



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:25 AM UTC

PDB ID : 8SZ3 / pdb_00008sz3
Title : Structure of human beta 1,3-N-acetylglucosaminyltransferase 2 with compound 7j
Authors : Sudom, A.; Min, X.
Deposited on : 2023-05-26
Resolution : 2.32 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

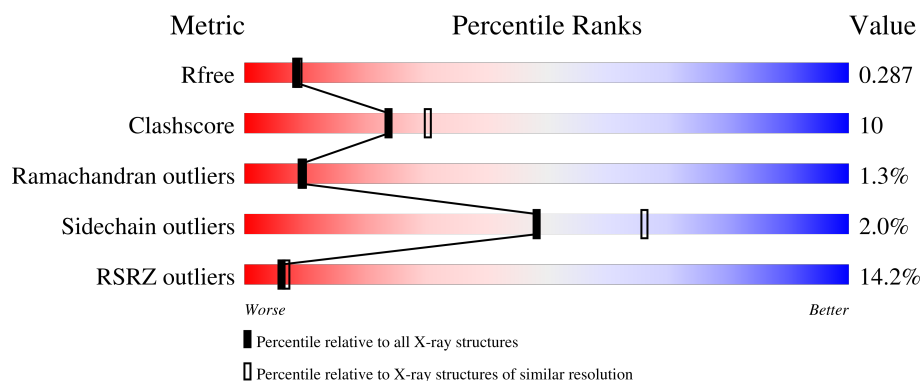
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	397	12% 58% 21% • 20%
1	B	397	11% 63% 17% • 19%
2	C	2	100%
2	D	2	100%
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5550 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 N-acetylglucosaminide beta-1,3-N-acetylglucosaminyltransferase 2.

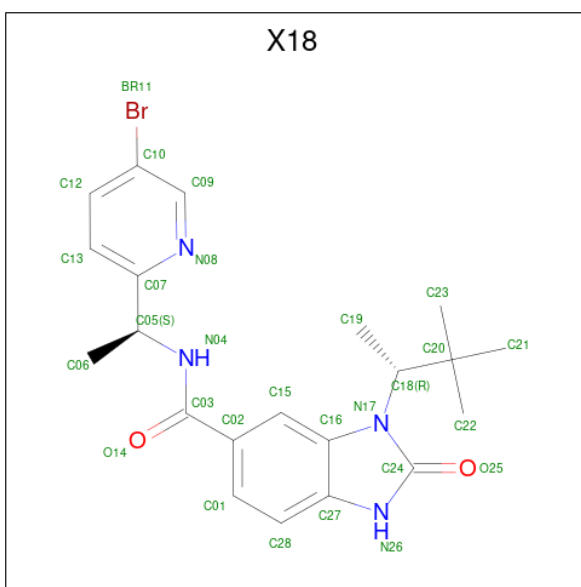
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2639	1698	453	476	12			
1	B	323	Total	C	N	O	S	0	0	0
			2668	1718	457	481	12			

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



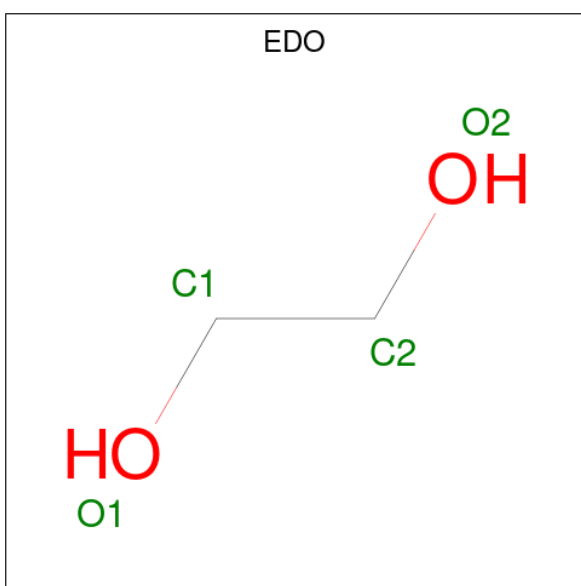
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is N-[(1S)-1-(5-bromopyridin-2-yl)ethyl]-3-[(2R)-3,3-dimethylbutan-2-yl]-2-oxo-2,3-dihydro-1H-benzimidazole-5-carboxamide (CCD ID: X18) (formula: C₂₁H₂₅BrN₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			28	1	21	4	2		
3	B	1	Total	Br	C	N	O	0	0
			28	1	21	4	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total 31	O 31	0	0
5	B	36	Total 36	O 36	0	0

i

- Molecule 1: N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase 2



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

Chain C:  100%

MAG1
MAG2

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

Chain D:  100%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.38Å 76.41Å 128.02Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	29.14 – 2.32 29.14 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.14-2.32) 98.6 (29.14-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.261 , 0.287 0.261 , 0.287	Depositor DCC
R_{free} test set	1630 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.864	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5550	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5750e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, X18, 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	0.17	0/2710	0.41	0/3668
1	B	0.14	0/2740	0.42	1/3710 (0.0%)
All	All	0.16	0/5450	0.41	1/7378 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	SER	N-CA-C	-5.77	105.35	113.20

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	2639	0	2582	61	0
1	B	2668	0	2616	48	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
3	A	28	0	0	1	0
3	B	28	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	0	0
4	B	4	0	6	2	0
5	A	31	0	0	2	0
5	B	36	0	0	1	0
All	All	5550	0	5310	109	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 (109) 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:354:ARG:NH2	5:A:501:HOH:O	2.01	0.92
1:A:322:ILE:HD11	1:A:342:LYS:HB3	1.56	0.86
1:A:335:TYR:HA	1:A:338:MET:HE2	1.65	0.77
1:B:255:ILE:HD13	1:B:373:MET:HE2	1.68	0.75
1:B:335:TYR:HA	1:B:338:MET:HE2	1.70	0.74
1:B:357:ASP:OD2	1:B:363:LYS:NZ	2.21	0.74
1:A:340:LEU:HD13	1:A:347:PRO:HG3	1.69	0.73
1:A:255:ILE:HD13	1:A:373:MET:HE2	1.71	0.72
1:A:302:PRO:HB2	1:A:347:PRO:HD2	1.79	0.65
1:A:145:LEU:HB3	1:A:241:VAL:HG12	1.80	0.64
1:A:141:LYS:HG2	1:A:237:ASP:HB3	1.80	0.63
1:B:360:GLU:O	1:B:362:ASN:N	2.31	0.63
1:B:371:ASP:OD1	1:B:371:ASP:N	2.32	0.62
1:A:91:SER:HB2	1:B:395:LEU:HD21	1.83	0.61
1:B:102:VAL:HA	1:B:105:VAL:HG12	1.81	0.61
1:B:141:LYS:HG3	1:B:237:ASP:HB3	1.82	0.61
1:A:360:GLU:HG2	1:A:361:LYS:H	1.65	0.60
1:A:366:ILE:H	1:A:366:ILE:HD12	1.67	0.60
1:B:262:LEU:HD21	1:B:270:LEU:HD12	1.84	0.59
1:A:322:ILE:HD12	1:A:343:LEU:HG	1.84	0.59
1:A:367:CYS:HA	1:A:370:VAL:HG23	1.84	0.58
1:B:259:LEU:HA	1:B:262:LEU:HD22	1.85	0.58
1:B:268:LYS:HD3	1:B:269:ASP:HB2	1.84	0.58
1:A:337:GLY:HA2	1:A:340:LEU:HD12	1.86	0.58
1:B:272:ILE:HD12	1:B:350:HIS:HD2	1.73	0.54
1:A:228:LEU:HB3	1:A:320:TYR:HB2	1.88	0.54
1:A:260:ASN:C	1:A:262:LEU:H	2.15	0.54
1:B:272:ILE:HD12	1:B:350:HIS:CD2	2.45	0.52
1:B:362:ASN:O	1:B:362:ASN:ND2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASN:HD21	1:A:367:CYS:HB2	1.75	0.51
1:B:259:LEU:HD21	1:B:310:LEU:HD21	1.93	0.51
1:A:284:ASP:HB3	1:A:287:LEU:HG	1.91	0.51
1:B:272:ILE:HG22	1:B:348:GLU:HB3	1.93	0.50
1:A:319:LEU:O	1:A:323:THR:HG23	2.12	0.50
1:B:133:ASP:OD2	1:B:134:GLN:N	2.45	0.50
1:B:284:ASP:HB3	1:B:287:LEU:HG	1.92	0.50
1:A:128:TYR:CE2	1:A:222:LEU:HD21	2.46	0.50
1:A:285:LYS:HE3	1:A:286:LYS:HD3	1.94	0.49
1:B:144:LEU:HB3	1:B:176:VAL:HG22	1.93	0.49
1:B:319:LEU:O	1:B:323:THR:HG23	2.12	0.49
1:A:147:ALA:HB1	1:A:181:LEU:HD11	1.93	0.49
1:A:272:ILE:HD11	1:A:310:LEU:HD23	1.94	0.49
1:B:189:ASP:OD2	1:B:214:ARG:NH1	2.40	0.49
1:A:358:ILE:HG22	1:A:363:LYS:HG2	1.95	0.49
1:A:358:ILE:HG23	1:A:359:GLU:HG2	1.93	0.49
1:A:141:LYS:NZ	1:A:239:GLU:HG2	2.28	0.49
1:B:147:ALA:HB1	1:B:181:LEU:HD11	1.94	0.48
1:A:101:ARG:NH1	1:A:105:VAL:HG11	2.28	0.48
1:A:293:GLU:H	1:A:293:GLU:CD	2.21	0.48
1:B:99:ASP:O	1:B:102:VAL:HG22	2.13	0.48
1:B:149:LYS:NZ	5:B:504:HOH:O	2.47	0.48
1:A:263:SER:O	1:A:266:LYS:N	2.47	0.48
1:B:137:LYS:O	1:B:177:VAL:HG11	2.14	0.47
1:A:376:HIS:CD2	1:A:377:SER:HB3	2.49	0.47
1:A:319:LEU:O	1:A:322:ILE:HG22	2.15	0.47
1:B:162:ARG:HG2	1:B:178:ARG:CZ	2.45	0.47
1:B:354:ARG:NH1	1:B:358:ILE:HD12	2.31	0.46
1:A:162:ARG:HG2	1:A:178:ARG:CZ	2.46	0.46
1:A:260:ASN:C	1:A:262:LEU:N	2.73	0.46
1:B:137:LYS:HA	1:B:137:LYS:HD3	1.77	0.46
1:A:220:LEU:HD21	3:A:401:X18:C24	2.46	0.46
1:A:258:TYR:O	1:A:262:LEU:HG	2.16	0.46
1:A:281:PRO:HB3	1:A:291:ILE:HB	1.97	0.46
1:B:189:ASP:OD2	1:B:214:ARG:HD2	2.16	0.46
1:A:270:LEU:HD11	1:A:272:ILE:HD13	1.98	0.45
1:A:357:ASP:OD2	1:A:363:LYS:NZ	2.46	0.45
1:B:140:LYS:HE2	1:B:140:LYS:HB3	1.74	0.45
1:B:376:HIS:CD2	1:B:377:SER:HB3	2.51	0.45
1:A:99:ASP:O	1:A:102:VAL:HG22	2.16	0.45
1:B:260:ASN:C	1:B:262:LEU:H	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:NE	4:B:402:EDO:H12	2.31	0.45
1:A:360:GLU:HG2	1:A:361:LYS:N	2.30	0.45
1:A:254:HIS:NE2	1:A:371:ASP:O	2.50	0.45
1:B:109:PHE:HA	1:B:112:LEU:HD12	1.99	0.45
1:B:251:ASN:O	1:B:255:ILE:HG12	2.17	0.44
1:A:366:ILE:HG12	1:A:389:GLN:HB3	2.00	0.44
1:A:140:LYS:HB3	1:A:140:LYS:HE3	1.62	0.44
1:A:96:CYS:HA	1:A:125:CYS:HB2	2.00	0.44
1:B:220:LEU:HD21	3:B:401:X18:C24	2.48	0.44
1:A:133:ASP:OD1	1:A:134:GLN:N	2.51	0.43
1:B:148:ILE:HB	1:B:180:PHE:CD1	2.53	0.43
1:A:149:LYS:NZ	5:A:507:HOH:O	2.52	0.43
1:A:248:VAL:O	1:A:383:MET:HE2	2.19	0.43
1:A:272:ILE:HA	1:A:348:GLU:O	2.18	0.43
1:A:358:ILE:HG23	1:A:359:GLU:N	2.33	0.43
1:A:148:ILE:HB	1:A:180:PHE:CD1	2.54	0.42
1:B:342:LYS:HB2	1:B:342:LYS:HE2	1.85	0.42
1:A:110:ASN:HA	1:A:117:LYS:HE2	2.01	0.42
1:A:368:SER:O	1:A:372:LEU:HD23	2.18	0.42
1:A:147:ALA:O	1:A:243:LYS:HA	2.19	0.42
2:E:1:NAG:H61	2:E:2:NAG:N2	2.34	0.42
1:A:141:LYS:HD2	1:A:141:LYS:C	2.45	0.41
1:A:251:ASN:O	1:A:255:ILE:HG12	2.19	0.41
1:A:360:GLU:CG	1:A:361:LYS:H	2.32	0.41
1:A:329:TYR:HB2	1:A:338:MET:HE1	2.02	0.41
1:B:242:PHE:CZ	1:B:250:VAL:HG11	2.56	0.41
1:A:58:TYR:O	1:A:62:GLU:HG2	2.21	0.41
1:A:376:HIS:HA	1:A:377:SER:HA	1.77	0.41
1:B:137:LYS:NZ	1:B:206:GLN:O	2.49	0.41
1:B:165:TRP:CE3	1:B:250:VAL:HG22	2.56	0.41
1:A:211:TRP:HB2	1:A:213:TYR:CE1	2.55	0.41
1:B:142:PRO:HB3	1:B:177:VAL:HG23	2.03	0.41
1:B:157:ARG:O	1:B:161:ILE:HG13	2.21	0.41
1:B:96:CYS:HA	1:B:125:CYS:HB2	2.03	0.41
1:A:263:SER:C	1:A:265:THR:N	2.79	0.40
1:B:319:LEU:O	1:B:322:ILE:HG22	2.21	0.40
1:B:359:GLU:O	1:B:360:GLU:C	2.65	0.40
1:B:390:LEU:HD12	1:B:390:LEU:HA	1.97	0.40
1:B:154:HIS:CD2	4:B:402:EDO:H11	2.57	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	313/397 (79%)	295 (94%)	13 (4%)	5 (2%)	7	7
1	B	317/397 (80%)	298 (94%)	16 (5%)	3 (1%)	14	16
All	All	630/794 (79%)	593 (94%)	29 (5%)	8 (1%)	9	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLU
1	B	361	LYS
1	A	359	GLU
1	B	360	GLU
1	A	261	SER
1	A	357	ASP
1	B	359	GLU
1	A	267	ALA

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	294/362 (81%)	289 (98%)	5 (2%)	53	70
1	B	298/362 (82%)	291 (98%)	7 (2%)	44	62
All	All	592/724 (82%)	580 (98%)	12 (2%)	48	66

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	SER
1	A	141	LYS
1	A	229	ARG
1	A	262	LEU
1	A	363	LYS
1	B	110	ASN
1	B	169	SER
1	B	265	THR
1	B	360	GLU
1	B	361	LYS
1	B	370	VAL
1	B	371	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	191	HIS
1	A	365	ASN
1	A	391	GLN
1	B	174	GLN
1	B	253	HIS
1	B	260	ASN
1	B	391	GLN

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](#)

8 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	0.49	0	17,19,21	0.59	0
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	0.56	0
2	NAG	D	1	2,1	14,14,15	0.31	0	17,19,21	0.47	0
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	0.55	0
2	NAG	E	1	2,1	14,14,15	0.23	0	17,19,21	0.98	2 (11%)
2	NAG	E	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.31	0	17,19,21	0.51	0
2	NAG	F	2	2	14,14,15	0.44	0	17,19,21	0.65	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
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	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	2.03	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	2.45	115.47	112.19
2	E	2	NAG	C2-N2-C7	2.39	126.10	122.90
2	E	1	NAG	C2-N2-C7	2.24	125.90	122.90
2	F	2	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

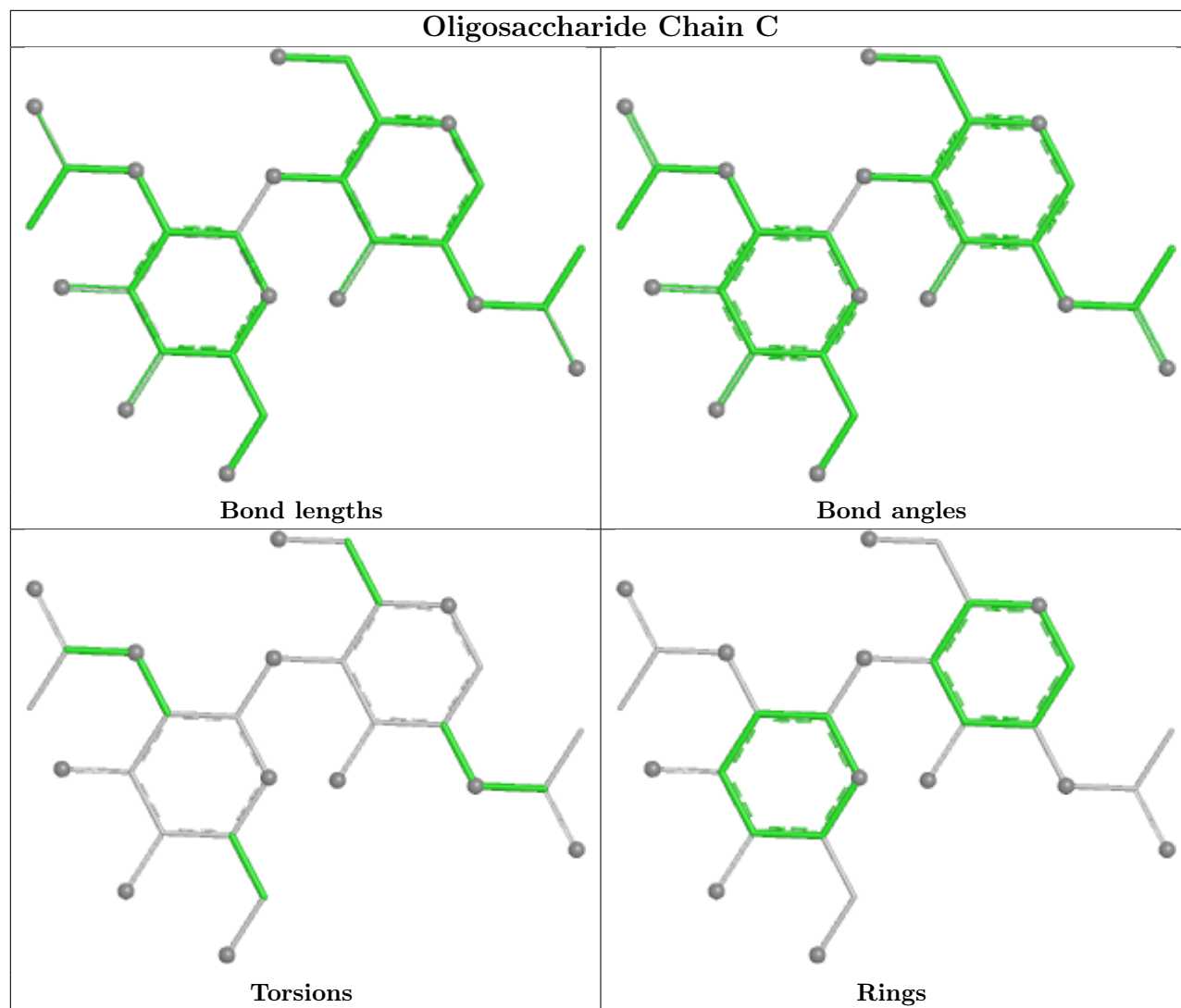
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7

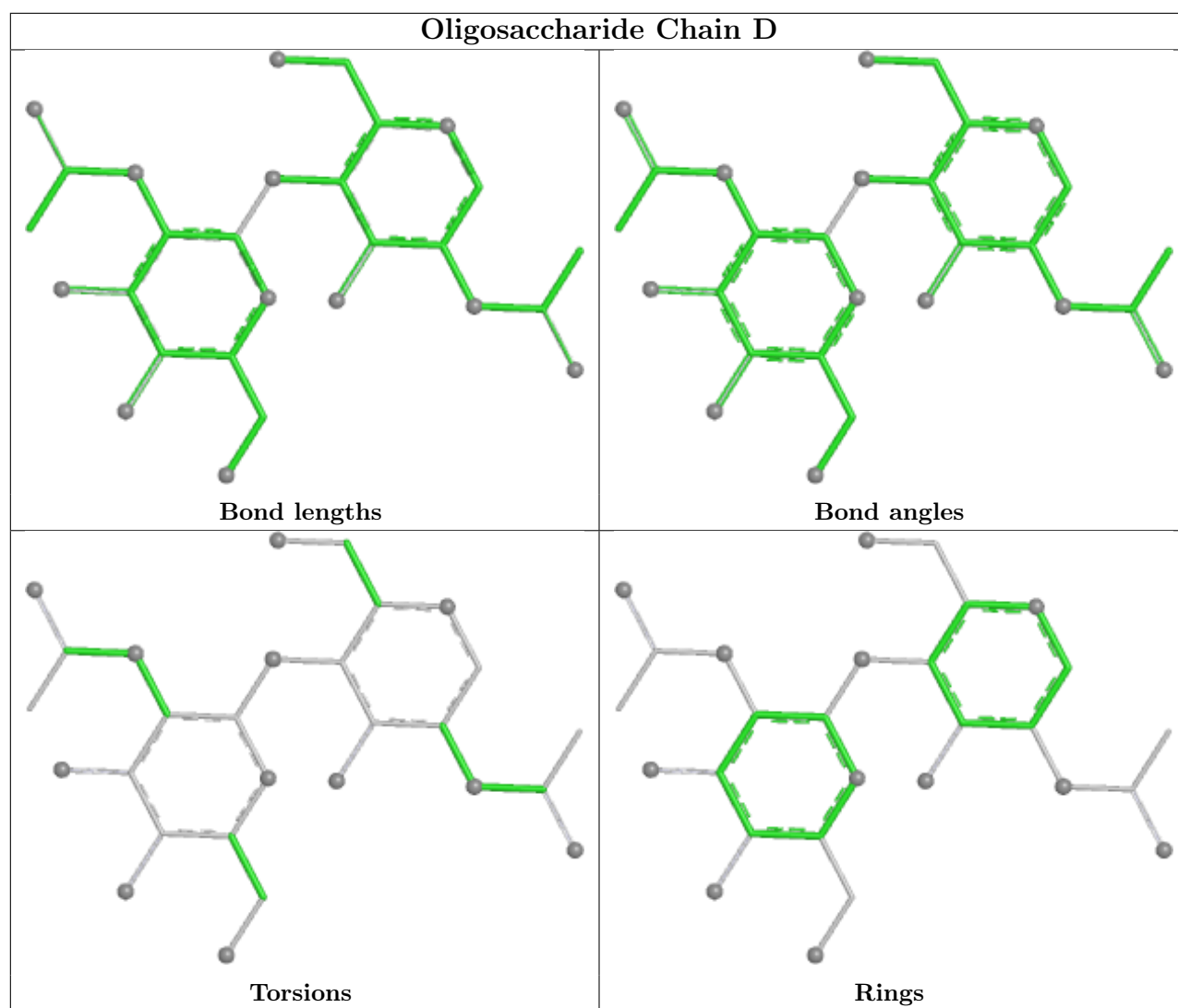
There are no ring outliers.

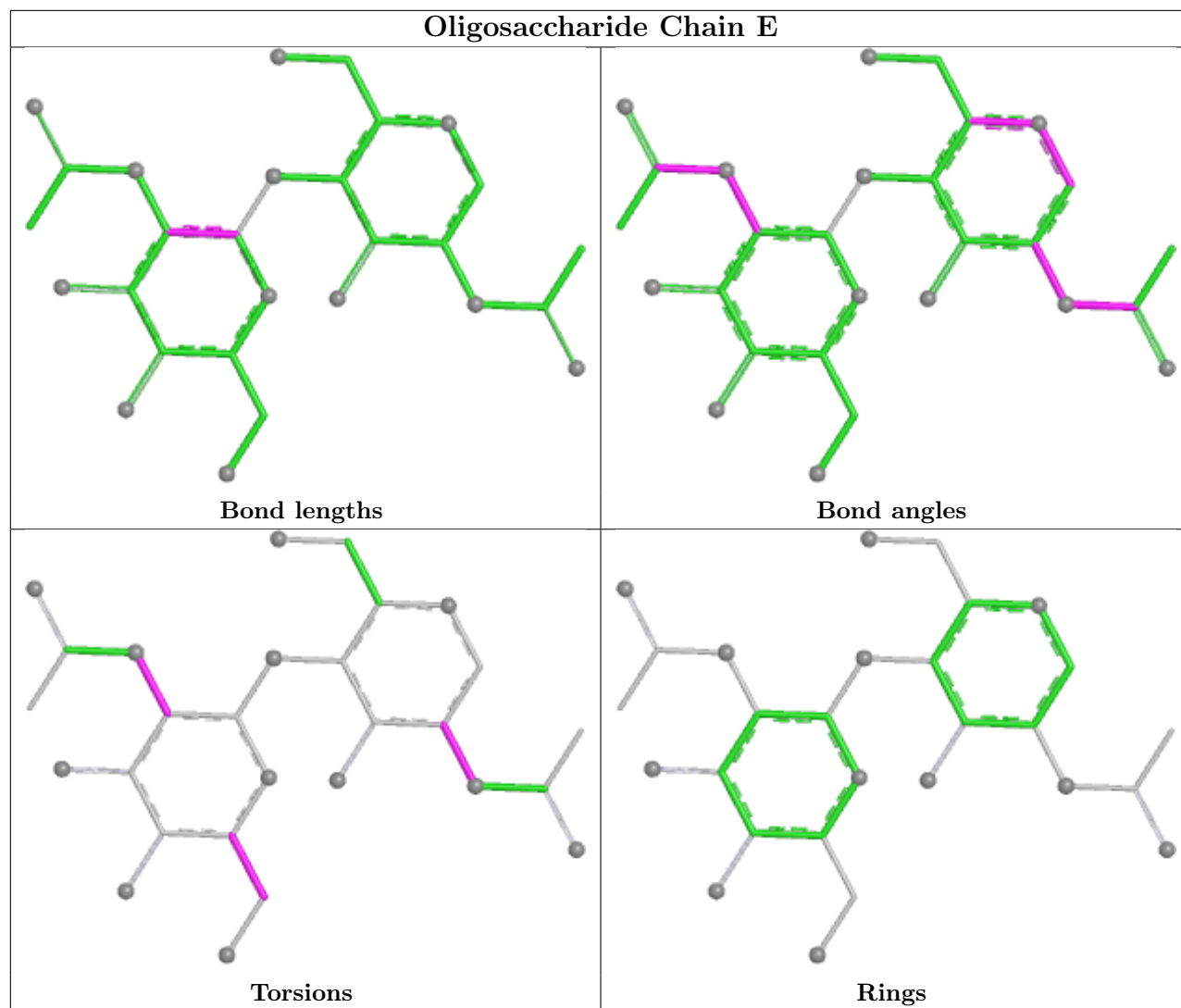
2 monomers are involved in 1 short contact:

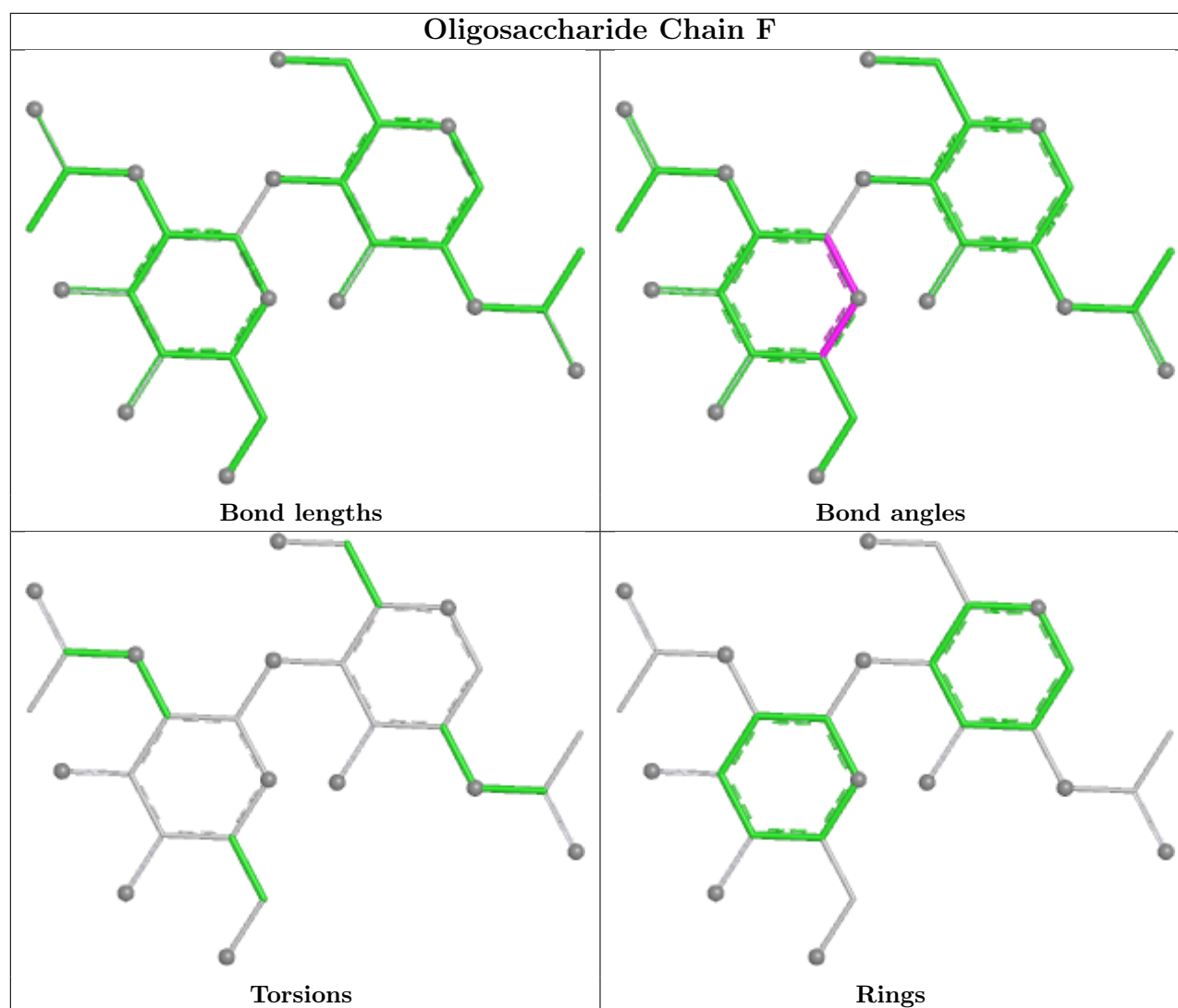
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	E	2	NAG	1	0

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](#)

4 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	EDO	A	402	-	3,3,3	0.40	0	2,2,2	0.46	0
3	X18	B	401	-	29,30,30	2.48	10 (34%)	42,45,45	1.88	10 (23%)
3	X18	A	401	-	29,30,30	2.44	9 (31%)	42,45,45	2.13	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	402	-	3,3,3	0.40	0	2,2,2	0.42	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
4	EDO	A	402	-	-	0/1/1/1	-
3	X18	B	401	-	-	1/22/22/22	0/3/3/3
3	X18	A	401	-	-	1/22/22/22	0/3/3/3
4	EDO	B	402	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	X18	C03-N04	6.52	1.49	1.34
3	B	401	X18	C03-N04	6.50	1.49	1.34
3	B	401	X18	C24-N26	6.26	1.43	1.37
3	A	401	X18	C24-N26	6.13	1.43	1.37
3	B	401	X18	C27-N26	5.22	1.48	1.38
3	A	401	X18	C27-N26	5.08	1.48	1.38
3	B	401	X18	C16-N17	4.70	1.49	1.40
3	A	401	X18	C16-N17	4.54	1.49	1.40
3	B	401	X18	C24-N17	2.73	1.44	1.38
3	A	401	X18	C24-N17	2.69	1.44	1.38
3	B	401	X18	C02-C03	2.57	1.55	1.50
3	A	401	X18	C02-C03	2.57	1.55	1.50
3	A	401	X18	O25-C24	-2.47	1.18	1.23
3	B	401	X18	O25-C24	-2.38	1.18	1.23
3	A	401	X18	BR11-C10	2.33	1.94	1.90
3	B	401	X18	BR11-C10	2.29	1.94	1.90
3	A	401	X18	O14-C03	-2.20	1.18	1.23
3	B	401	X18	O14-C03	-2.17	1.18	1.23
3	B	401	X18	C01-C28	2.03	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	X18	C09-N08-C07	5.99	122.29	118.00
3	A	401	X18	C19-C18-C20	-5.64	110.64	114.71
3	B	401	X18	C19-C18-C20	-5.30	110.89	114.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	X18	C05-C07-N08	5.29	120.83	116.03
3	A	401	X18	C09-N08-C07	4.97	121.55	118.00
3	A	401	X18	C13-C07-C05	-4.81	117.53	121.89
3	A	401	X18	C27-N26-C24	-4.39	107.58	110.27
3	B	401	X18	C27-N26-C24	-3.87	107.90	110.27
3	A	401	X18	C16-N17-C24	-3.53	106.87	109.24
3	B	401	X18	C16-N17-C24	-3.32	107.01	109.24
3	B	401	X18	C15-C16-C27	-3.05	119.06	121.55
3	A	401	X18	C15-C16-C27	-2.88	119.20	121.55
3	B	401	X18	C27-C16-N17	2.64	108.44	106.52
3	A	401	X18	C27-C16-N17	2.55	108.37	106.52
3	B	401	X18	C10-C09-N08	-2.50	119.26	122.37
3	A	401	X18	O25-C24-N26	-2.42	125.40	127.49
3	A	401	X18	C10-C09-N08	-2.28	119.54	122.37
3	B	401	X18	C15-C16-N17	2.23	132.50	128.59
3	A	401	X18	C15-C16-N17	2.19	132.43	128.59
3	B	401	X18	C05-C07-N08	2.16	117.99	116.03
3	B	401	X18	O25-C24-N26	-2.14	125.64	127.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	X18	C19-C18-N17-C16
3	B	401	X18	C19-C18-N17-C16

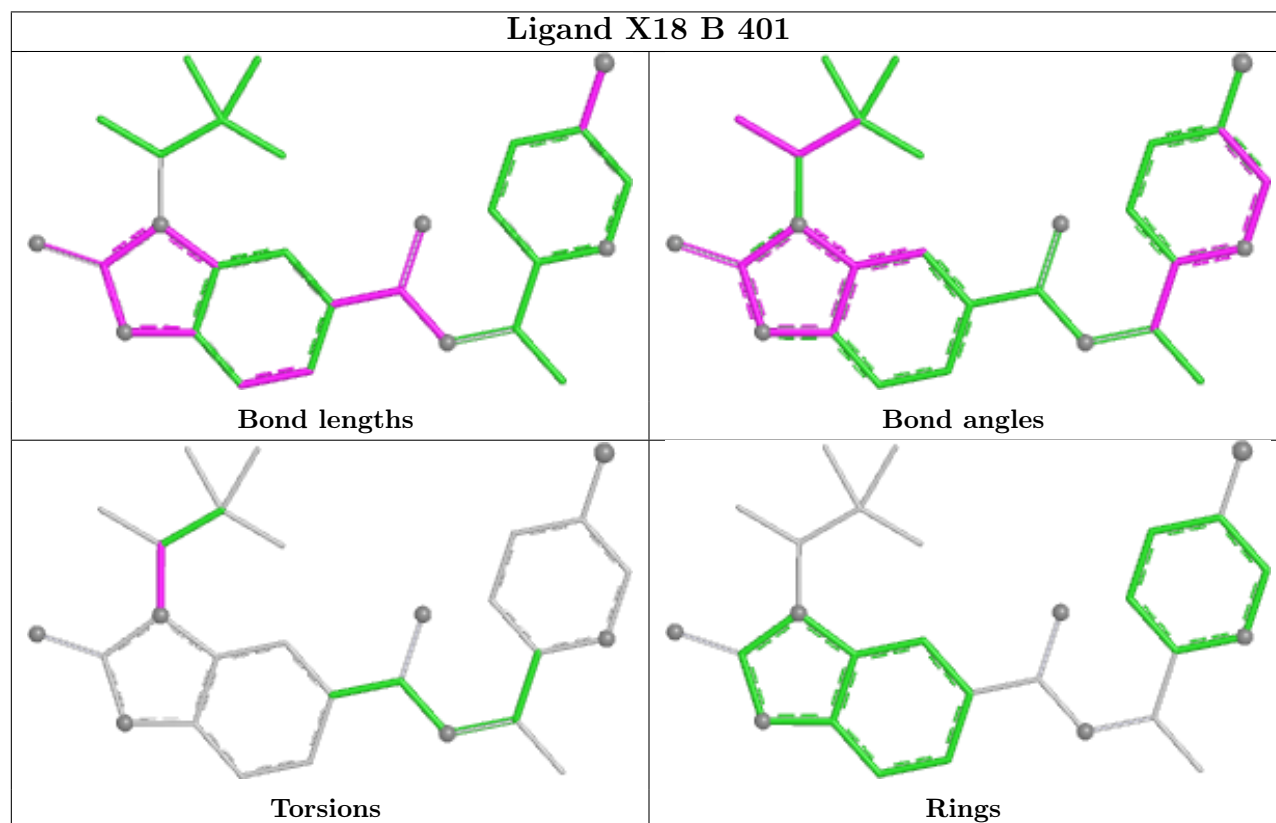
There are no ring outliers.

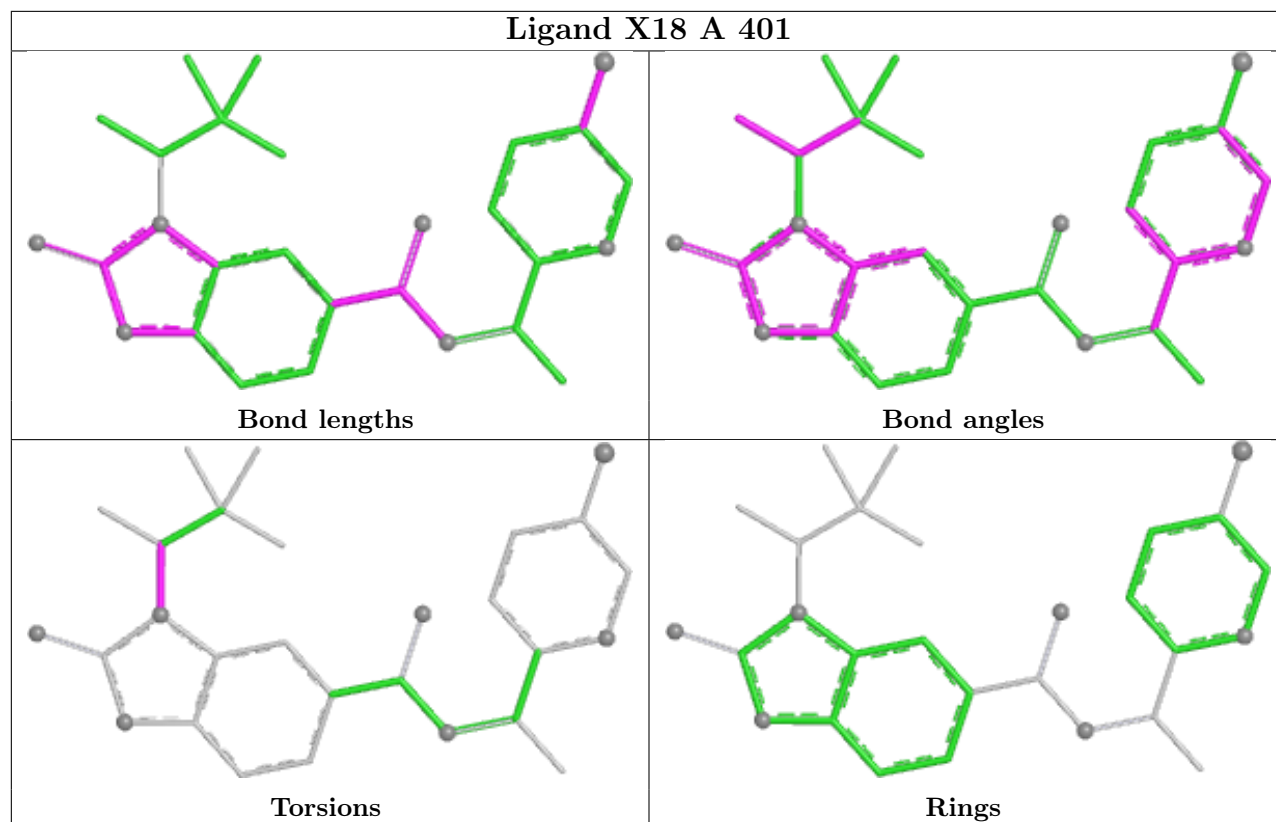
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	X18	1	0
3	A	401	X18	1	0
4	B	402	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	319/397 (80%)	1.20	47 (14%) 6 6	26, 48, 71, 95	0
1	B	323/397 (81%)	1.02	44 (13%) 7 7	24, 45, 65, 88	0
All	All	642/794 (80%)	1.11	91 (14%) 6 7	24, 46, 69, 95	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	GLU	5.8
1	A	260	ASN	5.7
1	A	262	LEU	4.8
1	B	360	GLU	4.5
1	A	366	ILE	4.3
1	A	259	LEU	4.1
1	A	397	CYS	3.8
1	B	262	LEU	3.6
1	B	397	CYS	3.6
1	A	396	LYS	3.6
1	A	344	GLY	3.5
1	A	279	ALA	3.4
1	B	269	ASP	3.4
1	A	71	ASN	3.3
1	A	258	TYR	3.3
1	A	395	LEU	3.2
1	B	255	ILE	3.2
1	A	358	ILE	3.2
1	B	279	ALA	3.0
1	A	269	ASP	3.0
1	B	264	LYS	3.0
1	B	361	LYS	3.0
1	A	268	LYS	2.9
1	B	139	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	56	GLU	2.8
1	B	257	ASN	2.8
1	A	340	LEU	2.8
1	A	139	ALA	2.8
1	B	366	ILE	2.8
1	A	265	THR	2.7
1	B	395	LEU	2.7
1	B	370	VAL	2.7
1	A	255	ILE	2.7
1	A	270	LEU	2.7
1	A	91	SER	2.6
1	A	174	GLN	2.6
1	A	361	LYS	2.6
1	B	104	SER	2.6
1	A	144	LEU	2.5
1	A	266	LYS	2.5
1	B	276	ILE	2.5
1	B	101	ARG	2.5
1	B	237	ASP	2.5
1	A	175	THR	2.4
1	A	356	PHE	2.4
1	A	314	HIS	2.4
1	B	253	HIS	2.4
1	B	266	LYS	2.4
1	B	345	LEU	2.4
1	A	257	ASN	2.4
1	A	238	THR	2.4
1	B	358	ILE	2.4
1	A	287	LEU	2.4
1	A	299	LEU	2.4
1	A	69	GLN	2.4
1	A	372	LEU	2.3
1	B	299	LEU	2.3
1	B	252	THR	2.3
1	B	259	LEU	2.3
1	B	373	MET	2.3
1	A	70	TYR	2.3
1	B	100	LEU	2.2
1	B	56	GLU	2.2
1	B	277	HIS	2.2
1	B	91	SER	2.2
1	B	143	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	362	ASN	2.2
1	B	260	ASN	2.2
1	A	368	SER	2.2
1	B	107	THR	2.2
1	B	265	THR	2.2
1	B	256	LEU	2.1
1	B	270	LEU	2.1
1	A	109	PHE	2.1
1	A	280	GLY	2.1
1	A	261	SER	2.1
1	A	369	TYR	2.1
1	B	198	LEU	2.1
1	B	108	GLY	2.1
1	B	393	ALA	2.1
1	B	140	LYS	2.1
1	A	315	LEU	2.1
1	A	276	ILE	2.1
1	B	258	TYR	2.1
1	B	286	LYS	2.0
1	B	278	ASN	2.0
1	B	356	PHE	2.0
1	A	232	SER	2.0
1	A	323	THR	2.0
1	A	277	HIS	2.0
1	B	364	ASN	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.

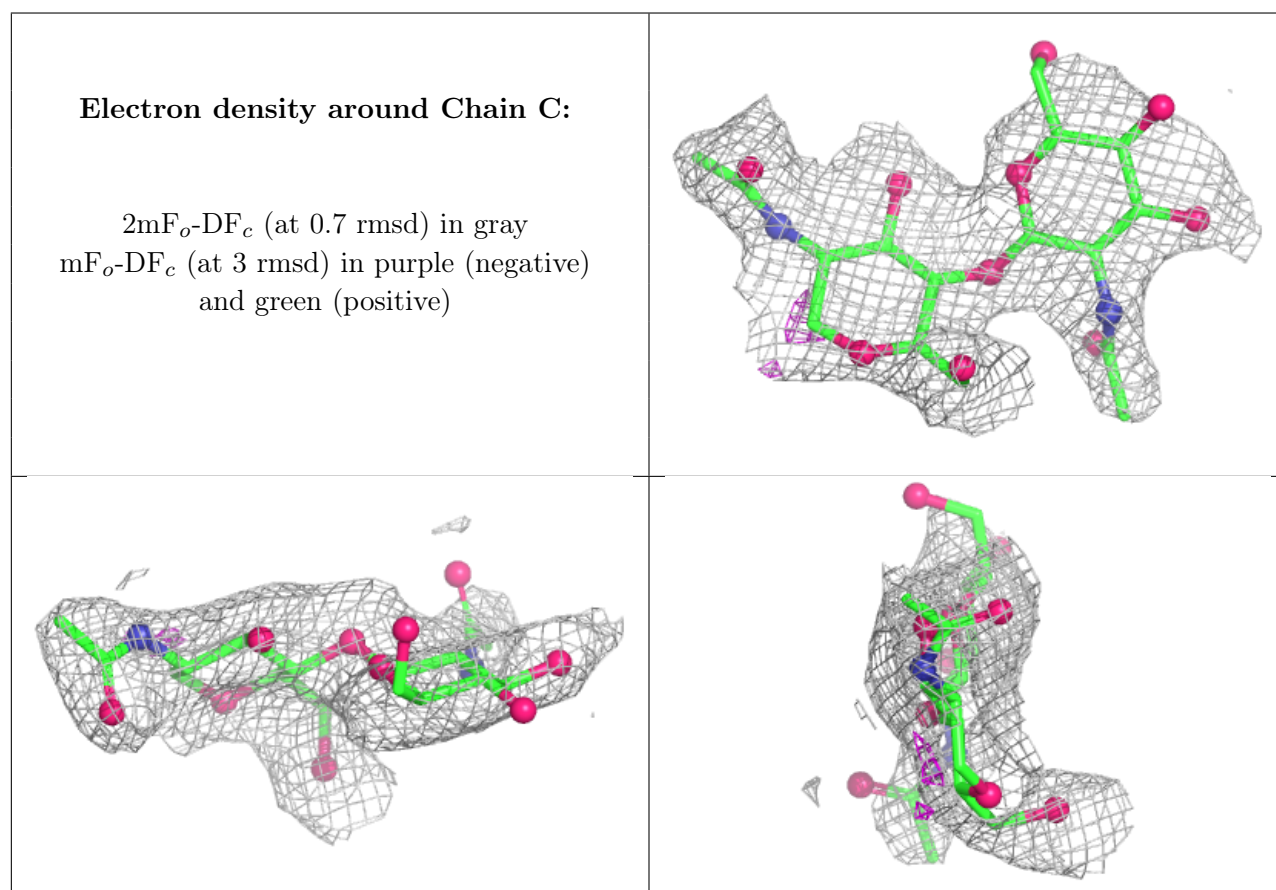
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	1	14/15	0.54	0.17	59,63,70,75	0
2	NAG	C	2	14/15	0.64	0.15	64,70,76,77	0
2	NAG	D	2	14/15	0.66	0.16	43,56,64,65	0

Continued on next page...

Continued from previous page...

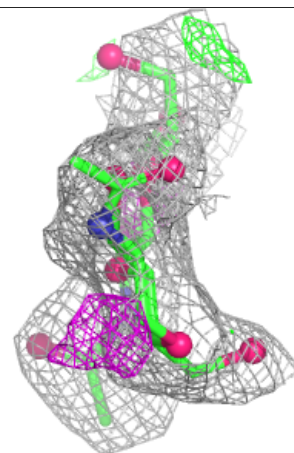
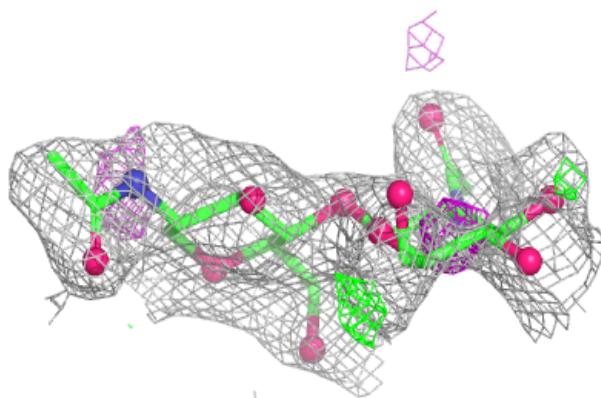
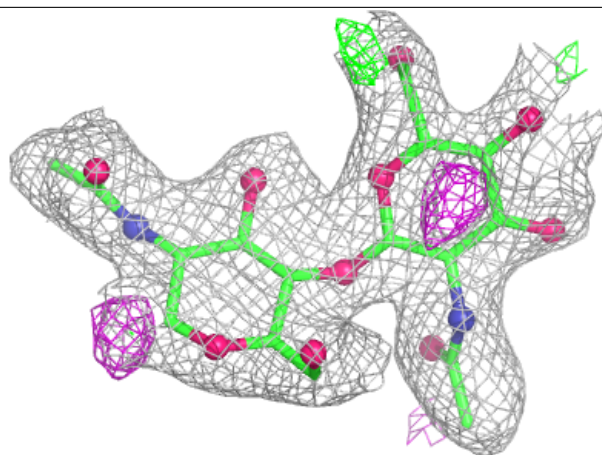
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	2	14/15	0.72	0.12	67,71,75,77	0
2	NAG	F	2	14/15	0.72	0.15	41,47,50,54	0
2	NAG	C	1	14/15	0.77	0.12	47,56,61,64	0
2	NAG	D	1	14/15	0.87	0.10	42,43,47,51	0
2	NAG	F	1	14/15	0.89	0.09	35,37,41,43	0

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



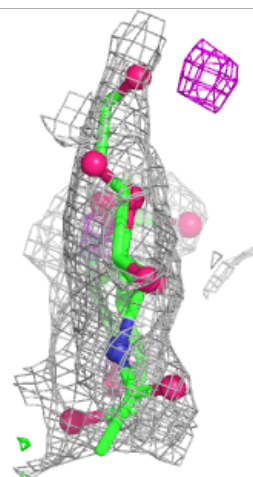
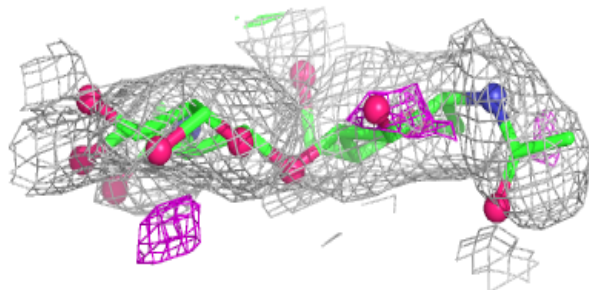
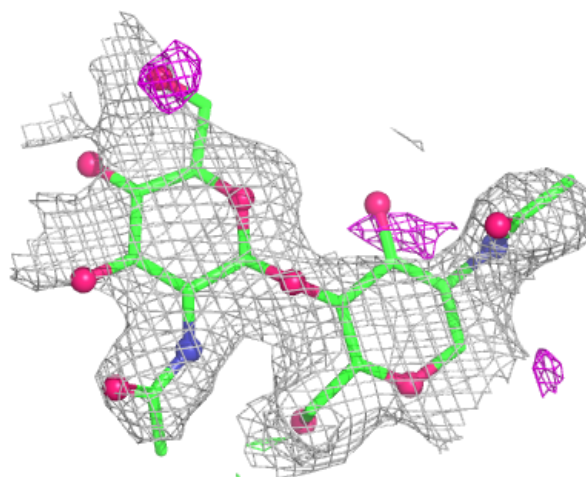
Electron density around Chain D:

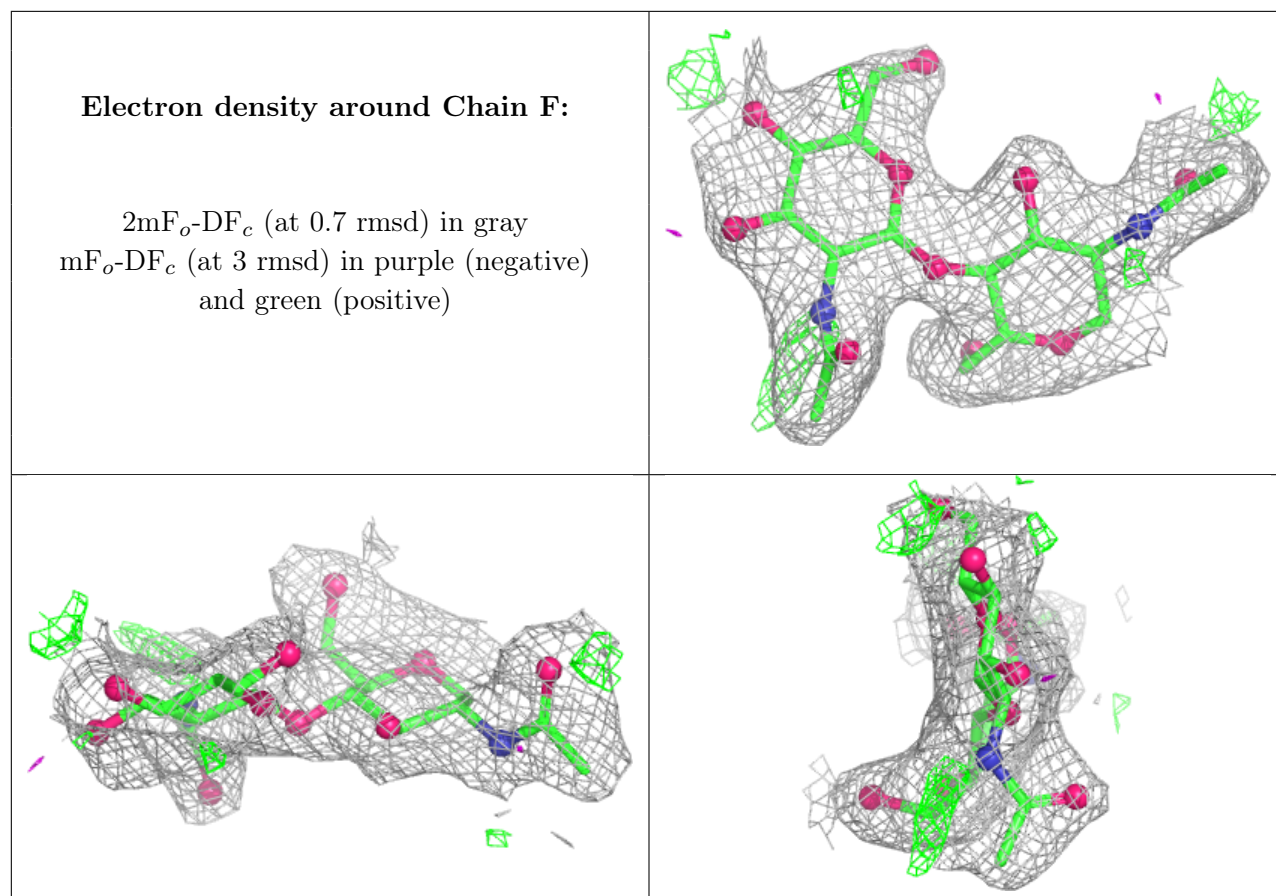
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

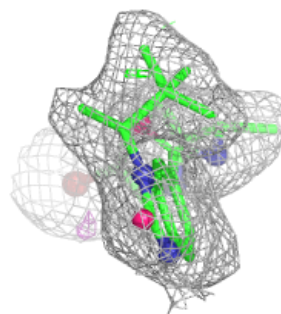
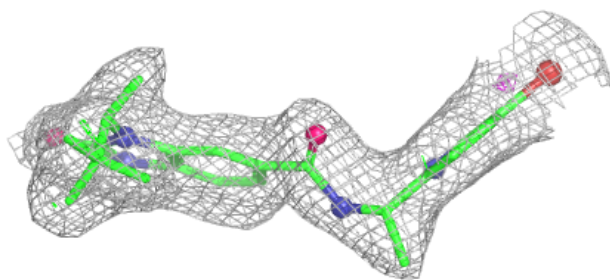
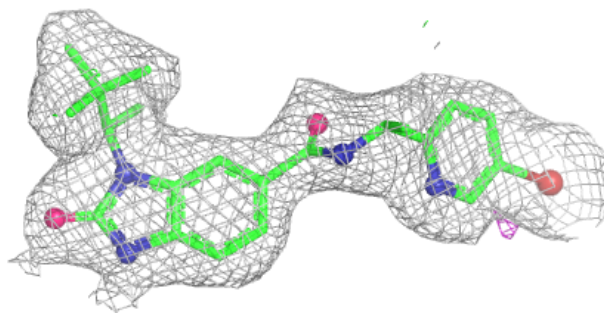
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	402	4/4	0.87	0.13	24,27,30,31	0
4	EDO	B	402	4/4	0.88	0.13	24,30,33,42	0
3	X18	A	401	28/28	0.93	0.09	21,28,42,67	0
3	X18	B	401	28/28	0.94	0.09	23,28,38,58	0

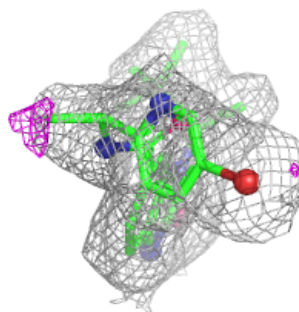
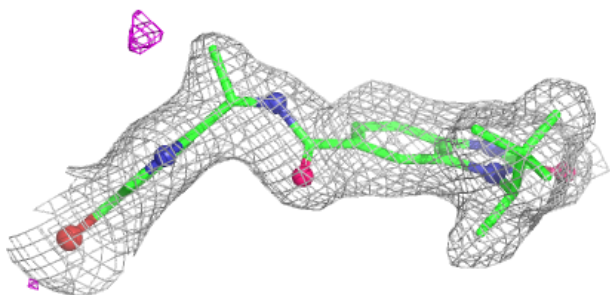
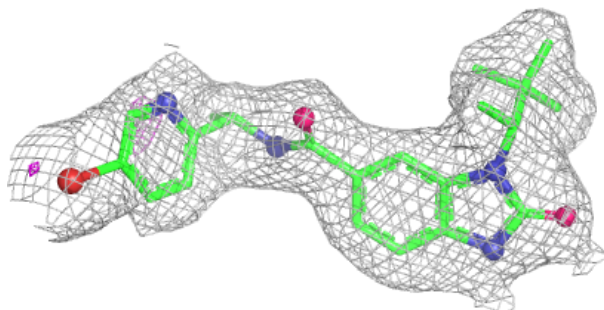
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X18 A 401:

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

**Electron density around X18 B 401:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.