



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 08:39 AM BST

PDB ID : 1W1X
Title : Structure of Neuraminidase from English duck subtype N6 complexed with 30 mM sialic acid (NANA, Neu5Ac), crystal soaked for 3 hours at 277 K.
Authors : Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.
Deposited on : 2004-06-24
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

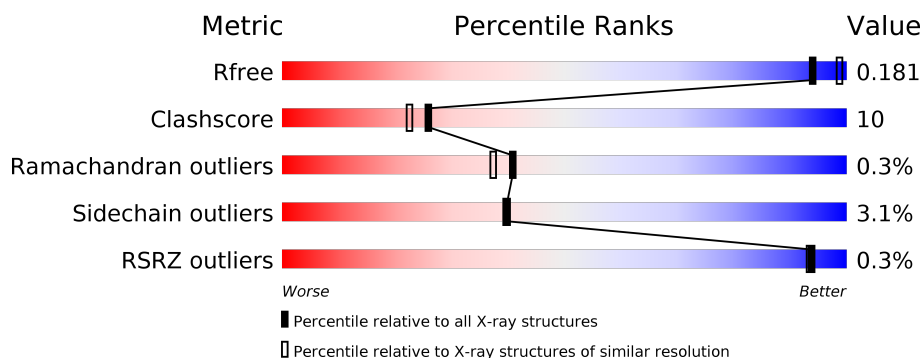
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.





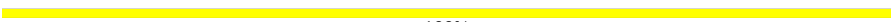
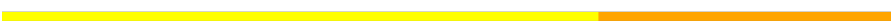
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	389	 84% 14% •
1	B	389	 81% 17% •
1	C	389	 81% 17% •
1	D	389	 83% 14% •
2	E	3	 100%
3	F	2	 100%

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Mol	Chain	Length	Quality of chain
3	J	2	 100%
4	G	3	 33% 67%
5	H	2	 100%
6	I	3	 67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	GOL	C	3488	-	X	-	-
11	GOL	D	4483	-	X	-	-
12	PEG	C	3476	-	-	X	-
3	NAG	F	1	-	-	X	-
3	NAG	J	1	-	-	X	-
4	NAG	G	2	-	-	X	-
6	BMA	I	2	-	-	X	-
6	MAN	I	3	-	-	X	-
7	SIA	A	1478	-	-	-	X
7	SIA	C	3478	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 14123 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	B	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	C	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			33	18	15			

- 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
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



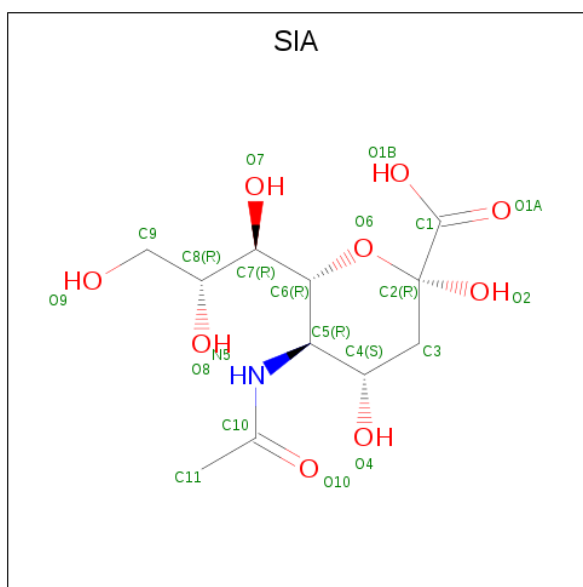
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	2	Total	C	O	0	0	0
			22	12	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 7 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).

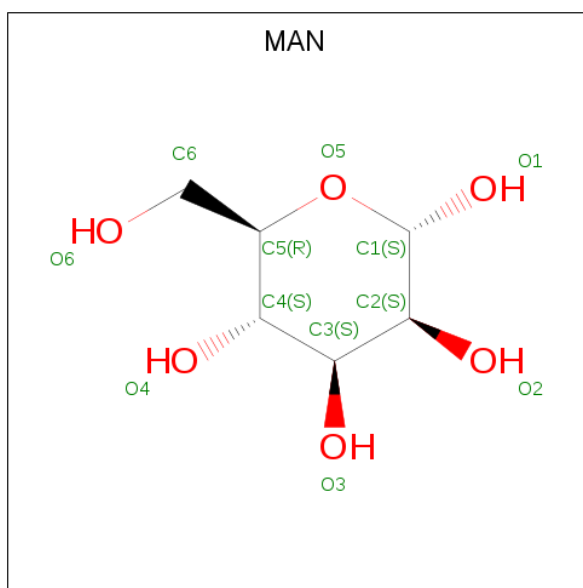


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			21	11	1	9		
7	A	1	Total	C	N	O	0	0
			21	11	1	9		
7	B	1	Total	C	N	O	0	0
			21	11	1	9		
7	B	1	Total	C	N	O	0	0
			21	11	1	9		
7	C	1	Total	C	N	O	0	0
			21	11	1	9		
7	C	1	Total	C	N	O	0	0
			21	11	1	9		
7	D	1	Total	C	N	O	0	0
			21	11	1	9		
7	D	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

- Molecule 9 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



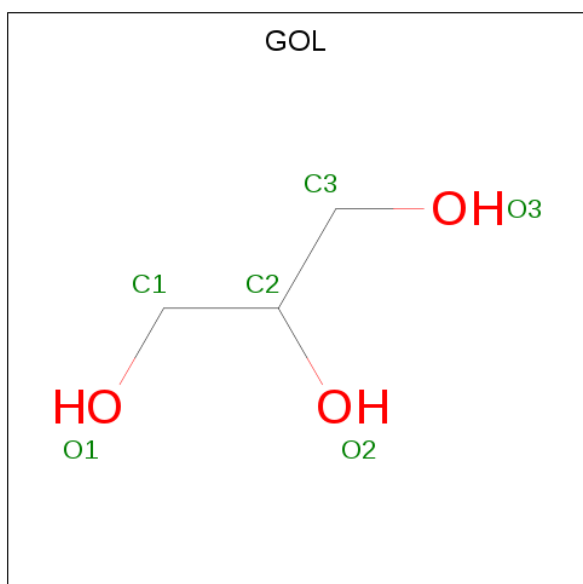
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	6	5		
9	B	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



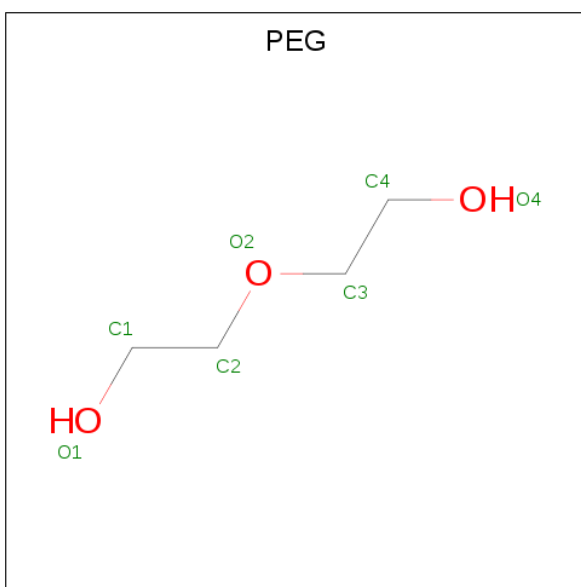
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



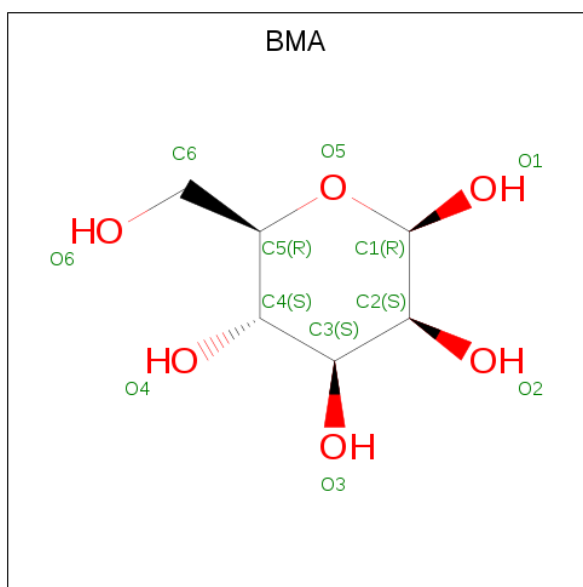
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		
11	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	C	O	0	0
			11	6	5		

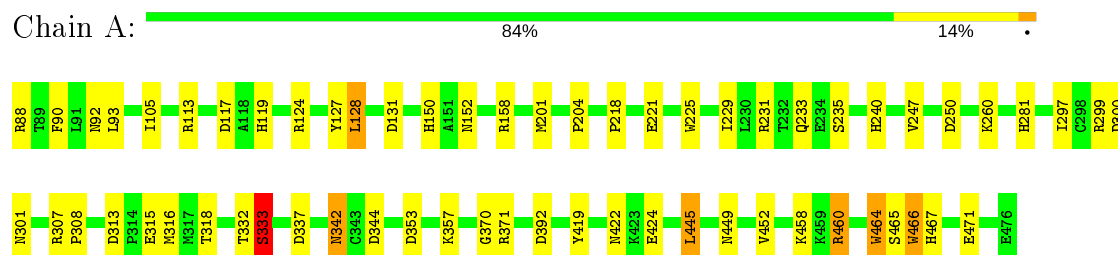
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	397	Total	O	0	0
			397	397		
14	B	385	Total	O	0	0
			385	385		
14	C	375	Total	O	0	0
			375	375		
14	D	408	Total	O	0	0
			408	408		

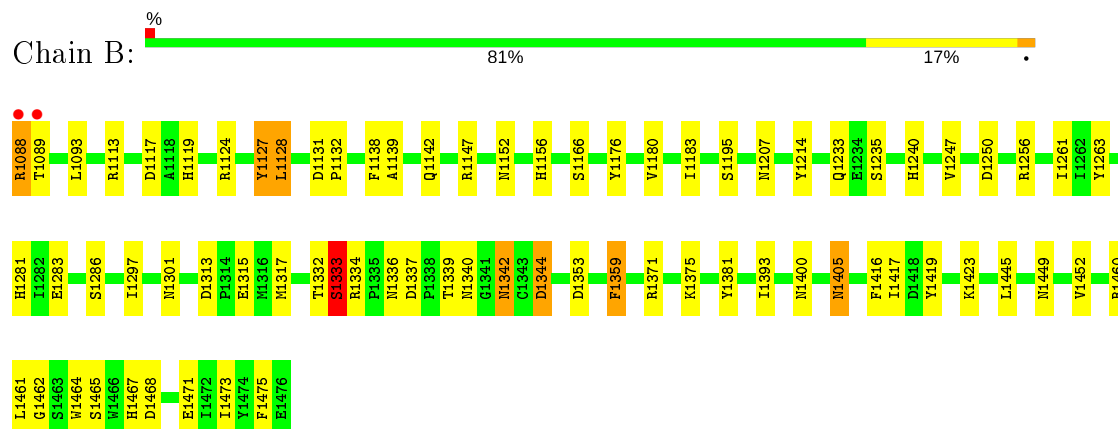
3 Residue-property plots

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.

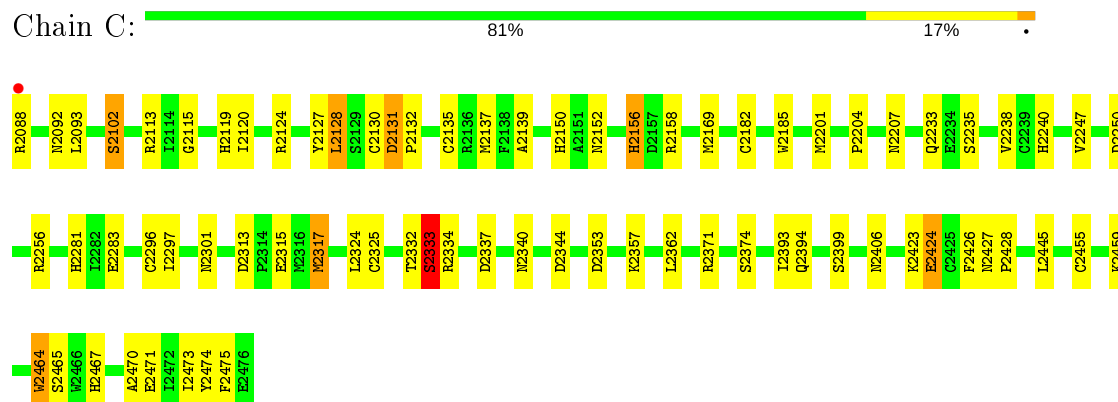
- Molecule 1: NEURAMINIDASE



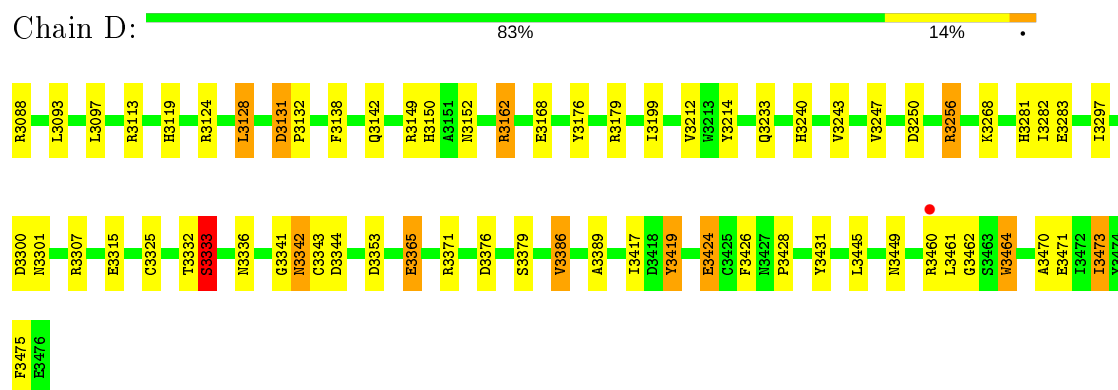
- Molecule 1: NEURAMINIDASE



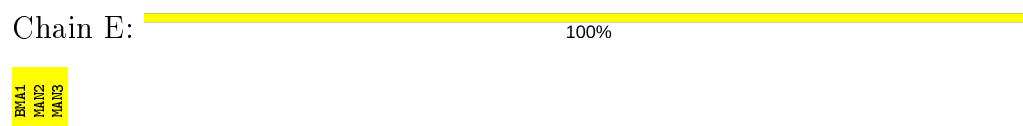
- Molecule 1: NEURAMINIDASE



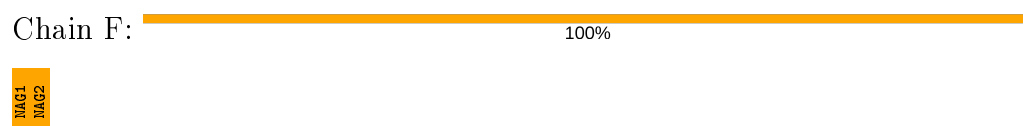
- Molecule 1: NEURAMINIDASE



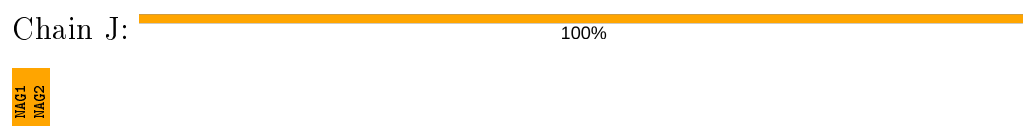
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose



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



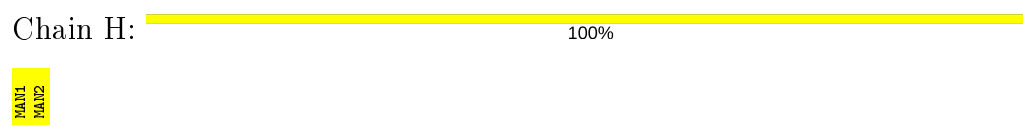
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose



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

Chain I:  67% 33%

MAG1
BGL2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.99Å 73.46Å 107.41Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	33.71 – 2.00 33.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.71-2.00) 99.3 (33.78-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.164 , 0.207 0.174 , 0.181	Depositor DCC
R_{free} test set	5604 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	1.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for l,k,-h 0.019 for h,-k,-l 0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14123	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CA, SIA, PEG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.30	7/3083 (0.2%)	1.04	14/4185 (0.3%)
1	B	1.31	10/3083 (0.3%)	1.01	14/4185 (0.3%)
1	C	1.28	7/3083 (0.2%)	1.01	8/4185 (0.2%)
1	D	1.28	10/3084 (0.3%)	1.03	15/4185 (0.4%)
All	All	1.29	34/12333 (0.3%)	1.02	51/16740 (0.3%)

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3475	PHE	CD1-CE1	7.32	1.53	1.39
1	C	2474	TYR	CE1-CZ	6.49	1.47	1.38
1	D	3268	LYS	CE-NZ	6.49	1.65	1.49
1	D	3176	TYR	CD2-CE2	6.48	1.49	1.39
1	B	1475	PHE	CD2-CE2	6.31	1.51	1.39

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3250	ASP	CB-CG-OD2	8.72	126.15	118.30
1	B	1117	ASP	CB-CG-OD2	7.89	125.40	118.30
1	C	2313	ASP	CB-CG-OD2	7.86	125.38	118.30
1	B	1337	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	231	ARG	NE-CZ-NH2	-7.68	116.46	120.30

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	3008	0	2888	47	0
1	B	3008	0	2888	50	0
1	C	3008	0	2888	65	0
1	D	3009	0	2887	46	0
2	E	33	0	30	8	0
3	F	28	0	25	11	0
3	J	28	0	26	9	0
4	G	39	0	36	11	0
5	H	22	0	20	5	0
6	I	36	0	33	13	0
7	A	42	0	36	4	0
7	B	42	0	36	2	0
7	C	42	0	36	5	0
7	D	42	0	36	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	11	0	10	2	0
9	B	11	0	10	2	0
9	C	33	0	30	9	0
10	A	28	0	26	4	0
10	B	14	0	13	2	0
10	C	14	0	13	2	0
10	D	14	0	13	1	0
11	A	6	0	8	2	0
11	B	6	0	8	2	0
11	C	6	0	8	1	0
11	D	6	0	8	2	0
12	C	7	0	10	8	0
13	D	11	0	10	2	0
14	A	397	0	0	2	0
14	B	385	0	0	4	0
14	C	375	0	0	7	0
14	D	408	0	0	10	0
All	All	14123	0	12032	243	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.

The worst 5 of 243 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:92:ASN:HD21	10:A:1484:NAG:C1	1.01	1.62
1:A:152:ASN:HD21	10:A:1485:NAG:C1	1.01	1.62
1:D:3152:ASN:HD21	10:D:4482:NAG:C1	1.08	1.54
1:B:1152:ASN:HD21	10:B:2484:NAG:C1	1.24	1.49
1:C:2152:ASN:HD21	10:C:3486:NAG:C1	1.27	1.46

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	387/389 (100%)	370 (96%)	16 (4%)	1 (0%)	41	37
1	B	387/389 (100%)	367 (95%)	19 (5%)	1 (0%)	41	37
1	C	387/389 (100%)	368 (95%)	18 (5%)	1 (0%)	41	37
1	D	387/389 (100%)	371 (96%)	15 (4%)	1 (0%)	41	37
All	All	1548/1556 (100%)	1476 (95%)	68 (4%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2333	SER
1	A	333	SER
1	B	1333	SER
1	D	3333	SER

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	331/331 (100%)	322 (97%)	9 (3%)	44	46
1	B	331/331 (100%)	320 (97%)	11 (3%)	38	37
1	C	331/331 (100%)	320 (97%)	11 (3%)	38	37
1	D	331/331 (100%)	321 (97%)	10 (3%)	41	41
All	All	1324/1324 (100%)	1283 (97%)	41 (3%)	40	40

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1405	ASN
1	C	2156	HIS
1	D	3424	GLU
1	B	1464	TRP
1	C	2102	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1400	ASN
1	B	1467	HIS
1	D	3340	ASN
1	B	1405	ASN
1	B	1408	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 ⓘ

15 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	BMA	E	1	2	11,11,12	0.26	0	15,15,17	0.64	0
2	MAN	E	2	2	11,11,12	0.26	0	15,15,17	0.65	0
2	MAN	E	3	2	11,11,12	0.27	0	15,15,17	0.63	0
3	NAG	F	1	3	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
4	NAG	G	1	1,4	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
4	BMA	G	3	4	11,11,12	0.27	0	15,15,17	0.64	0
5	MAN	H	1	5	11,11,12	0.25	0	15,15,17	0.64	0
5	MAN	H	2	5	11,11,12	0.26	0	15,15,17	0.64	0
6	NAG	I	1	6	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
6	BMA	I	2	6	11,11,12	0.26	0	15,15,17	0.64	0
6	MAN	I	3	6	11,11,12	0.26	0	15,15,17	0.64	0
3	NAG	J	1	1,3	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	1.01	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	BMA	E	1	2	-	2/2/19/22	0/1/1/1
2	MAN	E	2	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	C1-C2-N2	-3.23	104.97	110.49
3	J	2	NAG	C1-C2-N2	-3.22	104.99	110.49
6	I	1	NAG	C1-C2-N2	-3.21	105.01	110.49
4	G	1	NAG	C1-C2-N2	-3.21	105.01	110.49
3	F	1	NAG	C1-C2-N2	-3.21	105.01	110.49

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	MAN	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 52 short contacts:

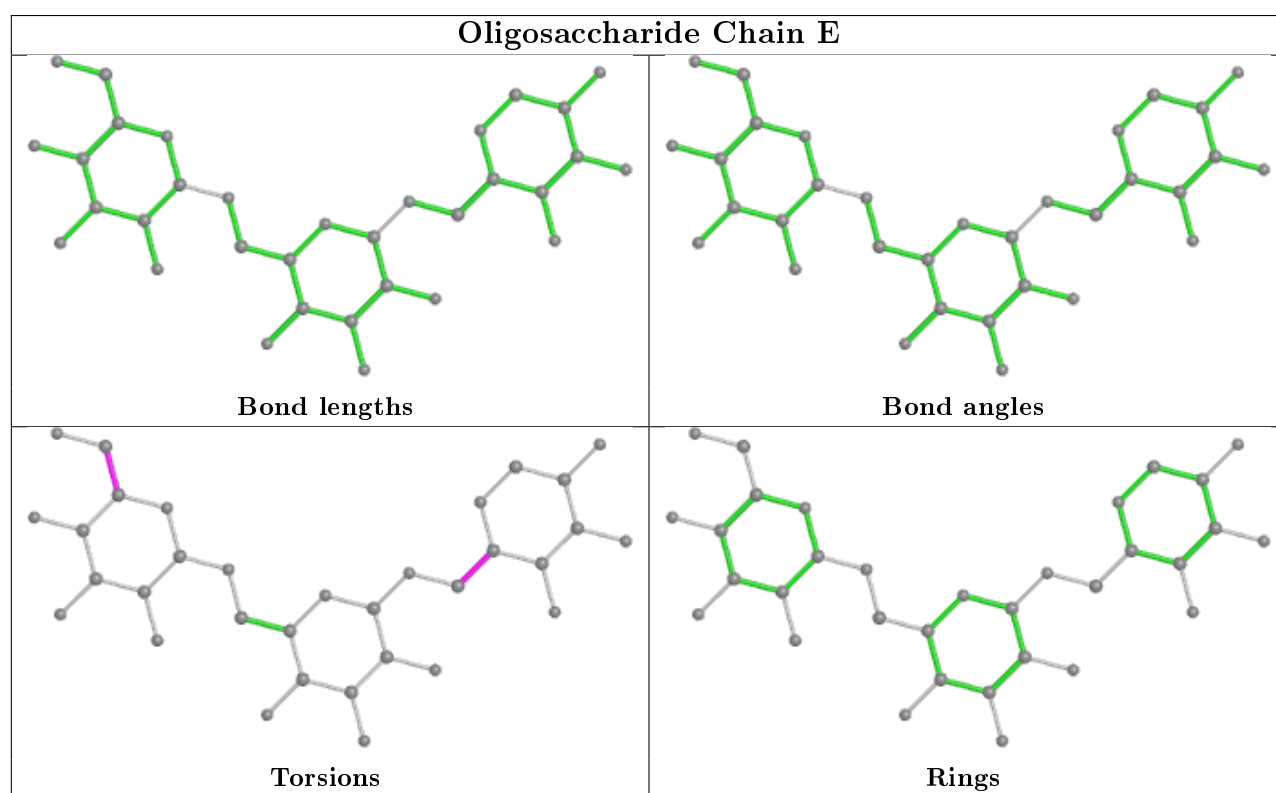
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	4	0
6	I	3	MAN	6	0
4	G	1	NAG	6	0
2	E	2	MAN	4	0
3	F	1	NAG	7	0
5	H	2	MAN	2	0
3	F	2	NAG	4	0

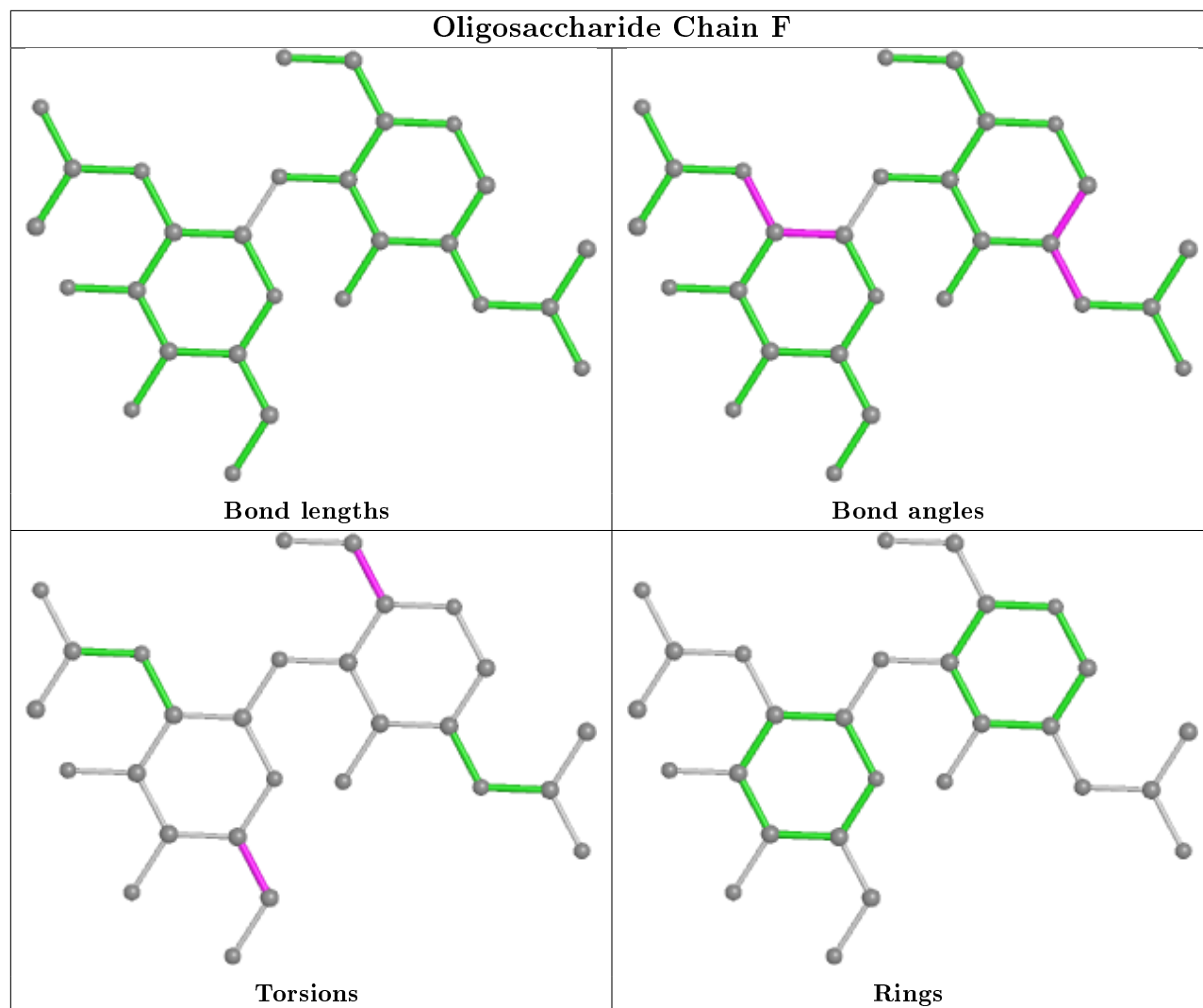
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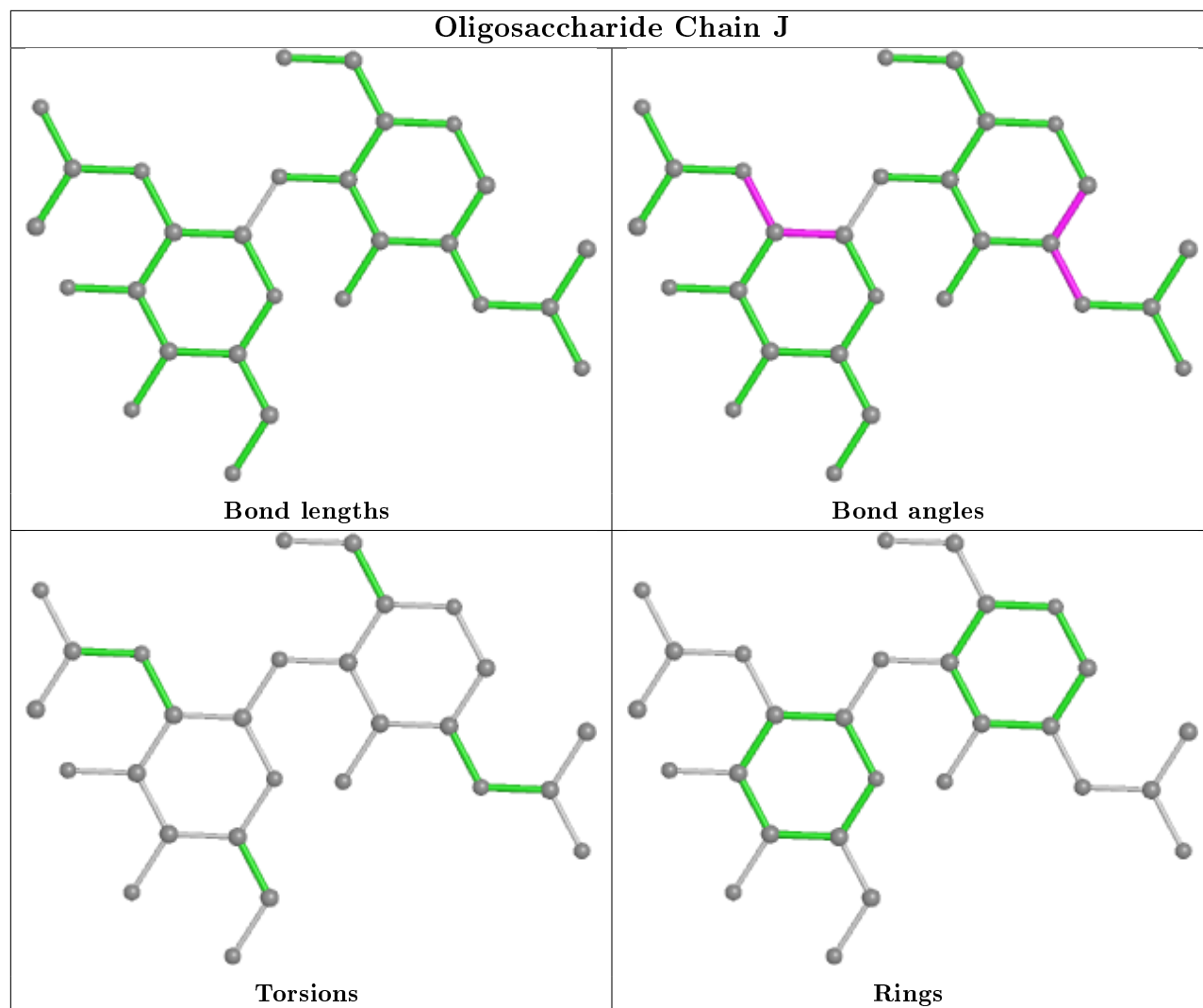
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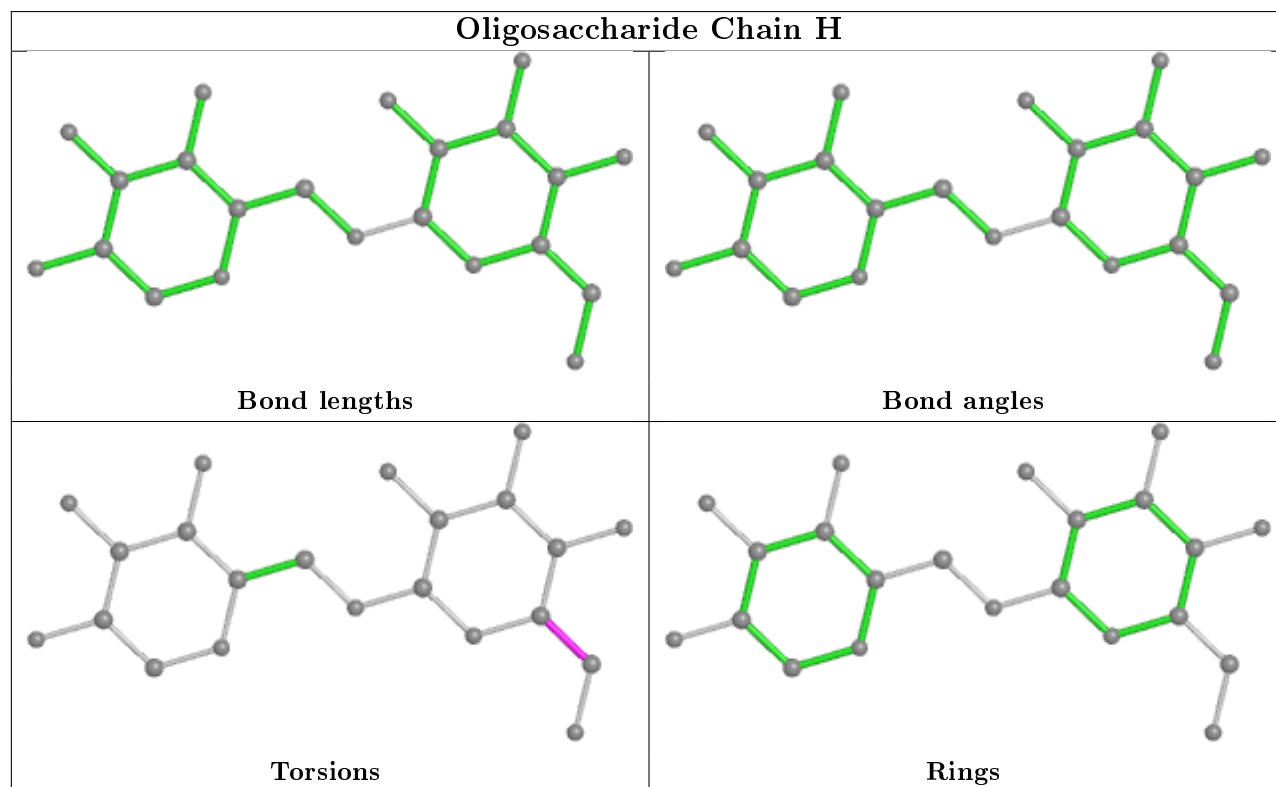
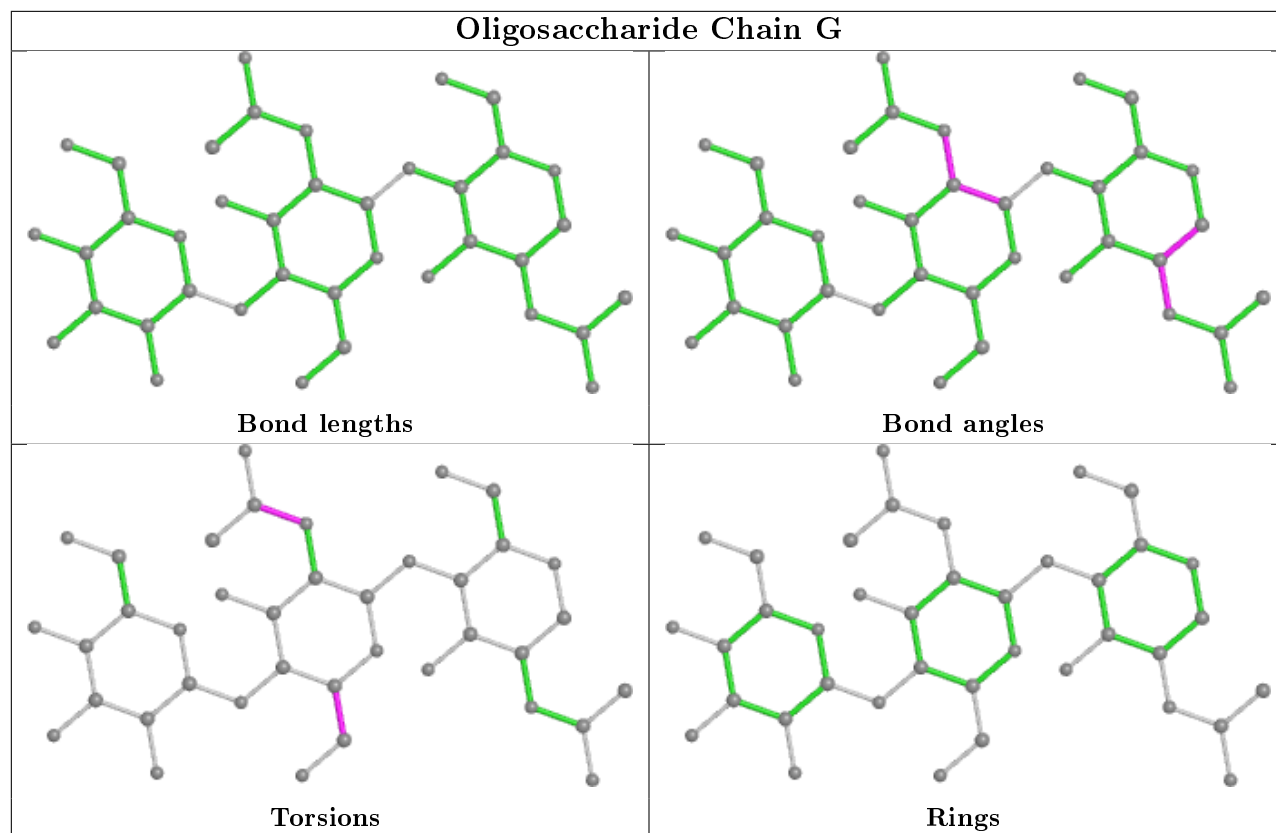
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	BMA	5	0
6	I	2	BMA	8	0
4	G	2	NAG	8	0
6	I	1	NAG	2	0
3	J	1	NAG	7	0
2	E	3	MAN	1	0
5	H	1	MAN	5	0
4	G	3	BMA	5	0

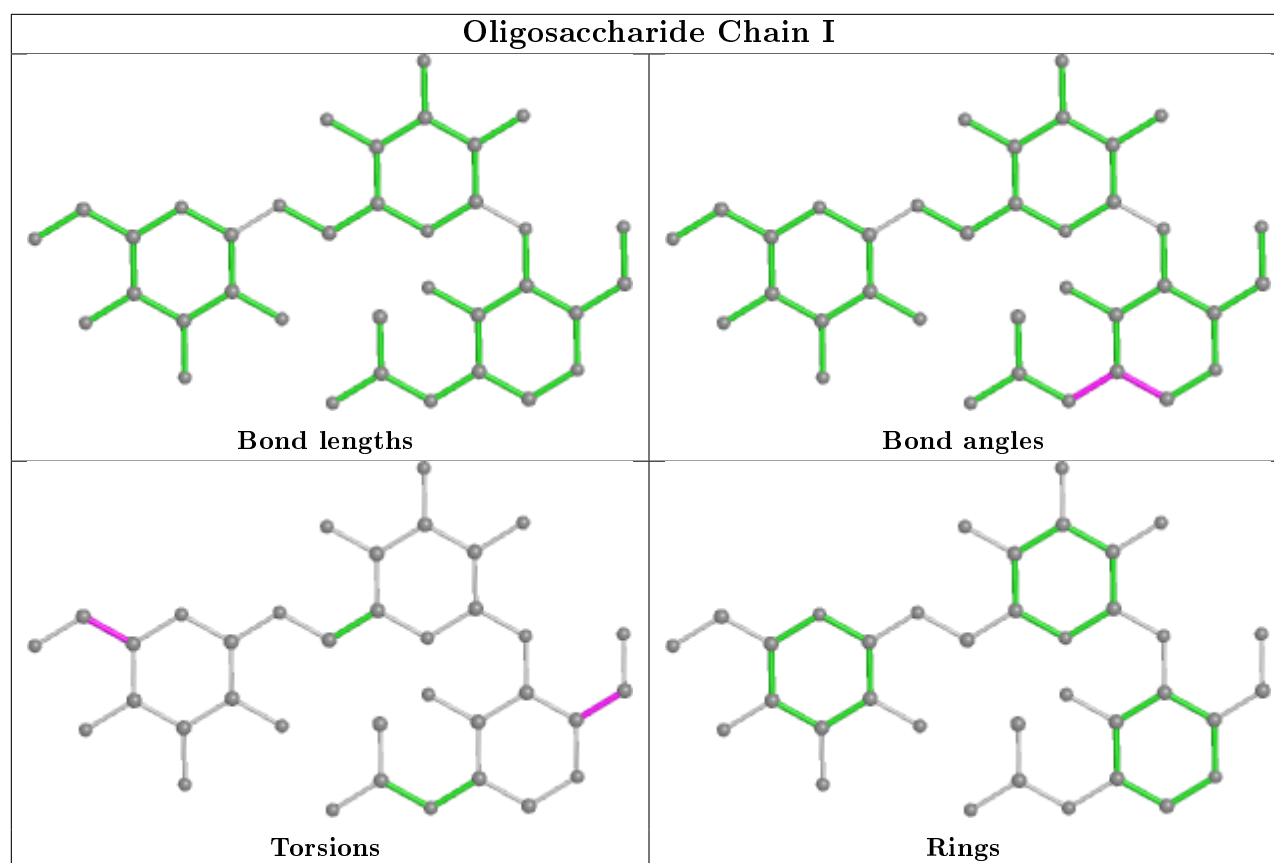
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\# Z > 2$
10	NAG	B	2484	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
12	PEG	C	3476	-	6,6,6	0.86	0	5,5,5	0.91	0
7	SIA	B	2478	-	18,21,21	0.74	1 (5%)	21,31,31	0.77	1 (4%)
7	SIA	C	3477	-	18,21,21	0.74	1 (5%)	21,31,31	0.79	1 (4%)
7	SIA	B	2477	-	18,21,21	0.74	1 (5%)	21,31,31	0.76	0
9	MAN	B	2483	-	11,11,12	0.27	0	15,15,17	0.63	0
11	GOL	B	2486	-	5,5,5	2.39	2 (40%)	5,5,5	2.44	2 (40%)
10	NAG	D	4482	1	14,14,15	0.26	0	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	A	1485	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
7	SIA	A	1477	-	18,21,21	0.75	1 (5%)	21,31,31	0.77	1 (4%)
7	SIA	A	1478	-	18,21,21	0.75	1 (5%)	21,31,31	0.77	1 (4%)
9	MAN	A	1483	-	11,11,12	0.27	0	15,15,17	0.63	0
10	NAG	C	3486	-	14,14,15	0.28	0	17,19,21	1.02	1 (5%)
9	MAN	C	3483	-	11,11,12	0.26	0	15,15,17	0.63	0
11	GOL	A	1487	-	5,5,5	1.73	2 (40%)	5,5,5	2.21	2 (40%)
7	SIA	C	3478	-	18,21,21	0.74	1 (5%)	21,31,31	0.77	1 (4%)
7	SIA	D	4477	-	18,21,21	0.75	1 (5%)	21,31,31	0.79	1 (4%)
11	GOL	D	4483	-	5,5,5	2.03	3 (60%)	5,5,5	2.39	2 (40%)
11	GOL	C	3488	-	5,5,5	1.88	3 (60%)	5,5,5	2.05	1 (20%)
9	MAN	C	3481	-	11,11,12	0.26	0	15,15,17	0.63	0
13	BMA	D	4480	-	11,11,12	0.27	0	15,15,17	0.63	0
9	MAN	C	3484	-	11,11,12	0.27	0	15,15,17	0.64	0
10	NAG	A	1484	1	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
7	SIA	D	4478	-	18,21,21	0.74	1 (5%)	21,31,31	0.77	1 (4%)

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
10	NAG	B	2484	1	-	2/6/23/26	0/1/1/1
12	PEG	C	3476	-	-	4/4/4/4	-
7	SIA	B	2478	-	-	0/14/38/38	0/1/1/1
7	SIA	C	3477	-	-	0/14/38/38	0/1/1/1
7	SIA	B	2477	-	-	4/14/38/38	0/1/1/1
9	MAN	B	2483	-	-	2/2/19/22	0/1/1/1
11	GOL	B	2486	-	-	1/4/4/4	-
10	NAG	D	4482	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1485	1	-	1/6/23/26	0/1/1/1
7	SIA	A	1477	-	-	2/14/38/38	0/1/1/1
7	SIA	A	1478	-	-	0/14/38/38	0/1/1/1
9	MAN	A	1483	-	-	1/2/19/22	0/1/1/1
10	NAG	C	3486	-	-	2/6/23/26	0/1/1/1
9	MAN	C	3483	-	-	2/2/19/22	0/1/1/1
11	GOL	A	1487	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SIA	C	3478	-	-	1/14/38/38	0/1/1/1
7	SIA	D	4477	-	-	0/14/38/38	0/1/1/1
11	GOL	D	4483	-	-	1/4/4/4	-
11	GOL	C	3488	-	-	2/4/4/4	-
9	MAN	C	3481	-	-	2/2/19/22	0/1/1/1
13	BMA	D	4480	-	-	0/2/19/22	0/1/1/1
9	MAN	C	3484	-	-	2/2/19/22	0/1/1/1
10	NAG	A	1484	1	-	0/6/23/26	0/1/1/1
7	SIA	D	4478	-	-	0/14/38/38	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	2486	GOL	O3-C3	3.56	1.57	1.42
7	A	1477	SIA	O2-C2	2.87	1.43	1.39
7	A	1478	SIA	O2-C2	2.87	1.43	1.39
11	C	3488	GOL	O3-C3	2.86	1.54	1.42
7	D	4477	SIA	O2-C2	2.85	1.43	1.39

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	2486	GOL	O3-C3-C2	4.48	131.67	110.20
11	D	4483	GOL	O3-C3-C2	4.16	130.14	110.20
11	A	1487	GOL	O3-C3-C2	4.04	129.55	110.20
11	C	3488	GOL	O3-C3-C2	3.56	127.27	110.20
10	C	3486	NAG	C1-C2-N2	-3.22	104.99	110.49

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2477	SIA	O6-C6-C7-C8
7	B	2477	SIA	O6-C6-C7-O7
7	A	1477	SIA	O6-C6-C7-O7
9	C	3481	MAN	O5-C5-C6-O6
9	C	3481	MAN	C4-C5-C6-O6

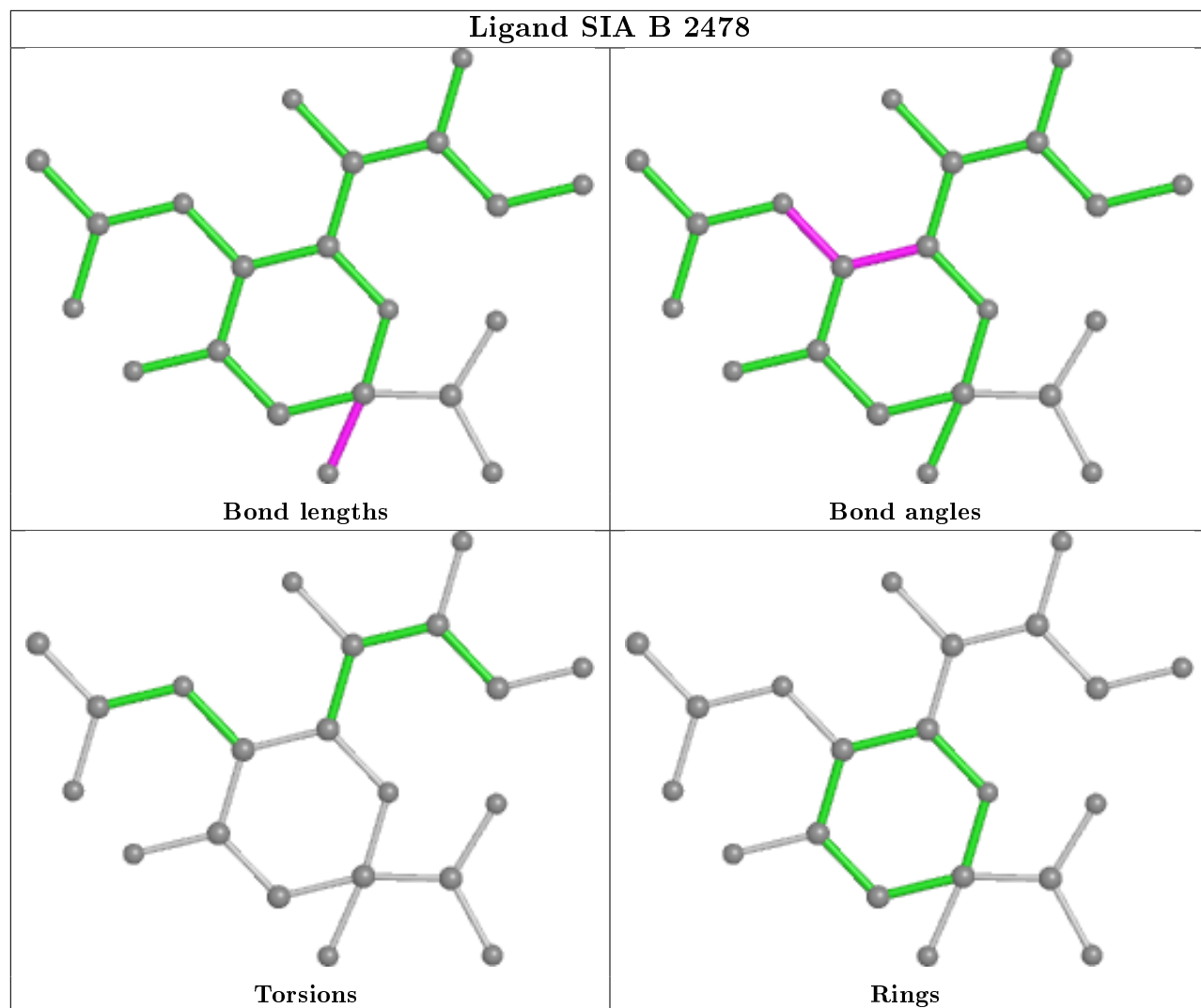
There are no ring outliers.

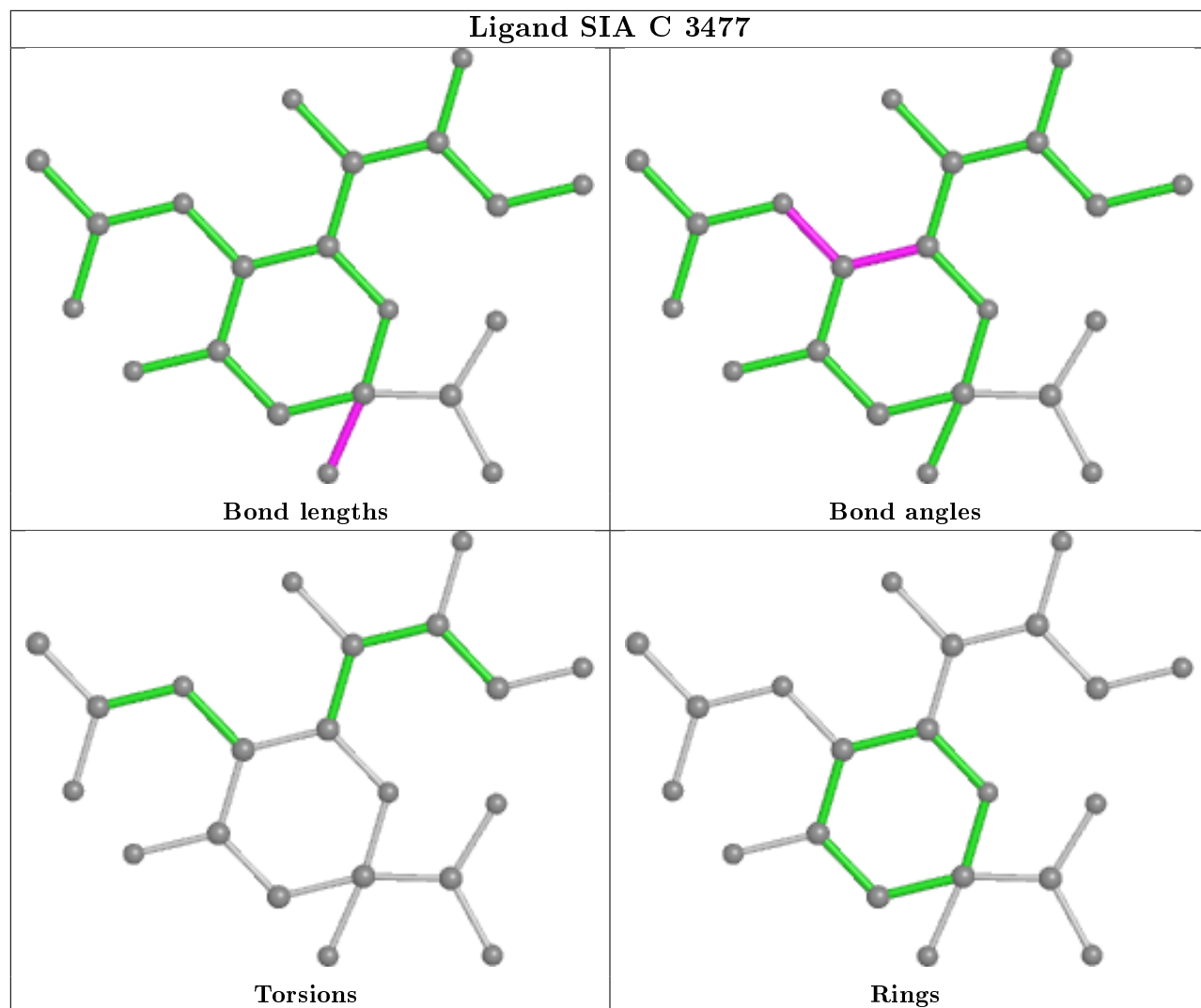
23 monomers are involved in 53 short contacts:

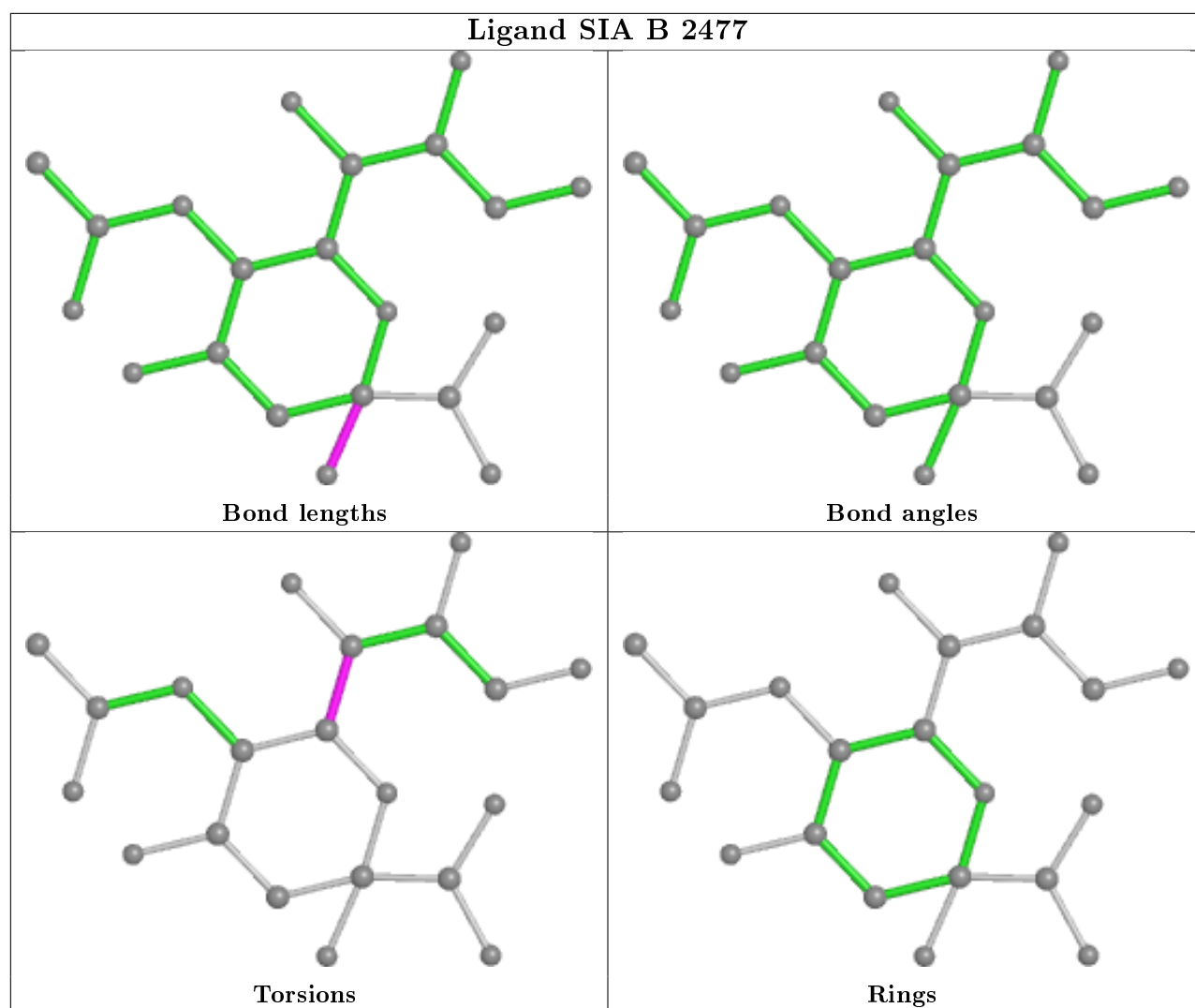
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	2484	NAG	2	0
12	C	3476	PEG	8	0
7	C	3477	SIA	2	0
7	B	2477	SIA	2	0
9	B	2483	MAN	2	0
11	B	2486	GOL	2	0
10	D	4482	NAG	1	0
10	A	1485	NAG	2	0
7	A	1477	SIA	3	0
7	A	1478	SIA	1	0
9	A	1483	MAN	2	0
10	C	3486	NAG	2	0
9	C	3483	MAN	2	0
11	A	1487	GOL	2	0
7	C	3478	SIA	3	0
7	D	4477	SIA	2	0
11	D	4483	GOL	2	0
11	C	3488	GOL	1	0
9	C	3481	MAN	4	0
13	D	4480	BMA	2	0
9	C	3484	MAN	3	0
10	A	1484	NAG	2	0
7	D	4478	SIA	1	0

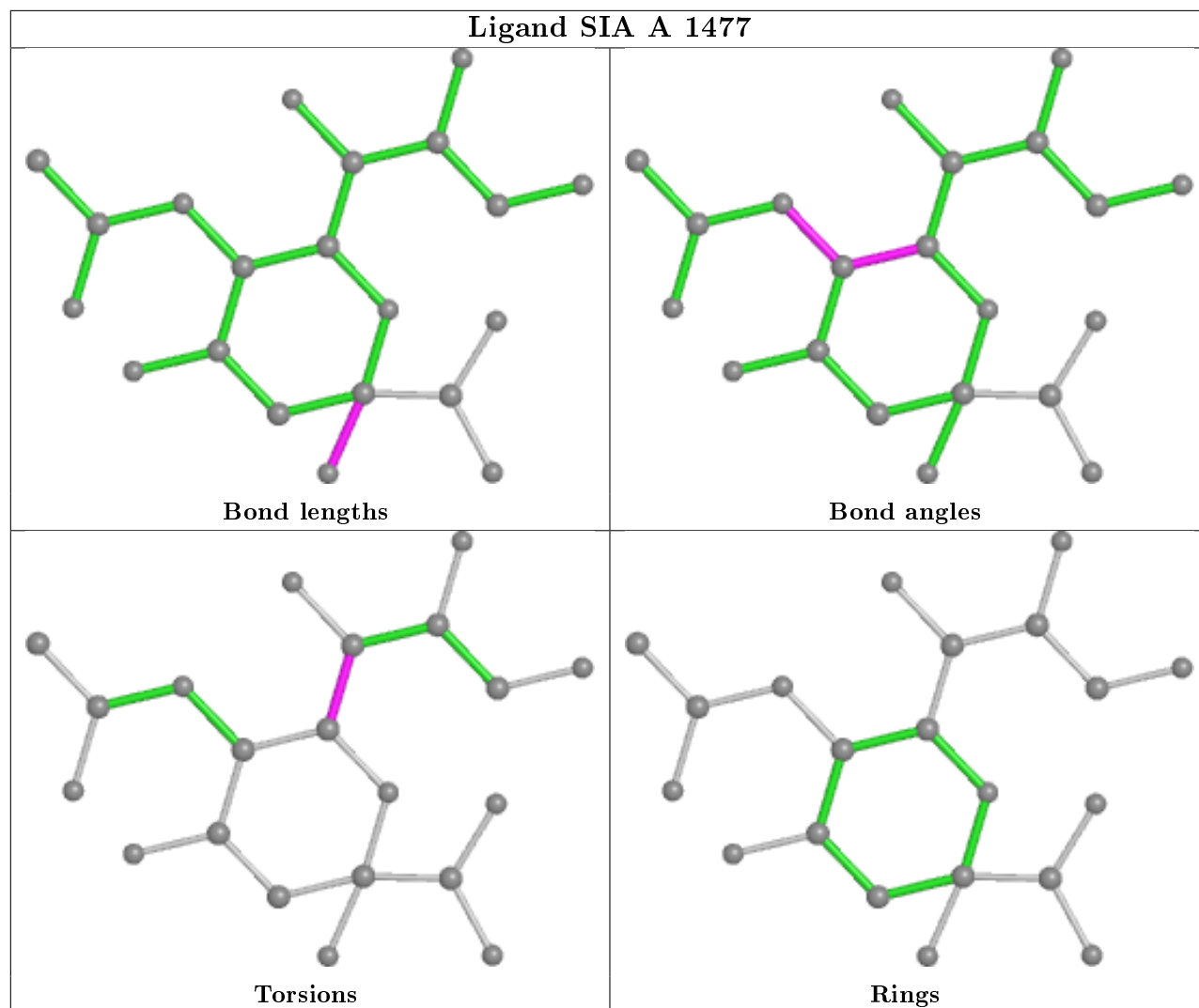
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

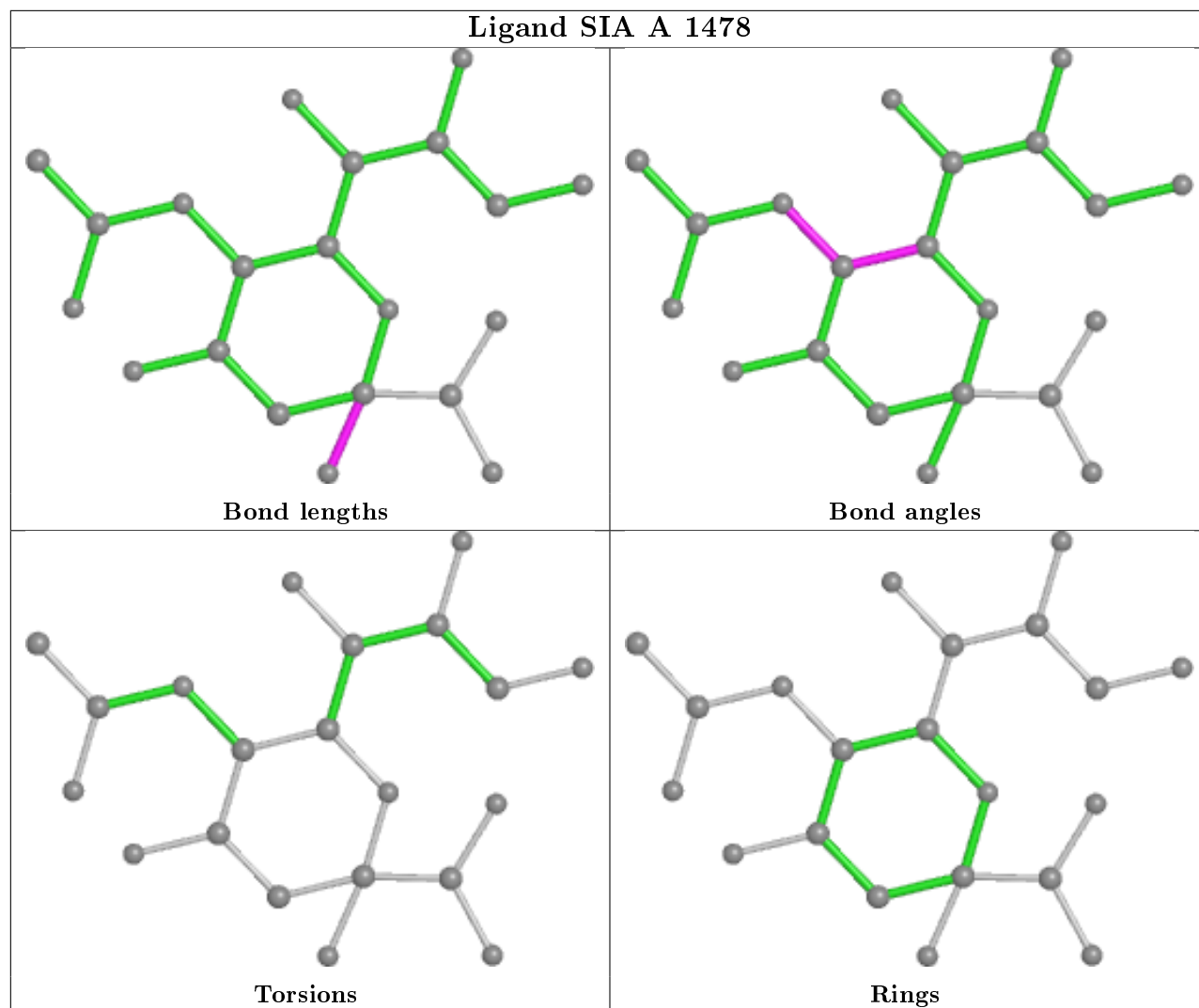
Ligand SIA B 2478

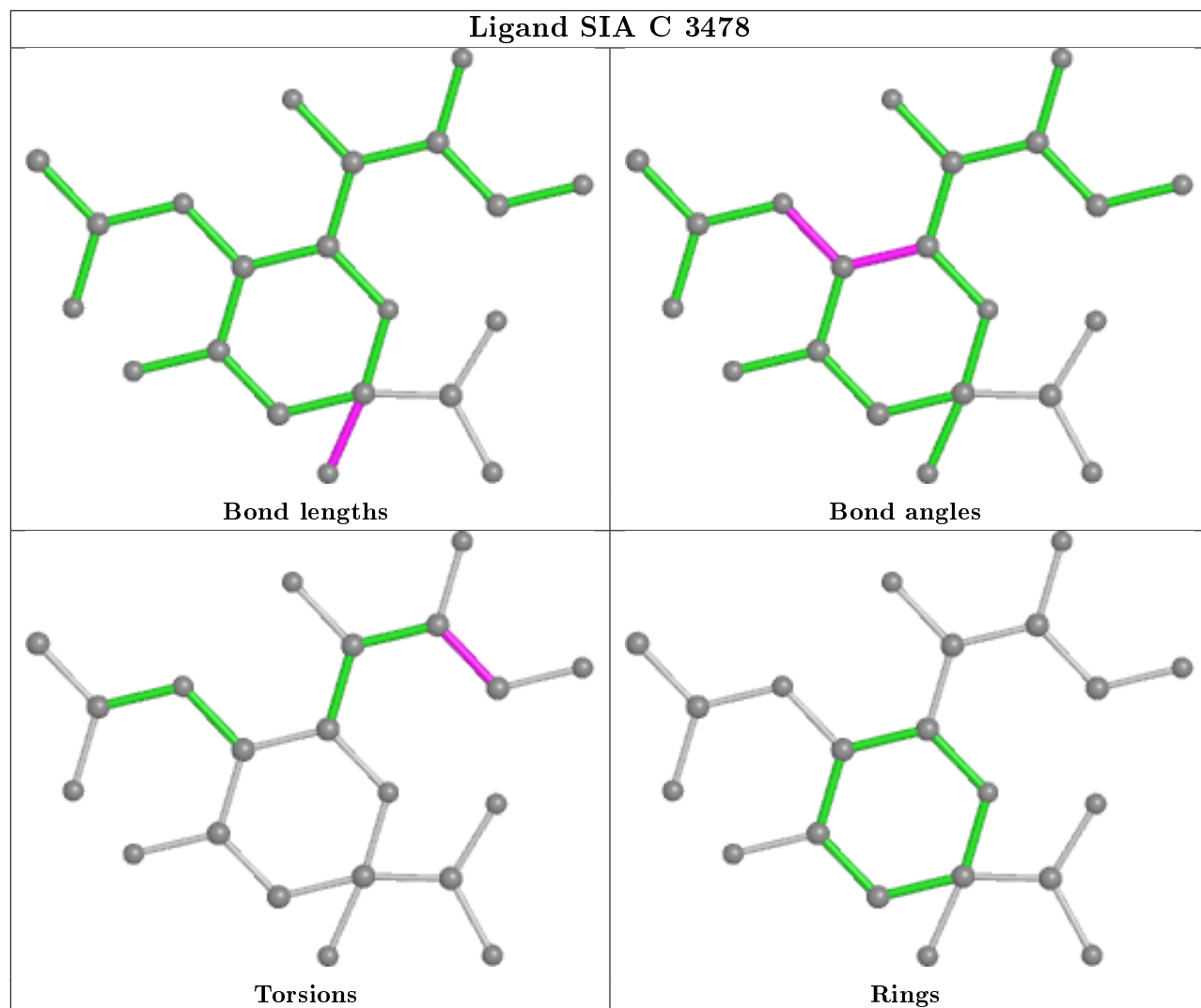


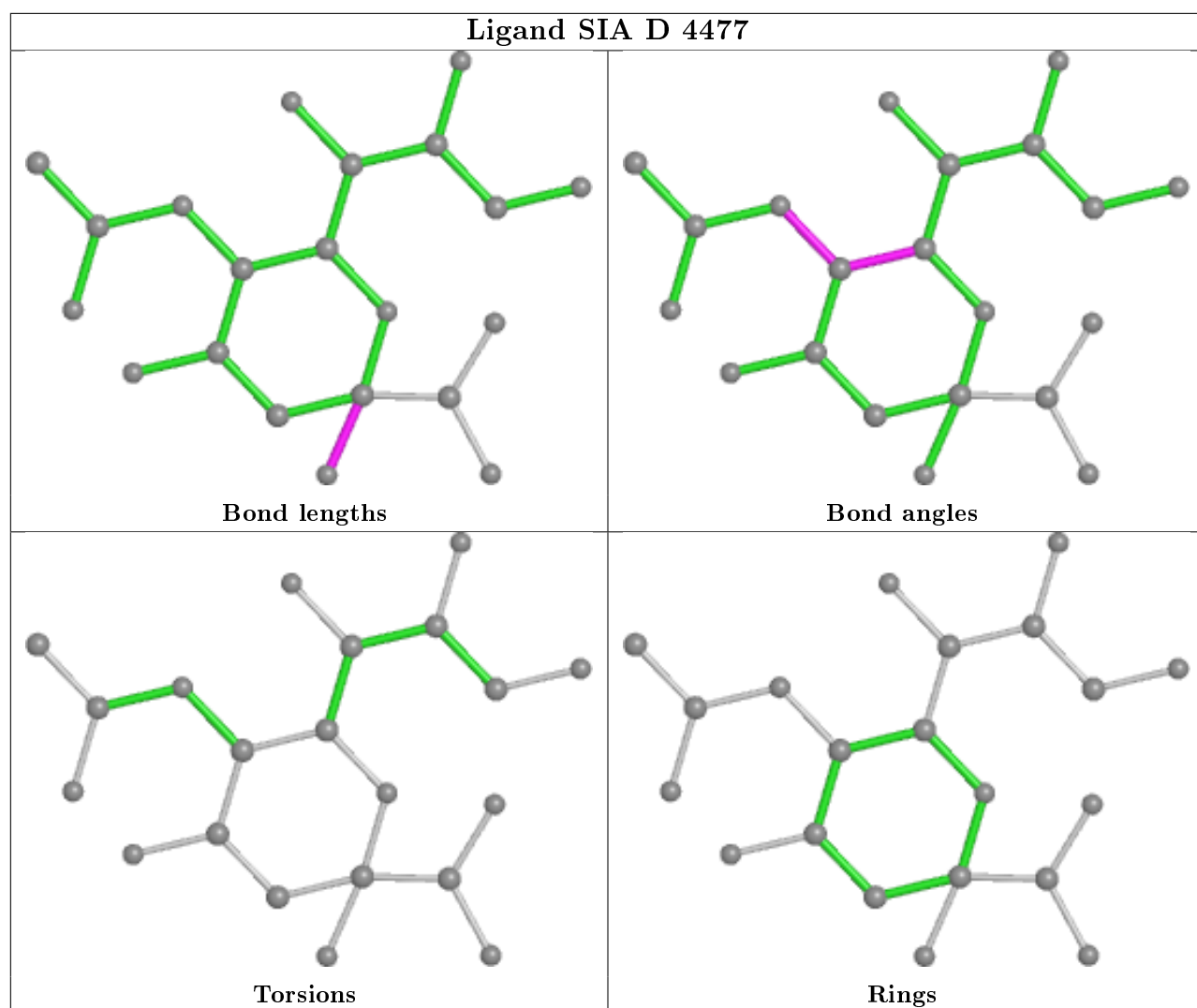


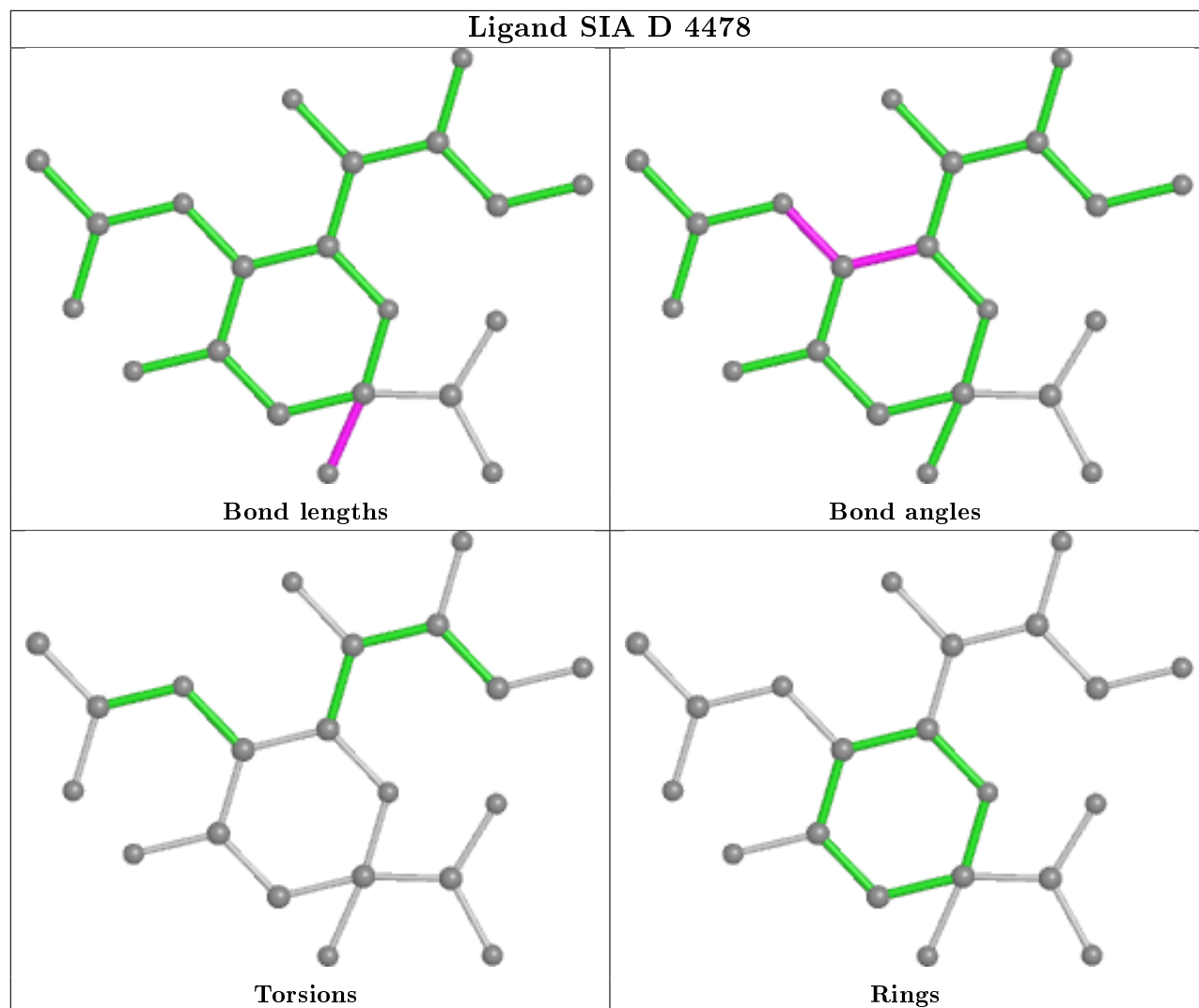












5.7 Other polymers [i](#)

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	389/389 (100%)	-0.41	0 100 100	11, 18, 26, 39	0
1	B	389/389 (100%)	-0.30	2 (0%) 91 90	12, 18, 27, 47	0
1	C	389/389 (100%)	-0.37	1 (0%) 94 93	12, 19, 28, 43	0
1	D	389/389 (100%)	-0.33	1 (0%) 94 93	11, 19, 27, 41	0
All	All	1556/1556 (100%)	-0.35	4 (0%) 94 93	11, 19, 27, 47	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1089	THR	3.1
1	B	1088	ARG	2.7
1	C	2088	ARG	2.6
1	D	3460	ARG	2.2

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

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

6.3 Carbohydrates [i](#)

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

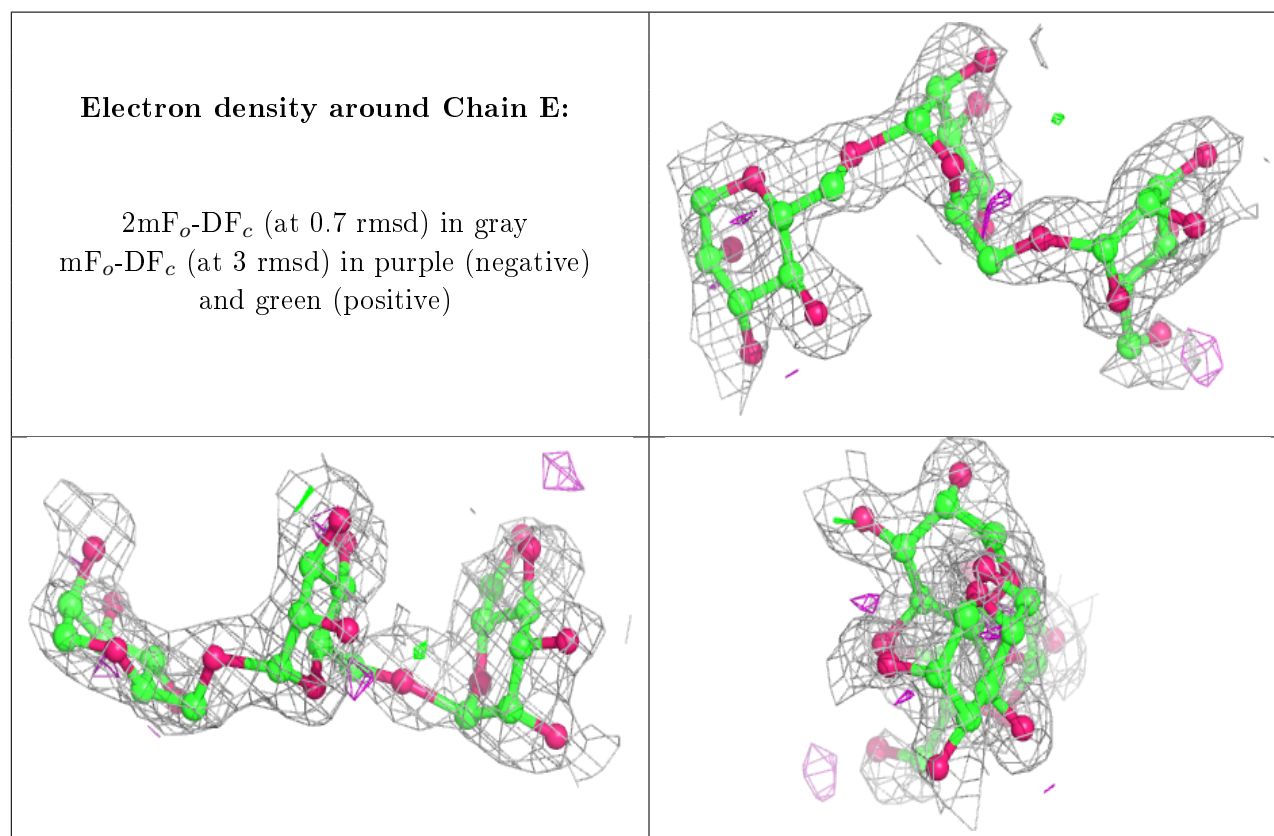
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	1	14/15	0.74	0.26	54,62,63,64	0
4	NAG	G	1	14/15	0.78	0.25	35,39,40,41	0
6	MAN	I	3	11/12	0.79	0.21	35,42,45,47	0

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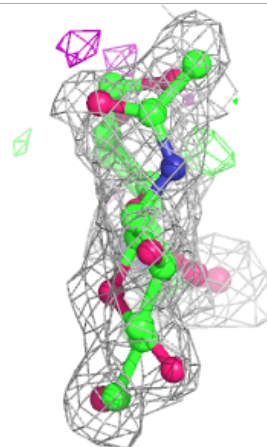
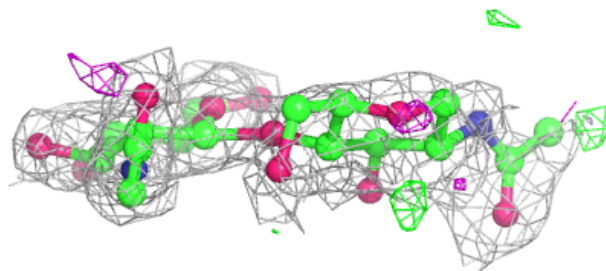
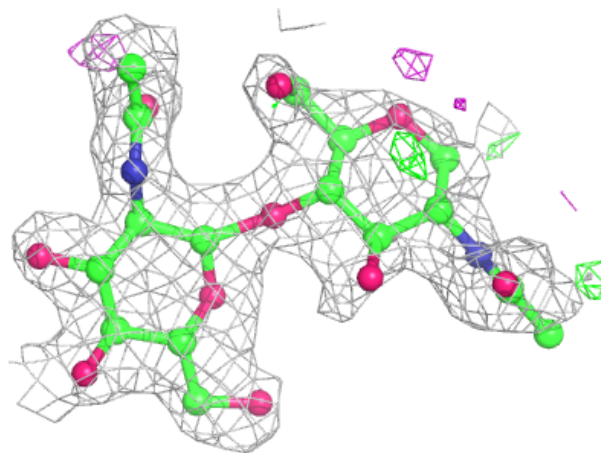
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	E	1	11/12	0.79	0.25	35,43,48,49	0
4	BMA	G	3	11/12	0.79	0.30	49,54,59,59	0
5	MAN	H	2	11/12	0.81	0.29	45,49,53,53	0
3	NAG	J	1	14/15	0.81	0.28	41,43,45,46	0
3	NAG	F	2	14/15	0.81	0.21	40,44,47,47	0
6	NAG	I	1	14/15	0.82	0.20	35,40,42,43	0
6	BMA	I	2	11/12	0.82	0.24	38,42,44,48	0
4	NAG	G	2	14/15	0.82	0.24	29,40,42,43	0
5	MAN	H	1	11/12	0.83	0.23	45,48,50,50	0
2	MAN	E	2	11/12	0.84	0.20	37,41,44,46	0
2	MAN	E	3	11/12	0.86	0.16	42,46,52,53	0
3	NAG	J	2	14/15	0.88	0.23	33,38,43,47	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.



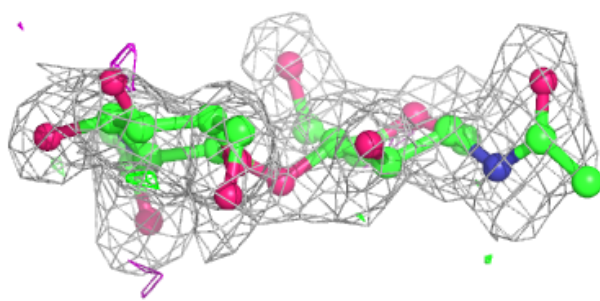
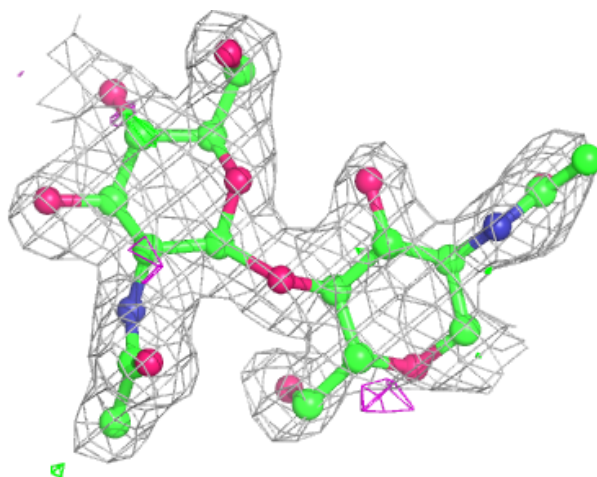
Electron density around Chain F:

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



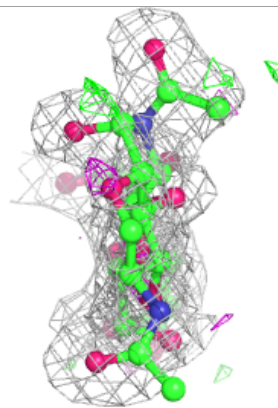
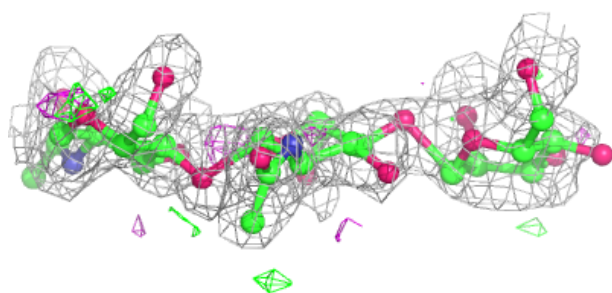
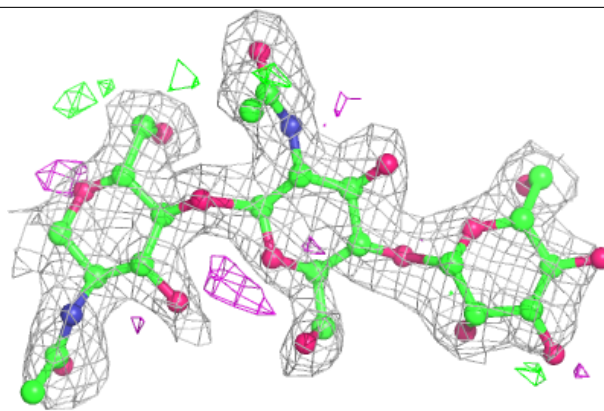
Electron density around Chain J:

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



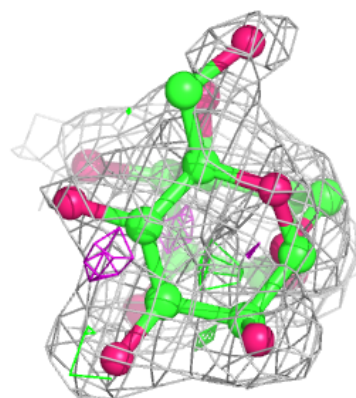
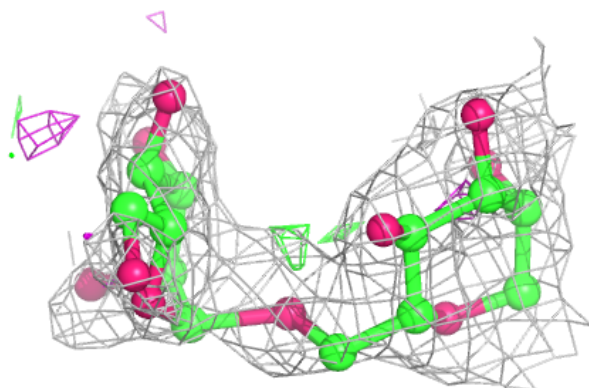
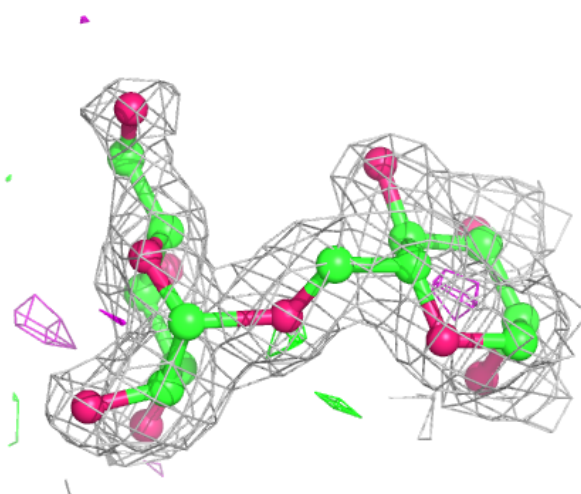
Electron density around Chain G:

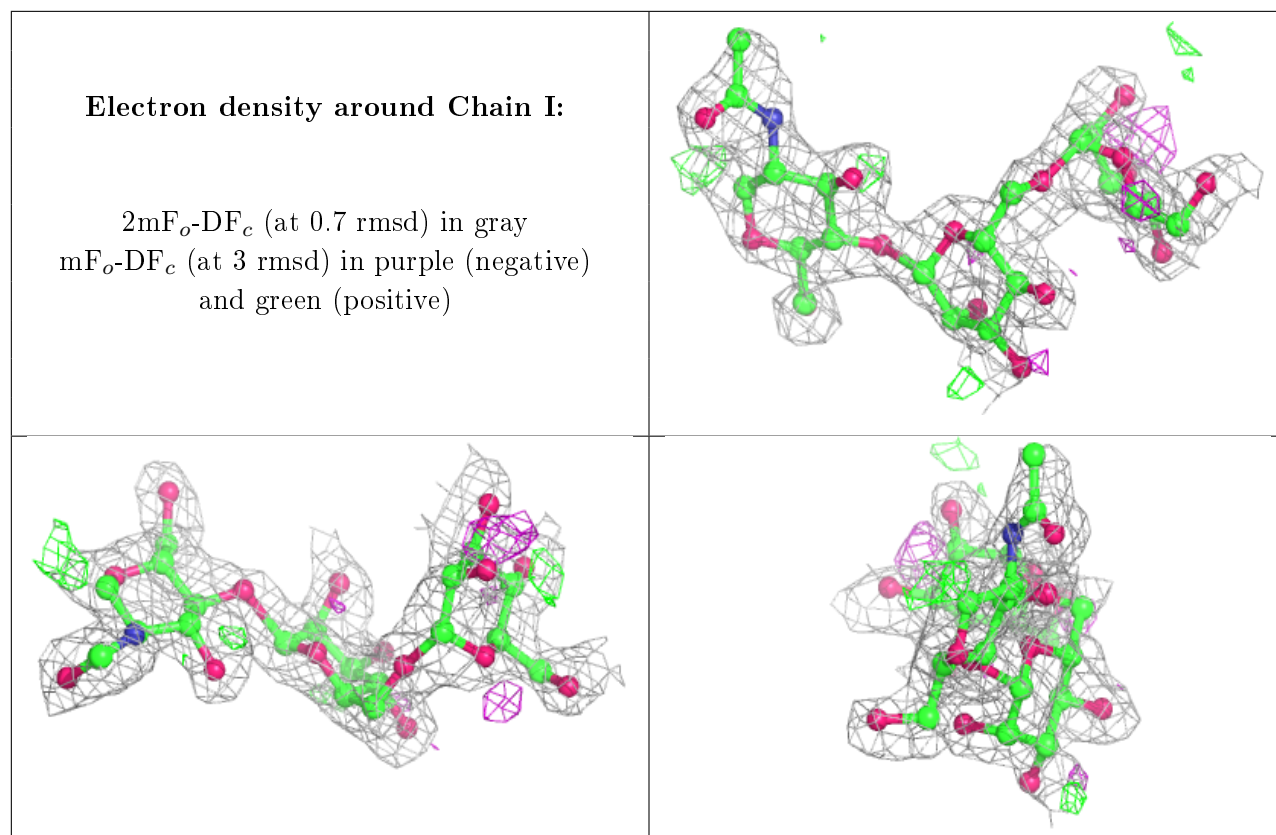
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





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(\AA^2)	Q<0.9
7	SIA	A	1478	21/21	0.59	0.54	29,36,40,45	21
7	SIA	C	3478	21/21	0.60	0.74	26,35,38,39	21
7	SIA	D	4478	21/21	0.66	0.30	30,40,43,47	21
7	SIA	B	2477	21/21	0.73	0.24	23,26,28,32	0
11	GOL	B	2486	6/6	0.74	0.21	22,30,33,33	0
13	BMA	D	4480	11/12	0.76	0.28	41,43,47,51	0
11	GOL	D	4483	6/6	0.76	0.21	22,31,33,35	0
7	SIA	B	2478	21/21	0.78	0.20	29,37,41,41	21
9	MAN	B	2483	11/12	0.80	0.26	48,51,53,54	0
11	GOL	A	1487	6/6	0.80	0.20	27,30,34,35	0
7	SIA	A	1477	21/21	0.80	0.21	23,26,29,33	0
9	MAN	C	3484	11/12	0.81	0.21	41,43,45,46	0
10	NAG	A	1484	14/15	0.82	0.19	36,42,44,45	0
9	MAN	C	3481	11/12	0.82	0.22	38,42,44,46	0

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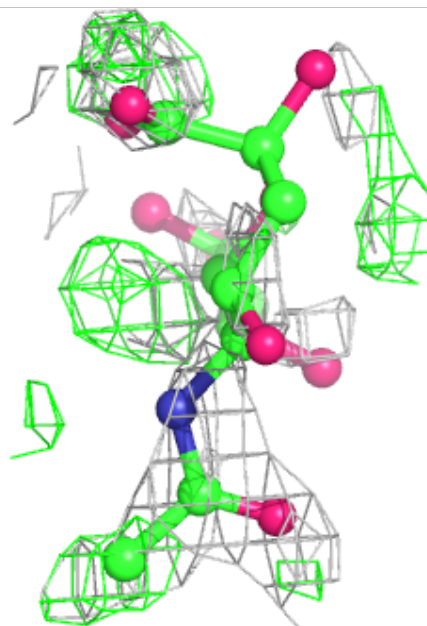
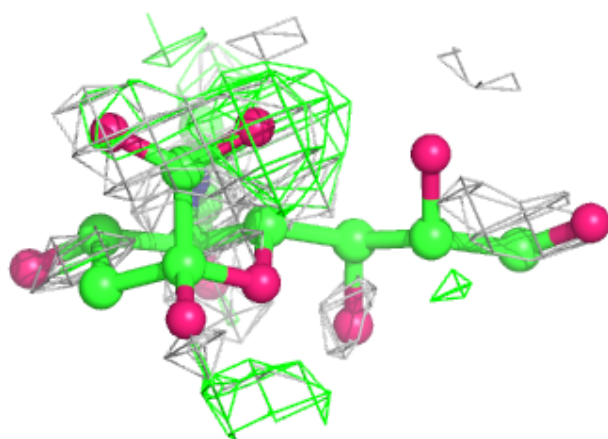
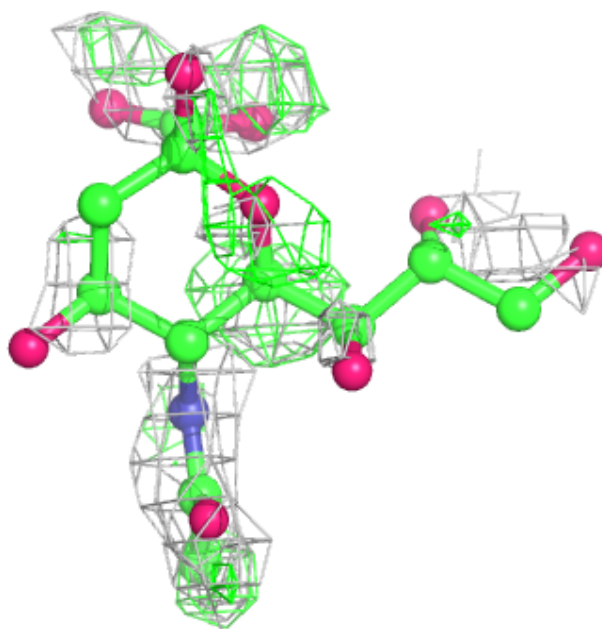
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SIA	C	3477	21/21	0.83	0.19	21,25,28,35	0
10	NAG	C	3486	14/15	0.85	0.17	27,30,34,37	0
7	SIA	D	4477	21/21	0.85	0.16	21,25,28,31	0
12	PEG	C	3476	7/7	0.86	0.21	28,38,46,49	0
11	GOL	C	3488	6/6	0.87	0.16	17,28,30,31	0
10	NAG	B	2484	14/15	0.87	0.15	21,33,39,43	0
9	MAN	A	1483	11/12	0.88	0.16	28,36,40,42	0
10	NAG	D	4482	14/15	0.89	0.16	25,33,37,38	0
10	NAG	A	1485	14/15	0.91	0.14	24,32,38,42	0
9	MAN	C	3483	11/12	0.91	0.16	41,46,48,50	0
8	CA	C	3479	1/1	0.94	0.38	16,16,16,16	0
8	CA	D	4479	1/1	0.96	0.35	11,11,11,11	0
8	CA	A	1479	1/1	0.97	0.43	6,6,6,6	0
8	CA	B	2479	1/1	0.97	0.41	14,14,14,14	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.

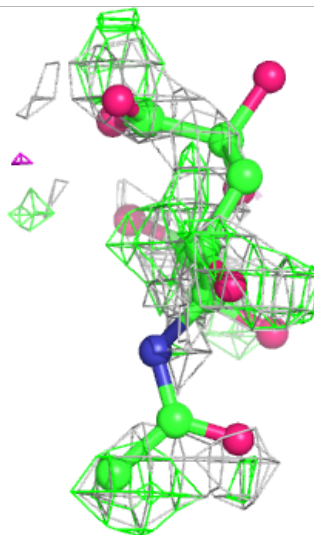
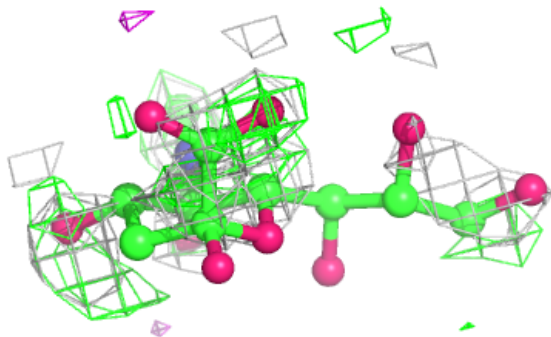
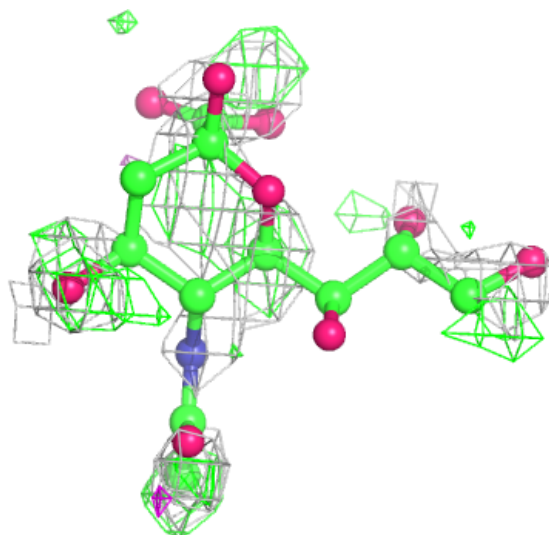
Electron density around SIA A 1478:

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



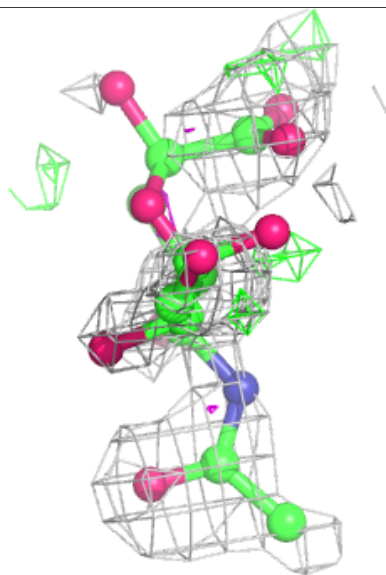
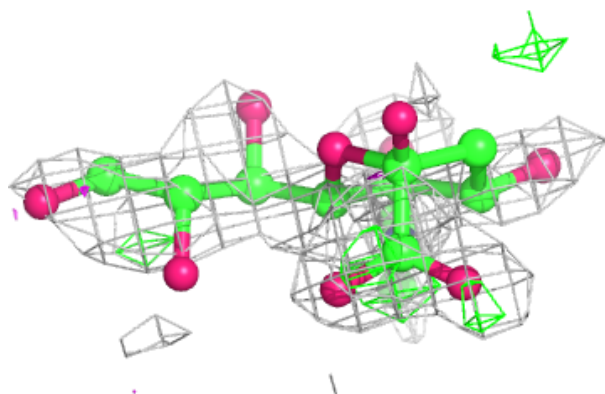
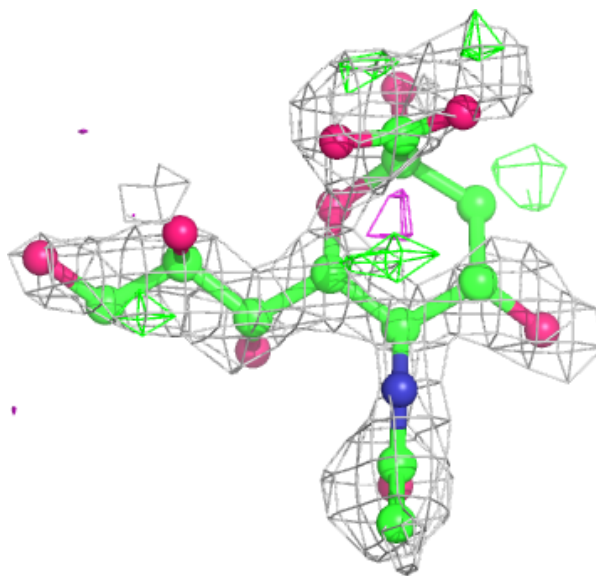
Electron density around SIA C 3478:

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



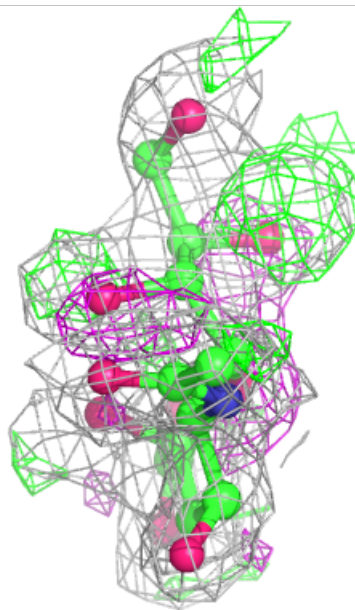
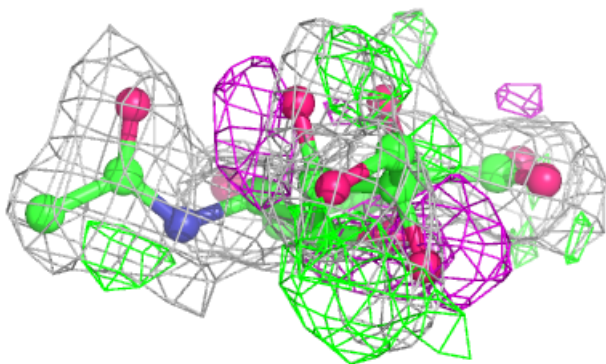
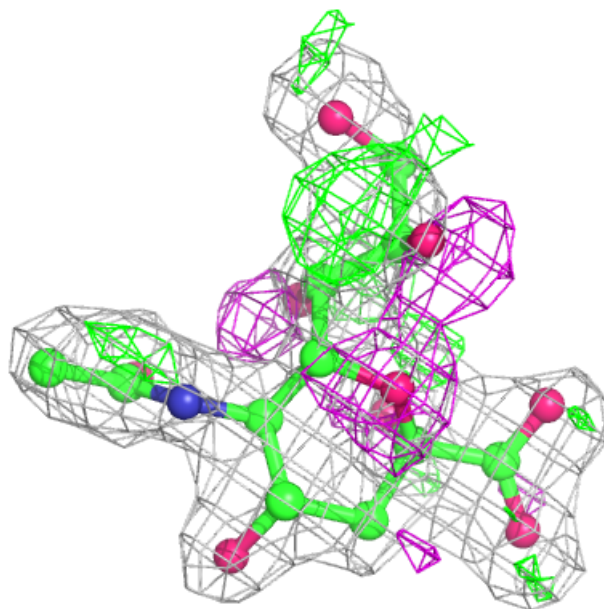
Electron density around SIA D 4478:

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



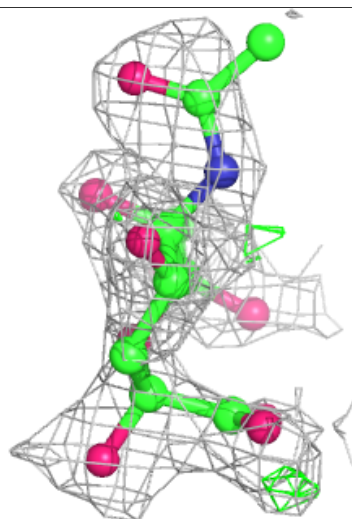
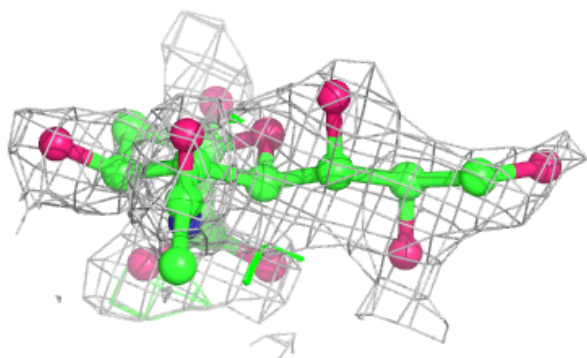
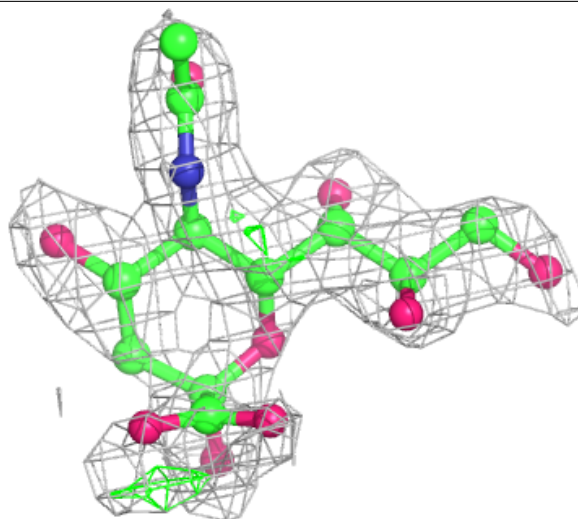
Electron density around SIA B 2477:

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



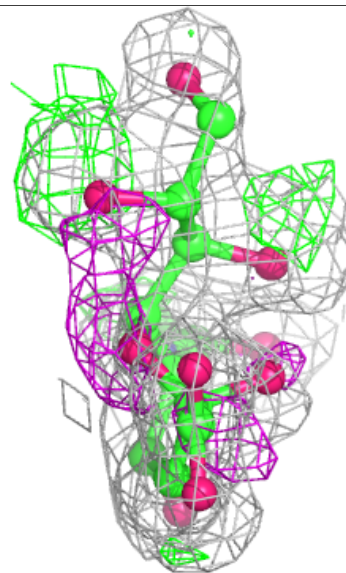
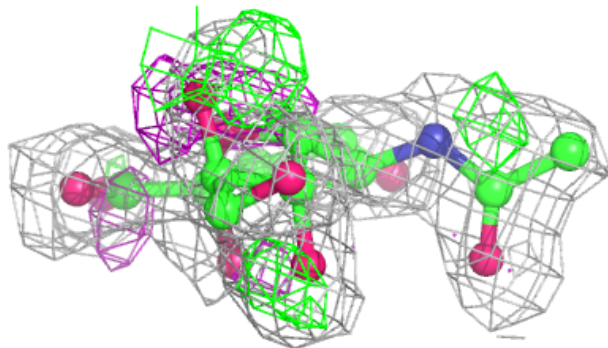
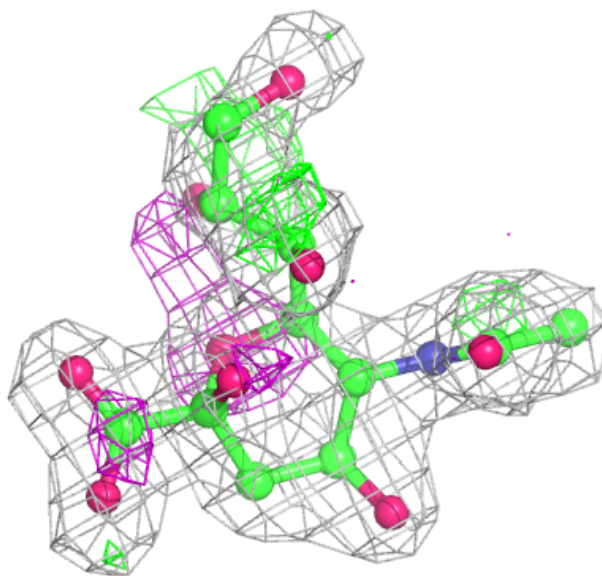
Electron density around SIA B 2478:

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



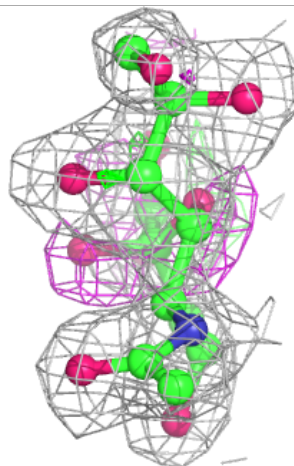
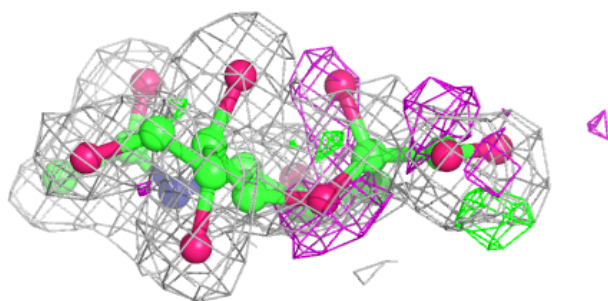
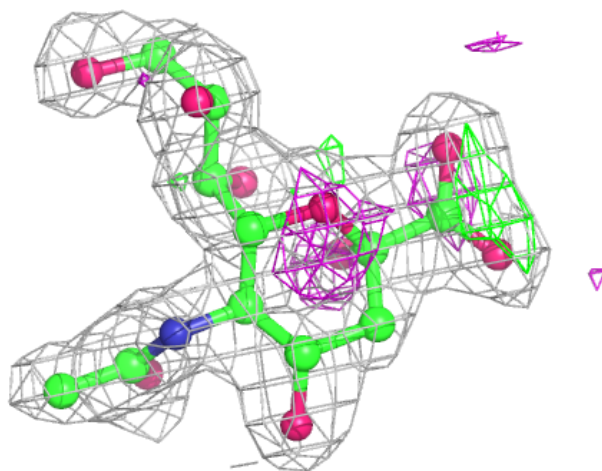
Electron density around SIA A 1477:

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



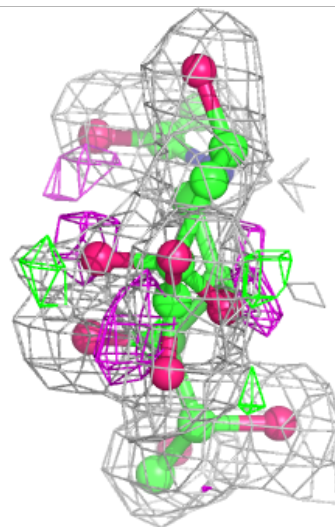
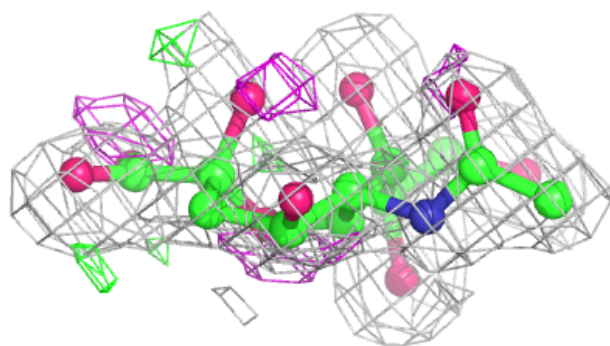
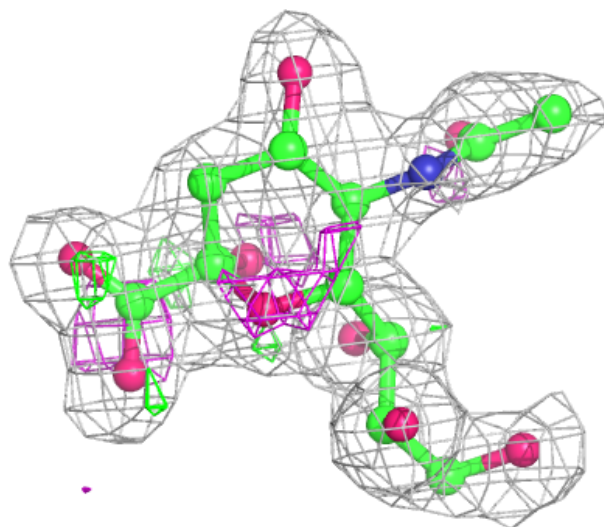
Electron density around SIA C 3477:

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



Electron density around SIA D 4477:

$2mF_o-DF_c$ (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.