



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:21 AM BST

PDB ID : 4O6D
Title : West Nile Virus Non-structural protein 1 (NS1) Form 1 crystal
Authors : Akey, D.L.; Smith, J.L.
Deposited on : 2013-12-20
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

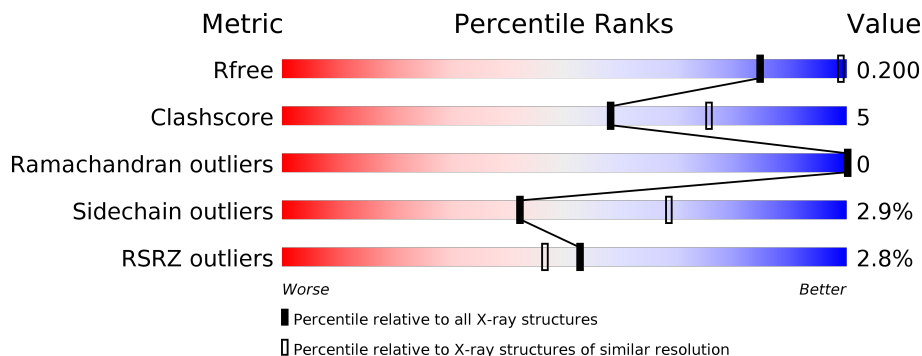
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	377	 3% 77% 13% 10%
2	B	377	 2% 79% 11% 10%
3	C	2	 100%
3	D	2	 100%
3	E	2	 100%
4	F	5	 40% 60%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OXN	A	407	-	-	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 5803 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 NS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2668	1656	474	521	17	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	ALA	-	expression tag	UNP U3N977
A	-23	GLU	-	expression tag	UNP U3N977
A	-22	HIS	-	expression tag	UNP U3N977
A	-21	HIS	-	expression tag	UNP U3N977
A	-20	HIS	-	expression tag	UNP U3N977
A	-19	HIS	-	expression tag	UNP U3N977
A	-18	HIS	-	expression tag	UNP U3N977
A	-16	SER	-	expression tag	UNP U3N977
A	-15	SER	-	expression tag	UNP U3N977
A	-14	GLY	-	expression tag	UNP U3N977
A	-13	VAL	-	expression tag	UNP U3N977
A	-12	ASP	-	expression tag	UNP U3N977
A	-11	LEU	-	expression tag	UNP U3N977
A	-10	GLY	-	expression tag	UNP U3N977
A	-9	THR	-	expression tag	UNP U3N977
A	-8	GLU	-	expression tag	UNP U3N977
A	-7	ASN	-	expression tag	UNP U3N977
A	-6	LEU	-	expression tag	UNP U3N977
A	-5	TYR	-	expression tag	UNP U3N977
A	-4	PHE	-	expression tag	UNP U3N977
A	-3	GLN	-	expression tag	UNP U3N977
A	-2	SER	-	expression tag	UNP U3N977
A	-1	ASN	-	expression tag	UNP U3N977

- Molecule 2 is a protein called NS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	341	2683	1665	477	524	17	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	UNK	-	expression tag	UNP U3N977
B	-23	UNK	-	expression tag	UNP U3N977
B	-22	UNK	-	expression tag	UNP U3N977
B	-21	UNK	-	expression tag	UNP U3N977
B	-20	UNK	-	expression tag	UNP U3N977
B	-19	UNK	-	expression tag	UNP U3N977
B	-18	HIS	-	expression tag	UNP U3N977
B	-16	SER	-	expression tag	UNP U3N977
B	-15	SER	-	expression tag	UNP U3N977
B	-14	GLY	-	expression tag	UNP U3N977
B	-13	VAL	-	expression tag	UNP U3N977
B	-12	ASP	-	expression tag	UNP U3N977
B	-11	LEU	-	expression tag	UNP U3N977
B	-10	GLY	-	expression tag	UNP U3N977
B	-9	THR	-	expression tag	UNP U3N977
B	-8	GLU	-	expression tag	UNP U3N977
B	-7	ASN	-	expression tag	UNP U3N977
B	-6	LEU	-	expression tag	UNP U3N977
B	-5	TYR	-	expression tag	UNP U3N977
B	-4	PHE	-	expression tag	UNP U3N977
B	-3	GLN	-	expression tag	UNP U3N977
B	-2	SER	-	expression tag	UNP U3N977
B	-1	ASN	-	expression tag	UNP U3N977

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



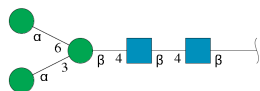
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0
3	D	2	28	16	2	10	0	0	0

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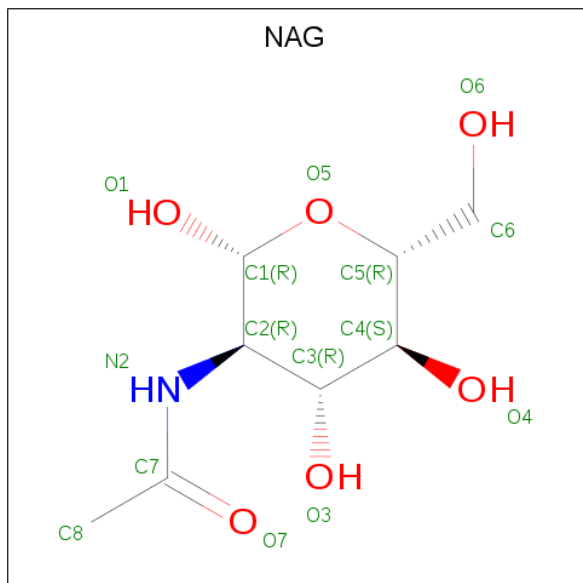
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
3	E	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



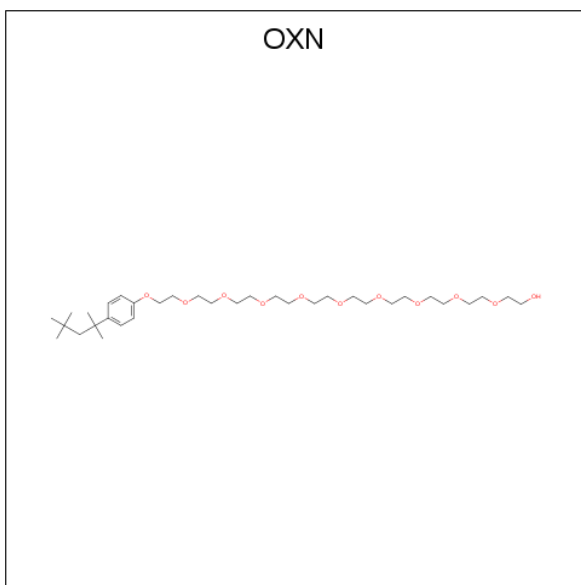
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
4	F	5	61	34	2	25	0	0	0

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



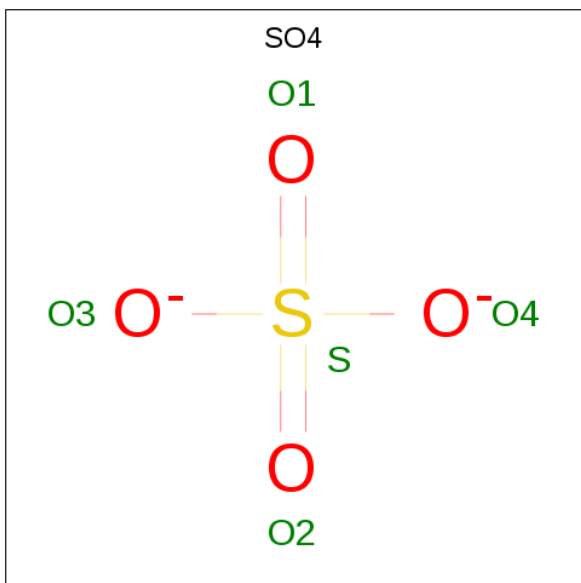
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
5	A	1	14	8	1	5	0	0

- Molecule 6 is OXTOXYNOL-10 (three-letter code: OXN) (formula: $C_{34}H_{62}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	14	1		
6	A	1	Total	C	O	0	0
			15	14	1		
6	A	1	Total	C	O	0	0
			25	16	9		
6	B	1	Total	C	O	0	0
			15	14	1		

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



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		

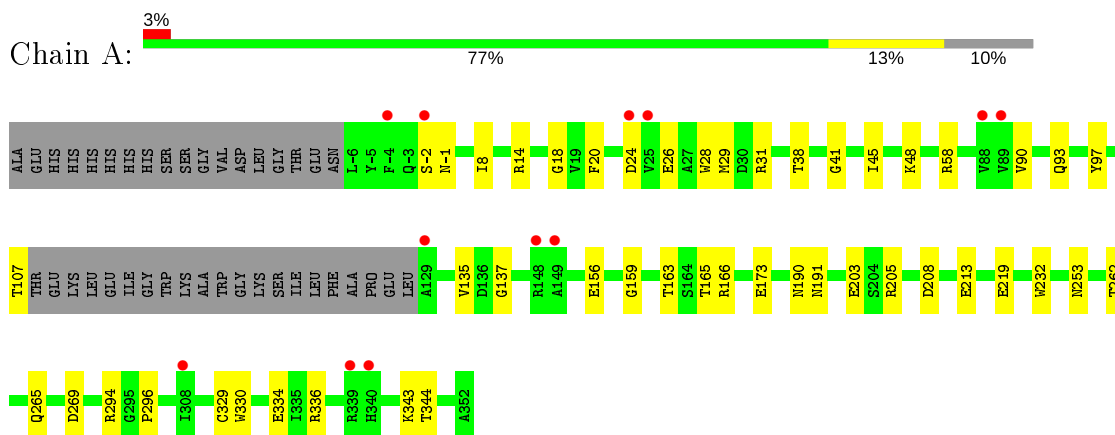
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	109	Total	O	0	0
			109	109		
8	B	104	Total	O	0	0
			104	104		

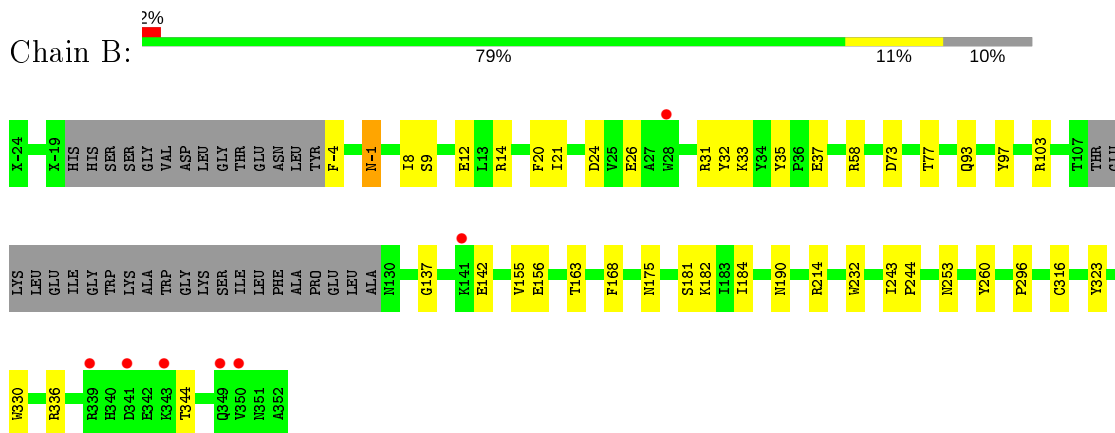
3 Residue-property plots [i](#)

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

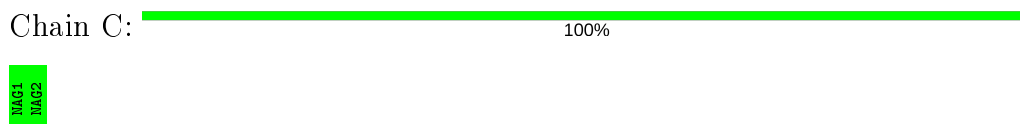
- Molecule 1: NS1



- Molecule 2: NS1



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



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

Chain D:  100%

GLU1
GLU2

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

Chain E:  100%

GLU1
GLU2

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

Chain F:  40% 60%

GLU1
GLU2
BGA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.69 Å 168.69 Å 92.89 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 2.59 48.70 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.79-2.59) 99.4 (48.70-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.58 Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.163 , 0.191 0.171 , 0.200	Depositor DCC
R_{free} test set	2358 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.3	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5803	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: MAN, OXN, BMA, NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2725	0.57	0/3697
2	B	0.40	0/2710	0.56	0/3676
All	All	0.40	0/5435	0.57	0/7373

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2668	0	2565	29	0
2	B	2683	0	2566	27	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
4	F	61	0	52	0	0
5	A	14	0	13	0	0
6	A	55	0	74	3	0
6	B	15	0	21	1	0
7	B	10	0	0	0	0
8	A	109	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	104	0	0	3	0
All	All	5803	0	5366	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ARG:NH1	2:B:137:GLY:O	2.22	0.73
1:A:203:GLU:OE2	1:A:205:ARG:NH2	2.25	0.69
6:A:408:OXN:H342	6:A:408:OXN:H291	1.78	0.65
2:B:-1:ASN:N	2:B:-1:ASN:OD1	2.29	0.65
1:A:190:ASN:ND2	8:A:591:HOH:O	2.30	0.65
2:B:296:PRO:O	2:B:336:ARG:NH1	2.25	0.62
2:B:142:GLU:N	2:B:142:GLU:OE1	2.31	0.61
2:B:31:ARG:NH2	8:B:526:HOH:O	2.34	0.60
1:A:262:THR:O	1:A:294:ARG:NH2	2.26	0.59
1:A:14:ARG:HD3	2:B:31:ARG:HG2	1.86	0.56
1:A:24:ASP:HA	1:A:28:TRP:HB2	1.88	0.56
6:A:407:OXN:H22	6:A:407:OXN:H72	1.88	0.56
2:B:103:ARG:NH2	2:B:175:ASN:OD1	2.39	0.55
1:A:24:ASP:OD1	2:B:14:ARG:NH1	2.40	0.54
2:B:73:ASP:O	2:B:77:THR:HG23	2.08	0.53
2:B:232:TRP:CD2	2:B:253:ASN:HB2	2.43	0.53
1:A:58:ARG:NH1	1:A:137:GLY:O	2.42	0.53
1:A:41:GLY:O	1:A:45:ILE:HG12	2.09	0.53
6:B:410:OXN:H73	6:B:410:OXN:H43	1.91	0.53
1:A:165:THR:OG1	2:B:12:GLU:OE2	2.23	0.52
1:A:159:GLY:N	1:A:166:ARG:O	2.42	0.51
1:A:18:GLY:HA3	2:B:21:ILE:O	2.11	0.51
1:A:329:CYS:HB2	8:A:589:HOH:O	2.11	0.51
1:A:232:TRP:CD2	1:A:253:ASN:HB2	2.45	0.50
2:B:26:GLU:OE1	2:B:214:ARG:NH2	2.39	0.50
1:A:296:PRO:O	1:A:336:ARG:NH1	2.26	0.50
1:A:344:THR:HA	8:A:555:HOH:O	2.12	0.49
2:B:323:TYR:HB2	2:B:330:TRP:HB2	1.94	0.48
8:A:550:HOH:O	2:B:190:ASN:HB3	2.16	0.46
6:A:407:OXN:H51	6:A:407:OXN:H10	1.78	0.45
1:A:205:ARG:HB2	1:A:213:GLU:HG3	1.99	0.45
2:B:181:SER:HA	2:B:184:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:CG	2:B:14:ARG:HH12	2.21	0.44
2:B:155:VAL:O	2:B:182:LYS:HD2	2.17	0.44
2:B:37:GLU:OE2	2:B:156:GLU:HG2	2.18	0.44
2:B:93:GLN:HG2	2:B:97:TYR:CE2	2.53	0.44
1:A:191:ASN:HB2	8:B:511:HOH:O	2.18	0.43
1:A:48:LYS:NZ	1:A:107:THR:HB	2.34	0.43
1:A:31:ARG:HD2	1:A:163:THR:O	2.19	0.43
1:A:29:MET:HE1	8:A:535:HOH:O	2.19	0.42
1:A:14:ARG:NH2	2:B:24:ASP:OD1	2.53	0.42
2:B:260:TYR:CZ	2:B:316:CYS:HB2	2.55	0.42
2:B:32:TYR:O	2:B:33:LYS:HD2	2.20	0.41
1:A:265:GLN:HB3	1:A:296:PRO:HA	2.02	0.41
1:A:24:ASP:CG	2:B:14:ARG:HH22	2.23	0.41
1:A:90:VAL:HG22	1:A:135:VAL:HB	2.02	0.41
1:A:93:GLN:HG2	1:A:97:TYR:CE2	2.56	0.41
2:B:35:TYR:O	2:B:168:PHE:HA	2.21	0.40
1:A:-1:ASN:HA	2:B:9:SER:OG	2.21	0.40
2:B:243:ILE:HA	2:B:244:PRO:HD3	1.95	0.40
1:A:173:GLU:CD	1:A:173:GLU:H	2.23	0.40
1:A:8:ILE:HG12	8:B:575:HOH:O	2.22	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	334/377 (89%)	311 (93%)	23 (7%)	0	100	100
2	B	331/377 (88%)	319 (96%)	12 (4%)	0	100	100
All	All	665/754 (88%)	630 (95%)	35 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	295/329 (90%)	284 (96%)	11 (4%)	34	60
2	B	295/324 (91%)	289 (98%)	6 (2%)	55	78
All	All	590/653 (90%)	573 (97%)	17 (3%)	42	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	20	PHE
1	A	26	GLU
1	A	38	THR
1	A	156	GLU
1	A	208	ASP
1	A	219	GLU
1	A	269	ASP
1	A	330	TRP
1	A	334	GLU
1	A	343	LYS
2	B	-4	PHE
2	B	-1	ASN
2	B	8	ILE
2	B	20	PHE
2	B	163	THR
2	B	344	THR

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

Mol	Chain	Res	Type
2	B	147	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

11 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
3	NAG	C	1	1,3	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	C	2	3	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	D	1	1,3	14,14,15	0.39	0	17,19,21	0.42	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	E	1	3,2	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	F	1	2,4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	F	2	4	14,14,15	0.26	0	17,19,21	0.37	0
4	BMA	F	3	4	11,11,12	0.91	1 (9%)	15,15,17	0.86	0
4	MAN	F	4	4	11,11,12	0.90	1 (9%)	15,15,17	1.14	2 (13%)
4	MAN	F	5	4	11,11,12	0.96	0	15,15,17	1.16	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4	MAN	C1-C2	2.16	1.57	1.52
4	F	3	BMA	C4-C3	2.06	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5	MAN	C1-O5-C5	2.69	115.83	112.19
4	F	4	MAN	C1-O5-C5	2.38	115.42	112.19
4	F	4	MAN	O2-C2-C3	-2.24	105.64	110.14

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
4	F	3	BMA	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6

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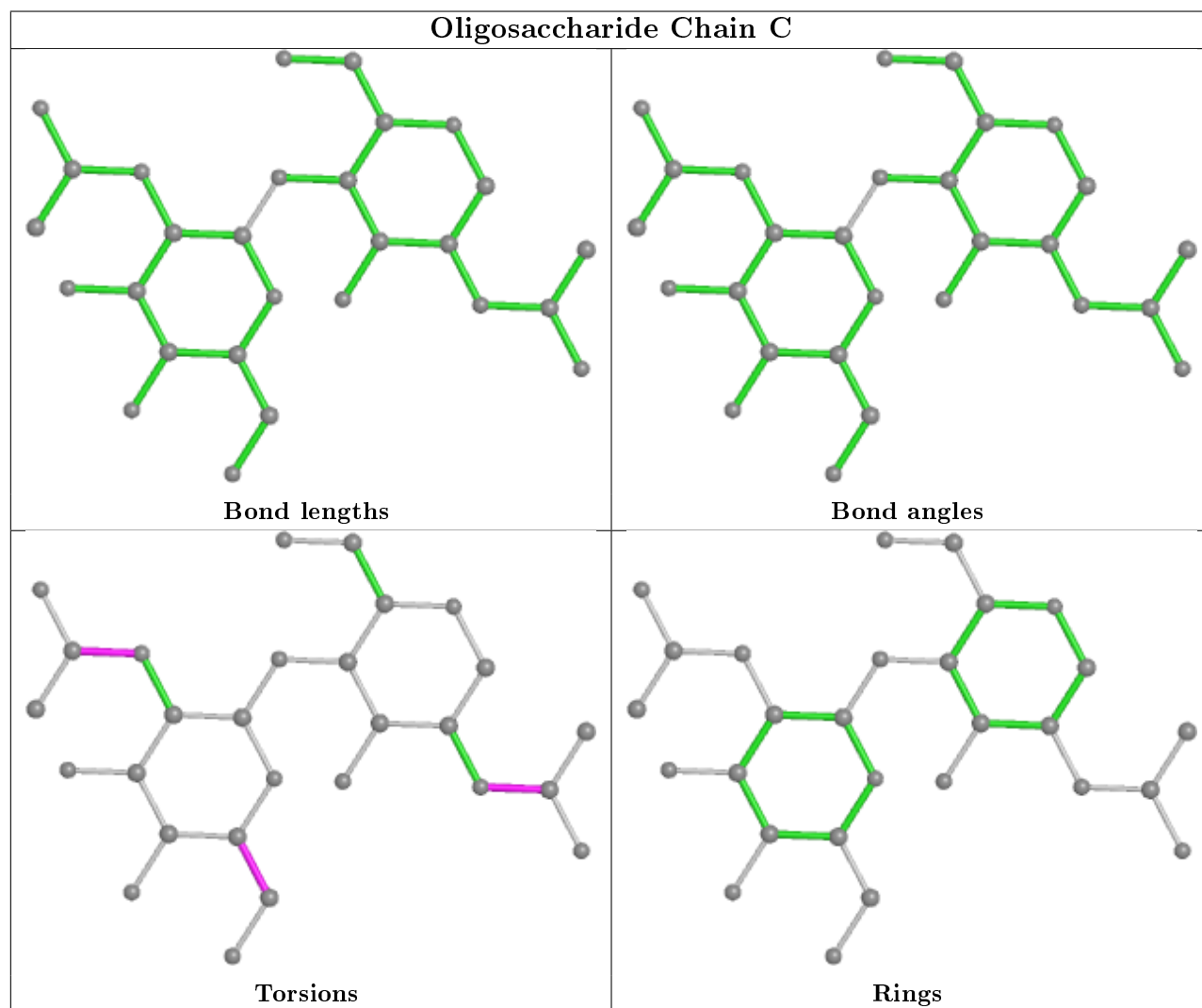
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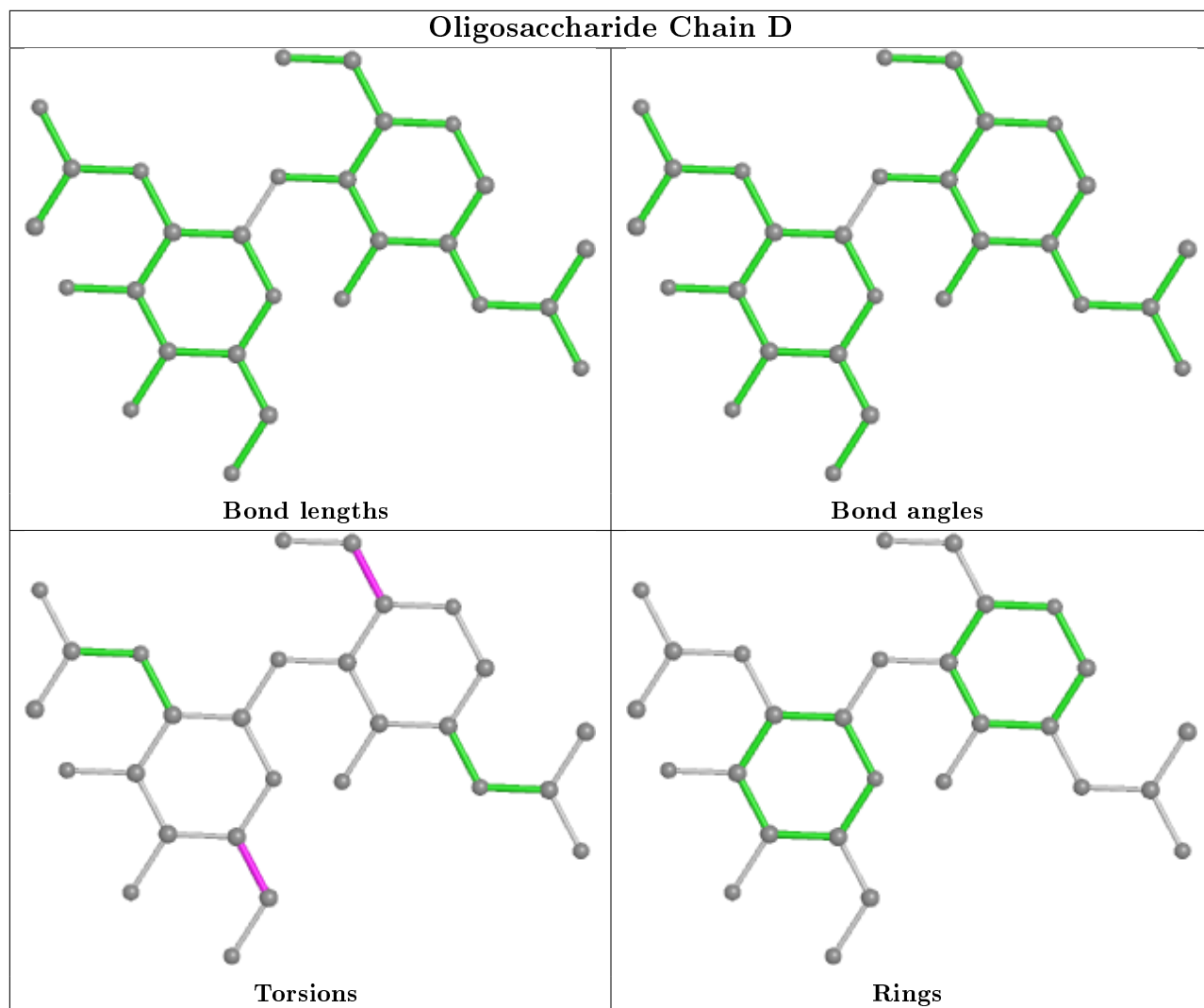
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6

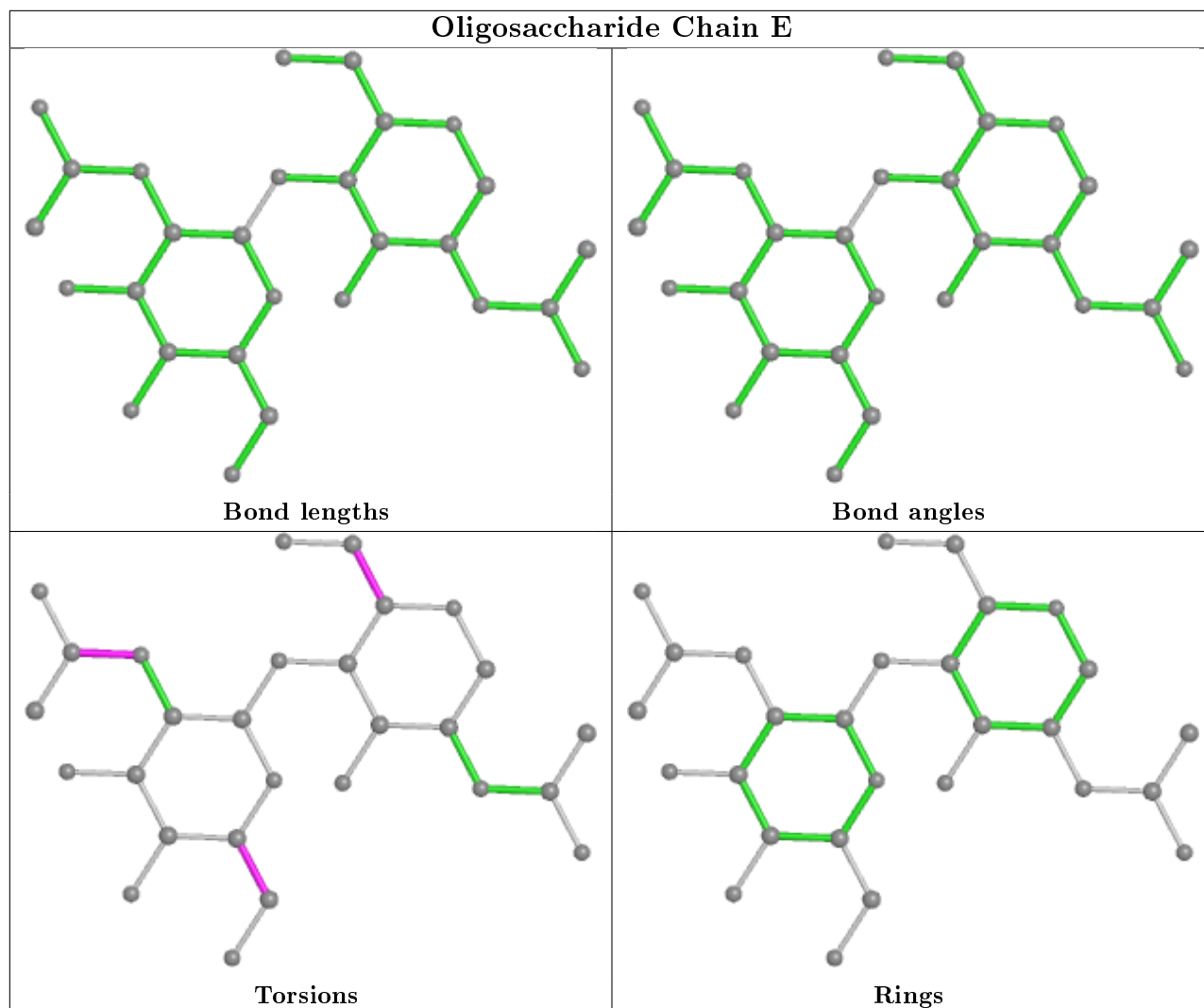
There are no ring outliers.

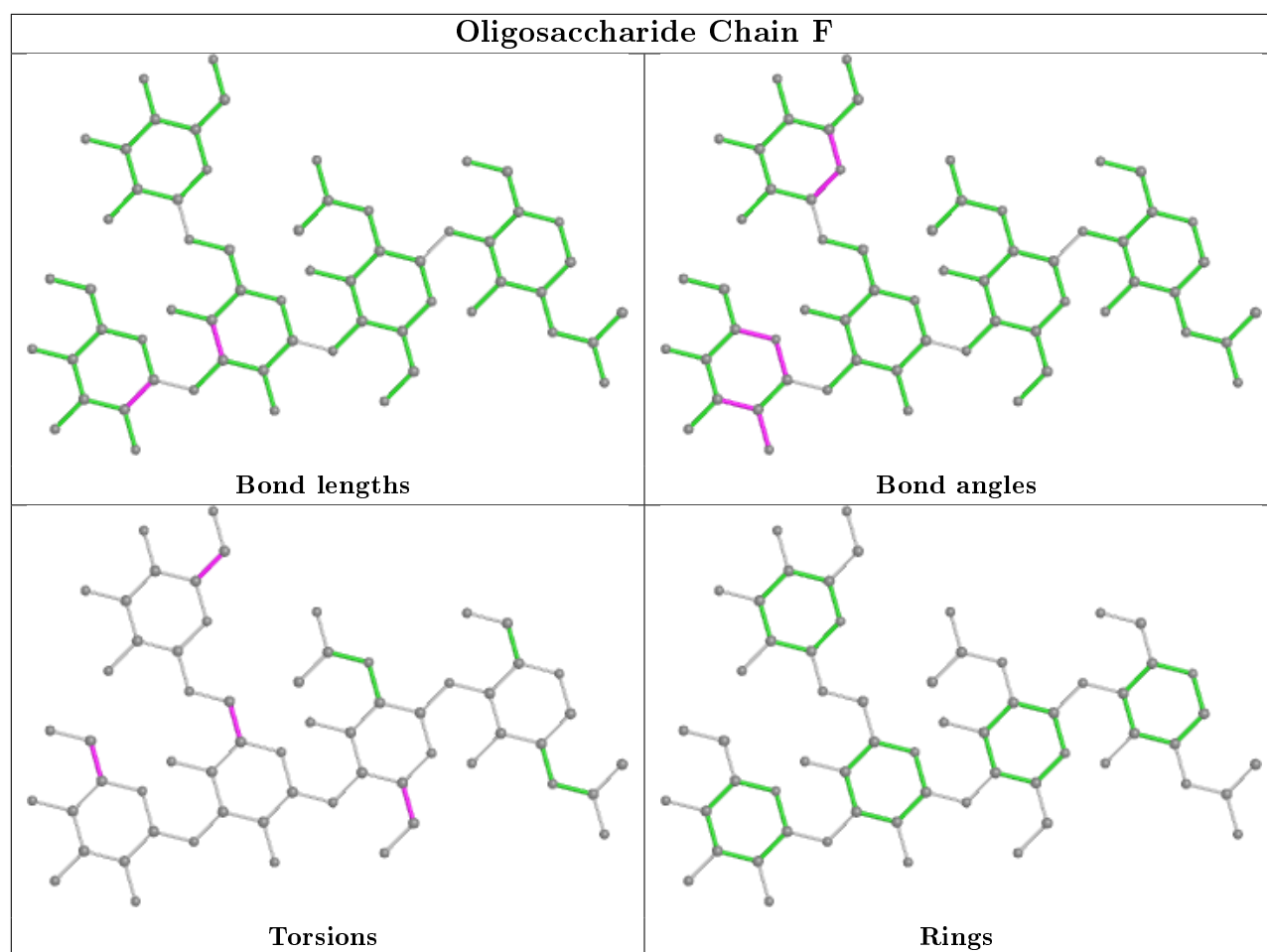
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	OXN	B	410	-	15,15,45	1.87	4 (26%)	23,23,53	1.00	1 (4%)
7	SO4	B	409	-	4,4,4	0.13	0	6,6,6	0.29	0
6	OXN	A	406	-	15,15,45	1.88	4 (26%)	23,23,53	1.16	2 (8%)
6	OXN	A	408	-	24,24,45	0.76	0	23,23,53	0.32	0
5	NAG	A	403	1	14,14,15	0.32	0	17,19,21	0.52	0
6	OXN	A	407	-	15,15,45	1.67	4 (26%)	23,23,53	1.46	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.10	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
6	OXN	B	410	-	-	4/12/12/43	0/1/1/1
6	OXN	A	408	-	-	16/22/22/43	-
6	OXN	A	406	-	-	1/12/12/43	0/1/1/1
5	NAG	A	403	1	-	0/6/23/26	0/1/1/1
6	OXN	A	407	-	-	3/12/12/43	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	410	OXN	C6-C9	4.43	1.60	1.53
6	A	406	OXN	C6-C9	4.09	1.60	1.53
6	A	407	OXN	C6-C9	3.75	1.59	1.53
6	A	406	OXN	O15-C12	2.96	1.43	1.37
6	B	410	OXN	O15-C12	2.95	1.43	1.37
6	A	406	OXN	C5-C1	2.85	1.63	1.55
6	A	406	OXN	C11-C12	2.75	1.44	1.38
6	B	410	OXN	C5-C1	2.74	1.63	1.55
6	B	410	OXN	C11-C12	2.59	1.43	1.38
6	A	407	OXN	O15-C12	2.58	1.43	1.37
6	A	407	OXN	C5-C1	2.46	1.62	1.55
6	A	407	OXN	C11-C12	2.38	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	407	OXN	C5-C6-C9	-3.54	104.11	111.93
6	A	407	OXN	C14-C9-C10	3.49	123.17	117.97
6	A	406	OXN	C14-C9-C10	2.95	122.36	117.97
6	A	407	OXN	C10-C9-C6	-2.63	116.72	121.53
6	B	410	OXN	C14-C9-C10	2.30	121.40	117.97
6	A	406	OXN	C7-C6-C9	-2.10	104.94	110.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	407	OXN	C1-C5-C6-C9
6	A	408	OXN	O30-C31-C32-O33
6	A	408	OXN	O18-C19-C20-O21
6	A	408	OXN	O39-C40-C41-O42
6	A	407	OXN	C1-C5-C6-C7
6	A	408	OXN	O33-C34-C35-O36
6	A	408	OXN	O27-C28-C29-O30
6	A	408	OXN	O21-C22-C23-O24
6	A	407	OXN	C1-C5-C6-C8
6	A	408	OXN	C22-C23-O24-C25
6	A	408	OXN	O24-C25-C26-O27
6	A	408	OXN	C34-C35-O36-C37
6	B	410	OXN	C1-C5-C6-C9
6	A	408	OXN	C23-C22-O21-C20
6	A	408	OXN	C41-C40-O39-C38
6	A	406	OXN	C1-C5-C6-C9
6	B	410	OXN	C1-C5-C6-C7
6	A	408	OXN	C29-C28-O27-C26
6	A	408	OXN	C38-C37-O36-C35
6	B	410	OXN	C7-C6-C9-C10
6	A	408	OXN	C25-C26-O27-C28
6	A	408	OXN	O36-C37-C38-O39
6	A	408	OXN	C28-C29-O30-C31
6	B	410	OXN	C7-C6-C9-C14

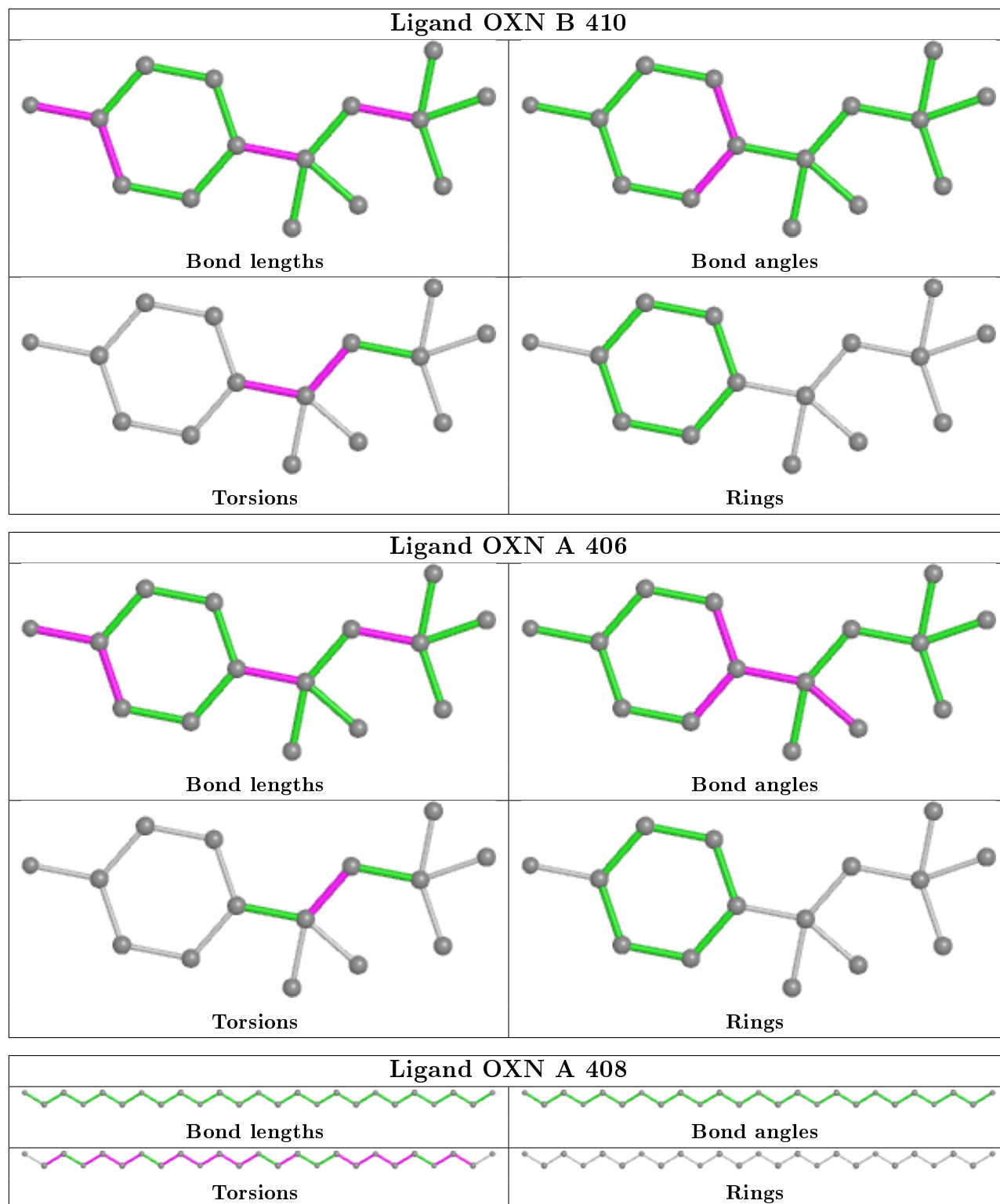
There are no ring outliers.

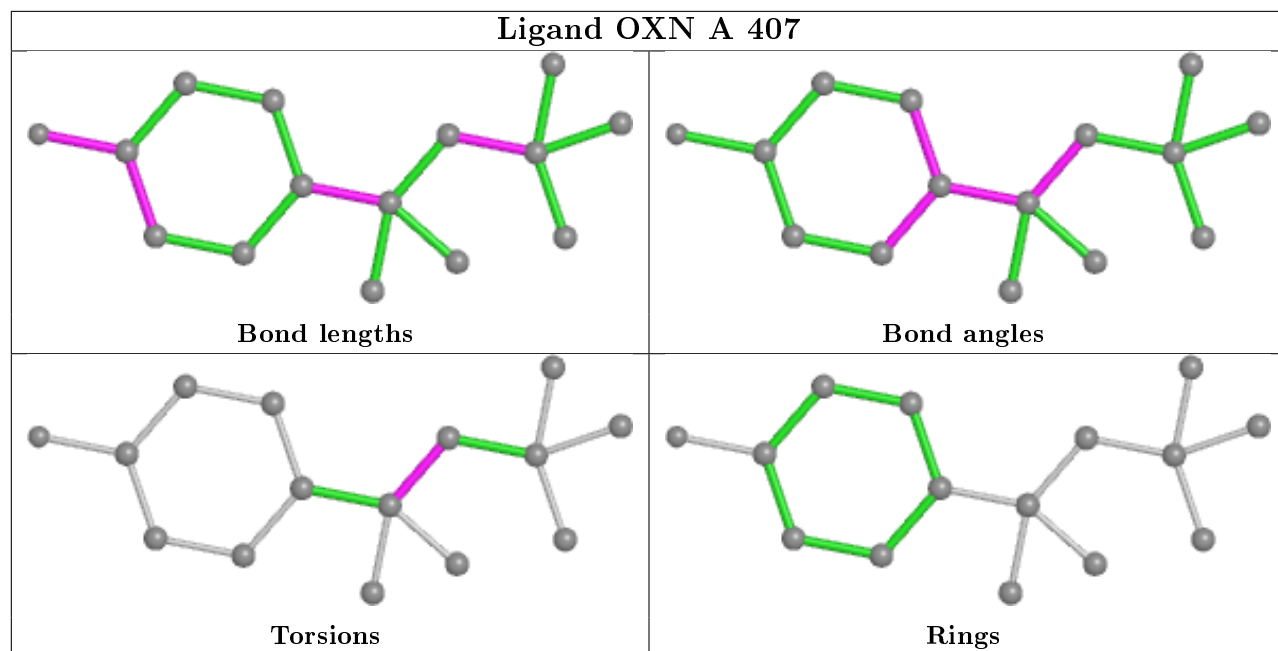
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	410	OXN	1	0
6	A	408	OXN	1	0
6	A	407	OXN	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	338/377 (89%)	0.24	12 (3%) 42 35	48, 80, 141, 197	0
2	B	335/377 (88%)	0.19	7 (2%) 63 58	49, 77, 130, 209	0
All	All	673/754 (89%)	0.22	19 (2%) 53 46	48, 79, 138, 209	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	28	TRP	6.0
1	A	25	VAL	3.9
2	B	141	LYS	3.4
1	A	339	ARG	3.3
1	A	340	HIS	3.3
2	B	341	ASP	3.2
2	B	339	ARG	3.1
1	A	149	ALA	2.7
1	A	24	ASP	2.7
1	A	88	VAL	2.6
1	A	-2	SER	2.6
1	A	129	ALA	2.5
1	A	308	ILE	2.3
1	A	89	VAL	2.2
2	B	349	GLN	2.1
1	A	148	ARG	2.1
2	B	350	VAL	2.1
2	B	343	LYS	2.1
1	A	-4	PHE	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

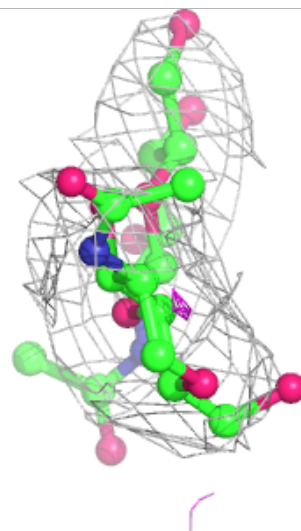
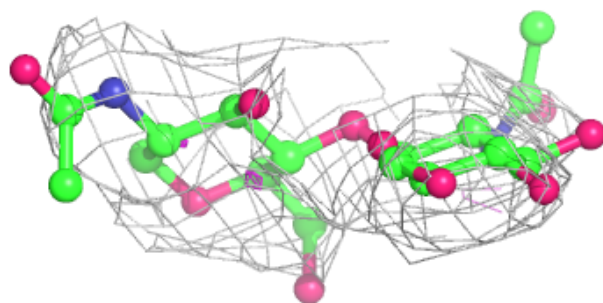
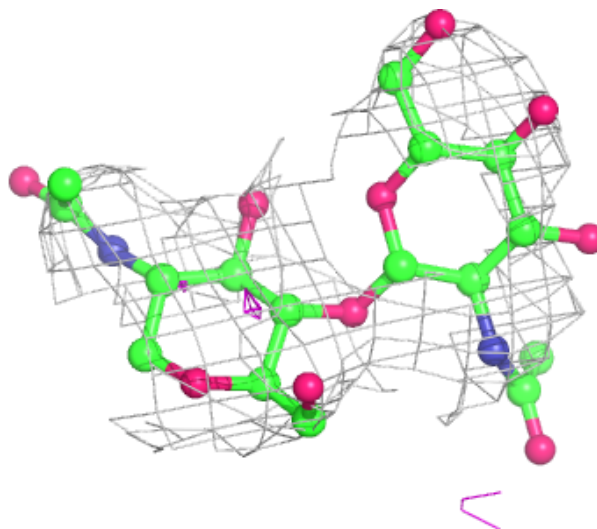
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	F	5	11/12	0.81	0.23	146,154,188,193	0
4	BMA	F	3	11/12	0.84	0.27	164,176,188,193	0
3	NAG	E	2	14/15	0.88	0.18	130,140,149,149	0
3	NAG	D	2	14/15	0.88	0.28	150,163,171,174	0
3	NAG	C	2	14/15	0.89	0.39	179,184,189,190	0
4	MAN	F	4	11/12	0.89	0.18	166,175,183,184	0
3	NAG	C	1	14/15	0.90	0.41	139,160,170,173	0
4	NAG	F	2	14/15	0.95	0.14	108,120,136,152	0
3	NAG	D	1	14/15	0.95	0.20	106,132,137,154	0
4	NAG	F	1	14/15	0.96	0.09	92,103,113,121	0
3	NAG	E	1	14/15	0.97	0.13	79,103,120,129	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.

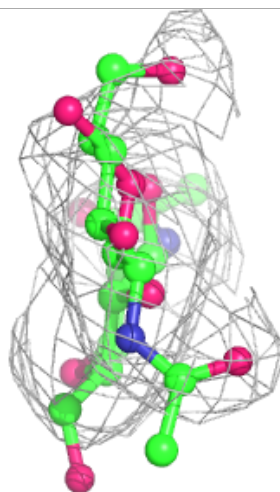
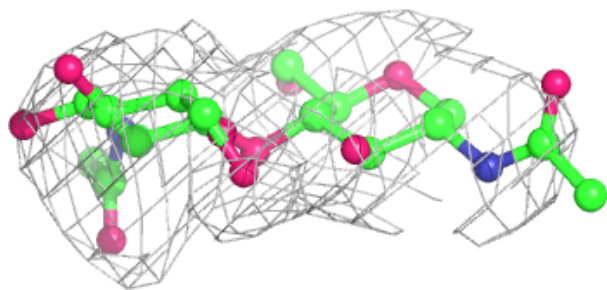
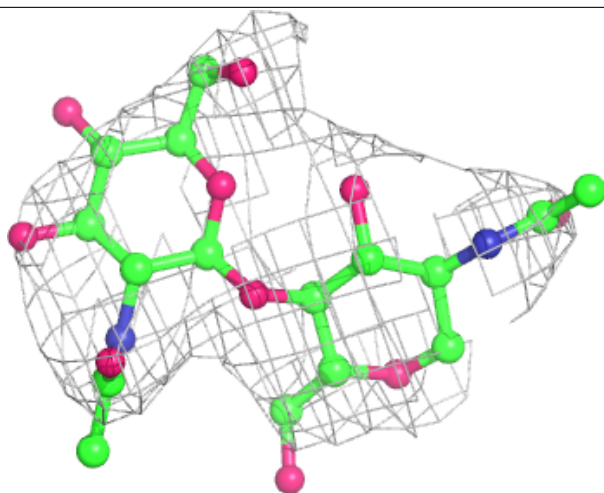
Electron density around Chain C:

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



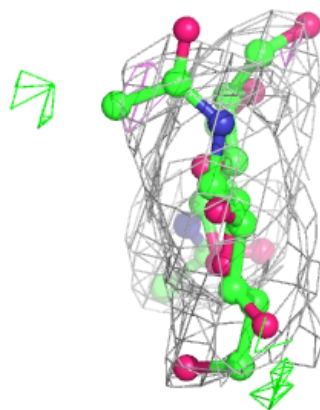
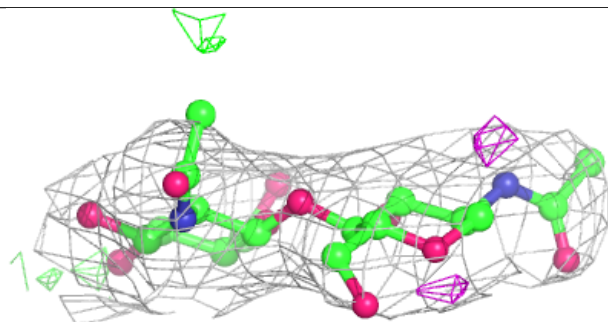
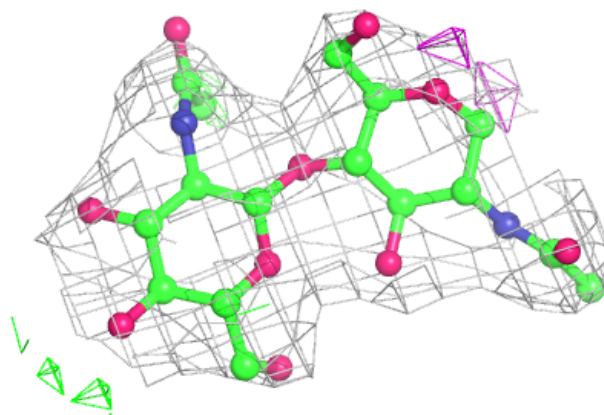
Electron density around Chain D:

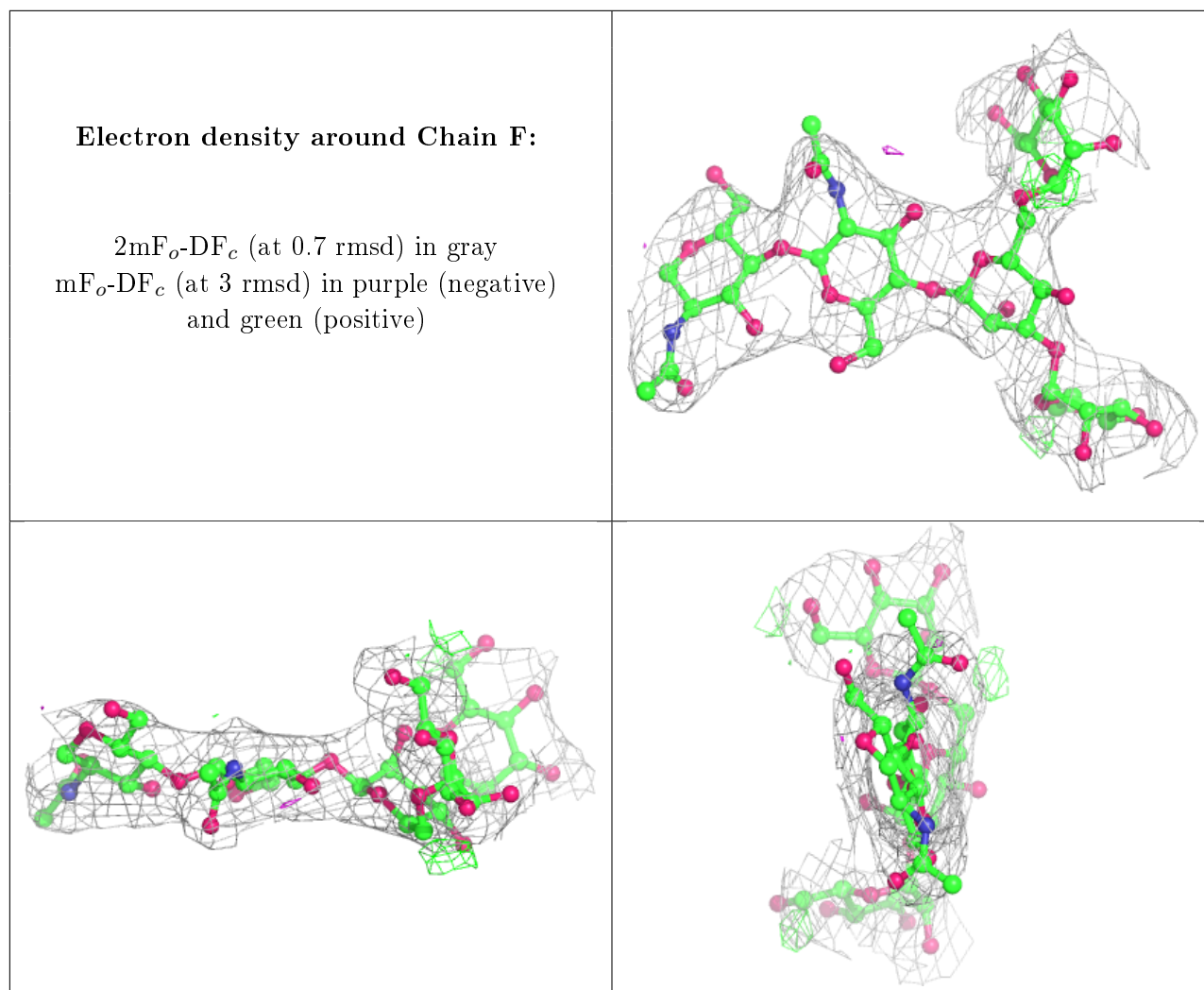
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





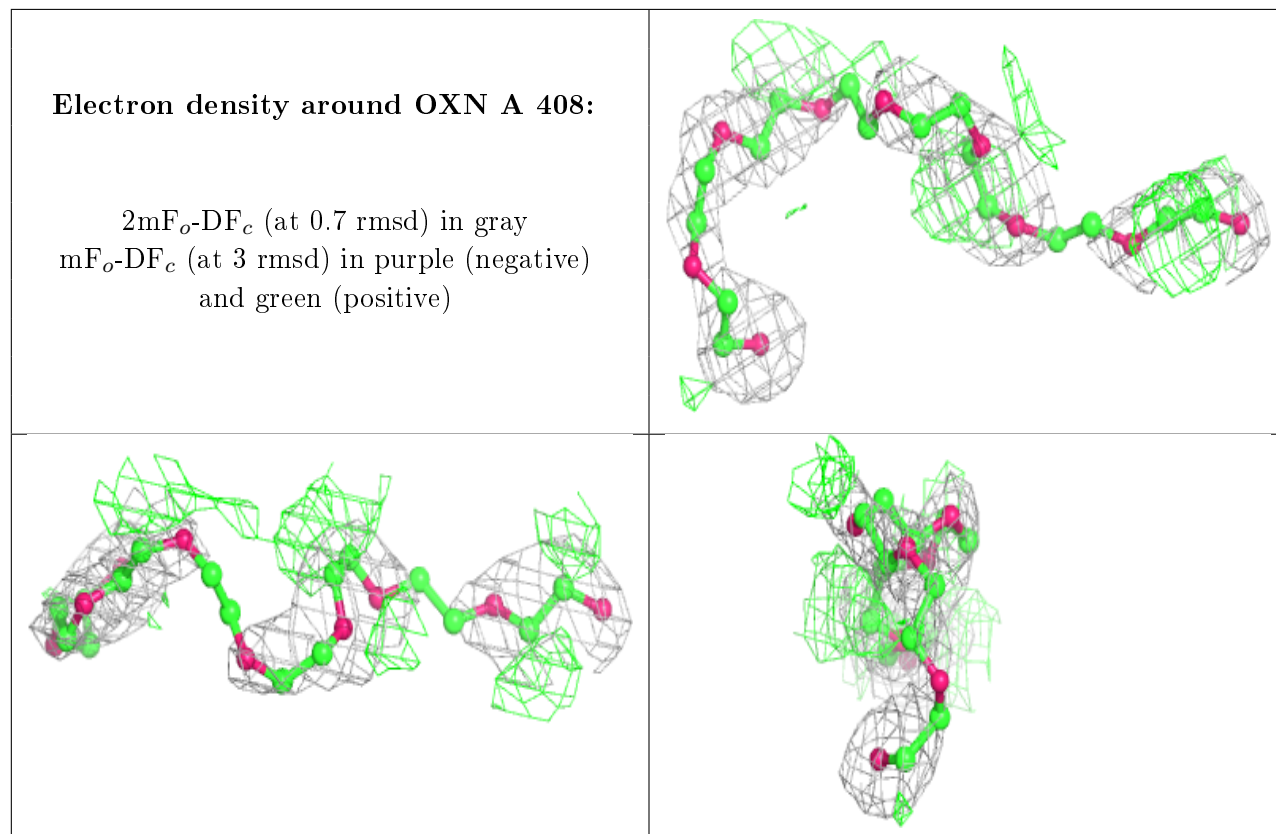
6.4 Ligands [i](#)

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
6	OXN	A	408	25/45	0.64	0.24	94,133,153,158	0
6	OXN	A	407	15/45	0.77	0.40	78,145,171,171	0
6	OXN	A	406	15/45	0.84	0.25	70,133,170,171	0
5	NAG	A	403	14/15	0.85	0.19	112,134,153,153	0
6	OXN	B	410	15/45	0.89	0.20	75,99,117,119	0
7	SO4	B	408	5/5	0.90	0.09	159,161,165,170	0
7	SO4	B	409	5/5	0.96	0.19	51,86,109,109	0

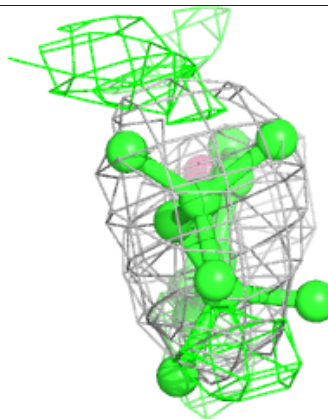
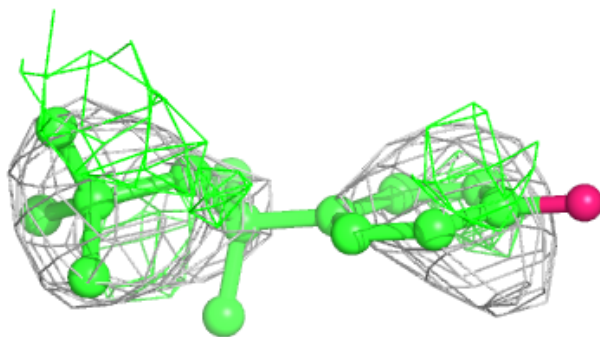
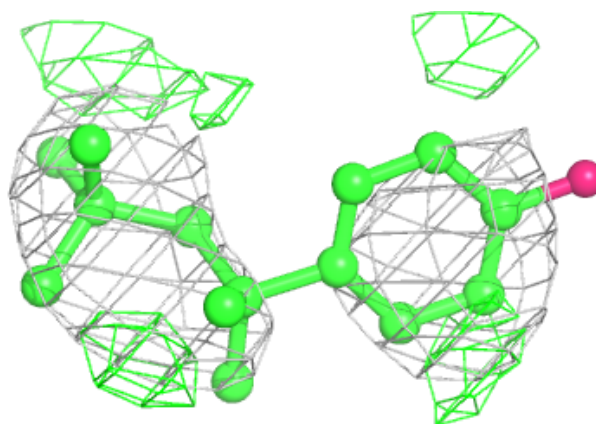
The following is a graphical depiction of the model fit to experimental electron density of all

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.

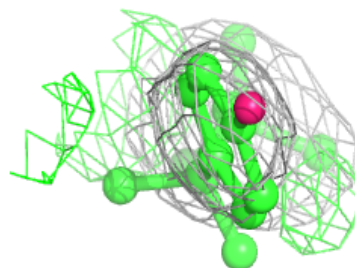
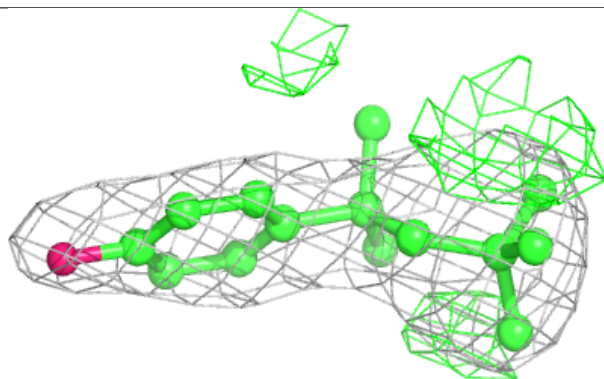
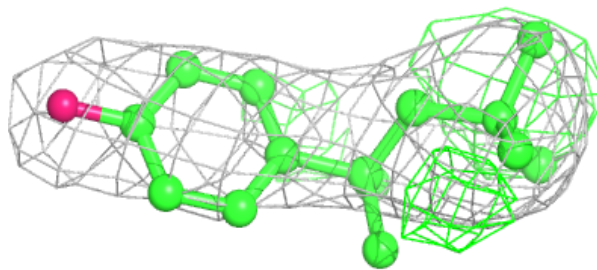


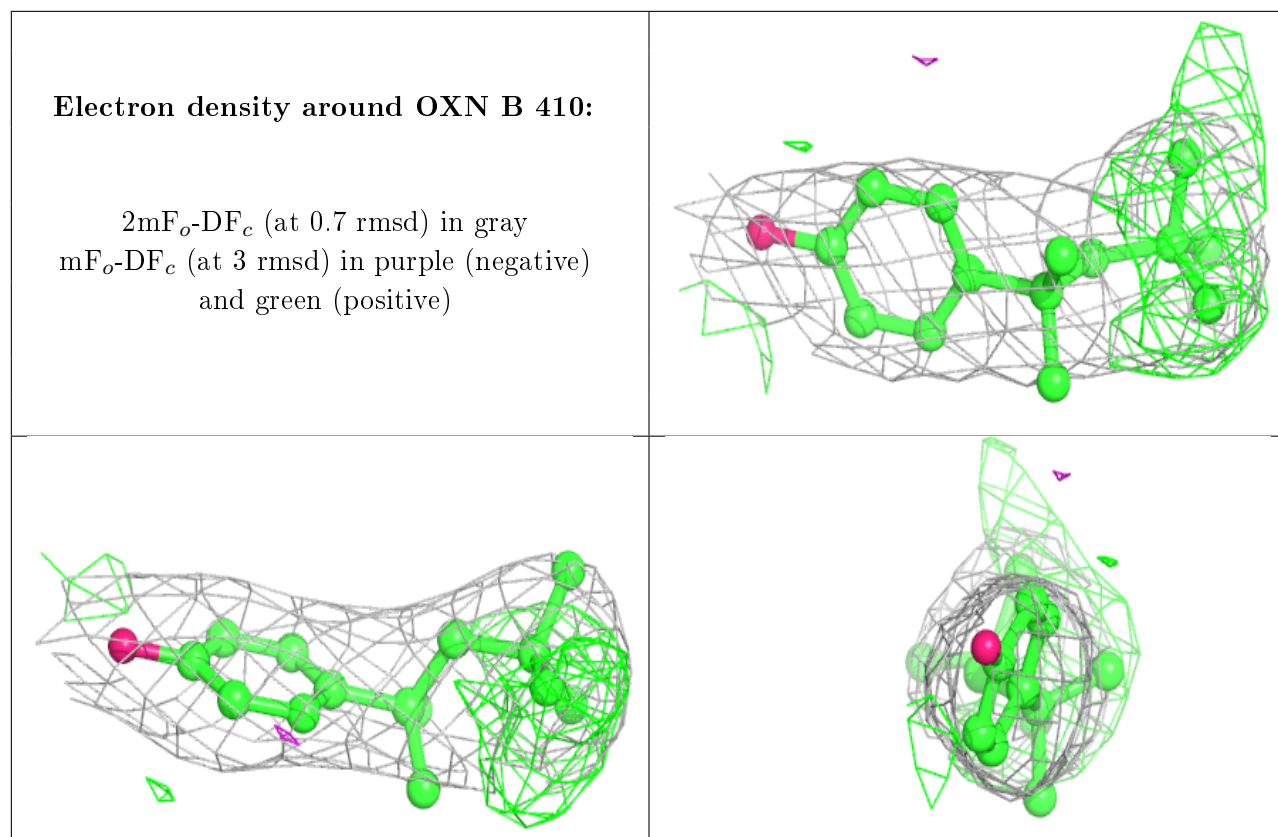
Electron density around OXN A 407:

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

**Electron density around OXN A 406:**

$2mF_o-DF_c$ (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.