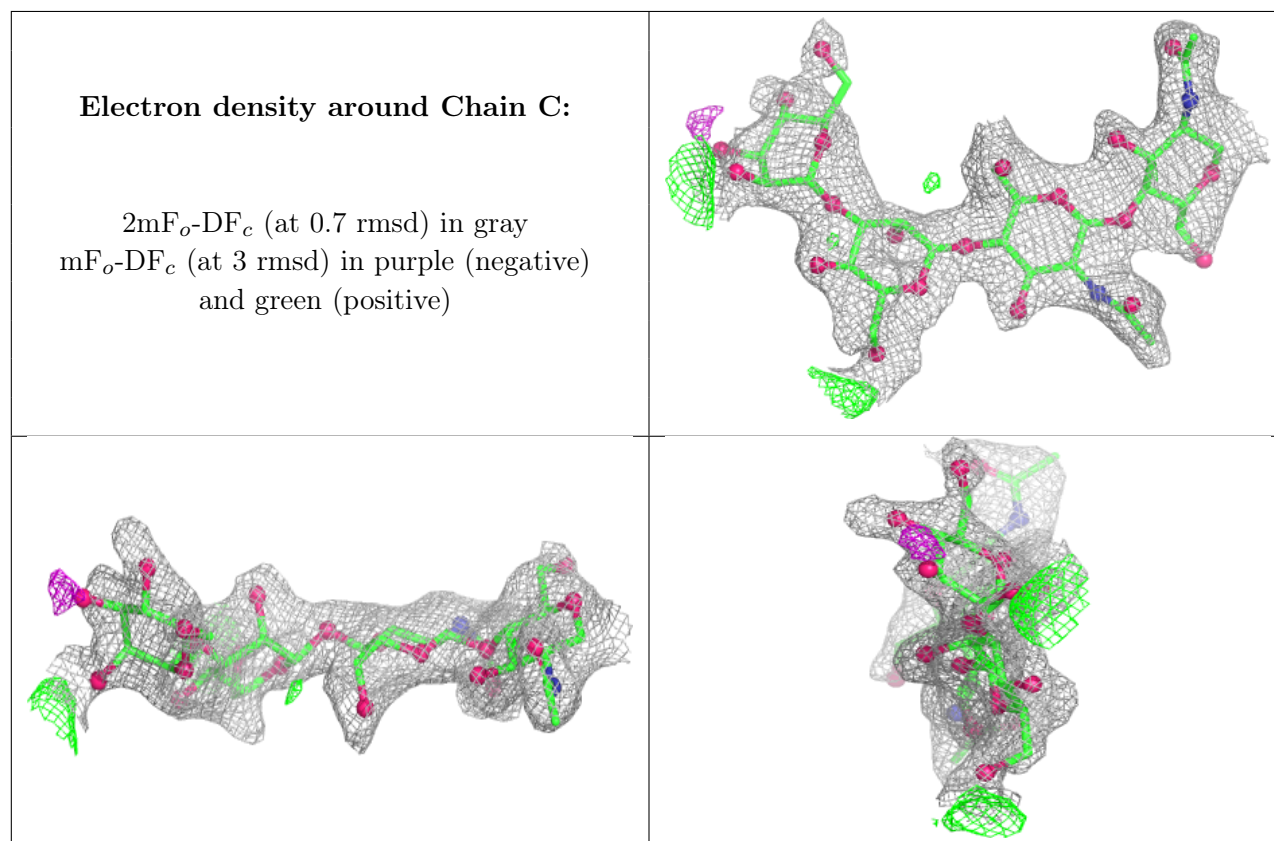
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	D	3	11/12	0.52	0.14	82,99,115,123	0
2	MAN	C	4	11/12	0.70	0.17	58,67,72,78	0
2	BMA	C	3	11/12	0.75	0.14	54,65,73,76	0

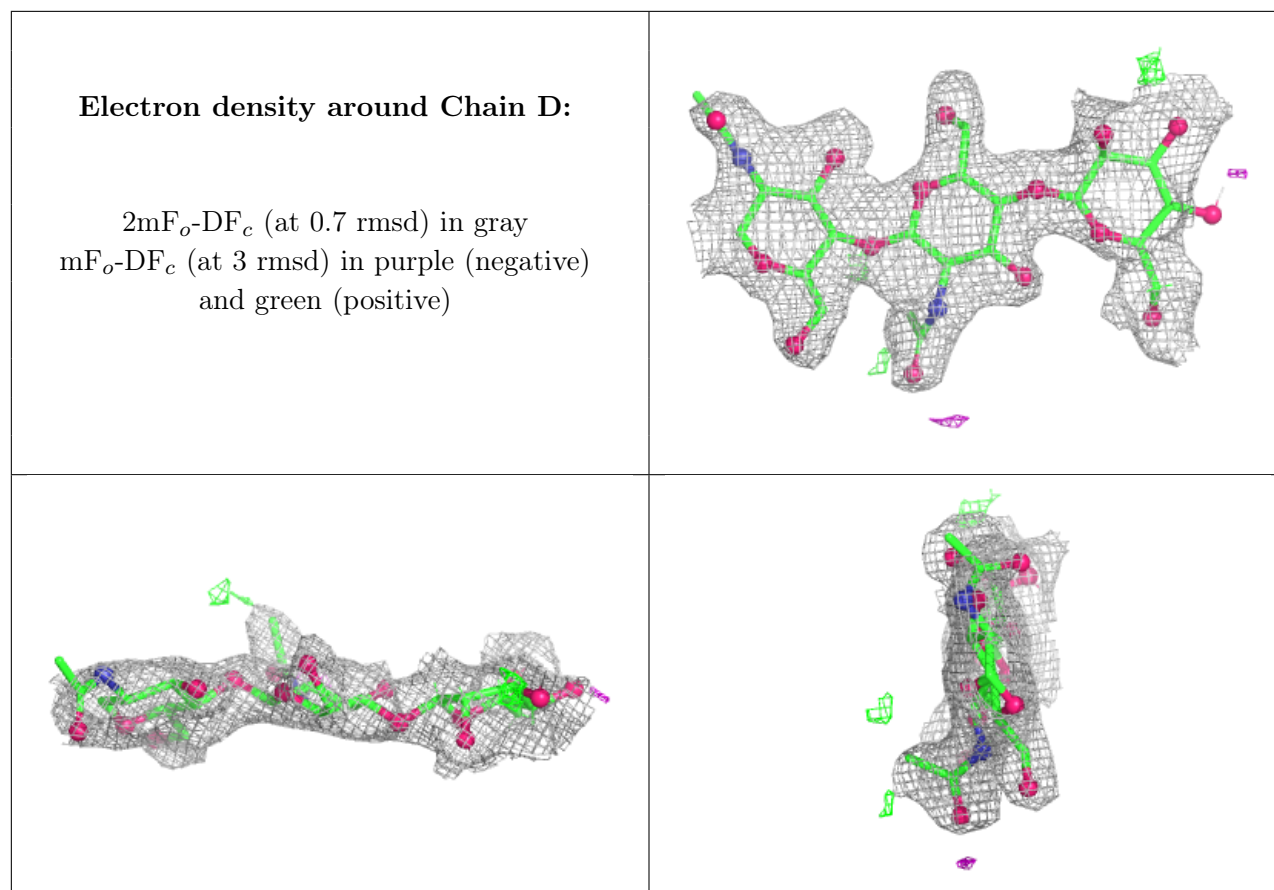
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	2	14/15	0.83	0.12	53,59,67,74	0
3	NAG	D	1	14/15	0.84	0.12	51,58,77,80	0
2	NAG	C	2	14/15	0.89	0.10	47,52,57,61	0
2	NAG	C	1	14/15	0.90	0.12	37,47,58,64	0

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.





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.

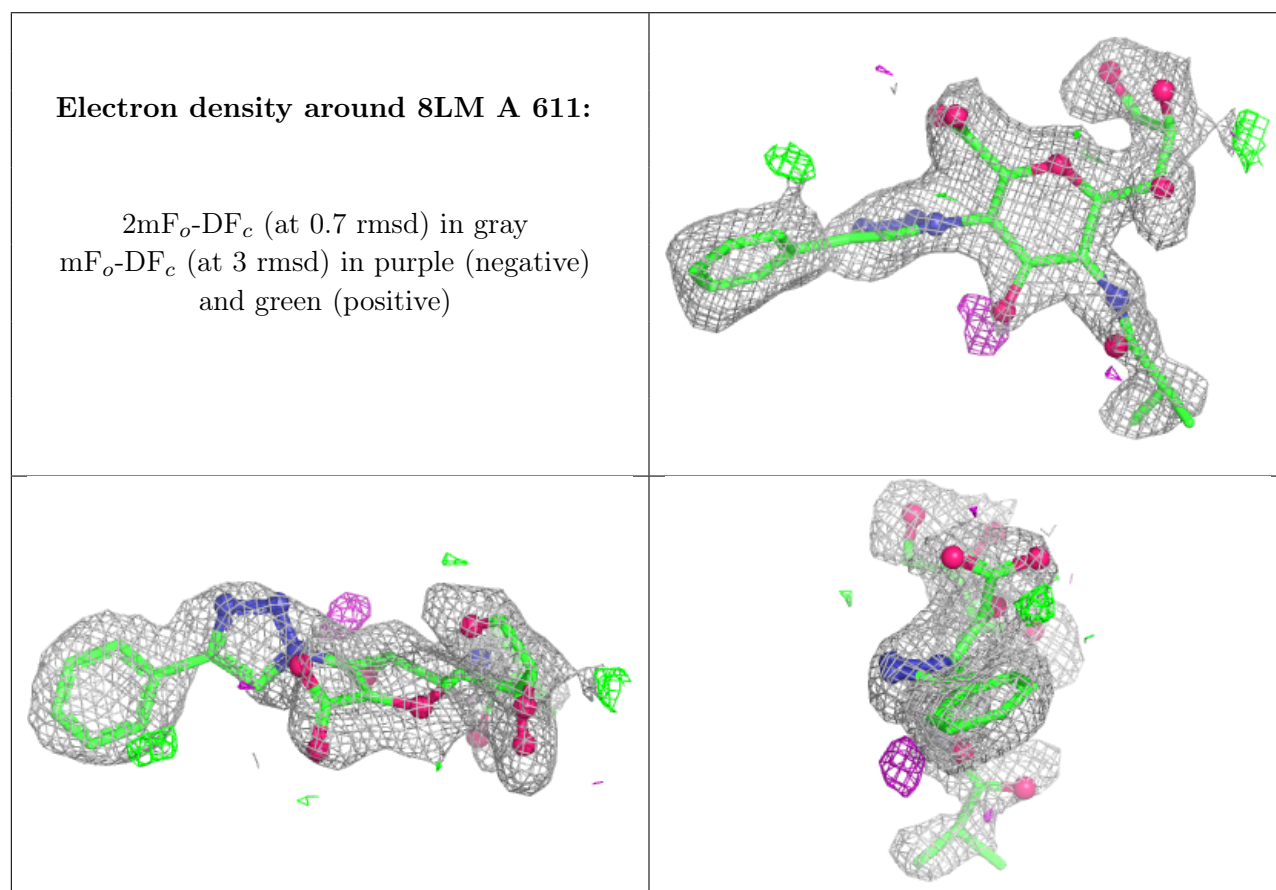
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	605	14/15	0.69	0.14	63,75,86,91	0
8	8LM	A	611	33/33	0.70	0.13	48,62,71,75	0
8	8LM	A	610	33/33	0.71	0.16	43,74,87,87	0
5	NAG	A	606	14/15	0.76	0.12	41,53,60,64	0
6	EDO	A	608	4/4	0.80	0.15	53,57,57,61	0
6	EDO	A	607	4/4	0.81	0.14	36,40,42,52	0
6	EDO	B	607	4/4	0.84	0.12	27,36,44,44	0
9	GOL	B	608	6/6	0.87	0.11	43,54,56,59	0
7	SO4	B	609	5/5	0.91	0.09	43,49,56,57	0
8	8LM	B	610	33/33	0.92	0.10	24,40,58,59	0
7	SO4	B	606	5/5	0.95	0.06	50,50,52,56	0
7	SO4	A	609	5/5	0.98	0.12	28,31,36,40	0
4	CA	A	601	1/1	0.99	0.03	29,29,29,29	0

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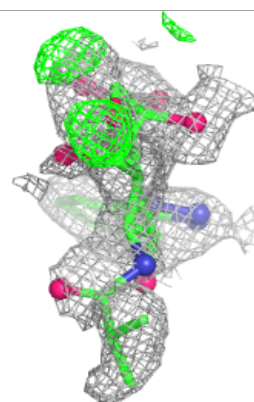
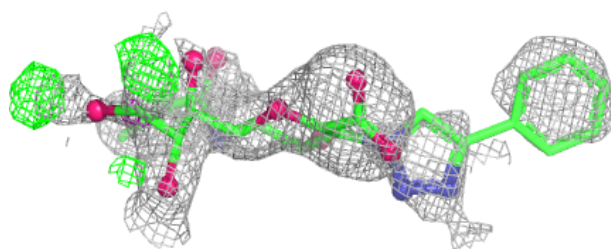
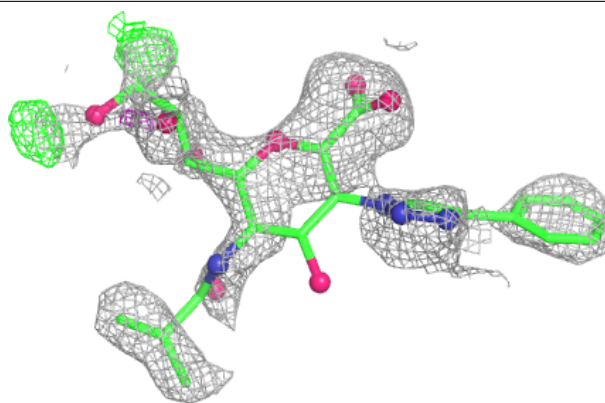
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	B	601	1/1	0.99	0.03	32,32,32,32	0

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.

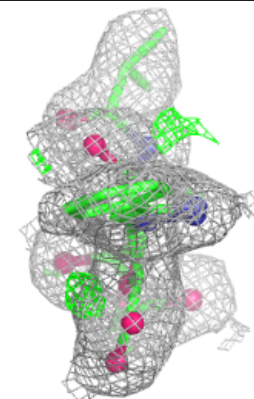
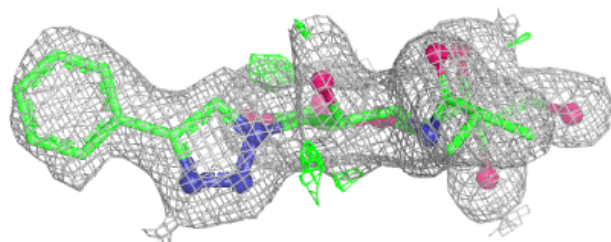
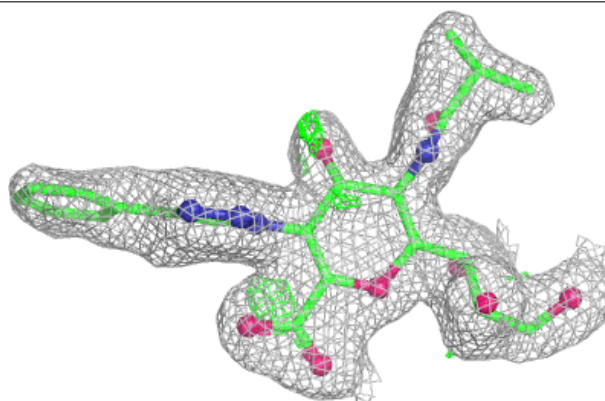


Electron density around 8LM A 610:

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

**Electron density around 8LM B 610:**

$2mF_o-DF_c$ (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.