



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 12, 2021 – 10:22 AM EDT

PDB ID : 7LAN
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)
COMPLEX WITH COMPOUND-30 AKA 7-[(3 {S},4 {R},6 {R})-4-benzyl-2
-oxa-7,13,14-triazatetracyclo[14.3.1.1[^]{3,6}.1[^]{11,14}]docosa-1(19),11(21),12
,16(20),17-pentaen-10-yl]-3 {H}-triazolo[4,5-b]pyridin-5-amine
Authors : Khan, J.A.
Deposited on : 2021-01-06
Resolution : 2.28 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 : 2.18
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) : 2.18

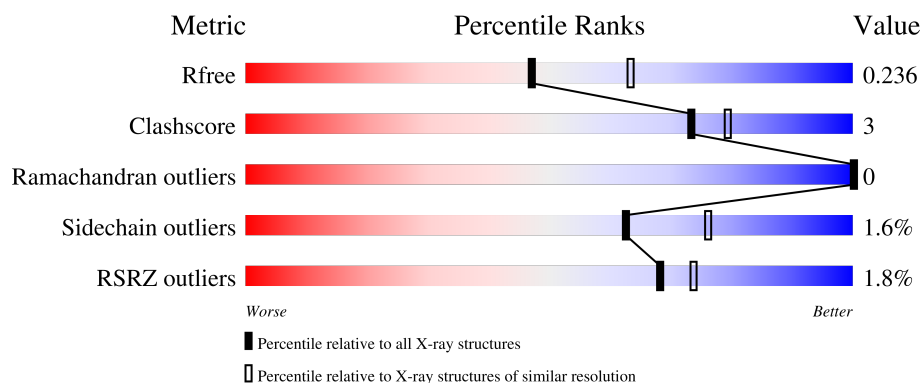
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	105	<div> <div>92%</div> <div>5% ..</div> </div>
1	D	105	<div> <div>95%</div> <div>..</div> </div>
1	F	105	<div> <div>90%</div> <div>7% ..</div> </div>
1	H	105	<div> <div>92%</div> <div>5% ..</div> </div>
2	B	466	<div> <div>94%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	466	 2% 95% 5%
2	G	466	 2% 92% 7%
2	I	466	 2% 95% 5%
3	C	2	 100%
3	K	2	 100%
3	M	2	 50% 50%
4	J	6	 33% 67%
4	L	6	 33% 67%
4	N	6	 50% 50%
4	O	6	 67% 33%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 19728 atoms, of which 123 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 Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	3	0	0
			821	520	145	151	5			
1	D	104	Total	C	N	O	S	5	0	0
			835	528	147	155	5			
1	F	103	Total	C	N	O	S	3	0	0
			821	520	145	151	5			
1	H	103	Total	C	N	O	S	0	0	0
			809	515	144	145	5			

- Molecule 2 is a protein called Isoform H14 of Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	32	0	0
			3636	2298	654	658	26			
2	E	465	Total	C	N	O	S	36	0	0
			3651	2311	659	654	27			
2	G	464	Total	C	N	O	S	32	0	0
			3662	2314	664	657	27			
2	I	464	Total	C	N	O	S	36	0	0
			3636	2302	655	652	27			

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



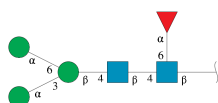
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

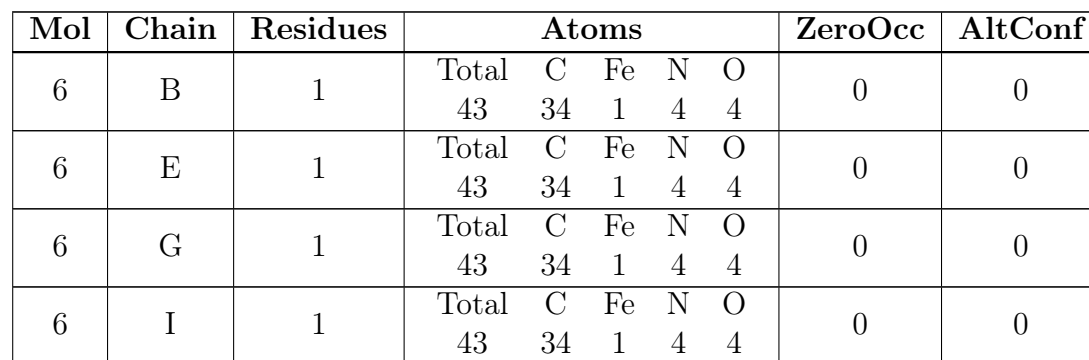


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	6	Total	C	N	O	0	0	0
			71	40	2	29			
4	L	6	Total	C	N	O	0	0	0
			71	40	2	29			
4	N	6	Total	C	N	O	0	0	0
			71	40	2	29			
4	O	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl	0	0
			1 1		
5	B	1	Total Cl	0	0
			1 1		
5	F	1	Total Cl	0	0
			1 1		
5	G	1	Total Cl	0	0
			1 1		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



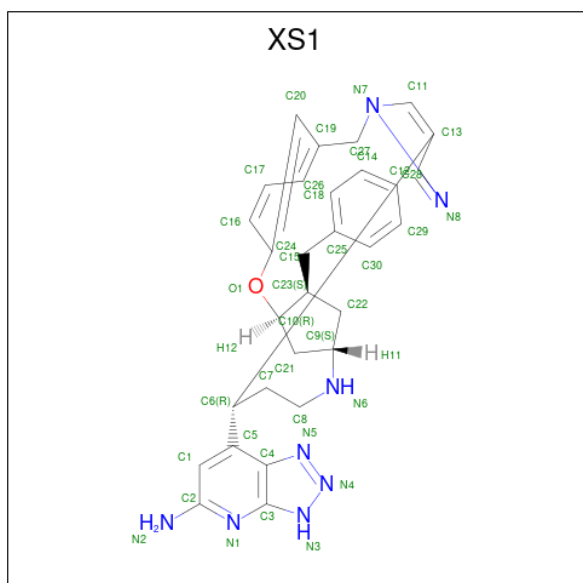
-
- Chemical structure of NAG (N-Acetylglucosamine) in a chair conformation. The pyranose ring has carbons labeled C1(R) through C6(R). C1(R) is bonded to O1 (HO) with a dashed bond. C2(R) is bonded to N2 (HN) with a wedged bond. C3(R) is bonded to O3 (OH) with a dashed bond. C4(S) is bonded to O4 (OH) with a wedged bond. C5(R) is bonded to O5 (O) and C6 (C6) with a dashed bond. C6 is bonded to O6 (OH) with a wedged bond. The N2 group is bonded to C7, which is double-bonded to O7 and single-bonded to C8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	E	1	Total Ca 1 1	0	0
8	G	1	Total Ca 1 1	0	0
8	I	1	Total Ca 1 1	0	0

- Molecule 9 is 7-[(3R,4S,6S,10R)-4-benzyl-2-oxa-7,13,14-triazatetracyclo[14.3.1.1^{3,6}.1^{11,14}]docosa-1(20),11(21),12,16,18-pentaen-10-yl]-3H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (three-letter code: XS1) (formula: C₃₀H₃₂N₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	27	0
			60	24	27	8	1		
9	E	1	Total	C	H	N	O	32	0
			71	30	32	8	1		
9	G	1	Total	C	H	N	O	32	0
			71	30	32	8	1		
9	I	1	Total	C	H	N	O	32	0
			71	30	32	8	1		

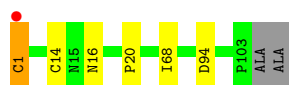
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	59	Total	O	0	0
			59	59		
10	B	162	Total	O	0	0
			162	162		
10	D	61	Total	O	0	0
			61	61		
10	E	213	Total	O	0	0
			213	213		
10	F	56	Total	O	0	0
			56	56		
10	G	188	Total	O	0	0
			188	188		
10	H	47	Total	O	0	0
			47	47		
10	I	180	Total	O	0	0
			180	180		

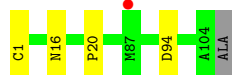
3 Residue-property plots [i](#)

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.

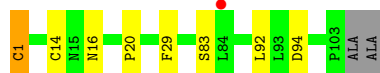
- Molecule 1: Myeloperoxidase light chain



- Molecule 1: Myeloperoxidase light chain



- Molecule 1: Myeloperoxidase light chain



- Molecule 1: Myeloperoxidase light chain

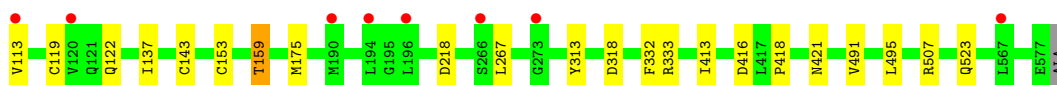


- Molecule 2: Isoform H14 of Myeloperoxidase





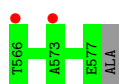
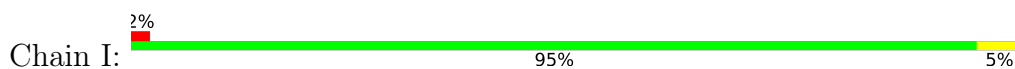
- Molecule 2: Isoform H14 of Myeloperoxidase



- Molecule 2: Isoform H14 of Myeloperoxidase



- Molecule 2: Isoform H14 of Myeloperoxidase



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

Chain M:  50% 50%

MAG1
MAG2

- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  67% 33%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	144.21Å 150.39Å 231.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.45 – 2.28 47.45 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.45-2.28) 99.8 (47.45-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.239 0.195 , 0.236	Depositor DCC
R_{free} test set	5724 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19728	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: NAG, FUC, HEM, MAN, XS1, CA, CL, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/846	0.66	0/1154
1	D	0.48	0/860	0.67	0/1172
1	F	0.53	0/846	0.66	0/1154
1	H	0.50	0/834	0.67	0/1139
2	B	0.49	0/3721	0.61	0/5063
2	E	0.51	0/3736	0.61	0/5082
2	G	0.50	0/3747	0.61	0/5093
2	I	0.50	0/3722	0.60	0/5065
All	All	0.50	0/18312	0.62	0/24922

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	821	0	776	12	0
1	D	835	0	793	10	0
1	F	821	0	776	14	0
1	H	809	0	761	12	0
2	B	3636	0	3562	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3651	0	3598	11	0
2	G	3662	0	3617	18	0
2	I	3636	0	3566	11	0
3	C	28	0	25	0	0
3	K	28	0	25	0	0
3	M	28	0	25	0	0
4	J	71	0	61	0	0
4	L	71	0	61	0	0
4	N	71	0	61	0	0
4	O	71	0	61	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	B	43	0	30	8	0
6	E	43	0	30	9	0
6	G	43	0	30	9	0
6	I	43	0	30	9	0
7	B	14	0	13	0	0
7	E	14	0	13	0	0
7	G	14	0	13	0	0
7	I	28	0	26	0	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
9	B	33	27	0	0	0
9	E	39	32	0	0	0
9	G	39	32	0	0	0
9	I	39	32	0	0	0
10	A	59	0	0	0	0
10	B	162	0	0	0	0
10	D	61	0	0	0	0
10	E	213	0	0	0	0
10	F	56	0	0	0	0
10	G	188	0	0	0	0
10	H	47	0	0	0	0
10	I	180	0	0	0	0
All	All	19605	123	17953	97	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 3.

The worst 5 of 97 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:F:94:ASP:CG	6:G:601:HEM:HMD3	1.41	1.41
1:D:94:ASP:CG	6:E:601:HEM:HMD3	1.41	1.39
1:D:94:ASP:OD2	6:E:601:HEM:CMD	1.71	1.38
1:F:94:ASP:CG	6:G:601:HEM:CMD	1.92	1.37
1:F:94:ASP:OD2	6:G:601:HEM:CMD	1.70	1.36

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	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
1	D	102/105 (97%)	98 (96%)	4 (4%)	0	100	100
1	F	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
1	H	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
2	B	462/466 (99%)	453 (98%)	9 (2%)	0	100	100
2	E	463/466 (99%)	452 (98%)	11 (2%)	0	100	100
2	G	462/466 (99%)	451 (98%)	11 (2%)	0	100	100
2	I	462/466 (99%)	453 (98%)	9 (2%)	0	100	100
All	All	2254/2284 (99%)	2202 (98%)	52 (2%)	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	87/90 (97%)	86 (99%)	1 (1%)	73	84
1	D	89/90 (99%)	88 (99%)	1 (1%)	73	84
1	F	87/90 (97%)	86 (99%)	1 (1%)	73	84
1	H	83/90 (92%)	82 (99%)	1 (1%)	71	82
2	B	390/411 (95%)	385 (99%)	5 (1%)	69	80
2	E	393/411 (96%)	387 (98%)	6 (2%)	65	77
2	G	395/411 (96%)	386 (98%)	9 (2%)	50	65
2	I	389/411 (95%)	382 (98%)	7 (2%)	59	72
All	All	1913/2004 (96%)	1882 (98%)	31 (2%)	62	76

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	122	GLN
2	I	267	LEU
2	G	229	ARG
2	I	526	GLN
2	I	159	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	121	GLN
2	E	121	GLN
2	G	121	GLN
2	I	114	ASN
2	I	121	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

30 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	3,2	14,14,15	0.35	0	17,19,21	1.13	1 (5%)
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.98	2 (11%)
4	NAG	J	1	2,4	14,14,15	0.33	0	17,19,21	0.74	1 (5%)
4	NAG	J	2	4	14,14,15	0.26	0	17,19,21	0.47	0
4	BMA	J	3	4	11,11,12	0.32	0	15,15,17	0.53	0
4	MAN	J	4	4	11,11,12	0.33	0	15,15,17	0.93	1 (6%)
4	MAN	J	5	4	11,11,12	0.38	0	15,15,17	0.92	1 (6%)
4	FUC	J	6	4	10,10,11	0.32	0	14,14,16	0.86	1 (7%)
3	NAG	K	1	3,2	14,14,15	0.28	0	17,19,21	0.83	1 (5%)
3	NAG	K	2	3	14,14,15	0.28	0	17,19,21	1.08	2 (11%)
4	NAG	L	1	2,4	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
4	NAG	L	2	4	14,14,15	0.28	0	17,19,21	0.51	0
4	BMA	L	3	4	11,11,12	0.36	0	15,15,17	0.65	0
4	MAN	L	4	4	11,11,12	0.30	0	15,15,17	1.01	1 (6%)
4	MAN	L	5	4	11,11,12	0.30	0	15,15,17	0.88	1 (6%)
4	FUC	L	6	4	10,10,11	0.41	0	14,14,16	0.81	1 (7%)
3	NAG	M	1	3,2	14,14,15	0.30	0	17,19,21	1.11	2 (11%)
3	NAG	M	2	3	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	N	1	2,4	14,14,15	0.40	0	17,19,21	1.05	1 (5%)
4	NAG	N	2	4	14,14,15	0.36	0	17,19,21	0.63	0
4	BMA	N	3	4	11,11,12	0.44	0	15,15,17	0.69	0
4	MAN	N	4	4	11,11,12	0.30	0	15,15,17	0.88	1 (6%)
4	MAN	N	5	4	11,11,12	0.30	0	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	N	6	4	10,10,11	0.33	0	14,14,16	0.53	0
4	NAG	O	1	2,4	14,14,15	0.30	0	17,19,21	0.68	0
4	NAG	O	2	4	14,14,15	0.28	0	17,19,21	0.48	0
4	BMA	O	3	4	11,11,12	0.28	0	15,15,17	0.69	0
4	MAN	O	4	4	11,11,12	0.32	0	15,15,17	1.10	1 (6%)
4	MAN	O	5	4	11,11,12	0.38	0	15,15,17	0.79	1 (6%)
4	FUC	O	6	4	10,10,11	0.38	0	14,14,16	0.69	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
3	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	1/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	FUC	J	6	4	-	-	0/1/1/1
3	NAG	K	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
4	NAG	L	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	MAN	L	4	4	-	1/2/19/22	0/1/1/1
4	MAN	L	5	4	-	0/2/19/22	0/1/1/1
4	FUC	L	6	4	-	-	0/1/1/1
3	NAG	M	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
4	NAG	N	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	MAN	N	4	4	-	1/2/19/22	0/1/1/1
4	MAN	N	5	4	-	0/2/19/22	0/1/1/1
4	FUC	N	6	4	-	-	0/1/1/1
4	NAG	O	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1
4	MAN	O	4	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	O	5	4	-	0/2/19/22	0/1/1/1
4	FUC	O	6	4	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	4	MAN	C1-O5-C5	3.90	117.47	112.19
4	N	1	NAG	O5-C1-C2	-3.56	105.66	111.29
4	L	4	MAN	C1-O5-C5	3.55	117.00	112.19
3	C	1	NAG	C1-C2-N2	-3.50	104.51	110.49
4	N	5	MAN	C1-O5-C5	3.43	116.83	112.19

There are no chirality outliers.

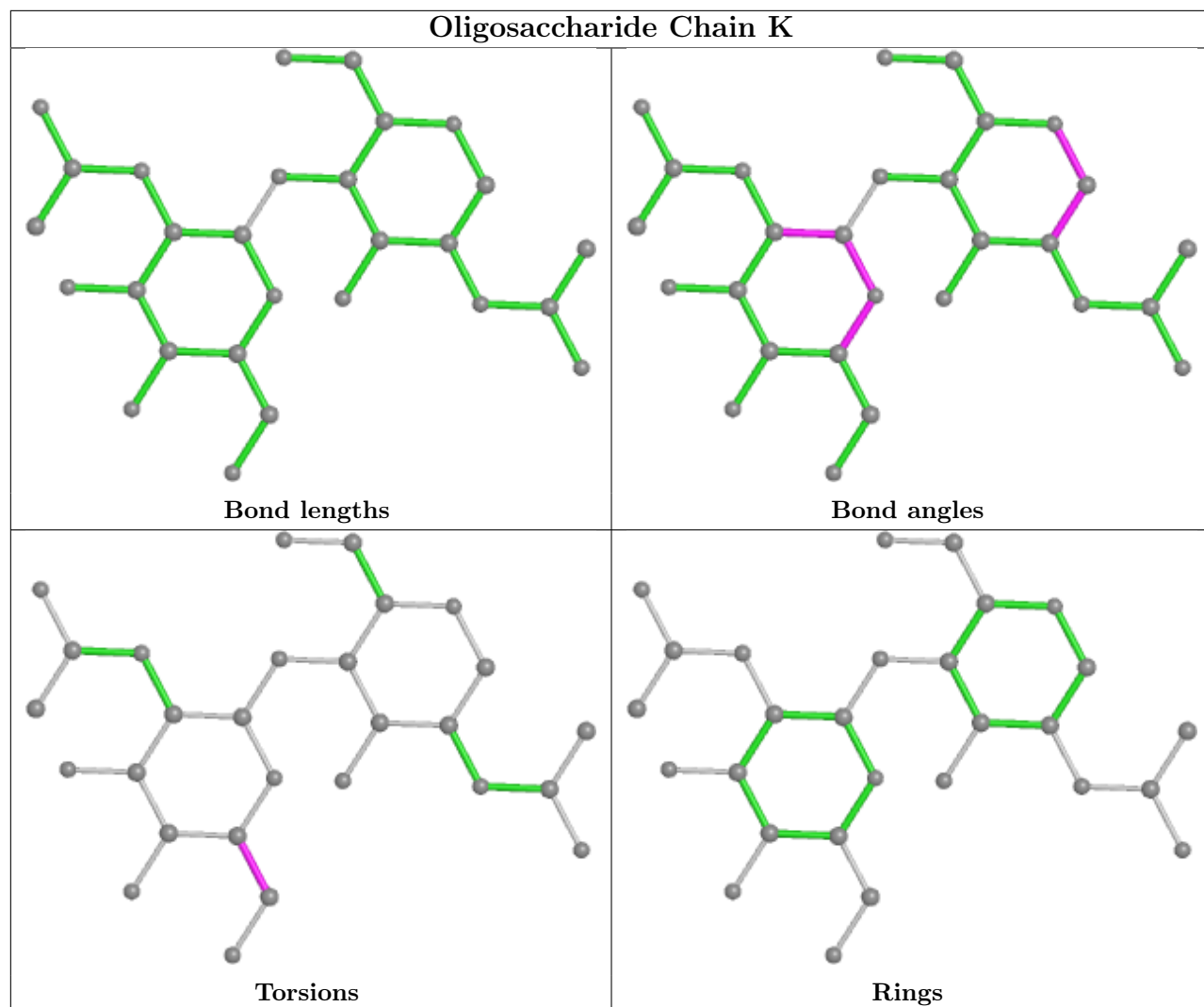
5 of 6 torsion outliers are listed below:

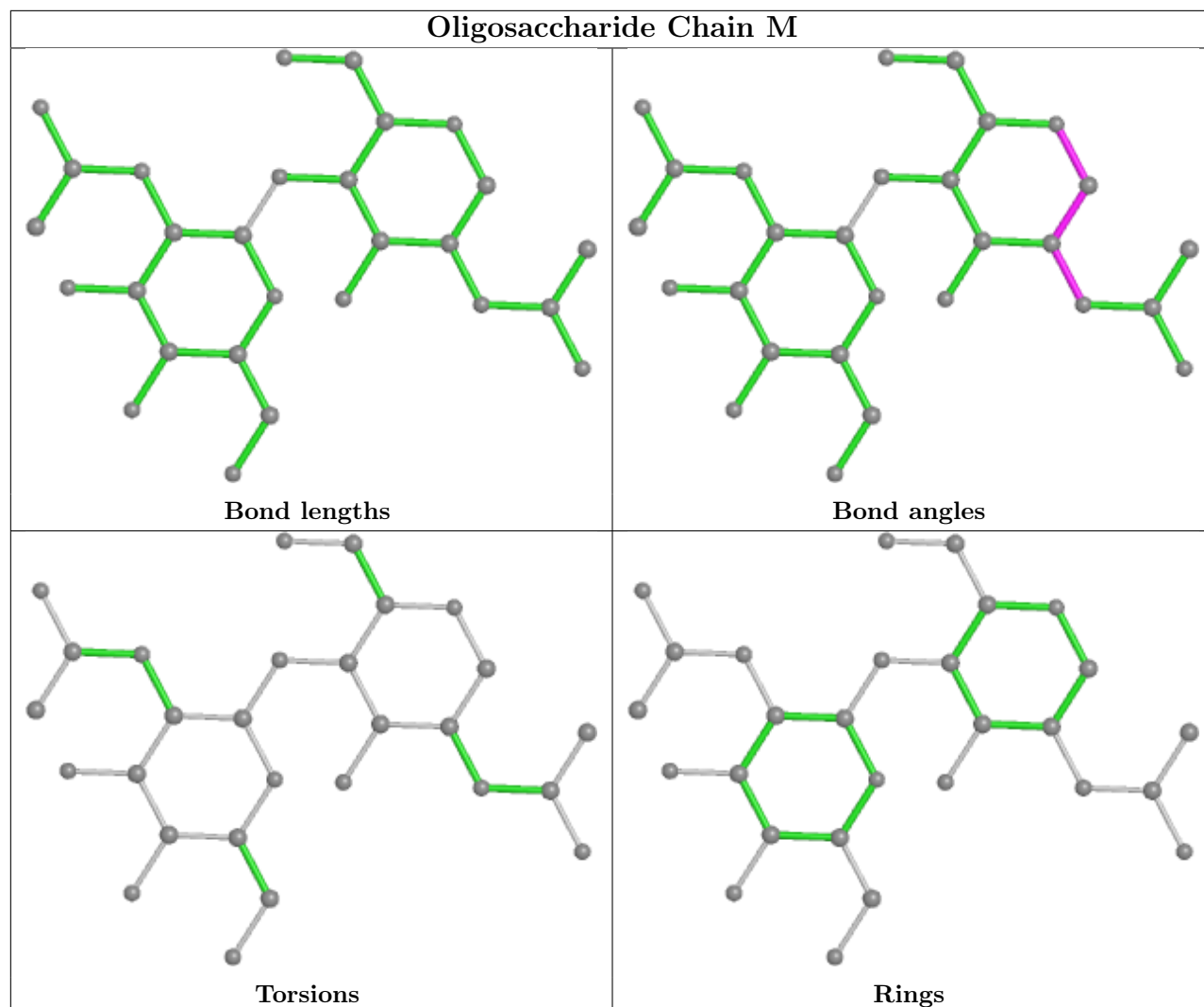
Mol	Chain	Res	Type	Atoms
4	J	4	MAN	O5-C5-C6-O6
4	L	4	MAN	O5-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
4	O	4	MAN	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6

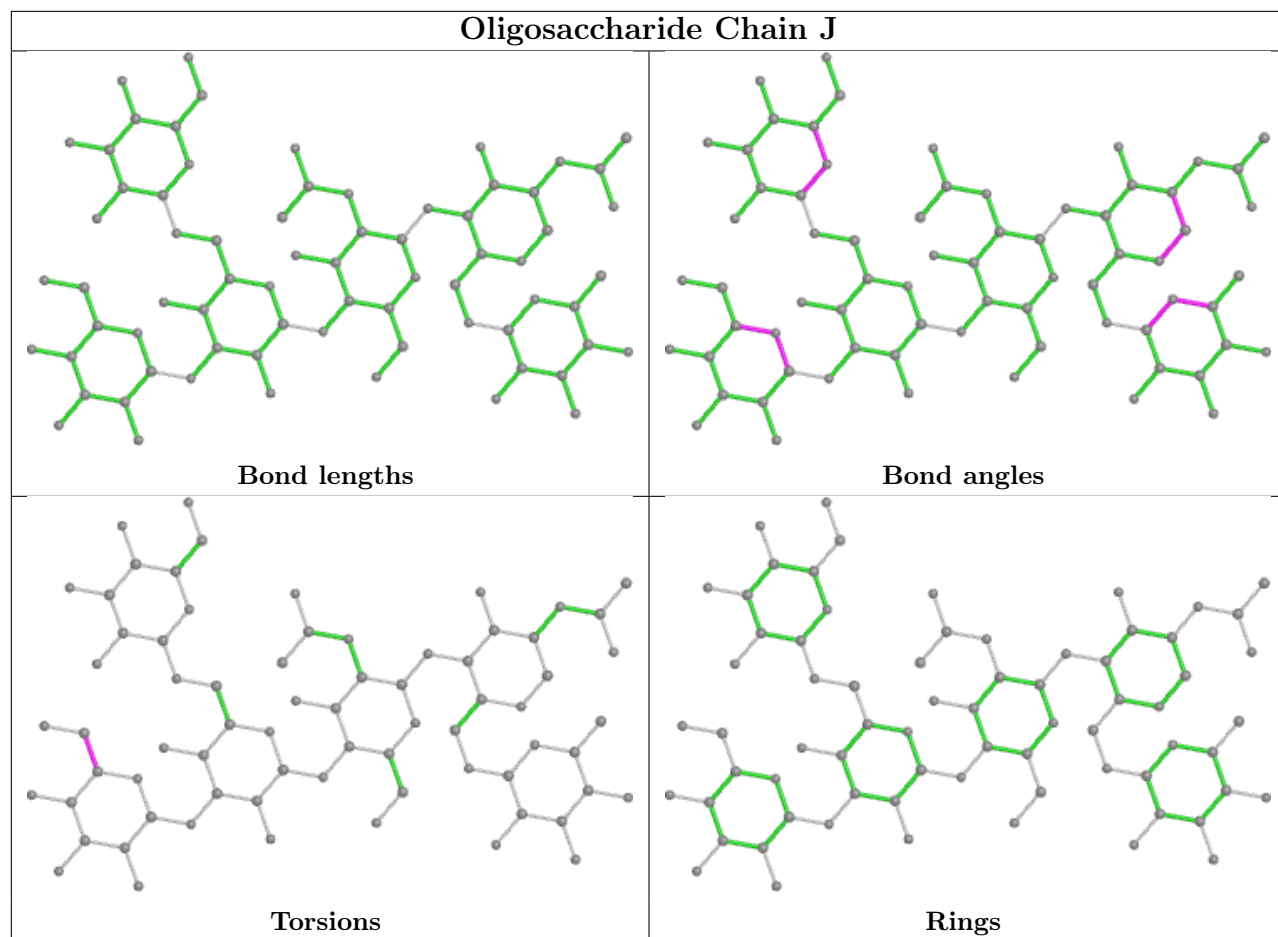
There are no ring outliers.

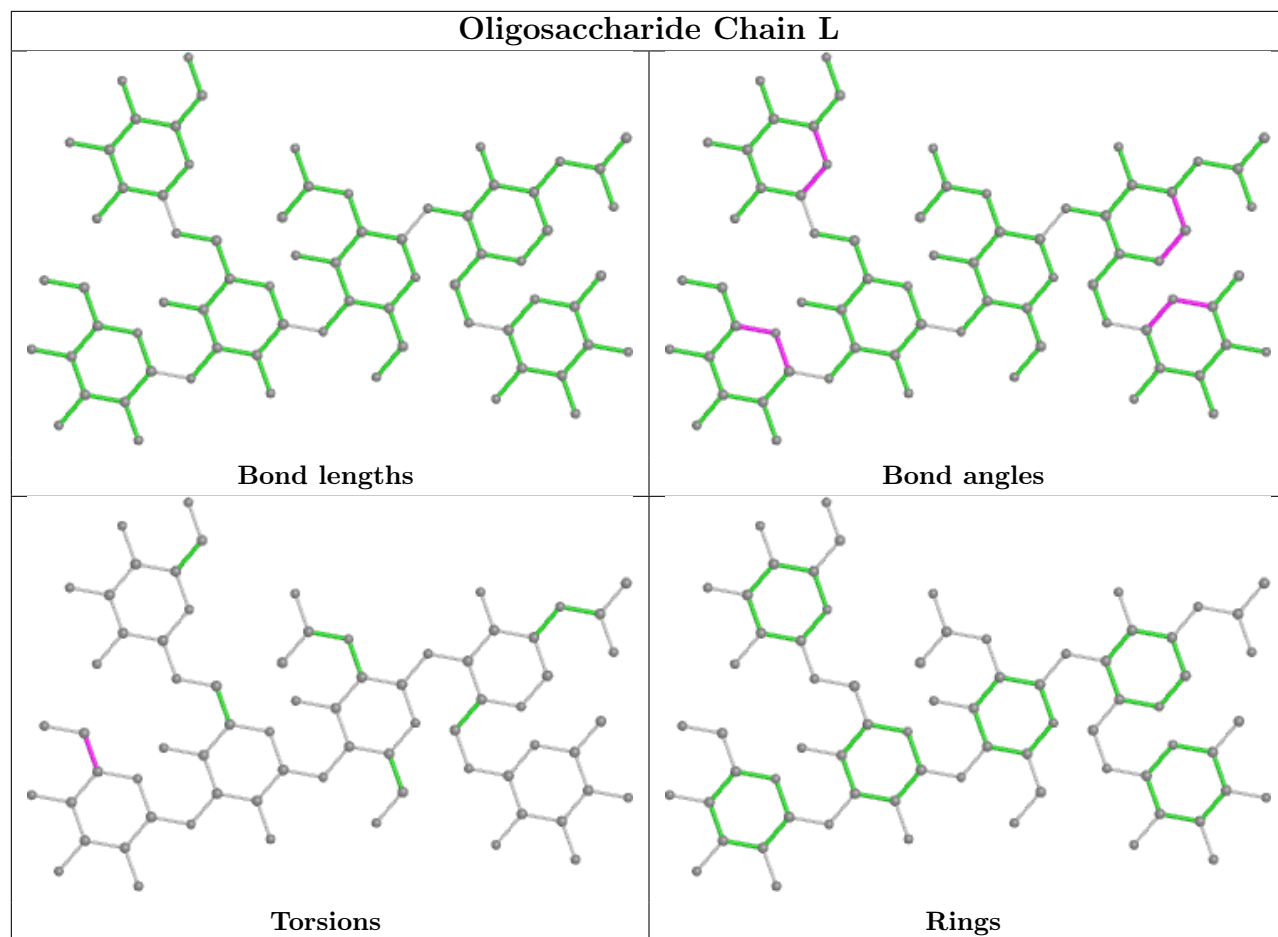
No monomer is involved in short contacts.

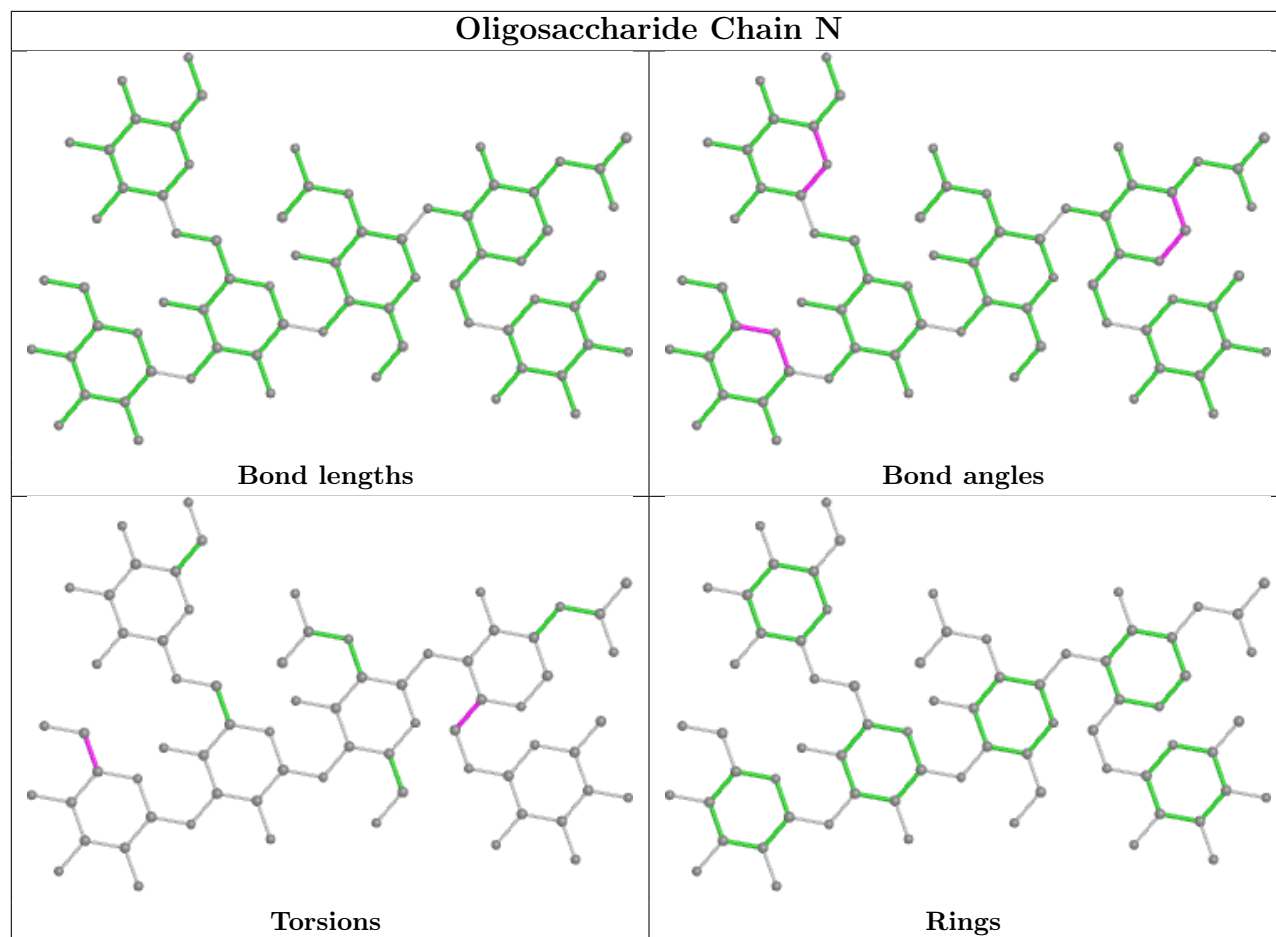
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

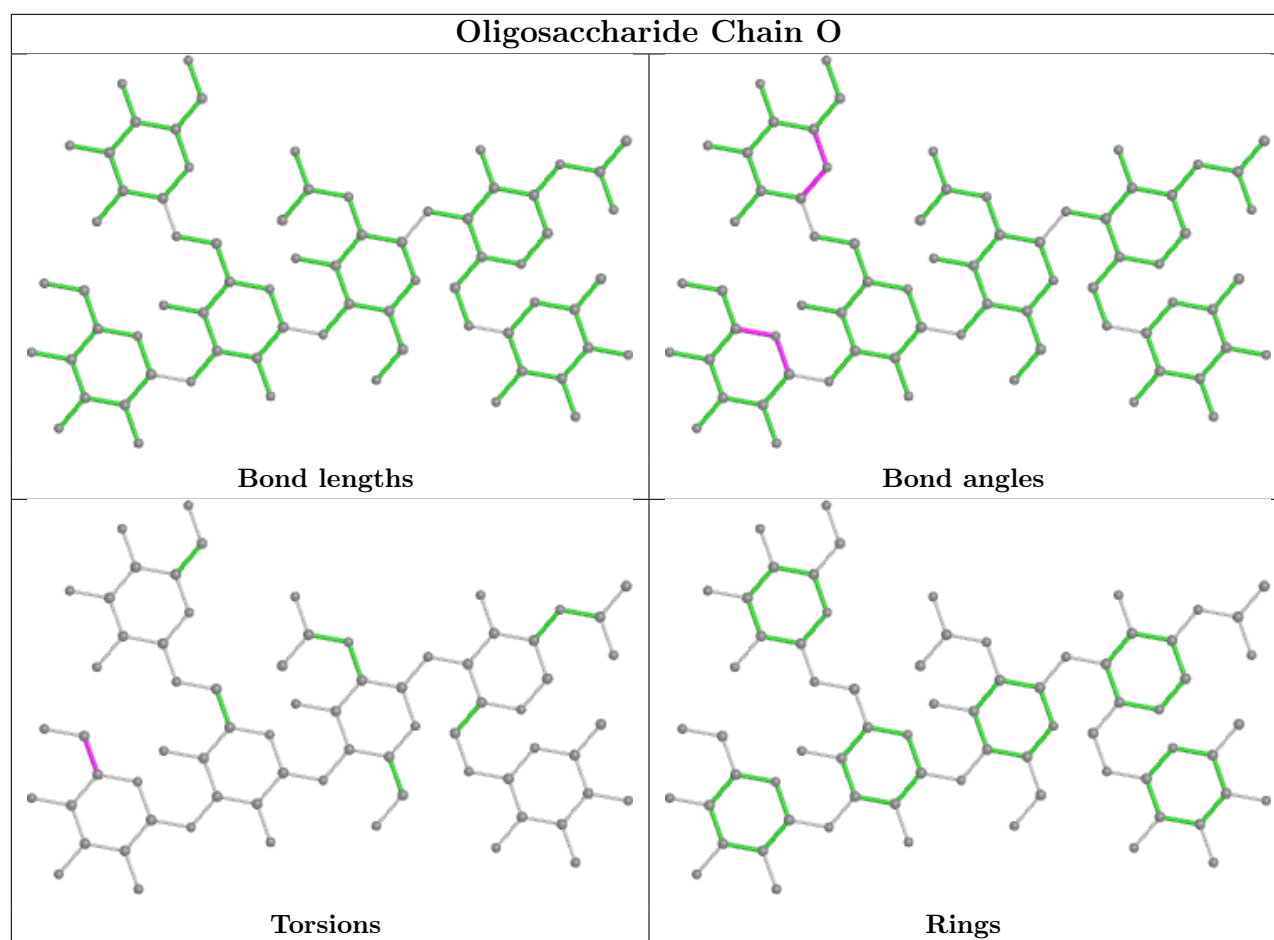












5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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
7	NAG	G	602	2	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
9	XS1	B	605	-	36,38,45	1.04	2 (5%)	36,55,64	1.54	7 (19%)
9	XS1	G	605	-	43,45,45	0.97	3 (6%)	47,64,64	1.29	5 (10%)
6	HEM	E	601	2	27,50,50	1.16	2 (7%)	17,82,82	2.00	8 (47%)
6	HEM	I	601	2	27,50,50	1.33	3 (11%)	17,82,82	2.04	7 (41%)
7	NAG	E	602	2	14,14,15	0.27	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	I	602	2	14,14,15	0.27	0	17,19,21	0.82	1 (5%)
9	XS1	E	604	-	43,45,45	1.01	3 (6%)	47,64,64	1.32	5 (10%)
7	NAG	I	603	2	14,14,15	0.25	0	17,19,21	0.75	1 (5%)
6	HEM	G	601	2,10	27,50,50	1.36	2 (7%)	17,82,82	2.08	5 (29%)
9	XS1	I	605	-	43,45,45	0.96	2 (4%)	47,64,64	1.28	5 (10%)
6	HEM	B	601	2,10	27,50,50	1.41	3 (11%)	17,82,82	1.63	3 (17%)
7	NAG	B	602	2	14,14,15	0.30	0	17,19,21	0.88	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
7	NAG	G	602	2	-	0/6/23/26	0/1/1/1
9	XS1	B	605	-	-	3/20/34/38	0/5/6/7
9	XS1	G	605	-	-	4/24/38/38	0/6/7/7
6	HEM	E	601	2	-	0/6/54/54	-
6	HEM	I	601	2	-	0/6/54/54	-
7	NAG	E	602	2	-	0/6/23/26	0/1/1/1
7	NAG	I	602	2	-	0/6/23/26	0/1/1/1
9	XS1	E	604	-	-	4/24/38/38	0/6/7/7
7	NAG	I	603	2	-	0/6/23/26	0/1/1/1
6	HEM	G	601	2,10	-	0/6/54/54	-
9	XS1	I	605	-	-	4/24/38/38	0/6/7/7
6	HEM	B	601	2,10	-	0/6/54/54	-
7	NAG	B	602	2	-	0/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	601	HEM	C3B-C2B	-4.64	1.33	1.40
6	B	601	HEM	C3B-C2B	-4.11	1.34	1.40
6	I	601	HEM	C3B-C2B	-4.05	1.34	1.40
6	E	601	HEM	C3B-C2B	-2.90	1.36	1.40
9	I	605	XS1	C1-C5	2.89	1.42	1.37

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	601	HEM	CBA-CAA-C2A	-4.78	103.67	112.49
6	I	601	HEM	CBA-CAA-C2A	-4.37	104.43	112.49
6	E	601	HEM	CBA-CAA-C2A	-4.21	104.72	112.49
9	E	604	XS1	C2-N1-C3	-4.05	113.00	119.22
6	B	601	HEM	CBA-CAA-C2A	-4.04	105.04	112.49

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	604	XS1	C22-C23-C24-C25
9	E	604	XS1	C10-C23-C24-C25
9	G	605	XS1	C22-C23-C24-C25
9	G	605	XS1	C10-C23-C24-C25
9	I	605	XS1	C22-C23-C24-C25

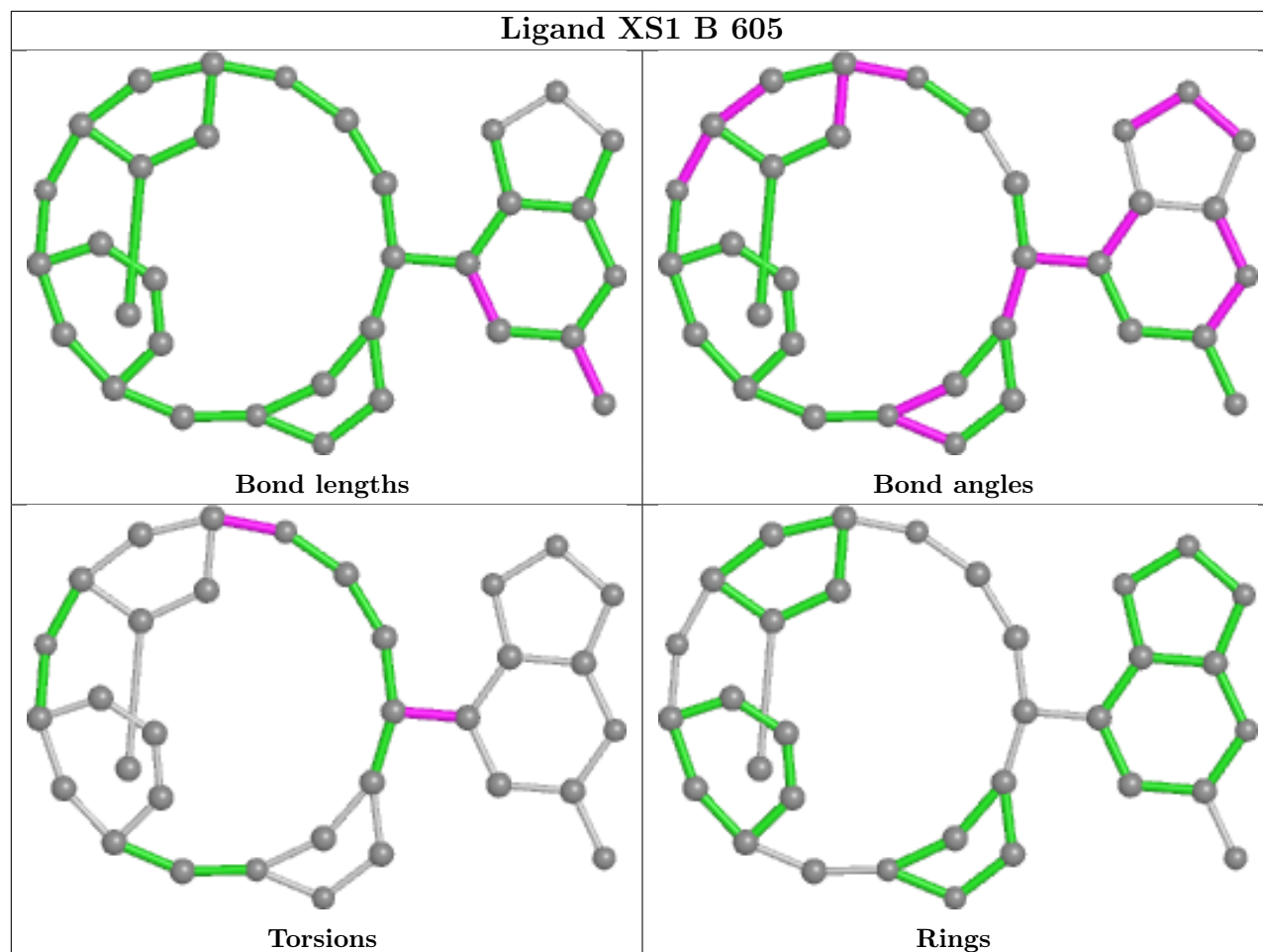
There are no ring outliers.

4 monomers are involved in 35 short contacts:

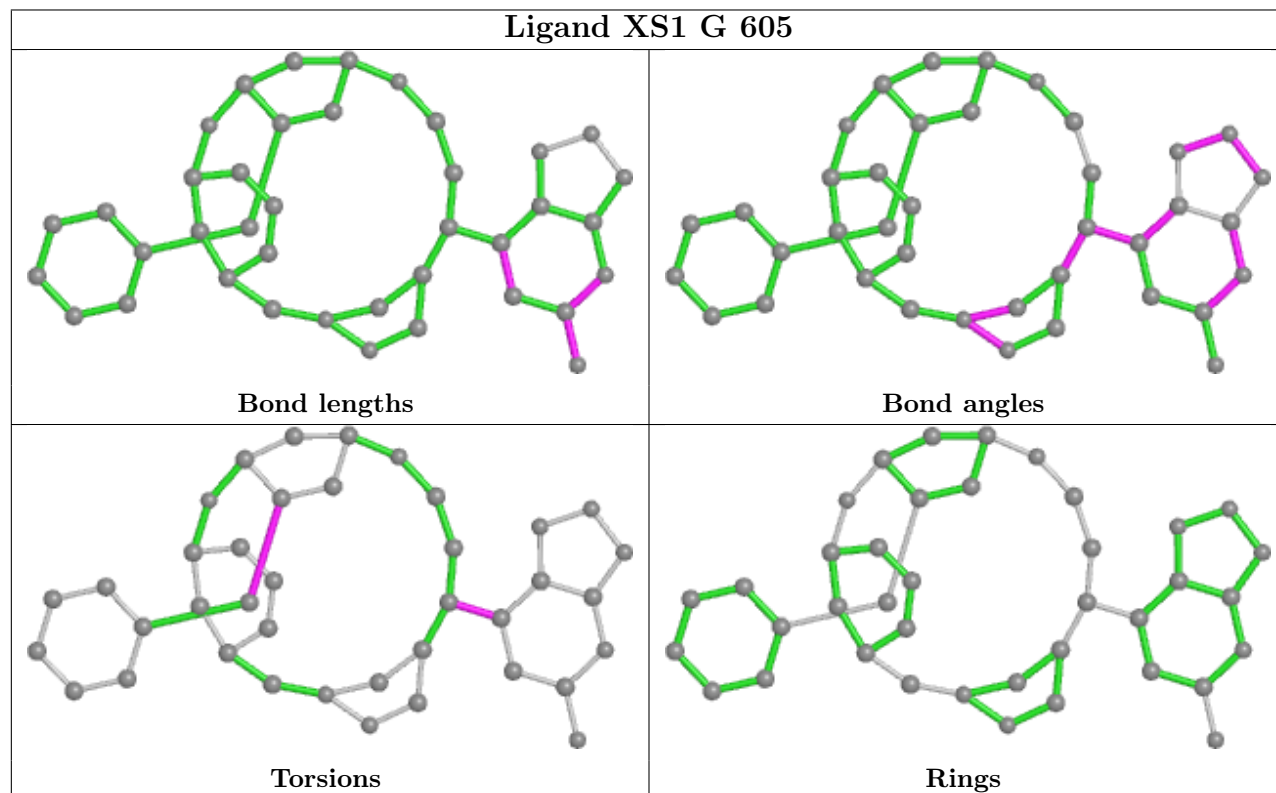
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	601	HEM	9	0
6	I	601	HEM	9	0
6	G	601	HEM	9	0
6	B	601	HEM	8	0

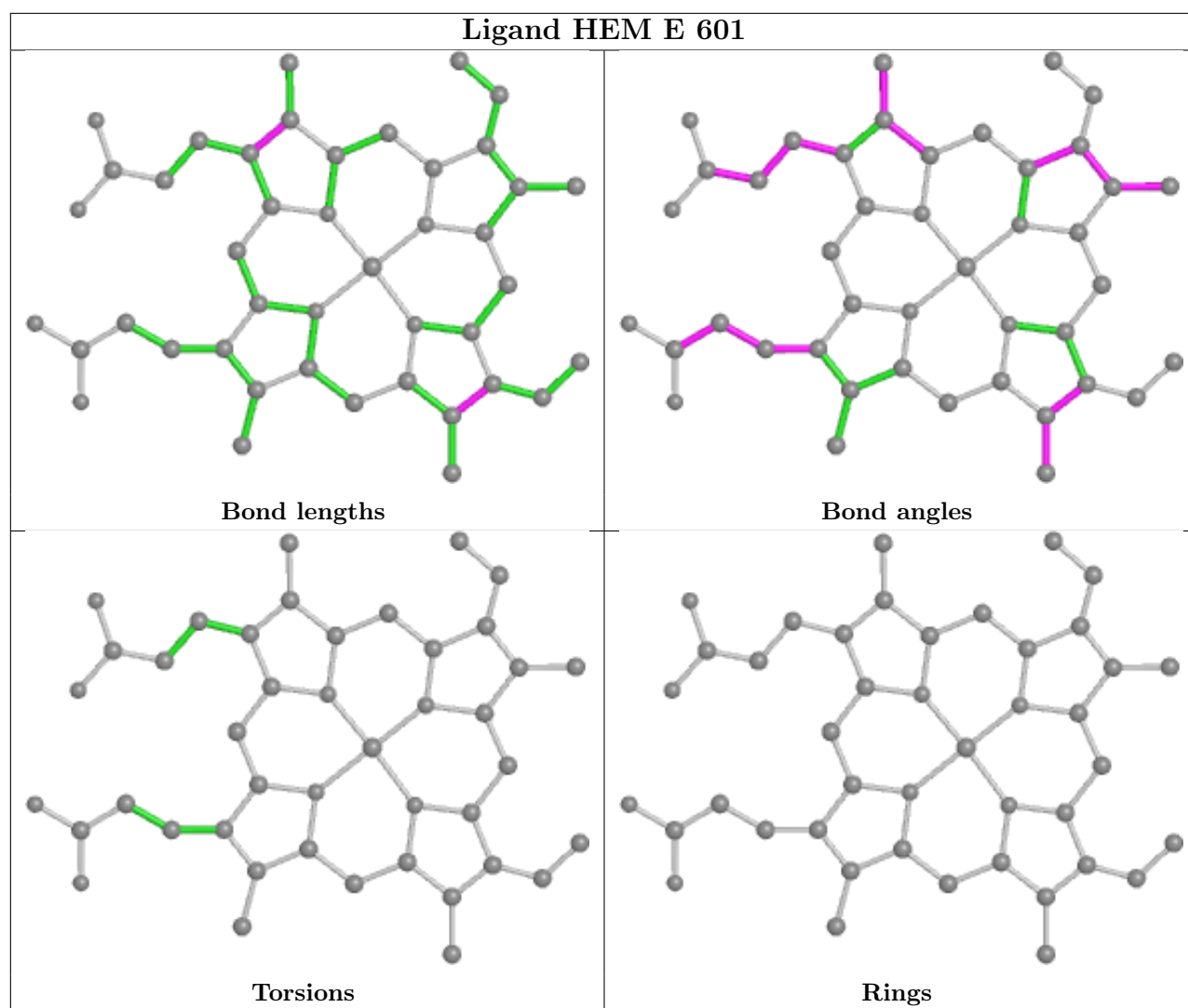
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 XS1 B 605

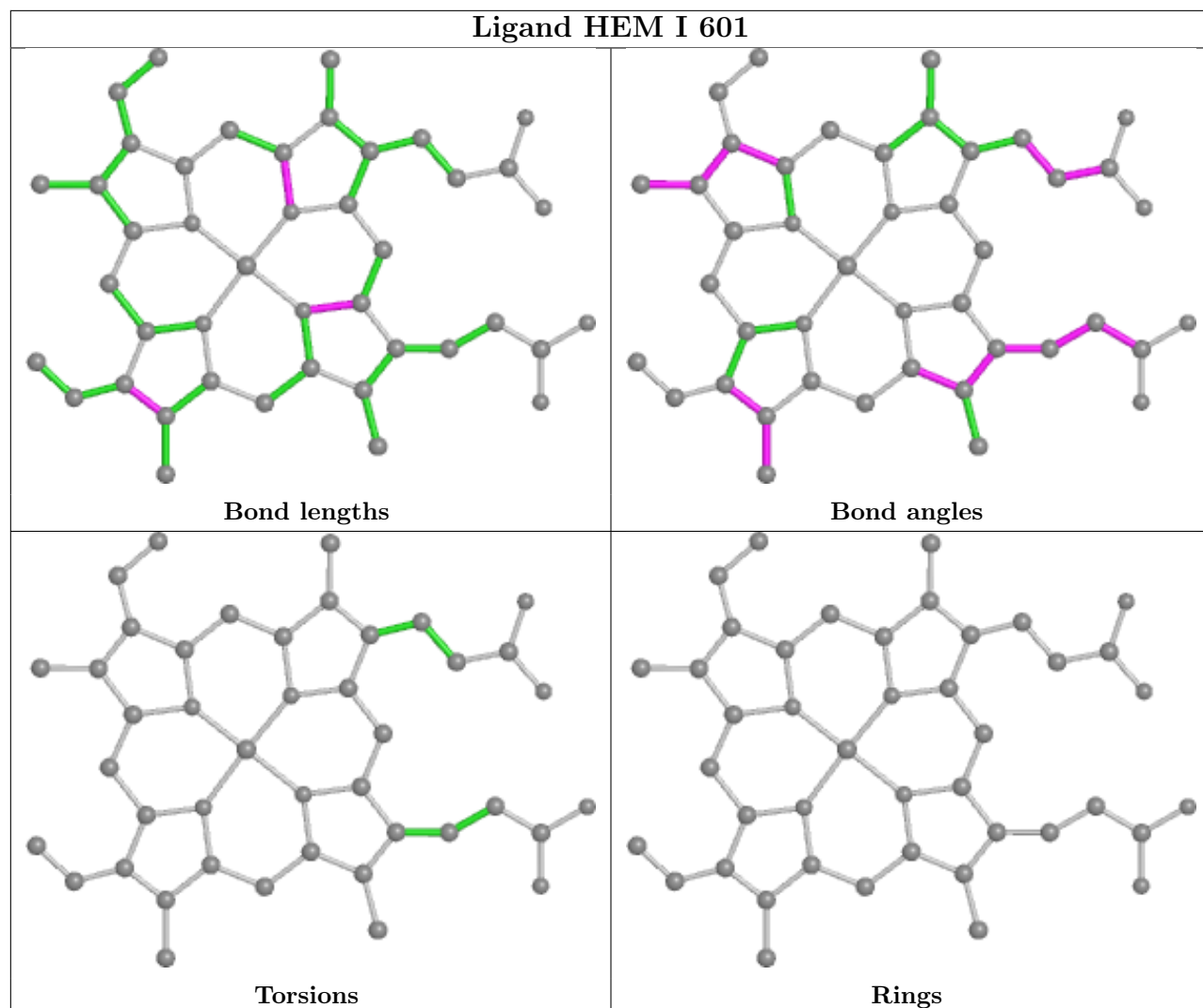


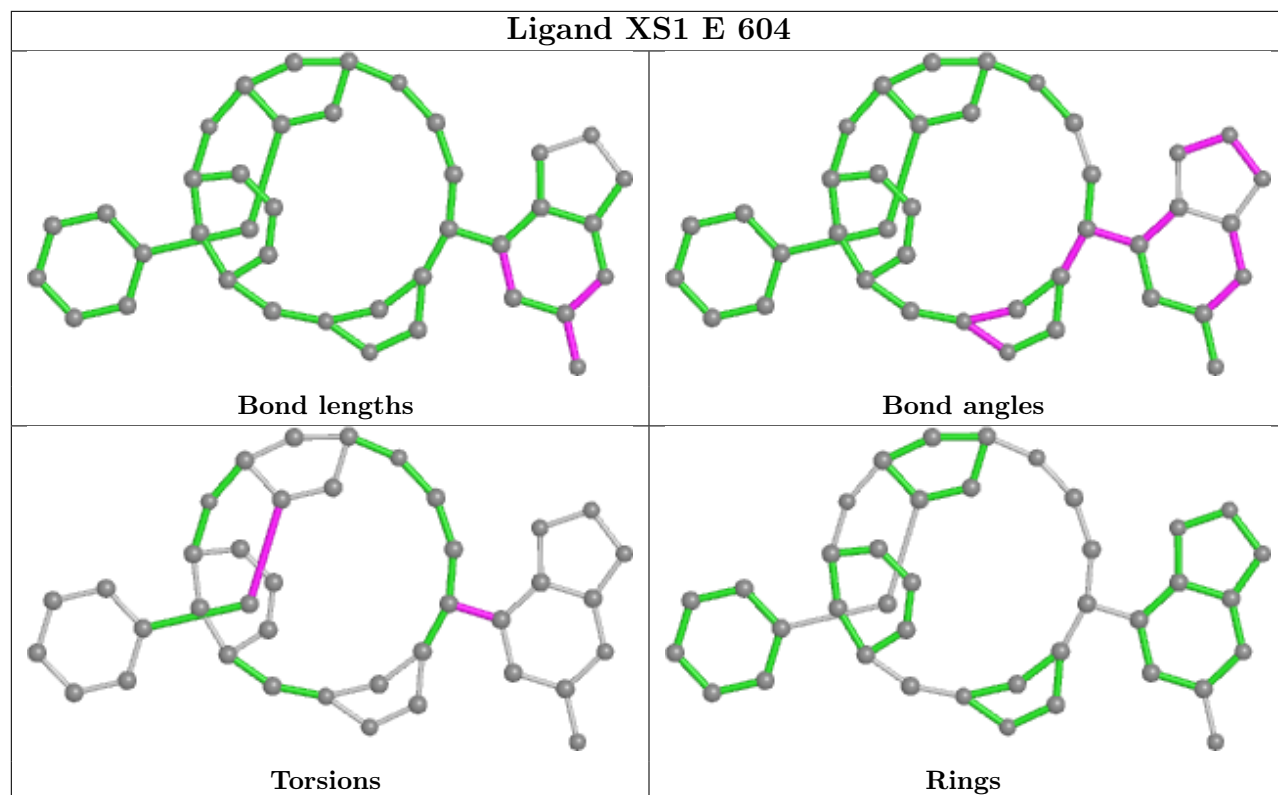
Ligand XS1 G 605

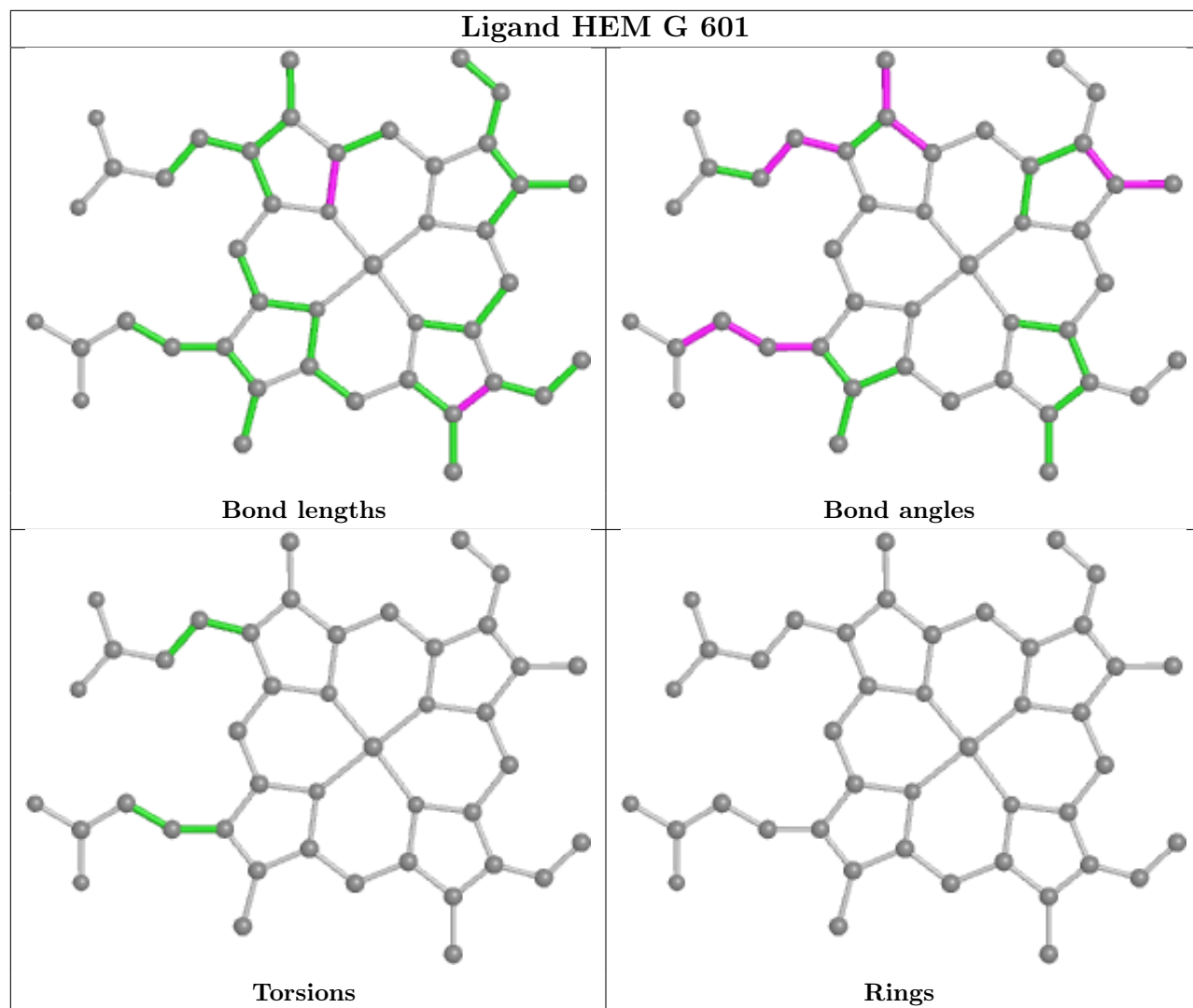




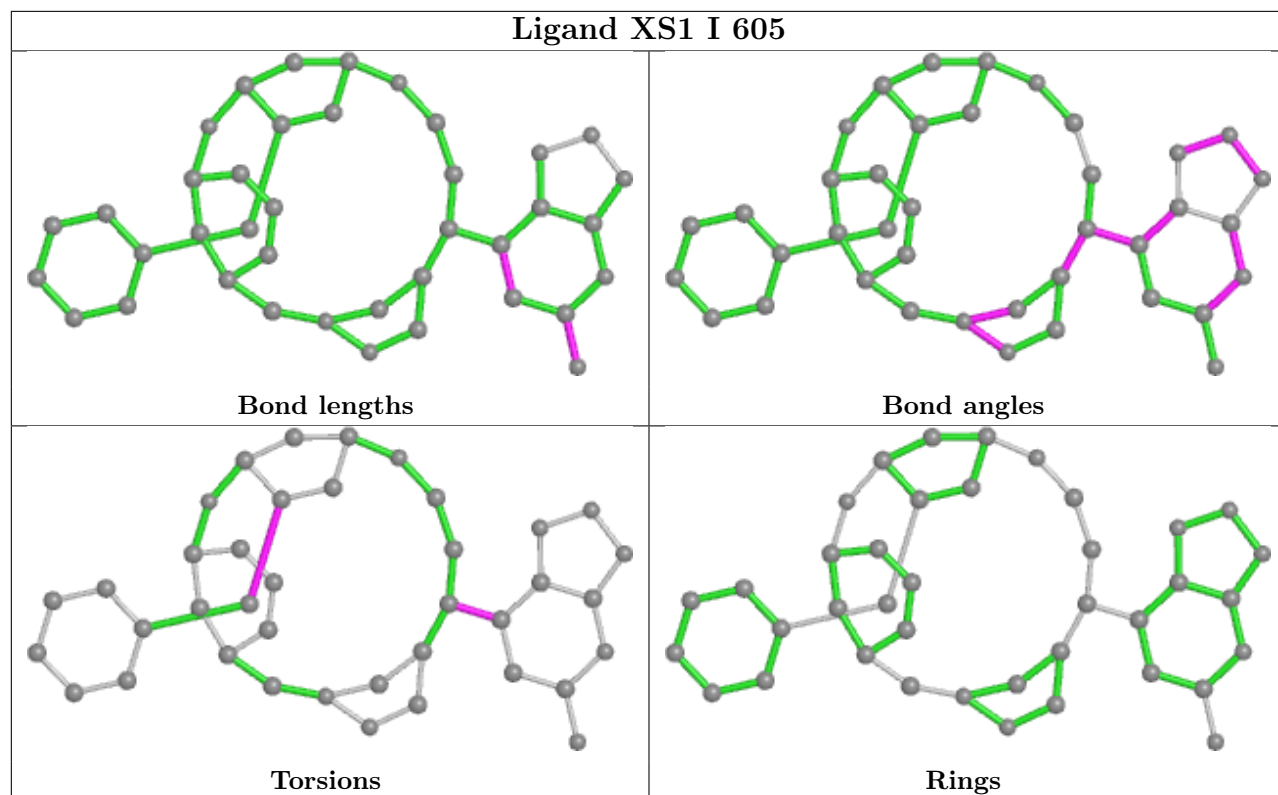
Ligand HEM I 601

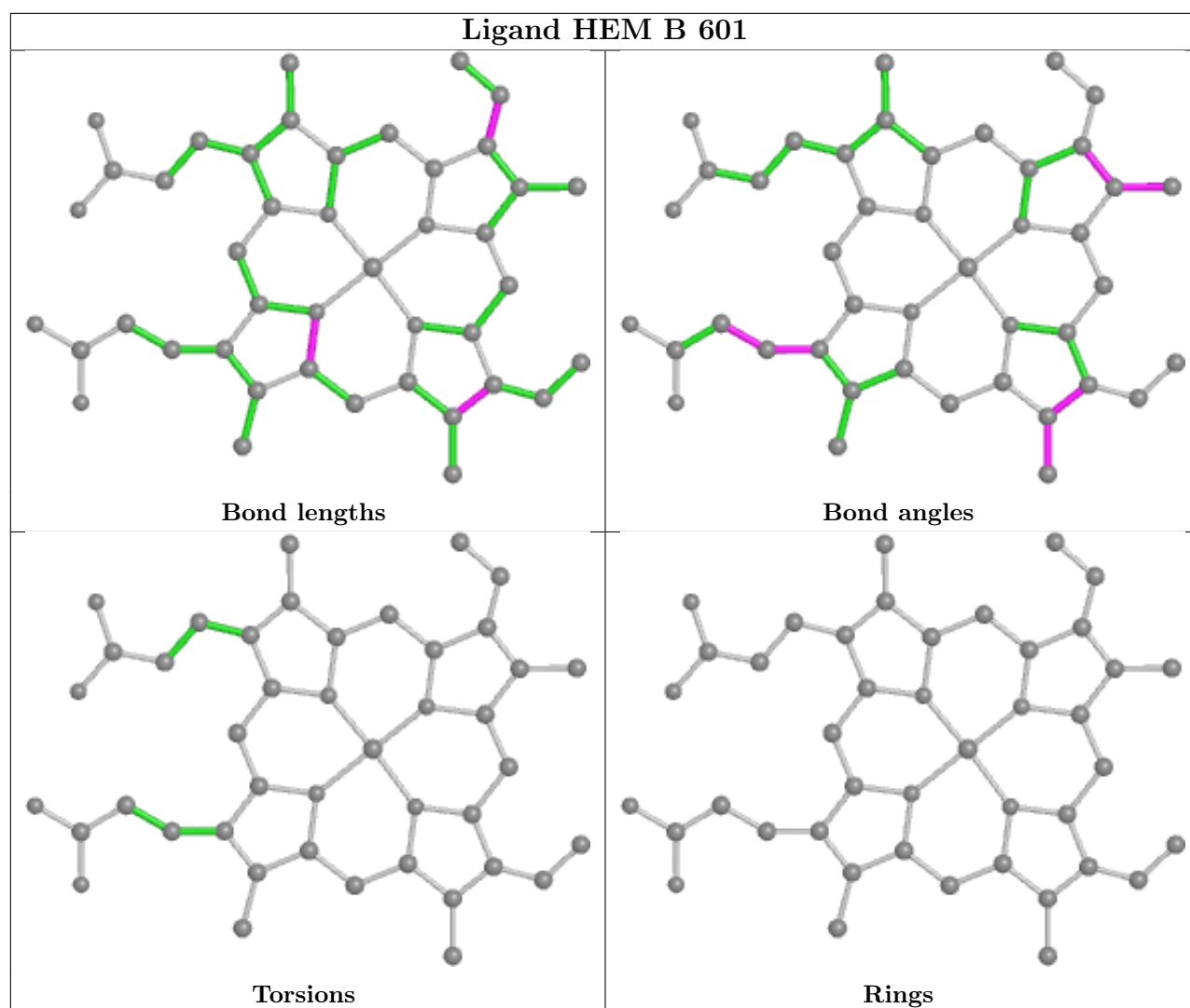






Ligand XS1 I 605





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	103/105 (98%)	-0.20	1 (0%) 82 86	29, 41, 65, 86	1 (0%)
1	D	104/105 (99%)	-0.27	1 (0%) 82 86	26, 37, 60, 85	2 (1%)
1	F	103/105 (98%)	-0.27	1 (0%) 82 86	27, 37, 63, 81	1 (0%)
1	H	103/105 (98%)	-0.29	0 100 100	27, 38, 60, 70	0
2	B	464/466 (99%)	-0.10	10 (2%) 62 68	26, 47, 69, 96	9 (1%)
2	E	465/466 (99%)	-0.15	8 (1%) 70 75	24, 41, 62, 82	12 (2%)
2	G	464/466 (99%)	-0.09	10 (2%) 62 68	26, 42, 63, 90	9 (1%)
2	I	464/466 (99%)	-0.18	9 (1%) 66 72	26, 45, 66, 79	11 (2%)
All	All	2270/2284 (99%)	-0.15	40 (1%) 68 74	24, 42, 66, 96	45 (1%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	190	MET	4.6
2	B	195	GLY	4.4
2	B	190	MET	4.4
2	B	372	VAL	4.0
2	E	113	VAL	3.8

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,

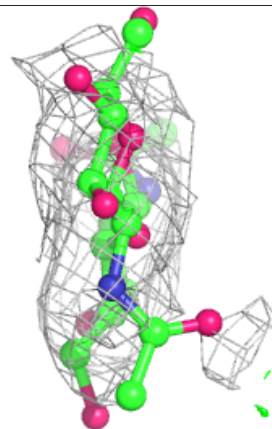
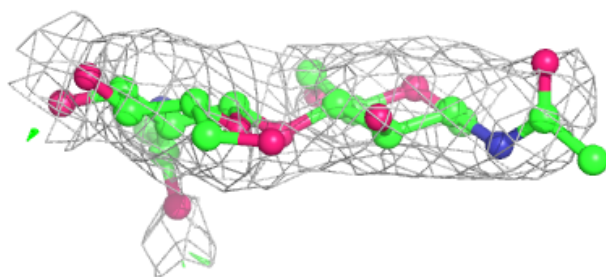
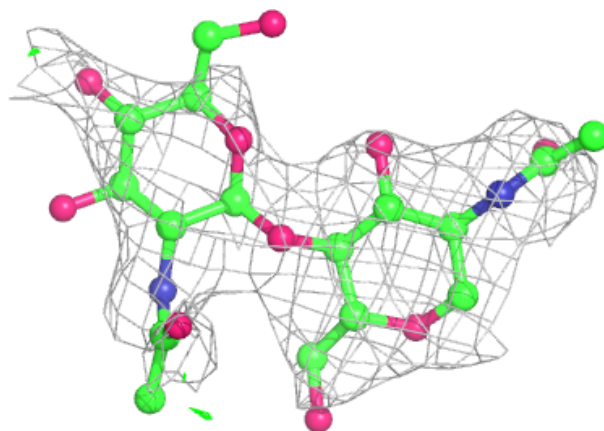
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	M	2	14/15	0.79	0.18	75,79,84,85	0
3	NAG	K	2	14/15	0.80	0.30	95,101,103,104	0
3	NAG	C	2	14/15	0.81	0.28	93,95,97,97	0
3	NAG	C	1	14/15	0.86	0.17	79,84,87,90	0
4	MAN	O	4	11/12	0.89	0.11	54,61,65,67	0
4	MAN	J	4	11/12	0.91	0.14	53,58,64,68	0
4	MAN	L	4	11/12	0.92	0.11	61,65,75,79	0
3	NAG	M	1	14/15	0.92	0.12	59,63,69,76	0
4	NAG	J	1	14/15	0.94	0.11	32,34,39,46	0
4	MAN	N	5	11/12	0.94	0.15	38,43,45,49	0
3	NAG	K	1	14/15	0.94	0.15	75,80,84,88	0
4	NAG	N	2	14/15	0.95	0.10	23,29,34,37	0
4	FUC	N	6	10/11	0.95	0.13	34,35,38,38	0
4	MAN	N	4	11/12	0.95	0.11	53,59,63,68	0
4	FUC	L	6	10/11	0.96	0.12	38,42,44,44	0
4	NAG	N	1	14/15	0.96	0.10	32,35,42,44	0
4	MAN	J	5	11/12	0.96	0.11	36,38,41,42	0
4	FUC	J	6	10/11	0.96	0.11	37,43,44,44	0
4	NAG	L	1	14/15	0.96	0.09	31,39,44,44	0
4	BMA	L	3	11/12	0.96	0.09	35,38,44,53	0
4	NAG	O	1	14/15	0.96	0.11	35,38,44,48	0
4	BMA	J	3	11/12	0.96	0.12	32,36,40,46	0
4	MAN	O	5	11/12	0.96	0.11	38,40,45,45	0
4	FUC	O	6	10/11	0.96	0.10	37,40,41,42	0
4	NAG	O	2	14/15	0.97	0.11	24,33,37,38	0
4	NAG	J	2	14/15	0.97	0.10	25,33,38,40	0
4	BMA	N	3	11/12	0.97	0.09	36,41,46,47	0
4	MAN	L	5	11/12	0.97	0.14	40,42,45,48	0
4	BMA	O	3	11/12	0.98	0.10	34,38,42,48	0
4	NAG	L	2	14/15	0.98	0.08	25,31,34,37	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.

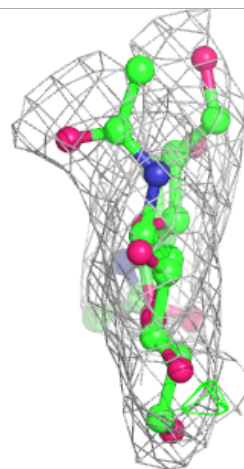
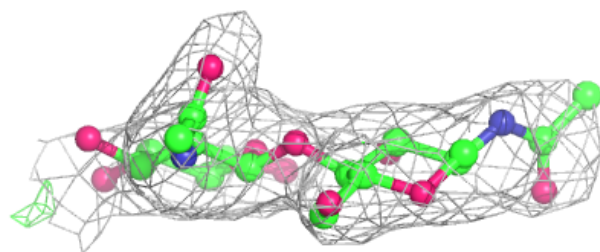
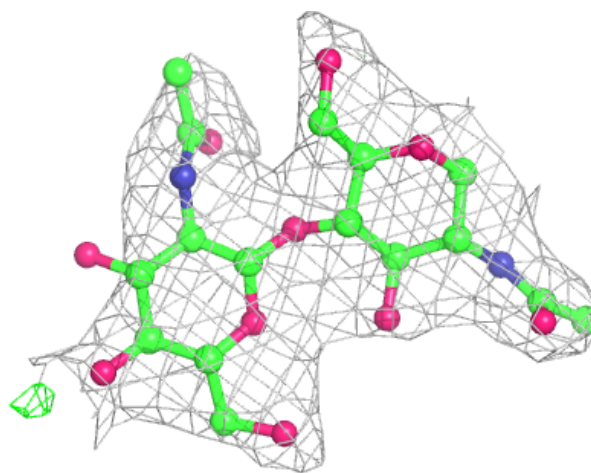
Electron density around Chain K:

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



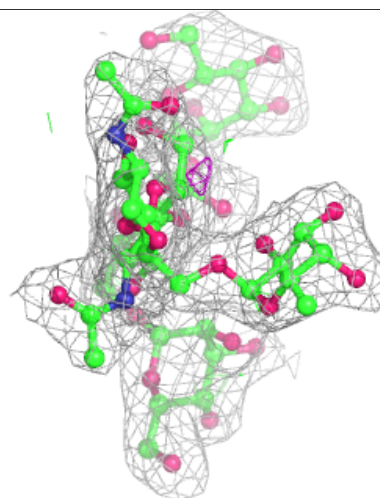
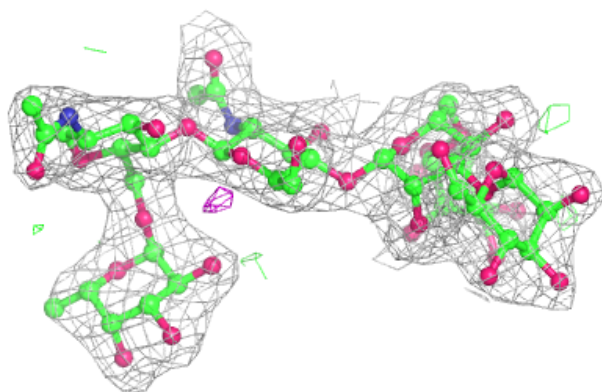
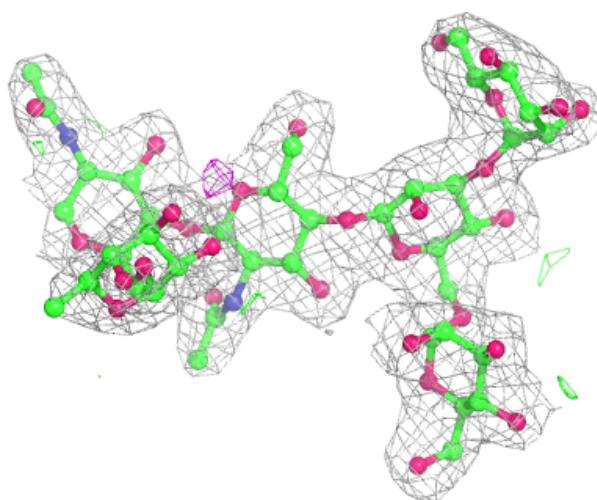
Electron density around Chain M:

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



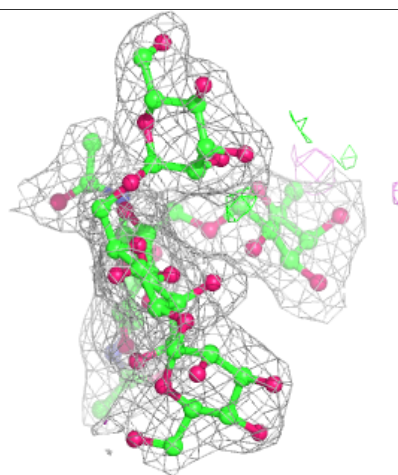
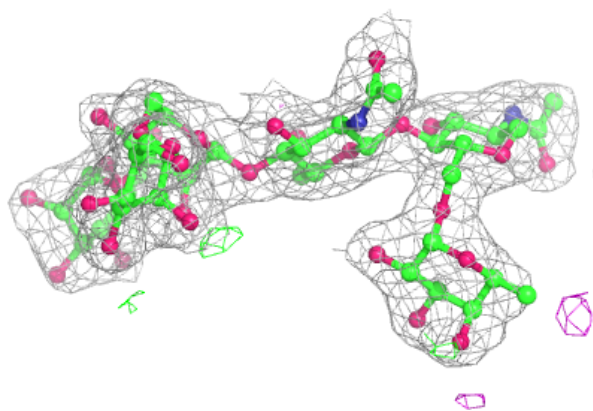
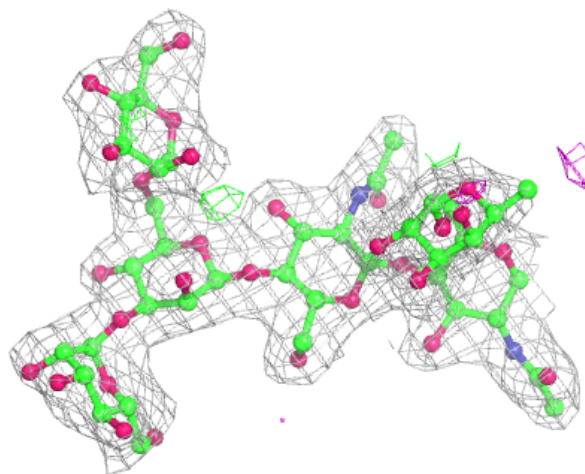
Electron density around Chain J:

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



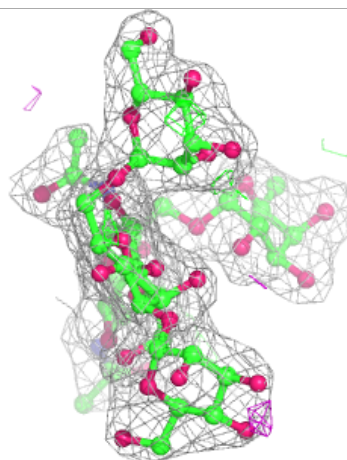
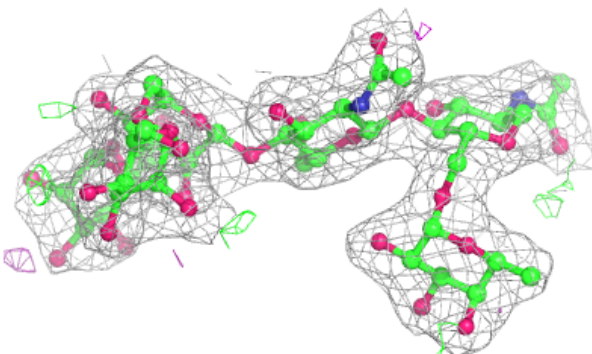
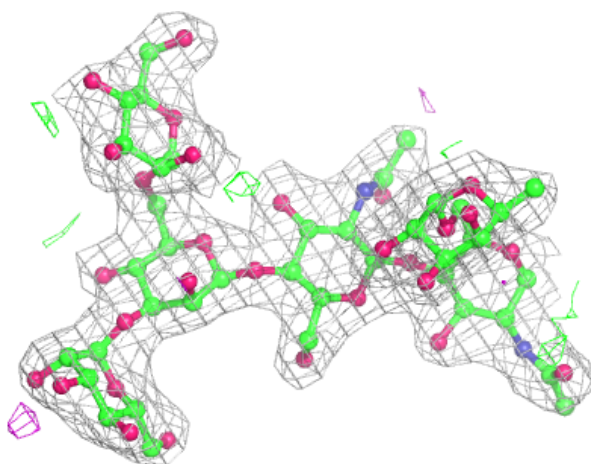
Electron density around Chain L:

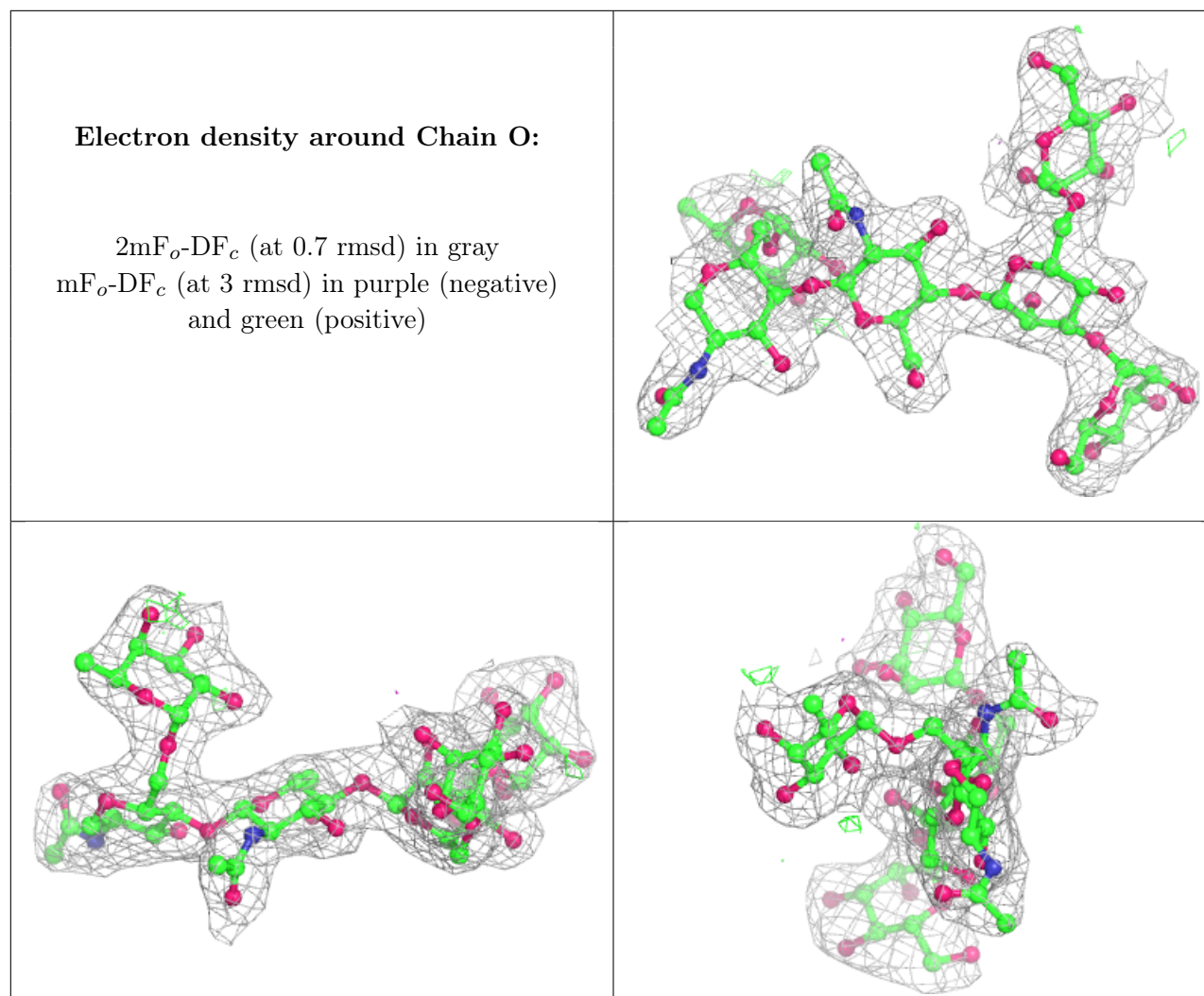
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o-DF_c$ (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
7	NAG	B	602	14/15	0.82	0.17	49,69,72,73	0
7	NAG	E	602	14/15	0.86	0.21	47,57,64,64	0
7	NAG	I	603	14/15	0.87	0.22	89,91,93,93	0
7	NAG	G	602	14/15	0.89	0.24	55,65,70,70	0
7	NAG	I	602	14/15	0.90	0.17	57,61,63,65	0
5	CL	B	604	1/1	0.90	0.17	65,65,65,65	0
9	XS1	G	605	39/39	0.92	0.14	26,36,46,48	32
9	XS1	I	605	39/39	0.93	0.13	37,42,58,60	32
9	XS1	B	605	33/39	0.95	0.12	42,46,52,53	27

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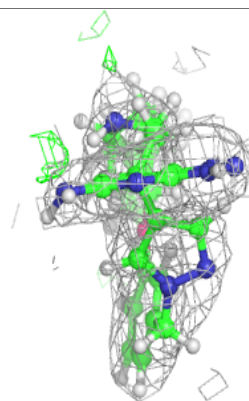
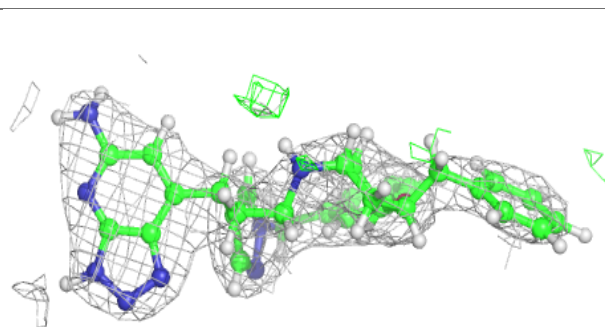
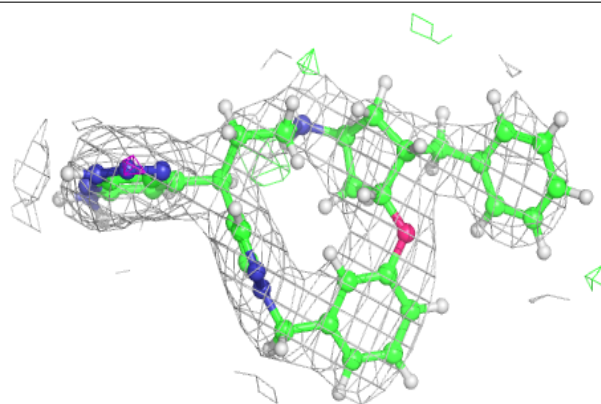
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	XS1	E	604	39/39	0.95	0.12	29,36,50,51	32
6	HEM	G	601	43/43	0.96	0.14	33,34,37,47	0
6	HEM	B	601	43/43	0.96	0.12	33,34,38,48	0
6	HEM	E	601	43/43	0.97	0.14	30,31,36,45	0
5	CL	G	604	1/1	0.97	0.22	58,58,58,58	0
6	HEM	I	601	43/43	0.97	0.12	35,36,40,46	0
8	CA	I	604	1/1	0.98	0.08	35,35,35,35	0
5	CL	A	201	1/1	0.99	0.10	30,30,30,30	0
5	CL	F	201	1/1	0.99	0.09	30,30,30,30	0
8	CA	B	603	1/1	0.99	0.09	38,38,38,38	0
8	CA	E	603	1/1	0.99	0.13	30,30,30,30	0
8	CA	G	603	1/1	0.99	0.14	30,30,30,30	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.

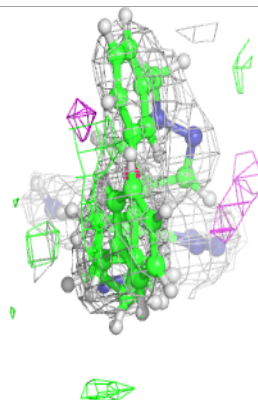
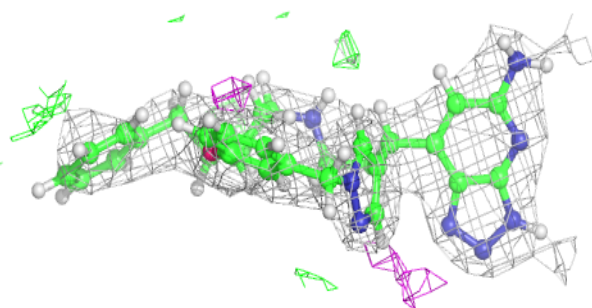
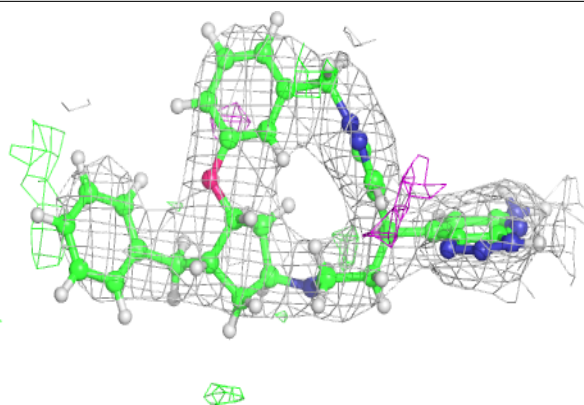
Electron density around XS1 G 605:

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

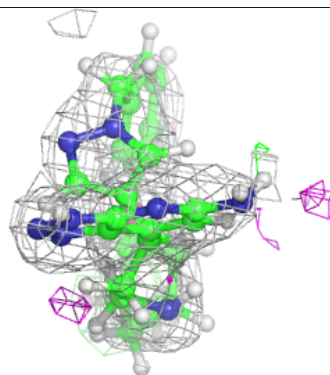
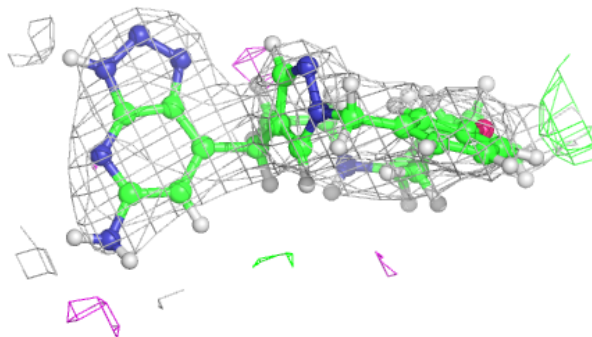
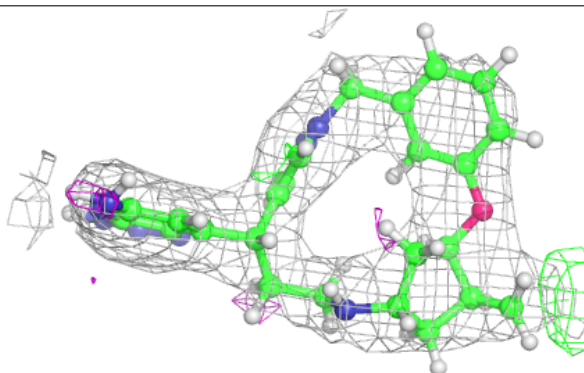


Electron density around XS1 I 605:

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

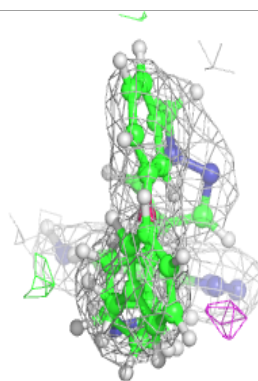
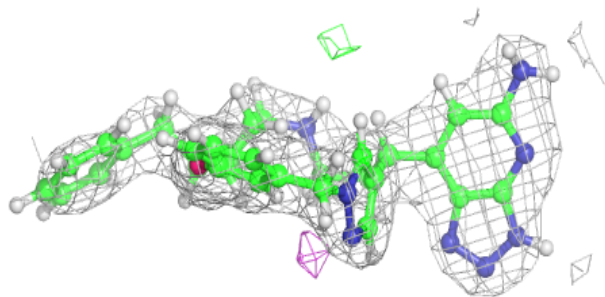
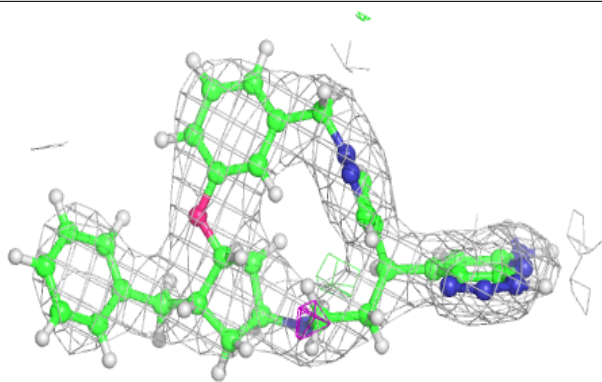
**Electron density around XS1 B 605:**

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



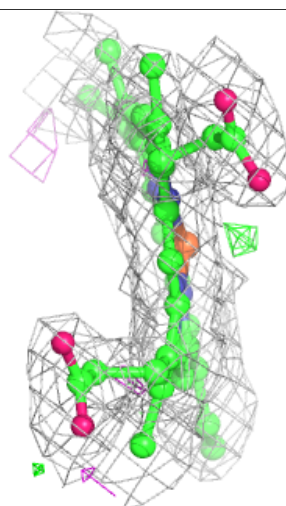
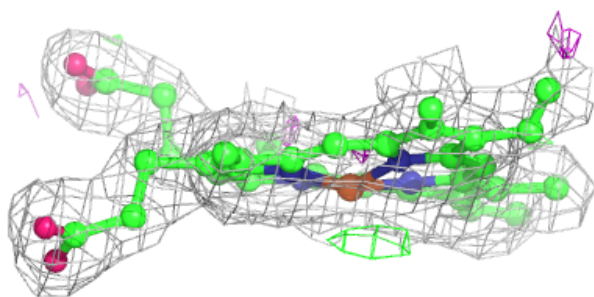
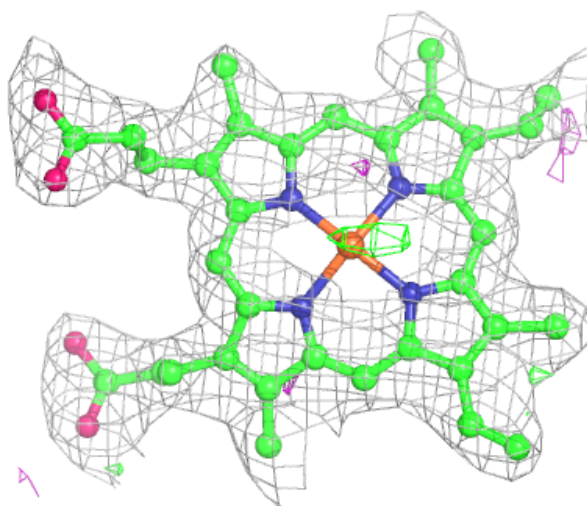
Electron density around XS1 E 604:

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



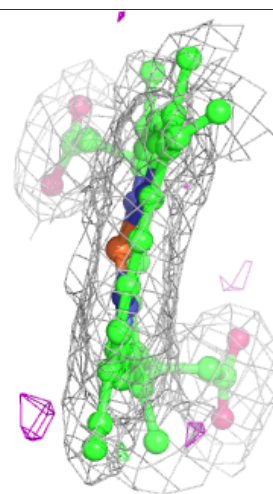
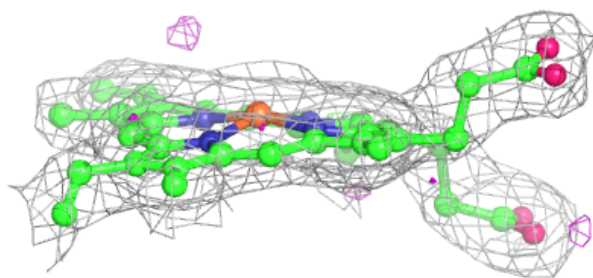
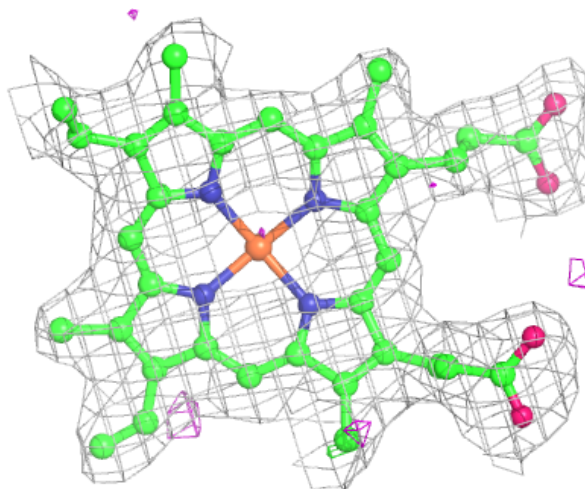
Electron density around HEM G 601:

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



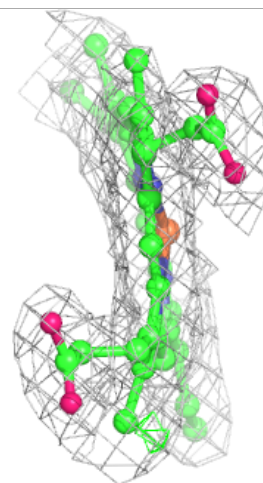
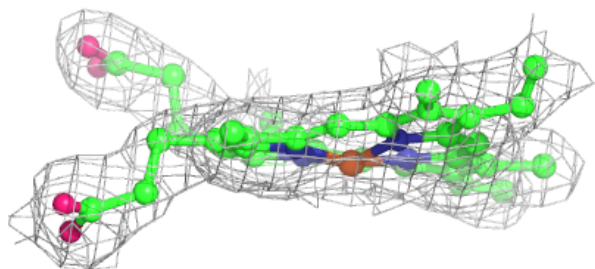
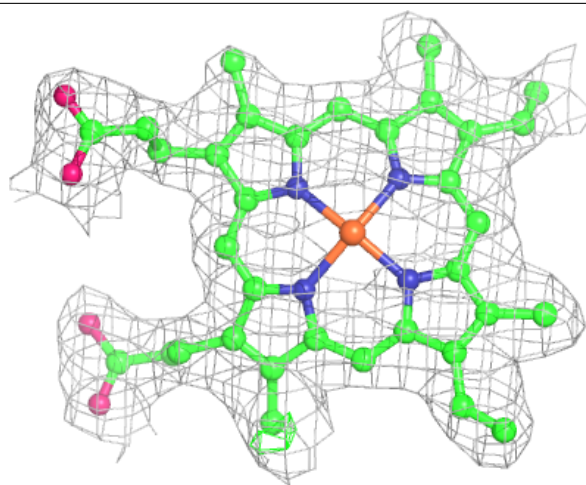
Electron density around HEM B 601:

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



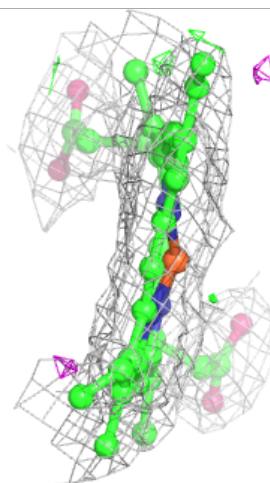
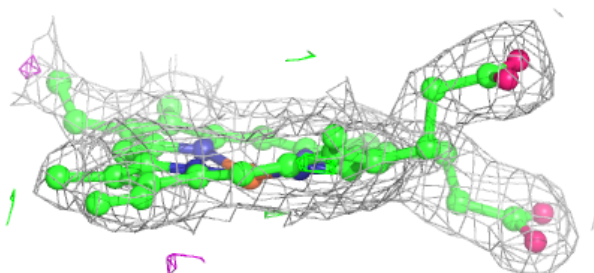
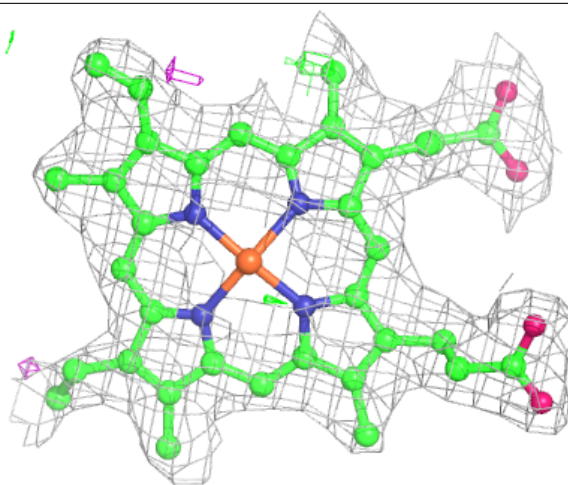
Electron density around HEM E 601:

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



Electron density around HEM I 601:

$2mF_o-DF_c$ (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.