



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:11 PM BST

PDB ID : 4M11
Title : Crystal Structure of Murine Cyclooxygenase-2 Complex with Meloxicam
Authors : Xu, S.; Banerjee, S.; Hermanson, D.J.; Marnett, L.J.
Deposited on : 2013-08-02
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

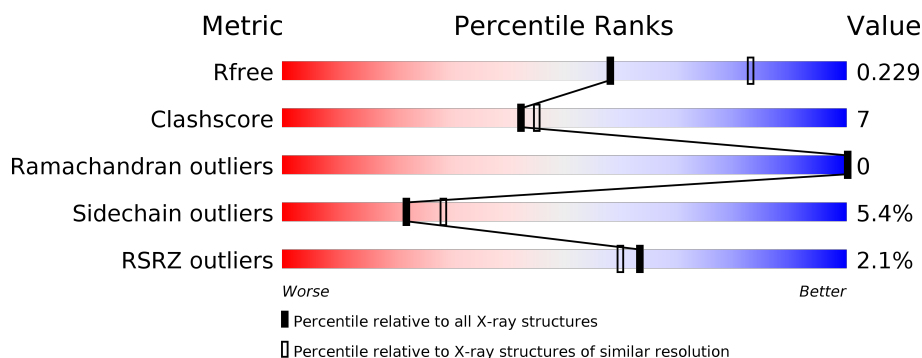
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	552	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 81%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> </div> <div>81% 17% .</div>
1	B	552	<div> <div style="width: 3%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> </div> <div>3% 82% 16% .</div>
1	C	552	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 14%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> </div> <div>2% 84% 14% .</div>
1	D	552	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 86%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> </div> <div>2% 86% 12% .</div>
2	E	2	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> </div> <div>50% 50%</div>
2	F	2	<div> <div style="width: 100%; background-color: green;"></div> </div> <div>100%</div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 50%50%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19520 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 Prostaglandin G/H synthase 2.

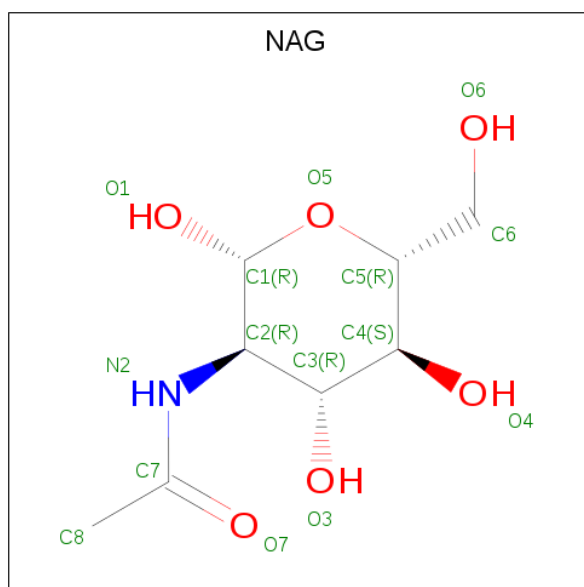
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



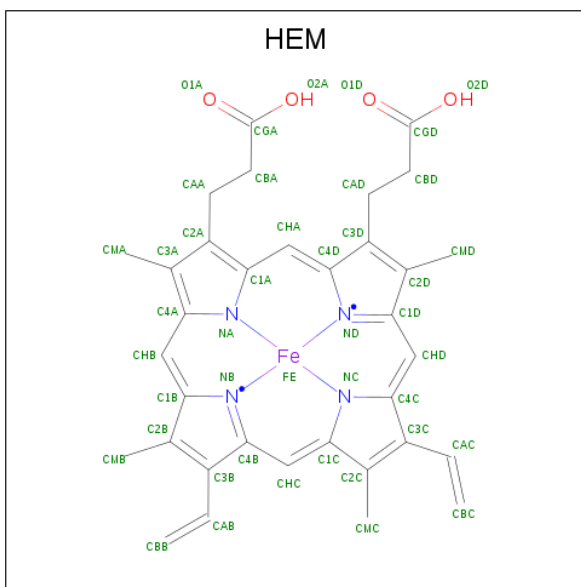
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



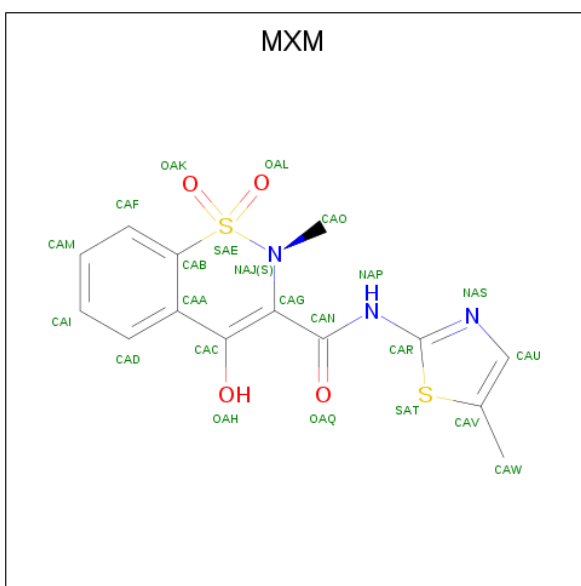
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



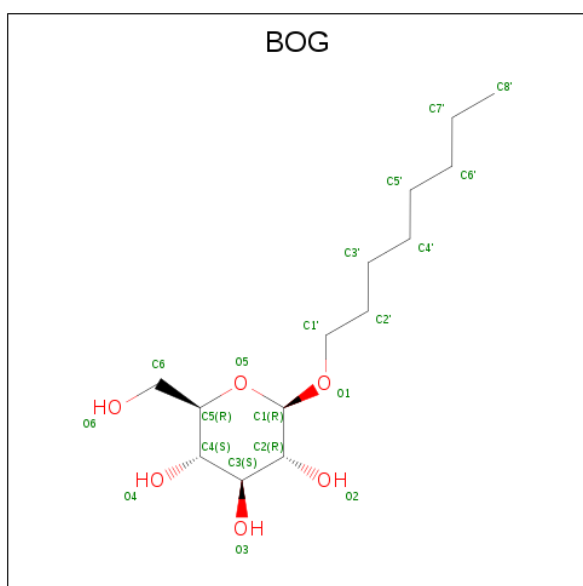
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 4-hydroxy-2-methyl-N-(5-methyl-1,3-thiazol-2-yl)-2H-1,2-benzothiazine-3-carboxamide 1,1-dioxide (three-letter code: MXM) (formula: $C_{14}H_{13}N_3O_4S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	1
			46	28	6	8	4		
5	B	1	Total	C	N	O	S	0	1
			46	28	6	8	4		
5	C	1	Total	C	N	O	S	0	1
			46	28	6	8	4		
5	D	1	Total	C	N	O	S	0	1
			46	28	6	8	4		

- Molecule 6 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			20	14	6		
6	C	1	Total	C	O	0	0
			20	14	6		

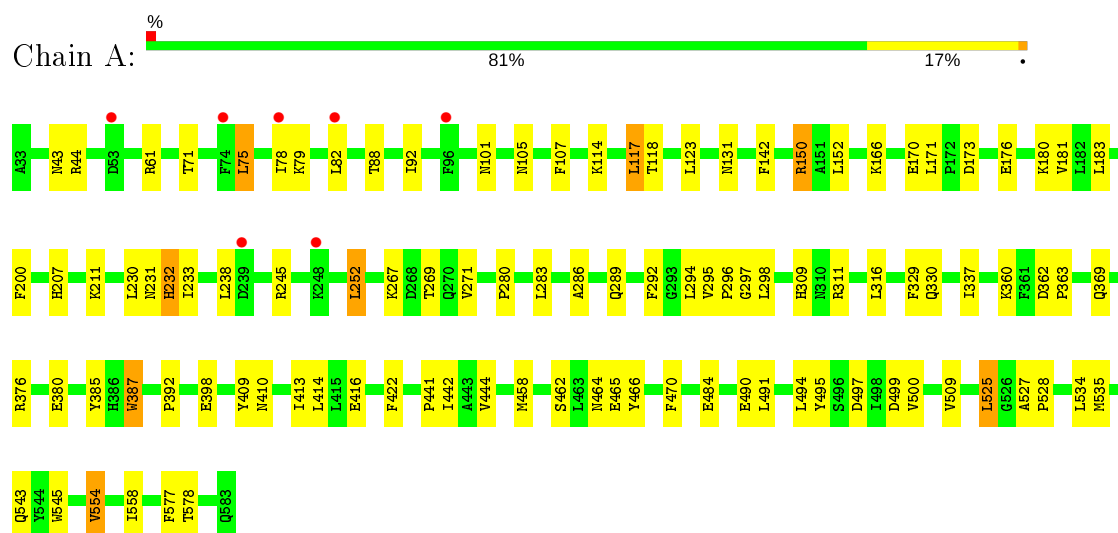
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	232	Total	O	0	0
			232	232		
7	B	216	Total	O	0	0
			216	216		
7	C	261	Total	O	0	0
			261	261		
7	D	295	Total	O	0	0
			295	295		

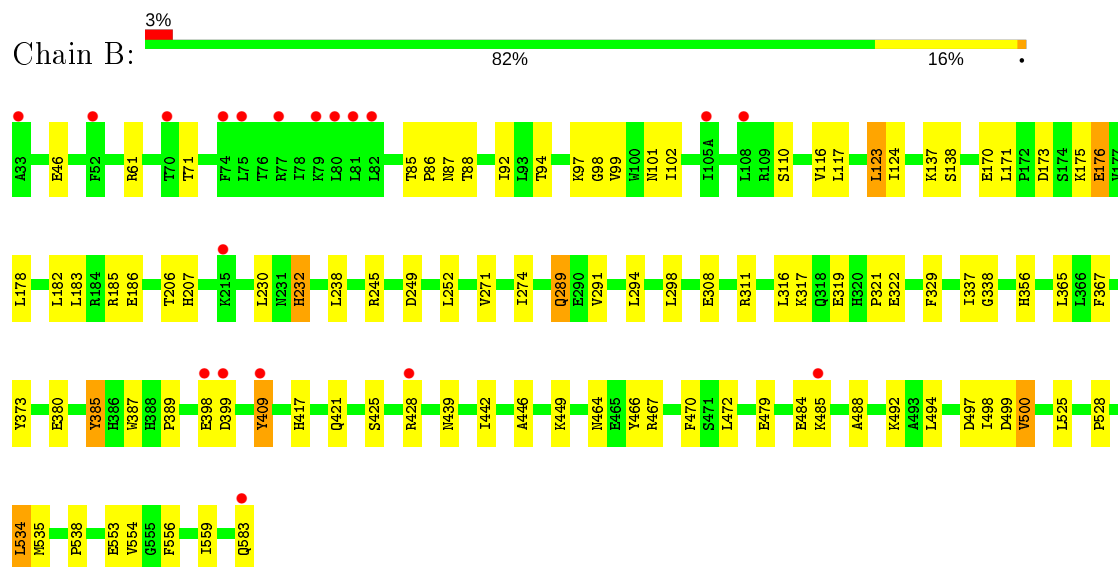
3 Residue-property plots [i](#)

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.

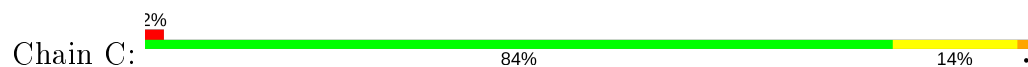
- Molecule 1: Prostaglandin G/H synthase 2

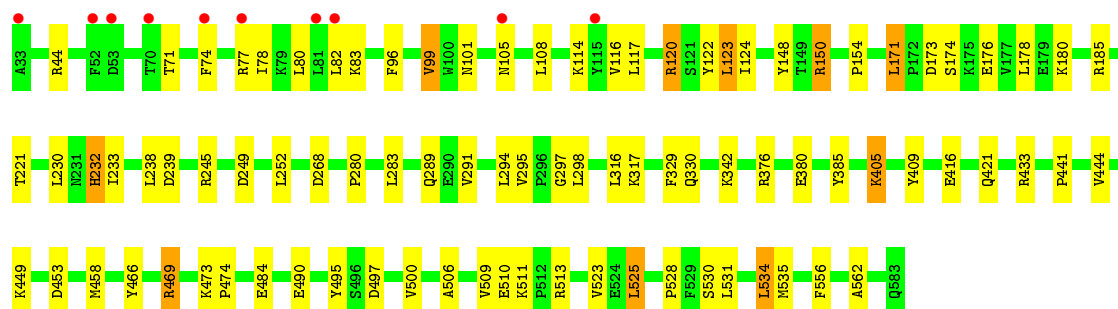


- Molecule 1: Prostaglandin G/H synthase 2

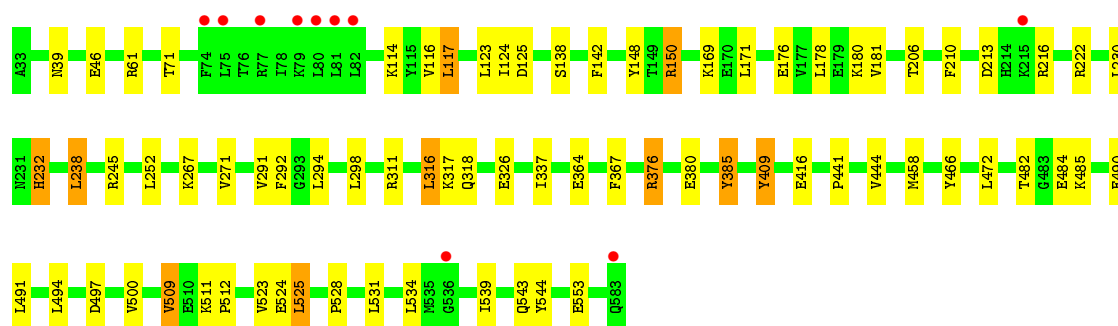
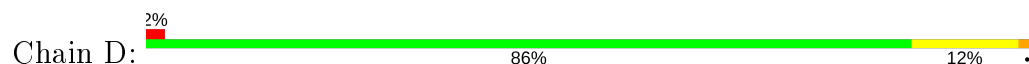


- Molecule 1: Prostaglandin G/H synthase 2





- Molecule 1: Prostaglandin G/H synthase 2



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	121.63Å 133.54Å 180.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.45 49.95 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.95-2.45) 91.0 (49.95-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.202 , 0.231 0.202 , 0.229	Depositor DCC
R_{free} test set	5338 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19520	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2060e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, MXM, NAG, BOG

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	0.42	2/4601 (0.0%)	0.51	0/6239
1	B	0.37	0/4601	0.48	0/6239
1	C	0.34	0/4601	0.49	0/6239
1	D	0.35	0/4601	0.48	0/6239
All	All	0.37	2/18404 (0.0%)	0.49	0/24956

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	PRO	N-CD	5.40	1.55	1.47
1	A	387	TRP	NE1-CE2	-5.38	1.30	1.37

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	4474	0	4372	65	0
1	B	4474	0	4373	69	0
1	C	4474	0	4373	57	0
1	D	4474	0	4373	42	0
2	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
3	A	28	0	26	1	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	1	0
4	A	43	0	30	2	0
4	B	43	0	30	2	0
4	C	43	0	30	2	0
4	D	43	0	30	2	0
5	A	46	0	26	3	0
5	B	46	0	25	7	0
5	C	46	0	26	9	0
5	D	46	0	26	5	0
6	B	20	0	25	1	0
6	C	20	0	25	2	0
7	A	232	0	0	9	0
7	B	216	0	0	9	0
7	C	261	0	0	9	0
7	D	295	0	0	11	0
All	All	19520	0	17968	251	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 7.

All (251) 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:B:97:LYS:HD3	1:B:356:HIS:CG	2.07	0.88
1:B:97:LYS:HD3	1:B:356:HIS:CD2	2.08	0.88
1:D:294:LEU:HD23	1:D:409:TYR:HE1	1.39	0.86
1:D:294:LEU:HD23	1:D:409:TYR:CE1	2.12	0.84
1:C:74:PHE:HD1	1:C:77:ARG:NH2	1.78	0.81
1:A:118:THR:HG21	1:A:369:GLN:HE21	1.45	0.80
1:D:142:PHE:O	1:D:376:ARG:NH2	2.15	0.80
1:D:148:TYR:O	7:D:829:HOH:O	2.02	0.77
1:A:44:ARG:N	7:A:824:HOH:O	1.79	0.77
1:C:123:LEU:O	1:C:469:ARG:NH2	2.17	0.77
1:B:321:PRO:O	7:B:907:HOH:O	2.02	0.76
1:A:166:LYS:HE2	1:A:499:ASP:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG21	1:A:369:GLN:NE2	2.03	0.74
1:C:96:PHE:HB3	1:C:99:VAL:CG1	2.17	0.74
1:B:479:GLU:OE1	1:B:485:LYS:NZ	2.20	0.74
1:C:74:PHE:HD1	1:C:77:ARG:HH21	1.32	0.73
1:C:268:ASP:OD2	7:C:878:HOH:O	2.07	0.72
1:C:473:LYS:NZ	1:C:474:PRO:O	2.22	0.72
1:C:154:PRO:O	7:C:853:HOH:O	2.08	0.72
1:C:150:ARG:NH2	1:C:458:MET:O	2.24	0.70
1:A:44:ARG:CA	7:A:824:HOH:O	2.31	0.70
1:D:216:ARG:NH1	2:H:2:NAG:O7	2.24	0.70
1:B:94:THR:O	1:B:356:HIS:NE2	2.25	0.69
1:C:44:ARG:N	7:C:852:HOH:O	2.22	0.69
1:D:61:ARG:NH1	7:D:752:HOH:O	2.26	0.68
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.76	0.68
1:B:97:LYS:O	1:B:101:ASN:ND2	2.28	0.67
1:C:453:ASP:OD2	7:C:748:HOH:O	2.13	0.67
1:C:511:LYS:O	7:C:901:HOH:O	2.12	0.66
1:A:88:THR:O	1:A:92:ILE:HD12	1.96	0.66
1:B:85:THR:HG22	1:B:87:ASN:H	1.60	0.65
1:B:373:TYR:O	7:B:892:HOH:O	2.15	0.65
1:B:398:GLU:OE1	7:B:882:HOH:O	2.15	0.65
1:B:425:SER:O	1:B:428:ARG:HG2	1.98	0.64
3:D:601:NAG:N2	7:D:883:HOH:O	2.29	0.64
4:C:605:HEM:HBC2	4:C:605:HEM:HHD	1.80	0.63
1:C:280:PRO:HG2	1:C:283:LEU:HD12	1.79	0.63
1:C:295:VAL:HG12	1:C:297:GLY:H	1.64	0.62
1:C:405:LYS:HD2	1:C:405:LYS:H	1.64	0.62
4:A:605:HEM:HHD	4:A:605:HEM:HBC2	1.82	0.62
1:D:523:VAL:HA	5:D:606[B]:MXM:H4	1.80	0.62
1:B:479:GLU:HG2	1:B:488:ALA:HB1	1.80	0.61
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.83	0.61
1:B:446:ALA:O	7:B:849:HOH:O	2.16	0.61
1:A:101:ASN:O	1:A:105:ASN:ND2	2.34	0.60
1:B:479:GLU:HG2	1:B:488:ALA:CB	2.31	0.60
1:D:472:LEU:HD21	1:D:524:GLU:HG3	1.83	0.60
1:D:125:ASP:OD1	7:D:955:HOH:O	2.16	0.60
1:D:497:ASP:HB3	1:D:500:VAL:HG23	1.84	0.60
4:B:605:HEM:HHD	4:B:605:HEM:HBC2	1.84	0.59
1:B:98:GLY:O	1:B:102:ILE:HD12	2.02	0.59
1:D:364:GLU:HB3	7:D:828:HOH:O	2.02	0.59
1:A:295:VAL:HG12	1:A:297:GLY:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ARG:NH2	1:D:458:MET:O	2.33	0.59
1:B:319:GLU:HG3	1:B:554:VAL:HG11	1.85	0.58
1:B:294:LEU:HD22	1:B:409:TYR:HD1	1.68	0.58
1:A:245:ARG:HD3	1:A:329:PHE:CD1	2.39	0.58
1:B:175:LYS:HG3	1:B:449:LYS:HE3	1.86	0.58
4:D:605:HEM:HHD	4:D:605:HEM:HBC2	1.84	0.58
1:C:249:ASP:CG	1:C:317:LYS:HE3	2.25	0.57
1:C:185:ARG:NH1	6:C:607:BOG:H3'1	2.20	0.57
1:C:96:PHE:O	1:C:99:VAL:HG13	2.04	0.57
5:C:606[A]:MXM:OAQ	5:C:606[A]:MXM:NAS	2.35	0.57
1:A:166:LYS:HE2	1:A:499:ASP:CB	2.34	0.56
5:B:606[B]:MXM:OAH	5:B:606[B]:MXM:NAP	2.25	0.56
4:B:605:HEM:HMB1	4:B:605:HEM:HBB2	1.88	0.56
1:C:523:VAL:HA	5:C:606[A]:MXM:H4	1.87	0.56
4:D:605:HEM:HBB2	4:D:605:HEM:HMB1	1.88	0.56
1:A:180:LYS:HD3	1:A:490:GLU:HG3	1.88	0.55
1:A:78:ILE:O	1:A:82:LEU:HD13	2.07	0.55
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.88	0.55
1:C:96:PHE:HB3	1:C:99:VAL:HG13	1.87	0.55
1:A:413:ILE:HG12	3:A:604:NAG:H61	1.88	0.54
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.88	0.54
5:D:606[A]:MXM:NAP	5:D:606[A]:MXM:OAH	2.26	0.54
1:C:523:VAL:HA	5:C:606[B]:MXM:H3	1.90	0.54
4:A:605:HEM:HMB2	4:A:605:HEM:HBB2	1.89	0.54
1:B:175:LYS:CG	1:B:449:LYS:HE3	2.37	0.54
1:C:78:ILE:O	1:C:82:LEU:HD13	2.08	0.54
1:A:44:ARG:HA	7:A:824:HOH:O	1.99	0.53
1:A:311:ARG:NH2	7:A:707:HOH:O	2.34	0.53
1:D:441:PRO:HG2	1:D:444:VAL:HG22	1.91	0.53
1:A:554:VAL:HG22	7:A:837:HOH:O	2.09	0.53
1:C:101:ASN:O	1:C:105:ASN:ND2	2.38	0.53
1:C:96:PHE:HB3	1:C:99:VAL:HG11	1.88	0.53
5:C:606[B]:MXM:OAQ	5:C:606[B]:MXM:SAT	2.67	0.53
1:A:150:ARG:HG3	1:A:152:LEU:O	2.08	0.52
1:B:583:GLN:HA	7:B:850:HOH:O	2.07	0.52
1:C:171:LEU:HD12	7:C:943:HOH:O	2.08	0.52
1:A:294:LEU:HD12	1:A:409:TYR:CE2	2.45	0.52
1:A:554:VAL:O	1:A:558:ILE:HG13	2.10	0.52
1:A:294:LEU:HA	1:A:409:TYR:CE1	2.44	0.52
1:B:230:LEU:HG	1:B:337:ILE:HG12	1.91	0.52
1:A:543:GLN:NE2	7:A:812:HOH:O	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:HG3	1:B:421:GLN:CD	2.30	0.52
1:D:230:LEU:HG	1:D:337:ILE:HG12	1.91	0.52
1:D:180:LYS:HD3	1:D:490:GLU:HG3	1.92	0.52
1:A:398:GLU:OE2	7:A:826:HOH:O	2.19	0.52
1:C:245:ARG:HD3	1:C:329:PHE:CD1	2.45	0.52
1:D:482:THR:HG22	1:D:509:VAL:HG13	1.93	0.51
1:A:181:VAL:HG21	1:A:491:LEU:HD21	1.93	0.51
1:A:207:HIS:CE1	7:A:932:HOH:O	2.63	0.51
1:A:176:GLU:HG2	1:A:494:LEU:HD21	1.93	0.51
1:A:207:HIS:HE1	7:A:932:HOH:O	1.94	0.50
1:C:74:PHE:CD1	1:C:77:ARG:NH2	2.69	0.50
1:B:398:GLU:OE2	1:B:421:GLN:NE2	2.45	0.50
5:A:606[A]:MXM:OAQ	5:A:606[A]:MXM:NAS	2.40	0.50
1:A:183:LEU:HD22	1:A:442:ILE:HD13	1.94	0.50
1:A:294:LEU:HD23	1:A:295:VAL:HG23	1.94	0.50
1:A:495:TYR:O	1:A:497:ASP:N	2.44	0.49
1:B:294:LEU:HD22	1:B:409:TYR:CD1	2.47	0.49
5:D:606[B]:MXM:NAS	5:D:606[B]:MXM:OAQ	2.43	0.49
5:A:606[B]:MXM:OAQ	5:A:606[B]:MXM:SAT	2.70	0.49
1:B:497:ASP:HB3	1:B:500:VAL:HG23	1.94	0.49
5:B:606[A]:MXM:OAQ	5:B:606[A]:MXM:NAS	2.43	0.49
1:C:534:LEU:HD23	5:C:606[A]:MXM:H8	1.93	0.49
1:D:176:GLU:HG2	1:D:494:LEU:HD21	1.94	0.48
1:A:441:PRO:HG2	1:A:444:VAL:HG22	1.96	0.48
5:C:606[B]:MXM:NAP	5:C:606[B]:MXM:OAH	2.38	0.48
1:D:543:GLN:HB2	7:D:919:HOH:O	2.12	0.48
1:B:230:LEU:HD22	1:B:232:HIS:HE1	1.79	0.48
1:B:249:ASP:OD1	1:B:317:LYS:HE3	2.14	0.48
4:C:605:HEM:HBB2	4:C:605:HEM:HMB2	1.96	0.48
1:A:75:LEU:HD23	1:A:79:LYS:HE2	1.96	0.48
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.49	0.48
1:C:230:LEU:HD13	1:C:233:ILE:HD12	1.94	0.48
1:B:467:ARG:HB3	1:B:472:LEU:HB2	1.94	0.48
1:C:534:LEU:HD23	5:C:606[B]:MXM:H8	1.94	0.48
1:B:176:GLU:HG2	1:B:494:LEU:HD21	1.95	0.48
6:C:607:BOG:H2'1	6:C:607:BOG:H5'2	1.62	0.47
1:C:180:LYS:HB3	1:C:490:GLU:HG2	1.96	0.47
1:A:271:VAL:HG22	1:A:286:ALA:HB1	1.96	0.47
1:C:433:ARG:HD3	7:C:942:HOH:O	2.13	0.47
1:B:61:ARG:NH2	7:B:726:HOH:O	2.47	0.47
1:B:85:THR:HG23	1:B:86:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:NH1	1:B:367:PHE:HE2	2.13	0.47
1:A:577:PHE:CE1	1:D:267:LYS:HD2	2.49	0.47
1:B:178:LEU:HD22	1:B:449:LYS:HB2	1.97	0.47
1:B:124:ILE:HD11	1:B:528:PRO:HB2	1.95	0.47
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.97	0.47
1:B:88:THR:O	1:B:92:ILE:HG13	2.15	0.47
1:A:131:ASN:HA	1:A:150:ARG:HB2	1.96	0.47
1:A:166:LYS:CE	1:A:499:ASP:HB2	2.40	0.47
1:D:210:PHE:O	7:D:954:HOH:O	2.20	0.47
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.50	0.46
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.51	0.46
5:B:606[B]:MXM:SAT	5:B:606[B]:MXM:OAQ	2.73	0.46
1:D:169:LYS:HB2	1:D:169:LYS:HE2	1.71	0.46
1:A:296:PRO:HG3	1:A:410:ASN:O	2.15	0.46
1:C:173:ASP:HB3	1:C:176:GLU:HB2	1.98	0.46
1:B:173:ASP:HB3	1:B:176:GLU:HB2	1.96	0.46
1:C:80:LEU:HD23	1:C:83:LYS:HE3	1.98	0.46
1:D:46:GLU:HG2	7:D:963:HOH:O	2.16	0.45
1:D:124:ILE:HD11	1:D:528:PRO:HB2	1.98	0.45
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.45	0.45
1:A:252:LEU:HD22	1:A:309:HIS:CD2	2.51	0.45
1:B:97:LYS:HD3	1:B:356:HIS:CE1	2.51	0.45
1:B:525:LEU:O	1:B:528:PRO:HD2	2.16	0.45
1:D:181:VAL:HG21	1:D:491:LEU:HD21	1.98	0.45
1:B:97:LYS:HD2	1:B:97:LYS:HA	1.57	0.45
5:C:606[A]:MXM:OAQ	5:C:606[A]:MXM:H15	2.17	0.45
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.52	0.44
1:A:232:HIS:HB2	1:A:292:PHE:CE2	2.53	0.44
1:B:308:GLU:OE2	1:B:311:ARG:NH1	2.50	0.44
1:C:294:LEU:HG	1:C:295:VAL:HG23	1.98	0.44
5:C:606[B]:MXM:H15	5:C:606[B]:MXM:OAQ	2.16	0.44
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.18	0.44
1:A:387:TRP:CZ2	5:A:606[A]:MXM:H3	2.52	0.44
1:B:110:SER:OG	1:B:365:LEU:HD21	2.16	0.44
1:D:39:ASN:HA	7:D:972:HOH:O	2.17	0.44
1:A:211:LYS:NZ	1:A:231:ASN:OD1	2.45	0.44
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.53	0.44
1:B:534:LEU:HD23	5:B:606[A]:MXM:H8	1.99	0.44
1:C:122:TYR:CE2	1:C:123:LEU:HD13	2.52	0.44
1:A:527:ALA:HB3	1:A:528:PRO:HD3	2.00	0.44
1:B:123:LEU:HA	1:B:123:LEU:HD13	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:O	1:C:531:LEU:HD23	2.19	0.43
1:C:405:LYS:CD	1:C:405:LYS:H	2.27	0.43
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.53	0.43
1:B:479:GLU:CG	1:B:488:ALA:HB1	2.48	0.43
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.91	0.43
1:C:495:TYR:O	1:C:497:ASP:N	2.51	0.43
1:A:173:ASP:HB3	1:A:176:GLU:HB2	2.00	0.43
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.78	0.43
1:B:464:ASN:ND2	1:B:499:ASP:OD1	2.43	0.43
1:A:462:SER:OG	1:A:465:GLU:HG2	2.19	0.42
1:B:185:ARG:HD3	6:B:607:BOG:H8'2	2.01	0.42
1:C:174:SER:OG	1:C:449:LYS:NZ	2.45	0.42
1:C:342:LYS:HG2	1:C:562:ALA:HB3	2.00	0.42
1:D:311:ARG:NH1	7:D:873:HOH:O	2.32	0.42
1:A:497:ASP:HB3	1:A:500:VAL:CG2	2.48	0.42
1:C:123:LEU:HA	1:C:123:LEU:HD12	1.86	0.42
1:C:421:GLN:OE1	7:C:815:HOH:O	2.21	0.42
1:B:46:GLU:CD	1:B:137:LYS:HZ1	2.23	0.42
1:D:364:GLU:HG2	1:D:367:PHE:CE2	2.54	0.42
1:B:417:HIS:O	7:B:811:HOH:O	2.22	0.42
1:C:44:ARG:HH11	1:C:44:ARG:HG2	1.85	0.42
1:C:150:ARG:NH1	7:C:721:HOH:O	2.52	0.42
1:D:117:LEU:HA	1:D:117:LEU:HD12	1.90	0.42
1:D:238:LEU:HD23	1:D:238:LEU:HA	1.93	0.42
1:B:398:GLU:HG3	1:B:421:GLN:OE1	2.20	0.42
1:B:338:GLY:HA3	1:B:559:ILE:HD13	2.02	0.42
5:B:606[A]:MXM:OAH	5:B:606[A]:MXM:NAP	2.53	0.42
1:C:506:ALA:O	1:C:510:GLU:HB2	2.20	0.42
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.79	0.42
1:D:245:ARG:NH2	1:D:326:GLU:OE2	2.40	0.42
1:C:441:PRO:HG2	1:C:444:VAL:HG22	2.01	0.42
1:B:178:LEU:HA	1:B:182:LEU:HD12	2.02	0.41
1:B:398:GLU:HB3	1:B:399:ASP:H	1.29	0.41
1:D:206:THR:HG21	1:D:385:TYR:CE1	2.55	0.41
1:A:330:GLN:HB3	1:B:138:SER:HB2	2.02	0.41
1:A:360:LYS:NZ	1:A:362:ASP:OD2	2.53	0.41
1:A:150:ARG:NH2	1:A:458:MET:O	2.43	0.41
1:B:245:ARG:HD3	1:B:329:PHE:CD1	2.56	0.41
1:B:289:GLN:OE1	1:B:291:VAL:HG22	2.20	0.41
1:C:230:LEU:HD22	1:C:232:HIS:HE1	1.85	0.41
5:D:606[B]:MXM:H15	5:D:606[B]:MXM:OAQ	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASN:O	1:A:44:ARG:HB2	2.21	0.41
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.55	0.41
1:B:553:GLU:HG3	7:B:751:HOH:O	2.19	0.41
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.89	0.41
1:C:124:ILE:HD11	1:C:528:PRO:HB2	2.01	0.41
1:C:108:LEU:HA	1:C:108:LEU:HD12	1.82	0.41
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.56	0.41
1:D:213:ASP:HB2	1:D:222:ARG:HG3	2.03	0.41
1:A:577:PHE:HE1	1:D:267:LYS:HD2	1.86	0.41
1:A:230:LEU:HD13	1:A:233:ILE:HD12	2.03	0.41
1:B:117:LEU:HA	1:B:117:LEU:HD12	1.84	0.41
1:B:322:GLU:N	1:B:322:GLU:OE2	2.42	0.41
1:B:554:VAL:HG23	7:B:867:HOH:O	2.21	0.41
1:C:148:TYR:CZ	1:C:221:THR:HB	2.56	0.41
1:C:525:LEU:O	1:C:528:PRO:HD2	2.21	0.41
1:B:389:PRO:HB3	1:B:439:ASN:HB3	2.01	0.41
1:D:232:HIS:HB2	1:D:292:PHE:CE2	2.56	0.41
1:D:531:LEU:HD13	5:D:606[B]:MXM:CAF	2.51	0.41
1:B:97:LYS:HD3	1:B:356:HIS:ND1	2.34	0.40
1:C:330:GLN:HB3	1:D:138:SER:HB2	2.03	0.40
1:D:525:LEU:O	1:D:528:PRO:HD2	2.21	0.40
1:D:539:ILE:HA	1:D:544:TYR:HB3	2.03	0.40
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.86	0.40
1:A:142:PHE:CE2	1:B:538:PRO:HG3	2.57	0.40
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.56	0.40
1:D:511:LYS:HA	1:D:512:PRO:HD3	1.96	0.40
1:A:464:ASN:HD22	1:A:499:ASP:HA	1.86	0.40
1:B:230:LEU:HA	1:B:232:HIS:CE1	2.57	0.40
1:C:530:SER:O	1:C:534:LEU:HD22	2.22	0.40
1:A:200:PHE:CE1	1:A:295:VAL:HG11	2.57	0.40
1:B:387:TRP:CZ2	5:B:606[A]:MXM:H3	2.57	0.40
1:B:534:LEU:HD23	5:B:606[B]:MXM:H8	2.04	0.40
1:C:294:LEU:HA	1:C:409:TYR:CE1	2.57	0.40
1:D:553:GLU:HG3	7:D:779:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/552 (100%)	531 (96%)	19 (4%)	0	100	100
1	B	550/552 (100%)	529 (96%)	21 (4%)	0	100	100
1	C	550/552 (100%)	534 (97%)	16 (3%)	0	100	100
1	D	550/552 (100%)	535 (97%)	15 (3%)	0	100	100
All	All	2200/2208 (100%)	2129 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/493 (100%)	468 (95%)	25 (5%)	24	31
1	B	493/493 (100%)	467 (95%)	26 (5%)	22	29
1	C	493/493 (100%)	464 (94%)	29 (6%)	19	25
1	D	493/493 (100%)	467 (95%)	26 (5%)	22	29
All	All	1972/1972 (100%)	1866 (95%)	106 (5%)	22	28

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	75	LEU

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Mol	Chain	Res	Type
1	A	107	PHE
1	A	114	LYS
1	A	117	LEU
1	A	150	ARG
1	A	170	GLU
1	A	171	LEU
1	A	232	HIS
1	A	238	LEU
1	A	252	LEU
1	A	267	LYS
1	A	289	GLN
1	A	298	LEU
1	A	316	LEU
1	A	376	ARG
1	A	385	TYR
1	A	416	GLU
1	A	484	GLU
1	A	509	VAL
1	A	525	LEU
1	A	534	LEU
1	A	535	MET
1	A	554	VAL
1	A	578	THR
1	B	71	THR
1	B	99	VAL
1	B	116	VAL
1	B	123	LEU
1	B	170	GLU
1	B	171	LEU
1	B	176	GLU
1	B	186	GLU
1	B	207	HIS
1	B	232	HIS
1	B	238	LEU
1	B	252	LEU
1	B	271	VAL
1	B	289	GLN
1	B	298	LEU
1	B	316	LEU
1	B	385	TYR
1	B	409	TYR
1	B	442	ILE

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Mol	Chain	Res	Type
1	B	484	GLU
1	B	492	LYS
1	B	498	ILE
1	B	500	VAL
1	B	534	LEU
1	B	535	MET
1	B	556	PHE
1	C	71	THR
1	C	99	VAL
1	C	114	LYS
1	C	116	VAL
1	C	120	ARG
1	C	123	LEU
1	C	150	ARG
1	C	171	LEU
1	C	178	LEU
1	C	232	HIS
1	C	238	LEU
1	C	239	ASP
1	C	252	LEU
1	C	289	GLN
1	C	291	VAL
1	C	298	LEU
1	C	316	LEU
1	C	376	ARG
1	C	385	TYR
1	C	405	LYS
1	C	416	GLU
1	C	469	ARG
1	C	484	GLU
1	C	509	VAL
1	C	513	ARG
1	C	525	LEU
1	C	534	LEU
1	C	535	MET
1	C	556	PHE
1	D	71	THR
1	D	114	LYS
1	D	116	VAL
1	D	117	LEU
1	D	123	LEU
1	D	150	ARG

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Mol	Chain	Res	Type
1	D	171	LEU
1	D	178	LEU
1	D	232	HIS
1	D	238	LEU
1	D	252	LEU
1	D	271	VAL
1	D	291	VAL
1	D	298	LEU
1	D	316	LEU
1	D	317	LYS
1	D	318	GLN
1	D	376	ARG
1	D	385	TYR
1	D	409	TYR
1	D	416	GLU
1	D	484	GLU
1	D	485	LYS
1	D	509	VAL
1	D	525	LEU
1	D	534	LEU

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

Mol	Chain	Res	Type
1	A	207	HIS
1	A	270	GLN
1	A	369	GLN
1	B	386	HIS
1	B	421	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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	E	1	1,2	14,14,15	0.61	1 (7%)	17,19,21	0.44	0
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	0.56	0
2	NAG	F	1	1,2	14,14,15	0.51	0	17,19,21	0.47	0
2	NAG	F	2	2	14,14,15	0.51	0	17,19,21	0.74	0
2	NAG	G	1	1,2	14,14,15	0.41	0	17,19,21	0.56	0
2	NAG	G	2	2	14,14,15	0.22	0	17,19,21	0.59	0
2	NAG	H	1	1,2	14,14,15	0.54	0	17,19,21	0.46	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.54	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.01	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

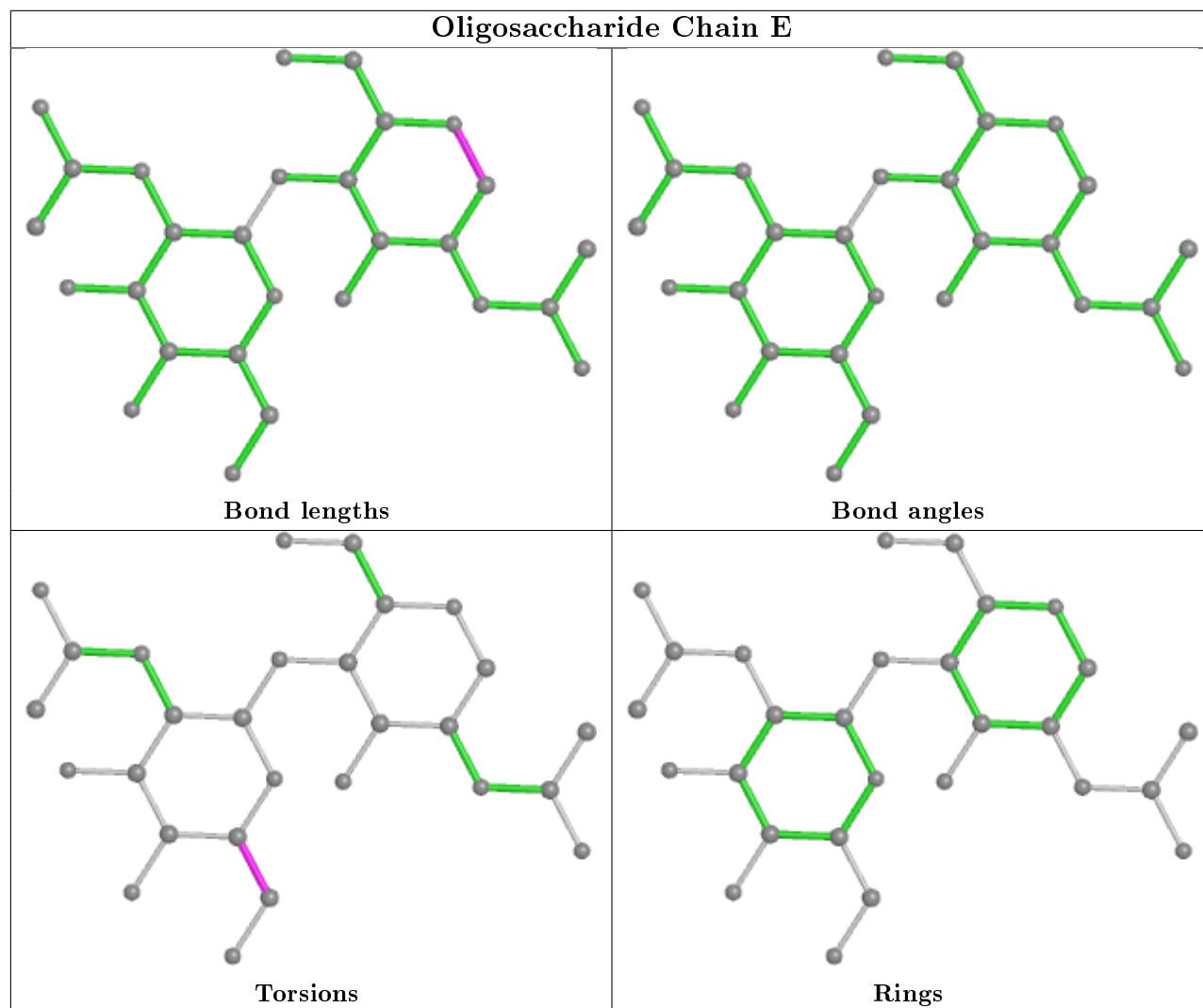
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

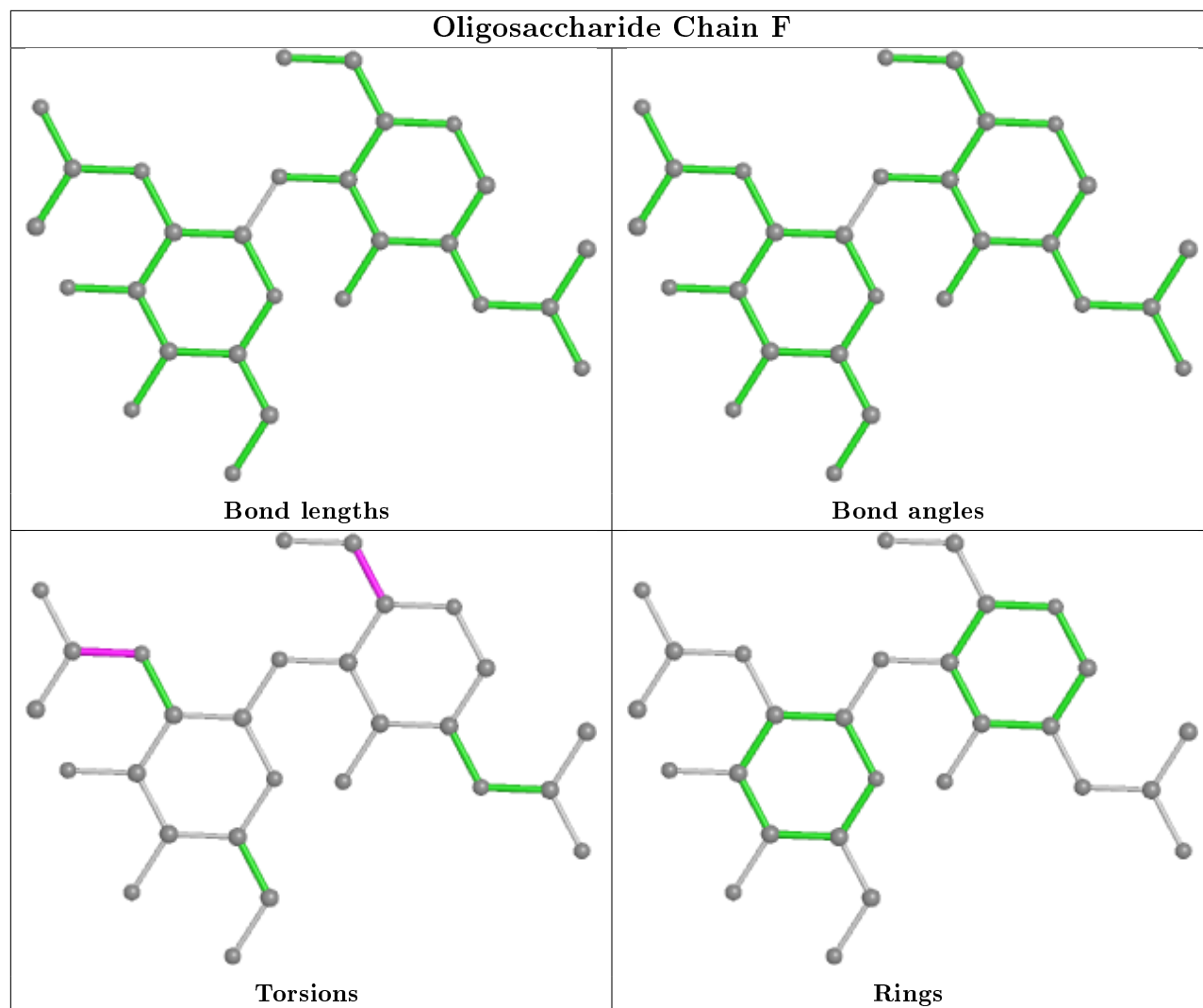
There are no ring outliers.

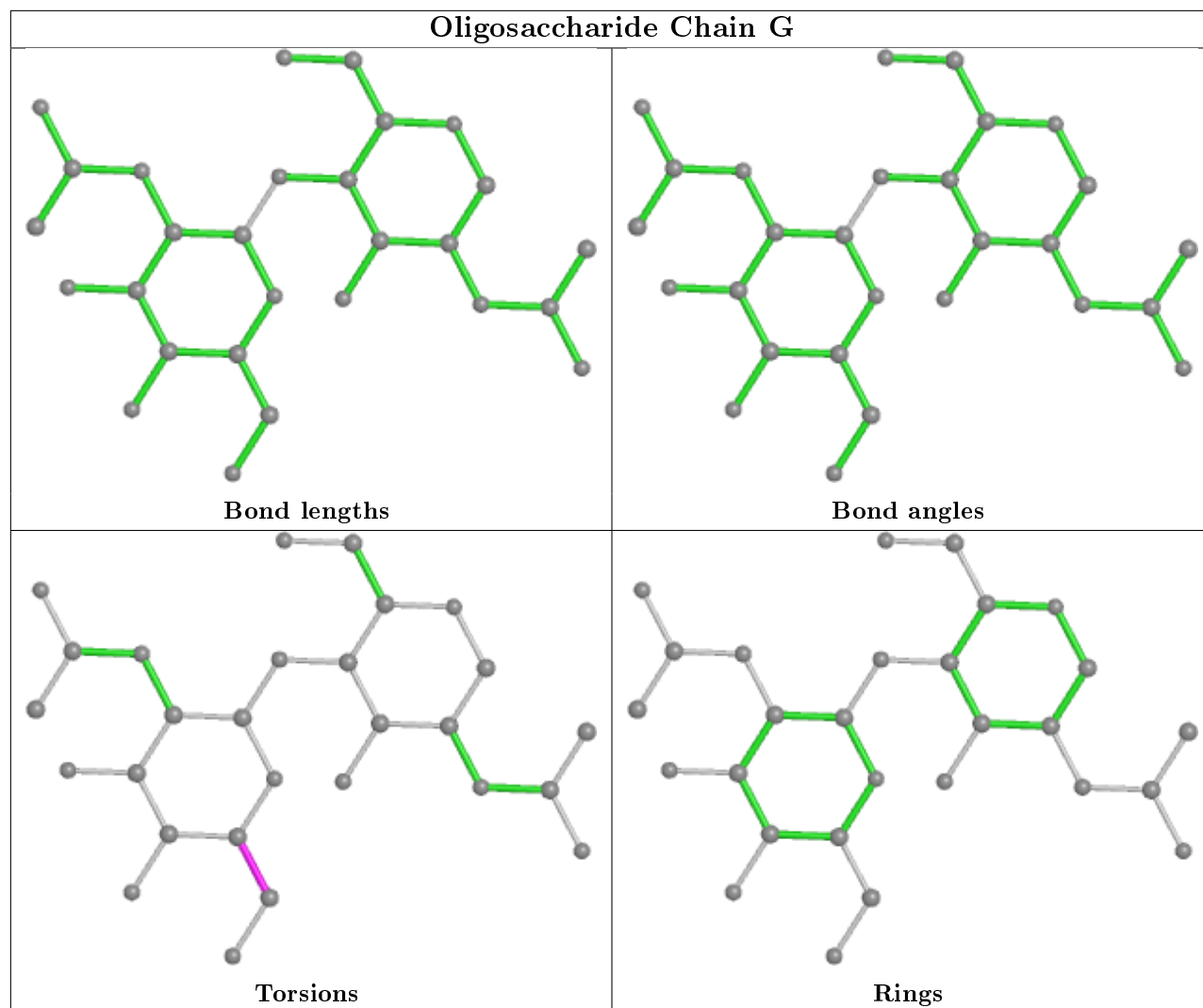
1 monomer is involved in 1 short contact:

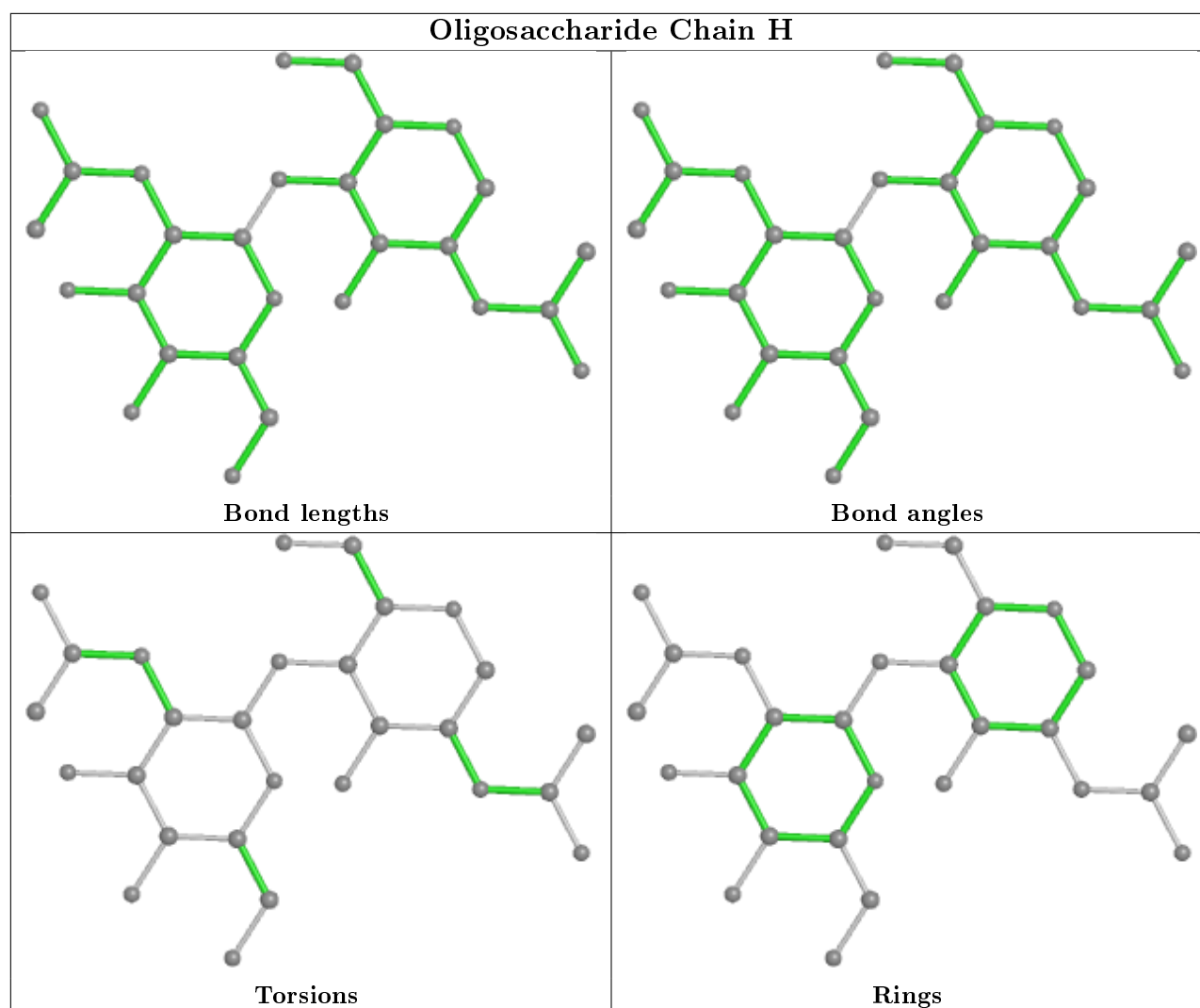
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	1	0

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









5.6 Ligand geometry ⓘ

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MXM	C	606[A]	-	23,25,25	6.38	12 (52%)	32,38,38	5.30	20 (62%)
3	NAG	C	601	1	14,14,15	0.48	0	17,19,21	0.51	0
3	NAG	A	601	1	14,14,15	1.00	1 (7%)	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	601	1	14,14,15	0.67	0	17,19,21	0.49	0
3	NAG	C	604	1	14,14,15	0.89	1 (7%)	17,19,21	0.78	0
4	HEM	A	605	1,7	27,50,50	2.15	5 (18%)	17,82,82	1.75	4 (23%)
3	NAG	B	604	1	14,14,15	0.46	0	17,19,21	0.54	0
4	HEM	B	605	1,7	27,50,50	2.15	5 (18%)	17,82,82	1.62	4 (23%)
5	MXM	A	606[A]	-	23,25,25	5.41	11 (47%)	32,38,38	4.72	19 (59%)
6	BOG	C	607	-	20,20,20	1.63	3 (15%)	25,25,25	1.50	5 (20%)
5	MXM	A	606[B]	-	23,25,25	6.23	10 (43%)	32,38,38	5.06	16 (50%)
3	NAG	D	601	1	14,14,15	0.92	1 (7%)	17,19,21	0.79	0
6	BOG	B	607	-	20,20,20	1.44	2 (10%)	25,25,25	1.65	3 (12%)
4	HEM	D	605	1,7	27,50,50	2.16	6 (22%)	17,82,82	1.67	3 (17%)
3	NAG	D	604	1	14,14,15	0.29	0	17,19,21	0.62	0
4	HEM	C	605	1	27,50,50	2.12	5 (18%)	17,82,82	1.69	4 (23%)
5	MXM	B	606[B]	-	23,25,25	5.23	10 (43%)	32,38,38	4.70	15 (46%)
5	MXM	B	606[A]	-	23,25,25	5.29	10 (43%)	32,38,38	4.67	18 (56%)
5	MXM	D	606[A]	-	23,25,25	6.69	12 (52%)	32,38,38	4.85	19 (59%)
3	NAG	A	604	1	14,14,15	0.77	1 (7%)	17,19,21	0.63	0
5	MXM	D	606[B]	-	23,25,25	6.87	11 (47%)	32,38,38	5.18	18 (56%)
5	MXM	C	606[B]	-	23,25,25	6.93	12 (52%)	32,38,38	4.94	19 (59%)

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
5	MXM	C	606[A]	-	-	0/6/32/32	0/3/3/3
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	604	1	-	2/6/23/26	0/1/1/1
4	HEM	A	605	1,7	-	0/6/54/54	-
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
4	HEM	B	605	1,7	-	0/6/54/54	-
5	MXM	A	606[A]	-	-	0/6/32/32	0/3/3/3
6	BOG	C	607	-	-	9/11/31/31	0/1/1/1
5	MXM	A	606[B]	-	-	0/6/32/32	0/3/3/3
3	NAG	D	601	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BOG	B	607	-	-	6/11/31/31	0/1/1/1
4	HEM	D	605	1,7	-	0/6/54/54	-
3	NAG	D	604	1	-	2/6/23/26	0/1/1/1
4	HEM	C	605	1	-	0/6/54/54	-
5	MXM	B	606[B]	-	-	0/6/32/32	0/3/3/3
5	MXM	B	606[A]	-	-	0/6/32/32	0/3/3/3
5	MXM	D	606[A]	-	-	0/6/32/32	0/3/3/3
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	MXM	D	606[B]	-	-	0/6/32/32	0/3/3/3
5	MXM	C	606[B]	-	-	0/6/32/32	0/3/3/3

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	606[B]	MXM	SAE-NAJ	-23.20	1.33	1.64
5	D	606[A]	MXM	SAE-NAJ	-21.52	1.35	1.64
5	D	606[B]	MXM	SAE-NAJ	-20.94	1.36	1.64
5	C	606[A]	MXM	SAE-NAJ	-20.66	1.36	1.64
5	A	606[B]	MXM	SAE-NAJ	-17.48	1.40	1.64
5	B	606[A]	MXM	CAB-SAE	-16.42	1.52	1.75
5	A	606[B]	MXM	CAB-SAE	-15.62	1.53	1.75
5	A	606[A]	MXM	CAB-SAE	-15.48	1.53	1.75
5	D	606[B]	MXM	CAB-SAE	-13.68	1.56	1.75
5	D	606[B]	MXM	OAL-SAE	13.45	1.58	1.43
5	C	606[A]	MXM	OAL-SAE	12.97	1.57	1.43
5	D	606[A]	MXM	OAL-SAE	12.63	1.57	1.43
5	A	606[A]	MXM	SAE-NAJ	-12.45	1.47	1.64
5	D	606[A]	MXM	CAB-SAE	-12.39	1.58	1.75
5	C	606[B]	MXM	OAL-SAE	12.35	1.57	1.43
5	B	606[B]	MXM	CAB-SAE	-12.26	1.58	1.75
5	C	606[A]	MXM	CAB-SAE	-11.78	1.58	1.75
5	B	606[B]	MXM	CAV-SAT	-10.44	1.54	1.74
5	B	606[B]	MXM	SAE-NAJ	-10.42	1.50	1.64
5	A	606[B]	MXM	OAK-SAE	10.05	1.54	1.43
5	B	606[A]	MXM	SAE-NAJ	-10.02	1.50	1.64
5	C	606[A]	MXM	OAK-SAE	10.01	1.54	1.43
5	C	606[B]	MXM	CAB-SAE	-9.97	1.61	1.75
5	A	606[A]	MXM	OAL-SAE	9.97	1.54	1.43
5	D	606[B]	MXM	OAK-SAE	9.95	1.54	1.43
5	C	606[B]	MXM	CAV-SAT	-9.89	1.55	1.74
5	C	606[B]	MXM	OAK-SAE	9.85	1.54	1.43
5	B	606[A]	MXM	OAL-SAE	9.63	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606[B]	MXM	OAL-SAE	9.58	1.54	1.43
5	A	606[B]	MXM	OAL-SAE	9.50	1.54	1.43
5	D	606[A]	MXM	OAK-SAE	9.43	1.54	1.43
5	A	606[A]	MXM	OAK-SAE	9.25	1.53	1.43
5	B	606[A]	MXM	OAK-SAE	9.12	1.53	1.43
5	B	606[B]	MXM	OAK-SAE	9.05	1.53	1.43
5	A	606[B]	MXM	CAV-SAT	-8.58	1.58	1.74
5	D	606[B]	MXM	CAV-SAT	-7.27	1.60	1.74
5	D	606[A]	MXM	CAG-NAJ	-5.98	1.37	1.44
5	B	606[A]	MXM	CAG-CAC	5.59	1.44	1.36
5	A	606[A]	MXM	CAG-CAC	5.56	1.44	1.36
4	B	605	HEM	C3D-C2D	5.46	1.53	1.37
4	A	605	HEM	C3D-C2D	5.45	1.53	1.37
5	B	606[B]	MXM	CAG-CAC	5.40	1.43	1.36
4	D	605	HEM	C3D-C2D	5.39	1.53	1.37
4	C	605	HEM	C3D-C2D	5.39	1.53	1.37
5	A	606[B]	MXM	CAG-CAC	5.28	1.43	1.36
5	C	606[A]	MXM	CAG-CAC	5.13	1.43	1.36
5	D	606[B]	MXM	CAG-CAC	5.11	1.43	1.36
5	C	606[B]	MXM	CAG-CAC	5.06	1.43	1.36
5	D	606[B]	MXM	CAG-NAJ	-4.98	1.38	1.44
5	D	606[A]	MXM	CAG-CAC	4.91	1.43	1.36
4	D	605	HEM	C3C-C2C	-4.88	1.33	1.40
5	C	606[B]	MXM	CAO-NAJ	4.82	1.54	1.48
5	B	606[B]	MXM	CAG-NAJ	-4.65	1.38	1.44
4	B	605	HEM	C3C-C2C	-4.61	1.34	1.40
4	C	605	HEM	C3C-C2C	-4.57	1.34	1.40
5	B	606[A]	MXM	CAG-NAJ	-4.52	1.39	1.44
5	D	606[A]	MXM	CAV-SAT	-4.51	1.65	1.74
5	D	606[A]	MXM	CAA-CAB	-4.50	1.35	1.40
4	A	605	HEM	C3C-C2C	-4.50	1.34	1.40
5	A	606[A]	MXM	CAG-NAJ	-4.32	1.39	1.44
5	D	606[B]	MXM	CAG-CAN	-4.23	1.37	1.46
5	D	606[B]	MXM	CAR-NAP	-4.15	1.29	1.36
5	D	606[A]	MXM	CAG-CAN	-4.14	1.37	1.46
5	C	606[B]	MXM	CAG-NAJ	-4.13	1.39	1.44
6	C	607	BOG	O2-C2	-4.11	1.33	1.43
5	D	606[B]	MXM	CAA-CAC	-4.06	1.39	1.45
5	C	606[B]	MXM	CAA-CAB	-4.05	1.36	1.40
6	B	607	BOG	O2-C2	-4.01	1.33	1.43
5	C	606[B]	MXM	CAG-CAN	-3.96	1.37	1.46
4	C	605	HEM	C3C-CAC	3.88	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	C3B-C2B	-3.86	1.35	1.40
4	C	605	HEM	C3B-CAB	3.86	1.55	1.47
4	A	605	HEM	C3B-CAB	3.81	1.55	1.47
4	B	605	HEM	C3B-CAB	3.81	1.55	1.47
4	D	605	HEM	C3B-CAB	3.77	1.55	1.47
5	B	606[A]	MXM	CAV-SAT	-3.74	1.67	1.74
5	D	606[A]	MXM	CAO-NAJ	3.73	1.52	1.48
4	D	605	HEM	C3B-C2B	-3.72	1.35	1.40
4	B	605	HEM	C3B-C2B	-3.70	1.35	1.40
4	A	605	HEM	C3C-CAC	3.66	1.55	1.47
5	C	606[A]	MXM	CAG-NAJ	-3.57	1.40	1.44
4	B	605	HEM	C3C-CAC	3.54	1.55	1.47
4	D	605	HEM	C3C-CAC	3.54	1.55	1.47
5	C	606[A]	MXM	CAG-CAN	-3.51	1.38	1.46
5	A	606[B]	MXM	CAG-NAJ	-3.47	1.40	1.44
5	D	606[A]	MXM	CAA-CAC	-3.41	1.40	1.45
5	C	606[A]	MXM	CAV-SAT	-3.29	1.68	1.74
5	B	606[B]	MXM	CAA-CAB	-3.26	1.37	1.40
4	C	605	HEM	C3B-C2B	-3.25	1.35	1.40
5	A	606[A]	MXM	CAV-SAT	-3.24	1.68	1.74
5	C	606[B]	MXM	CAA-CAC	-3.20	1.40	1.45
5	A	606[B]	MXM	CAA-CAB	-3.20	1.37	1.40
5	C	606[A]	MXM	CAA-CAC	-3.17	1.40	1.45
5	B	606[B]	MXM	CAG-CAN	-3.16	1.39	1.46
5	D	606[B]	MXM	CAA-CAB	-3.16	1.37	1.40
5	A	606[B]	MXM	CAA-CAC	-3.14	1.40	1.45
5	C	606[A]	MXM	CAA-CAB	-3.06	1.37	1.40
5	B	606[B]	MXM	CAA-CAC	-3.05	1.40	1.45
6	C	607	BOG	O3-C3	-3.04	1.35	1.43
5	D	606[A]	MXM	CAR-NAP	-3.03	1.31	1.36
3	A	601	NAG	C1-C2	2.98	1.56	1.52
5	A	606[A]	MXM	CAA-CAB	-2.94	1.37	1.40
5	B	606[A]	MXM	CAA-CAB	-2.87	1.37	1.40
5	A	606[B]	MXM	CAG-CAN	-2.87	1.40	1.46
3	C	604	NAG	O5-C1	-2.82	1.39	1.43
3	D	601	NAG	O5-C1	2.75	1.48	1.43
6	B	607	BOG	O3-C3	-2.68	1.36	1.43
5	A	606[A]	MXM	CAG-CAN	-2.62	1.40	1.46
5	B	606[A]	MXM	CAG-CAN	-2.56	1.40	1.46
5	A	606[A]	MXM	CAA-CAC	-2.52	1.41	1.45
3	A	604	NAG	O5-C1	-2.50	1.39	1.43
5	C	606[A]	MXM	CAR-NAP	-2.48	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606[A]	MXM	CAA-CAC	-2.28	1.42	1.45
6	C	607	BOG	O4-C4	-2.15	1.37	1.43
5	C	606[A]	MXM	CAO-NAJ	2.11	1.50	1.48
4	D	605	HEM	CAA-C2A	2.04	1.55	1.52
5	A	606[A]	MXM	CAU-CAV	-2.01	1.32	1.37
5	C	606[B]	MXM	CAR-NAP	-2.00	1.33	1.36

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	606[B]	MXM	CAO-NAJ-SAE	13.27	137.78	116.94
5	C	606[A]	MXM	OAL-SAE-OAK	-13.22	102.37	118.59
5	D	606[B]	MXM	OAL-SAE-OAK	-13.11	102.51	118.59
5	D	606[A]	MXM	OAL-SAE-OAK	-12.69	103.02	118.59
5	C	606[B]	MXM	OAL-SAE-OAK	-12.66	103.06	118.59
5	A	606[B]	MXM	CAO-NAJ-SAE	12.40	136.42	116.94
5	B	606[B]	MXM	CAO-NAJ-SAE	12.32	136.28	116.94
5	A	606[A]	MXM	CAO-NAJ-SAE	11.88	135.60	116.94
5	C	606[A]	MXM	CAO-NAJ-SAE	11.83	135.52	116.94
5	B	606[A]	MXM	CAO-NAJ-SAE	11.66	135.26	116.94
5	C	606[B]	MXM	CAO-NAJ-SAE	11.52	135.03	116.94
5	D	606[A]	MXM	CAO-NAJ-SAE	11.49	134.99	116.94
5	A	606[B]	MXM	CAB-SAE-NAJ	11.15	116.50	101.91
5	A	606[B]	MXM	CAB-CAA-CAC	-10.09	114.69	120.47
5	C	606[B]	MXM	CAB-SAE-NAJ	10.07	115.09	101.91
5	A	606[B]	MXM	OAL-SAE-OAK	-9.82	106.54	118.59
5	D	606[A]	MXM	CAB-CAA-CAC	-9.61	114.97	120.47
5	B	606[B]	MXM	OAL-SAE-OAK	-9.58	106.84	118.59
5	B	606[B]	MXM	CAG-NAJ-SAE	-9.50	100.25	113.15
5	B	606[A]	MXM	CAB-SAE-NAJ	9.42	114.24	101.91
5	A	606[A]	MXM	CAB-SAE-NAJ	9.39	114.20	101.91
5	A	606[B]	MXM	CAG-NAJ-SAE	-9.31	100.52	113.15
5	B	606[A]	MXM	OAL-SAE-OAK	-9.30	107.18	118.59
5	B	606[B]	MXM	CAB-SAE-NAJ	9.29	114.06	101.91
5	A	606[A]	MXM	OAL-SAE-OAK	-9.28	107.20	118.59
5	D	606[A]	MXM	CAB-SAE-NAJ	9.27	114.05	101.91
5	B	606[A]	MXM	CAG-NAJ-SAE	-9.21	100.64	113.15
5	A	606[A]	MXM	CAG-NAJ-SAE	-9.17	100.71	113.15
5	D	606[B]	MXM	CAB-CAA-CAC	-9.04	115.30	120.47
5	C	606[A]	MXM	CAB-SAE-NAJ	9.03	113.73	101.91
5	B	606[B]	MXM	CAB-CAA-CAC	-8.97	115.34	120.47
5	C	606[B]	MXM	CAB-CAA-CAC	-8.56	115.57	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	606[B]	MXM	CAB-SAE-NAJ	8.17	112.61	101.91
5	D	606[B]	MXM	CAG-NAJ-SAE	-7.98	102.32	113.15
5	A	606[A]	MXM	CAW-CAV-SAT	7.46	128.10	119.88
5	C	606[A]	MXM	OAL-SAE-NAJ	7.45	113.62	108.14
5	D	606[B]	MXM	OAL-SAE-NAJ	7.43	113.61	108.14
5	C	606[A]	MXM	CAB-CAA-CAC	-7.30	116.30	120.47
5	C	606[A]	MXM	OAK-SAE-NAJ	-7.29	102.78	108.14
5	A	606[A]	MXM	CAB-CAA-CAC	-7.29	116.30	120.47
5	B	606[A]	MXM	CAB-CAA-CAC	-7.29	116.30	120.47
5	A	606[B]	MXM	OAK-SAE-NAJ	-7.26	102.80	108.14
5	C	606[B]	MXM	CAO-NAJ-CAG	-7.21	105.16	115.09
5	D	606[A]	MXM	CAO-NAJ-CAG	-7.05	105.38	115.09
5	B	606[A]	MXM	CAW-CAV-SAT	6.96	127.56	119.88
5	C	606[A]	MXM	CAG-NAJ-SAE	-6.83	103.88	113.15
5	C	606[A]	MXM	CAW-CAV-SAT	6.61	127.17	119.88
5	A	606[B]	MXM	CAO-NAJ-CAG	-6.61	105.99	115.09
5	D	606[B]	MXM	OAK-SAE-NAJ	-6.59	103.30	108.14
5	D	606[A]	MXM	CAG-NAJ-SAE	-6.58	104.22	113.15
5	C	606[B]	MXM	CAG-NAJ-SAE	-6.54	104.28	113.15
5	A	606[A]	MXM	CAA-CAB-SAE	-6.47	109.47	117.26
5	C	606[A]	MXM	CAA-CAB-SAE	-6.46	109.49	117.26
5	B	606[A]	MXM	CAA-CAB-SAE	-6.41	109.54	117.26
5	B	606[B]	MXM	CAO-NAJ-CAG	-6.38	106.30	115.09
5	C	606[B]	MXM	OAK-SAE-NAJ	-6.18	103.59	108.14
5	D	606[A]	MXM	OAL-SAE-CAB	6.16	117.02	109.13
5	C	606[B]	MXM	CAA-CAB-SAE	-6.12	109.89	117.26
5	D	606[B]	MXM	CAO-NAJ-CAG	-6.02	106.81	115.09
5	C	606[A]	MXM	CAC-CAG-NAJ	-5.94	116.07	120.86
5	B	606[B]	MXM	OAH-CAC-CAG	-5.83	117.25	122.66
5	C	606[A]	MXM	CAO-NAJ-CAG	-5.82	107.08	115.09
5	D	606[B]	MXM	OAL-SAE-CAB	5.76	116.51	109.13
5	B	606[B]	MXM	CAA-CAB-SAE	-5.74	110.36	117.26
5	A	606[B]	MXM	OAL-SAE-NAJ	5.62	112.28	108.14
5	B	606[A]	MXM	OAH-CAC-CAG	-5.61	117.46	122.66
5	A	606[B]	MXM	CAA-CAB-SAE	-5.52	110.61	117.26
5	C	606[B]	MXM	OAL-SAE-CAB	5.19	115.79	109.13
5	D	606[A]	MXM	CAA-CAB-SAE	-5.04	111.19	117.26
5	A	606[A]	MXM	OAH-CAC-CAG	-5.02	118.00	122.66
5	D	606[B]	MXM	CAA-CAB-SAE	-5.01	111.22	117.26
5	B	606[B]	MXM	CAA-CAC-CAG	4.98	125.85	122.65
5	D	606[A]	MXM	CAW-CAV-SAT	4.95	125.33	119.88
5	C	606[A]	MXM	OAL-SAE-CAB	4.85	115.34	109.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606[B]	MXM	OAH-CAC-CAG	-4.78	118.23	122.66
5	A	606[A]	MXM	CAC-CAG-NAJ	-4.73	117.05	120.86
5	B	606[A]	MXM	CAC-CAG-NAJ	-4.67	117.09	120.86
5	C	606[A]	MXM	CAR-NAP-CAN	-4.63	115.19	126.64
5	C	606[A]	MXM	CAC-CAG-CAN	4.59	125.10	120.87
6	B	607	BOG	C1'-O1-C1	4.59	121.45	113.84
5	A	606[A]	MXM	CAO-NAJ-CAG	-4.52	108.87	115.09
5	B	606[A]	MXM	CAO-NAJ-CAG	-4.51	108.89	115.09
4	A	605	HEM	CBD-CAD-C3D	-4.50	104.18	112.48
5	D	606[B]	MXM	CAR-NAP-CAN	-4.46	115.61	126.64
5	D	606[A]	MXM	OAK-SAE-NAJ	-4.42	104.89	108.14
5	D	606[B]	MXM	CAC-CAG-NAJ	-4.34	117.36	120.86
5	C	606[B]	MXM	OAH-CAC-CAG	-4.31	118.66	122.66
4	D	605	HEM	CBD-CAD-C3D	-4.19	104.76	112.48
5	D	606[B]	MXM	CAW-CAV-SAT	4.11	124.41	119.88
5	A	606[A]	MXM	OAL-SAE-NAJ	4.10	111.16	108.14
4	C	605	HEM	CBD-CAD-C3D	-3.91	105.27	112.48
5	A	606[B]	MXM	OAK-SAE-CAB	-3.91	104.12	109.13
5	B	606[A]	MXM	OAL-SAE-NAJ	3.90	111.01	108.14
5	B	606[B]	MXM	OAK-SAE-NAJ	-3.87	105.30	108.14
5	A	606[A]	MXM	CAR-NAP-CAN	-3.83	117.16	126.64
5	B	606[A]	MXM	CAA-CAC-CAG	3.80	125.09	122.65
5	B	606[B]	MXM	OAL-SAE-NAJ	3.75	110.90	108.14
5	D	606[A]	MXM	OAH-CAC-CAG	-3.74	119.19	122.66
5	A	606[B]	MXM	CAW-CAV-SAT	3.71	123.97	119.88
5	C	606[A]	MXM	OAH-CAC-CAG	-3.67	119.25	122.66
5	B	606[A]	MXM	CAR-NAP-CAN	-3.66	117.58	126.64
5	C	606[B]	MXM	CAC-CAG-NAJ	-3.56	117.99	120.86
5	C	606[B]	MXM	OAL-SAE-NAJ	3.55	110.76	108.14
5	C	606[A]	MXM	OAQ-CAN-CAG	-3.52	115.01	122.03
6	B	607	BOG	O5-C5-C4	3.38	115.83	109.69
5	C	606[A]	MXM	CAF-CAB-SAE	3.31	125.79	120.56
4	C	605	HEM	CBA-CAA-C2A	-3.30	106.40	112.49
5	D	606[B]	MXM	OAH-CAC-CAG	-3.28	119.61	122.66
5	C	606[B]	MXM	CAW-CAV-SAT	3.26	123.47	119.88
5	C	606[B]	MXM	CAR-NAP-CAN	-3.25	118.59	126.64
4	B	605	HEM	CBD-CAD-C3D	-3.21	106.56	112.48
5	A	606[A]	MXM	CAA-CAC-CAG	3.21	124.71	122.65
5	D	606[A]	MXM	CAC-CAG-NAJ	-3.20	118.28	120.86
5	B	606[B]	MXM	CAW-CAV-SAT	3.20	123.41	119.88
5	D	606[A]	MXM	OAL-SAE-NAJ	3.18	110.48	108.14
6	C	607	BOG	C1'-O1-C1	3.16	119.08	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606[B]	MXM	OAL-SAE-CAB	3.13	113.14	109.13
5	C	606[A]	MXM	CAG-CAN-NAP	3.10	119.51	115.26
5	A	606[A]	MXM	OAK-SAE-NAJ	-3.08	105.87	108.14
5	A	606[A]	MXM	CAG-CAN-NAP	3.05	119.45	115.26
5	C	606[A]	MXM	CAA-CAC-CAG	3.00	124.58	122.65
5	A	606[A]	MXM	CAC-CAG-CAN	3.00	123.63	120.87
5	C	606[B]	MXM	CAD-CAA-CAB	2.96	121.23	118.05
6	B	607	BOG	O1-C1-C2	-2.96	103.68	108.30
5	B	606[A]	MXM	CAG-CAN-NAP	2.93	119.28	115.26
6	C	607	BOG	C1-O5-C5	2.89	119.37	113.69
5	C	606[B]	MXM	CAA-CAC-CAG	2.87	124.49	122.65
5	A	606[B]	MXM	CAA-CAC-CAG	2.86	124.48	122.65
5	C	606[B]	MXM	OAQ-CAN-CAG	-2.80	116.44	122.03
5	A	606[B]	MXM	CAR-NAP-CAN	-2.75	119.84	126.64
5	B	606[B]	MXM	CAF-CAB-SAE	2.74	124.89	120.56
5	B	606[A]	MXM	CAC-CAG-CAN	2.72	123.38	120.87
5	D	606[B]	MXM	CAC-CAG-CAN	2.67	123.33	120.87
5	D	606[A]	MXM	OAK-SAE-CAB	-2.54	105.88	109.13
4	D	605	HEM	CBA-CAA-C2A	-2.52	107.84	112.49
5	A	606[A]	MXM	OAQ-CAN-CAG	-2.51	117.03	122.03
4	A	605	HEM	CBA-CAA-C2A	-2.49	107.89	112.49
6	C	607	BOG	O5-C5-C4	2.47	114.19	109.69
5	D	606[A]	MXM	CAD-CAA-CAB	2.47	120.70	118.05
5	C	606[B]	MXM	CAF-CAB-SAE	2.41	124.38	120.56
5	B	606[B]	MXM	CAR-NAP-CAN	-2.41	120.69	126.64
4	C	605	HEM	CMB-C2B-C3B	2.38	129.14	124.68
5	A	606[B]	MXM	CAC-CAG-NAJ	-2.35	118.97	120.86
5	B	606[A]	MXM	OAQ-CAN-CAG	-2.33	117.38	122.03
4	B	605	HEM	CAA-CBA-CGA	-2.32	108.78	112.67
6	C	607	BOG	O2-C2-C3	-2.32	104.99	110.35
5	B	606[B]	MXM	OAL-SAE-CAB	2.31	112.09	109.13
4	A	605	HEM	CMB-C2B-C3B	2.30	128.98	124.68
5	A	606[A]	MXM	CAF-CAB-SAE	2.27	124.14	120.56
5	D	606[B]	MXM	CAD-CAA-CAB	2.24	120.45	118.05
4	B	605	HEM	CMB-C2B-C3B	2.23	128.85	124.68
5	C	606[B]	MXM	CAG-CAN-NAP	2.22	118.30	115.26
4	D	605	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
5	C	606[A]	MXM	CAD-CAA-CAB	2.18	120.39	118.05
5	D	606[A]	MXM	CAN-CAG-NAJ	2.16	120.98	116.30
5	B	606[A]	MXM	CAF-CAB-SAE	2.15	123.96	120.56
5	B	606[A]	MXM	OAK-SAE-NAJ	-2.13	106.57	108.14
4	C	605	HEM	C1D-C2D-C3D	-2.11	105.53	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	HEM	CBA-CAA-C2A	-2.10	108.61	112.49
5	D	606[A]	MXM	CAR-NAP-CAN	-2.10	121.44	126.64
5	D	606[A]	MXM	CAI-CAD-CAA	-2.10	115.85	119.81
5	D	606[A]	MXM	CAA-CAC-CAG	2.05	123.97	122.65
4	A	605	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
5	D	606[B]	MXM	OAK-SAE-CAB	-2.02	106.54	109.13
6	C	607	BOG	O3-C3-C2	-2.02	105.68	110.35
5	A	606[A]	MXM	CAW-CAV-CAU	-2.02	121.63	126.35
5	D	606[B]	MXM	CAI-CAD-CAA	-2.01	116.02	119.81

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	607	BOG	C4-C5-C6-O6
6	B	607	BOG	C4-C5-C6-O6
6	B	607	BOG	O5-C5-C6-O6
6	C	607	BOG	O5-C5-C6-O6
3	D	604	NAG	O5-C5-C6-O6
3	A	604	NAG	O5-C5-C6-O6
3	D	604	NAG	C4-C5-C6-O6
6	C	607	BOG	C2'-C3'-C4'-C5'
3	C	604	NAG	O5-C5-C6-O6
6	B	607	BOG	C3'-C4'-C5'-C6'
6	B	607	BOG	C4'-C5'-C6'-C7'
6	C	607	BOG	C3'-C4'-C5'-C6'
3	A	604	NAG	C4-C5-C6-O6
6	B	607	BOG	O1-C1'-C2'-C3'
6	C	607	BOG	O1-C1'-C2'-C3'
6	C	607	BOG	C1'-C2'-C3'-C4'
3	C	604	NAG	C4-C5-C6-O6
6	C	607	BOG	C2'-C1'-O1-C1
6	B	607	BOG	C2'-C1'-O1-C1
6	C	607	BOG	C2-C1-O1-C1'
6	C	607	BOG	C5'-C6'-C7'-C8'

There are no ring outliers.

16 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	606[A]	MXM	4	0

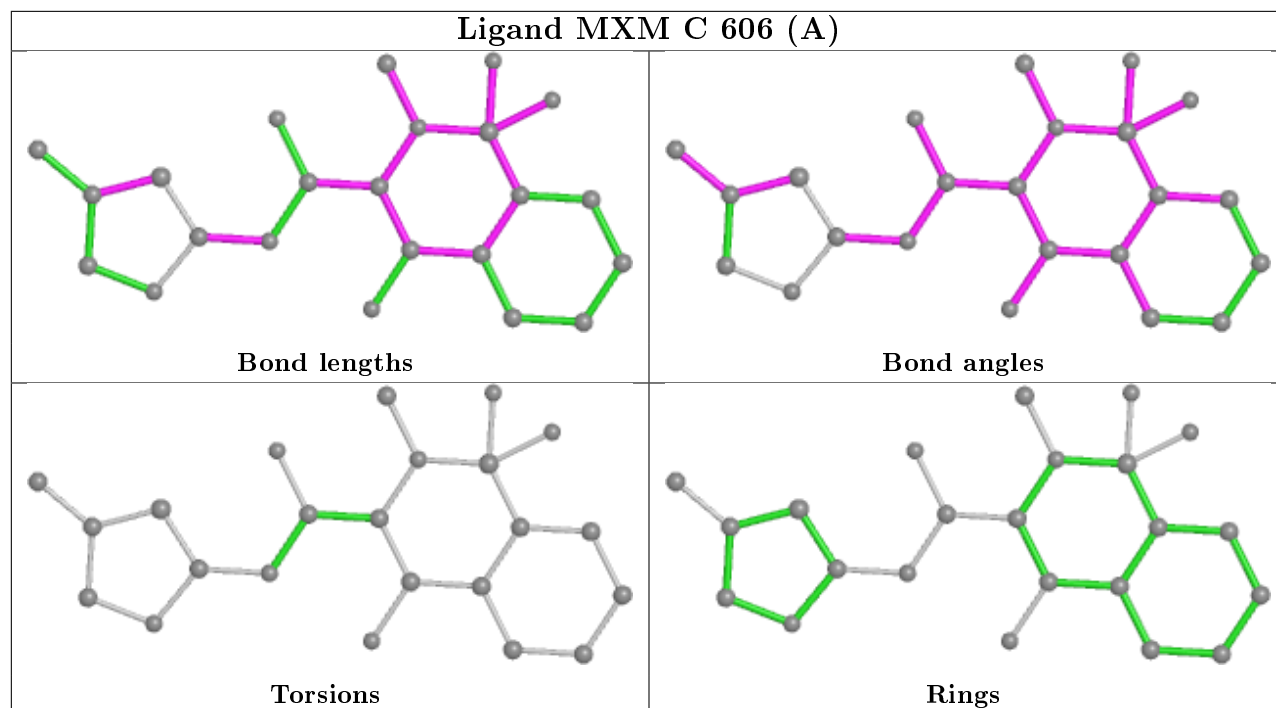
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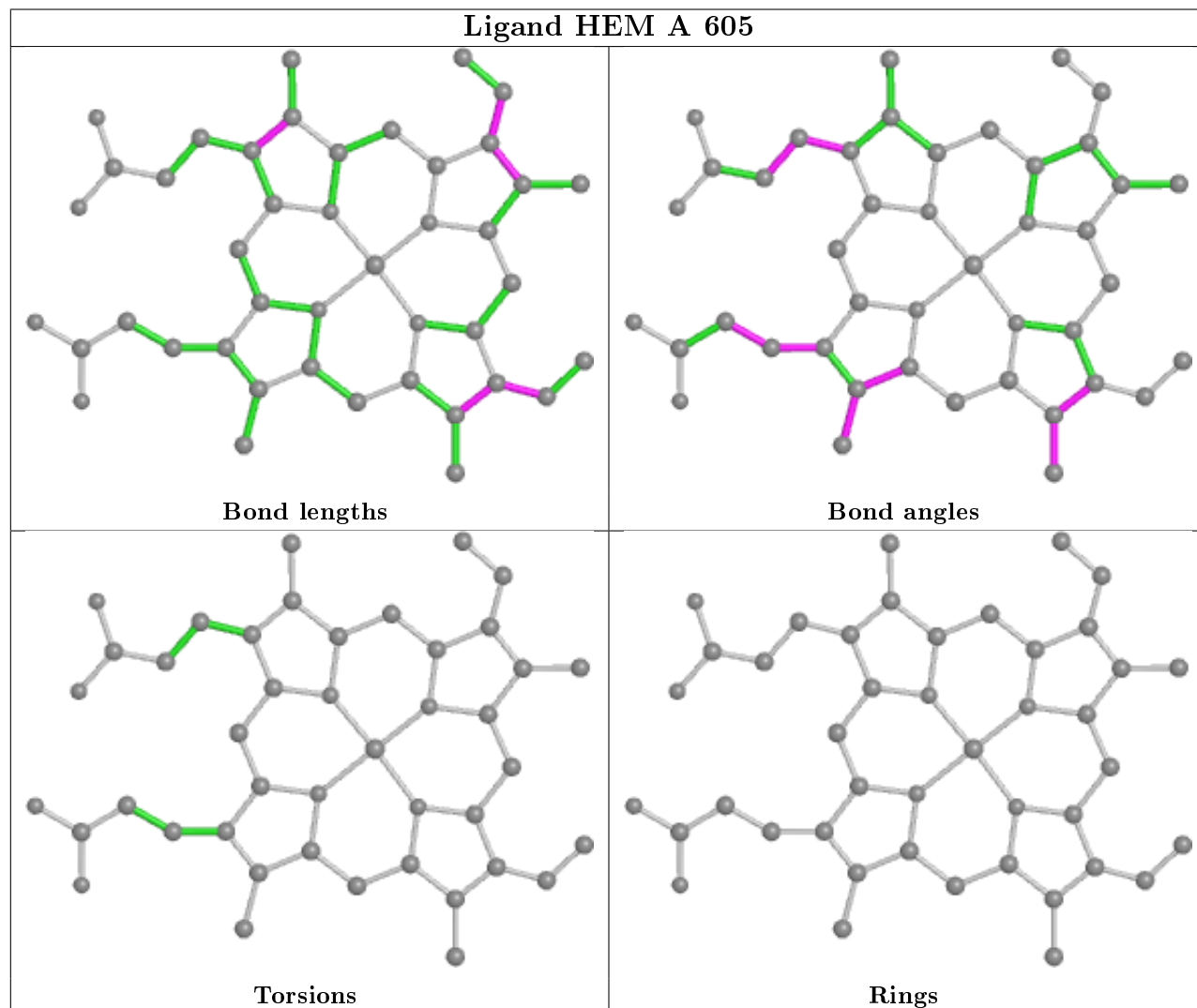
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	HEM	2	0
4	B	605	HEM	2	0
5	A	606[A]	MXM	2	0
6	C	607	BOG	2	0
5	A	606[B]	MXM	1	0
3	D	601	NAG	1	0
6	B	607	BOG	1	0
4	D	605	HEM	2	0
4	C	605	HEM	2	0
5	B	606[B]	MXM	3	0
5	B	606[A]	MXM	4	0
5	D	606[A]	MXM	1	0
3	A	604	NAG	1	0
5	D	606[B]	MXM	4	0
5	C	606[B]	MXM	5	0

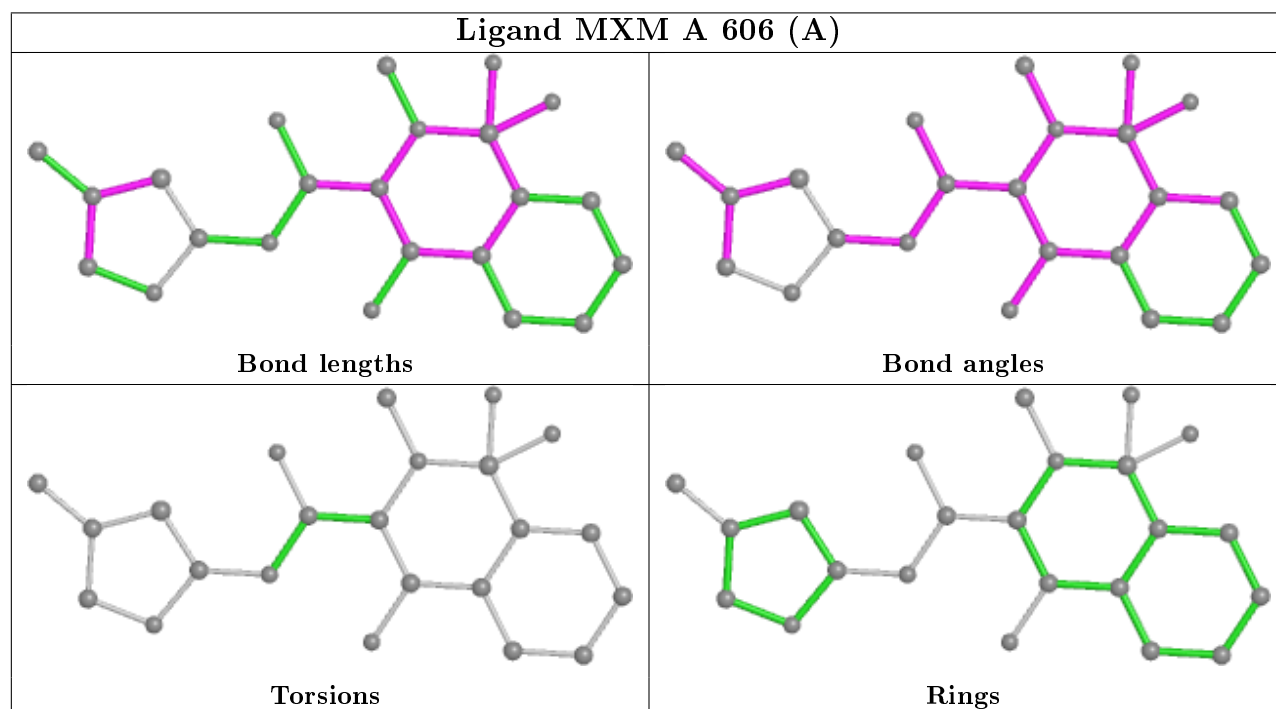
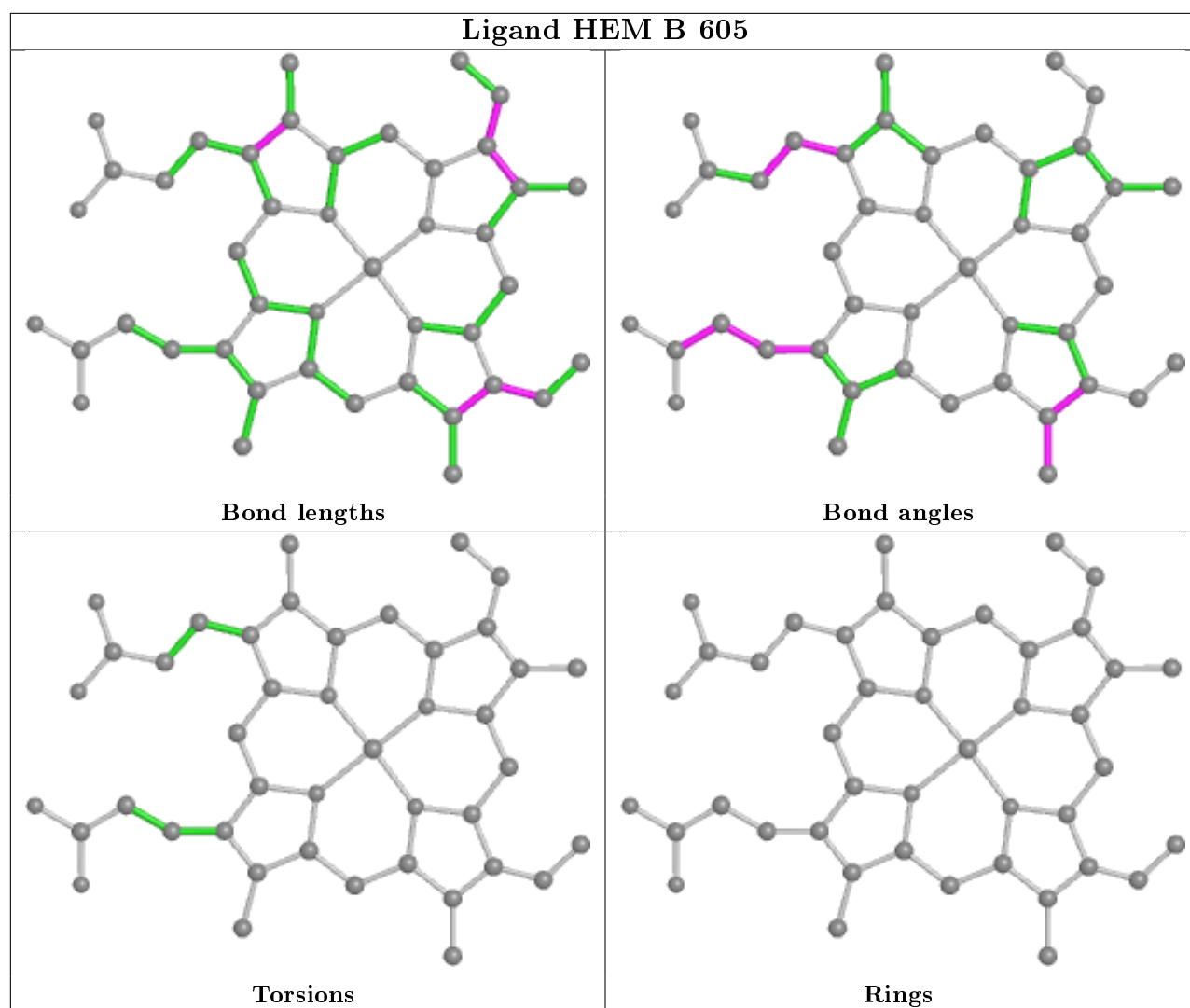
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

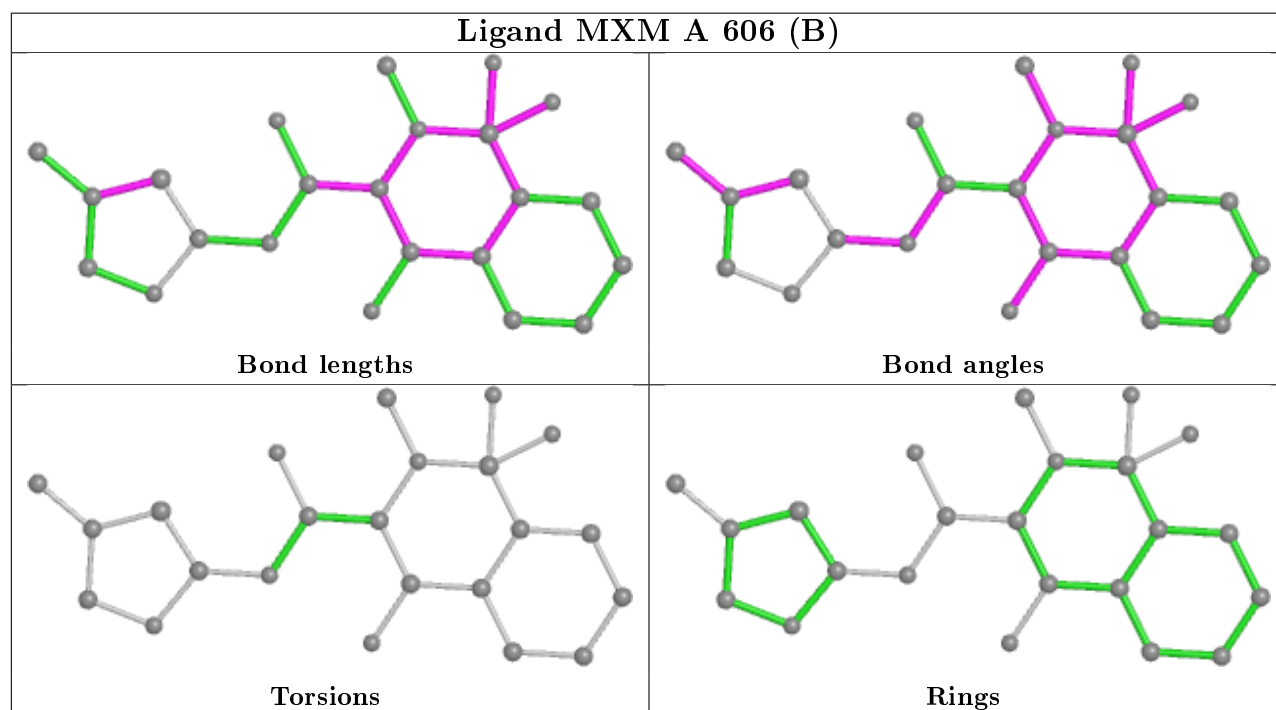
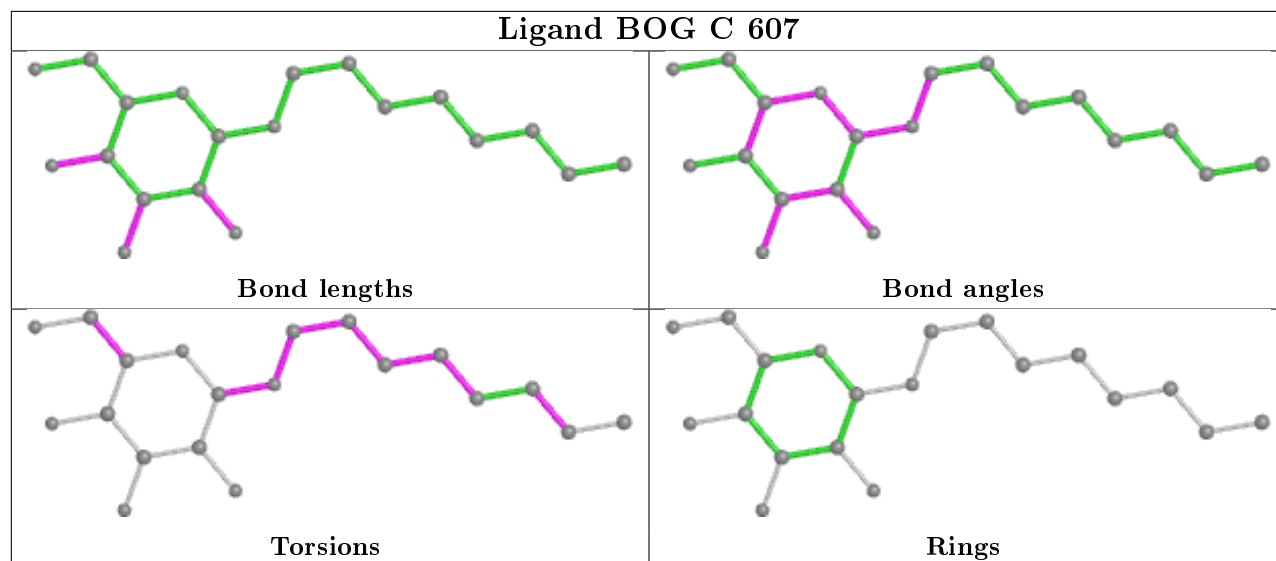
Ligand MXM C 606 (A)

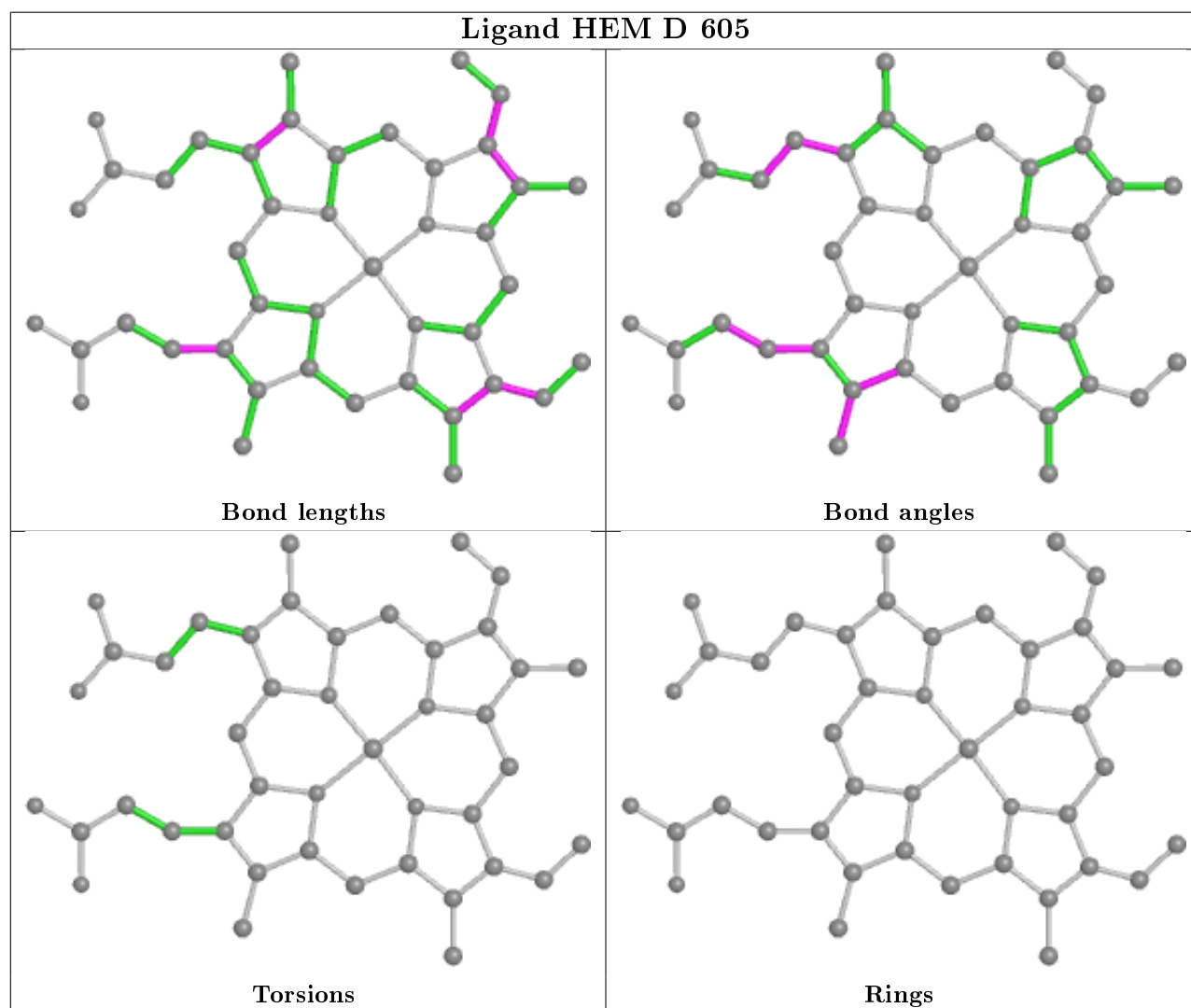
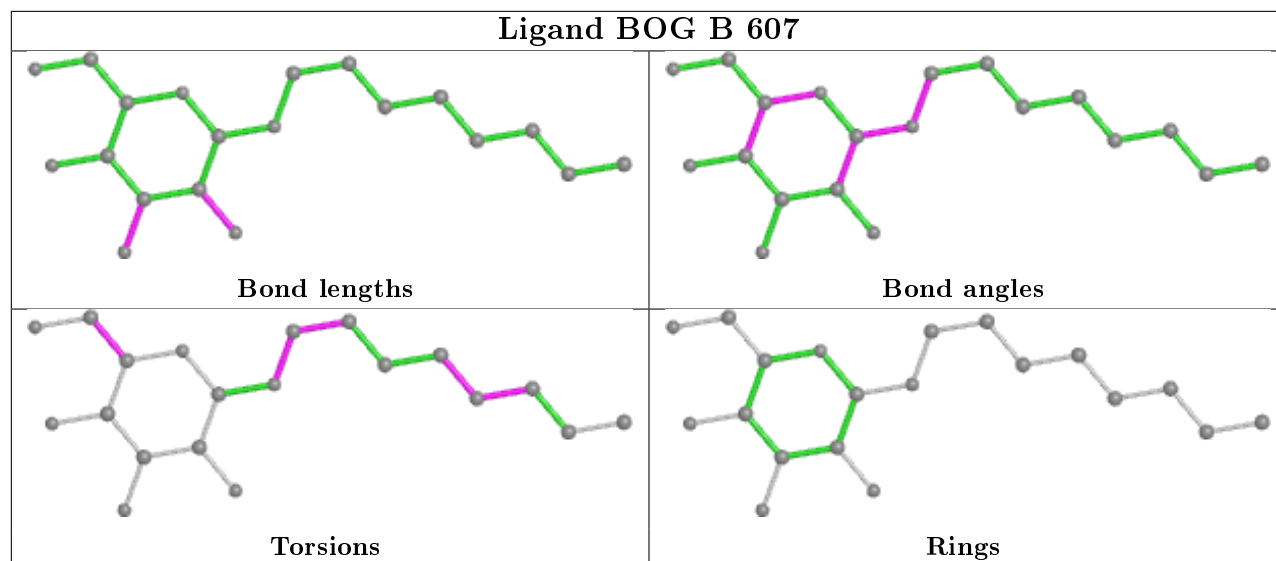


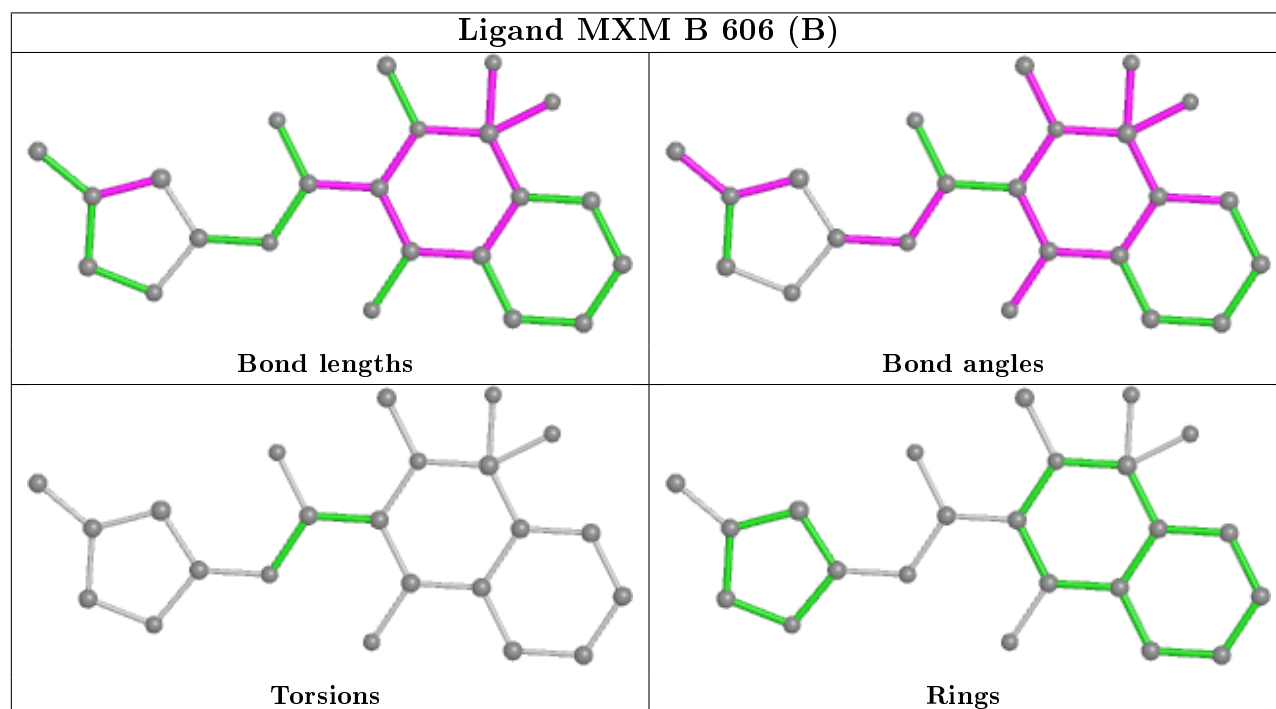
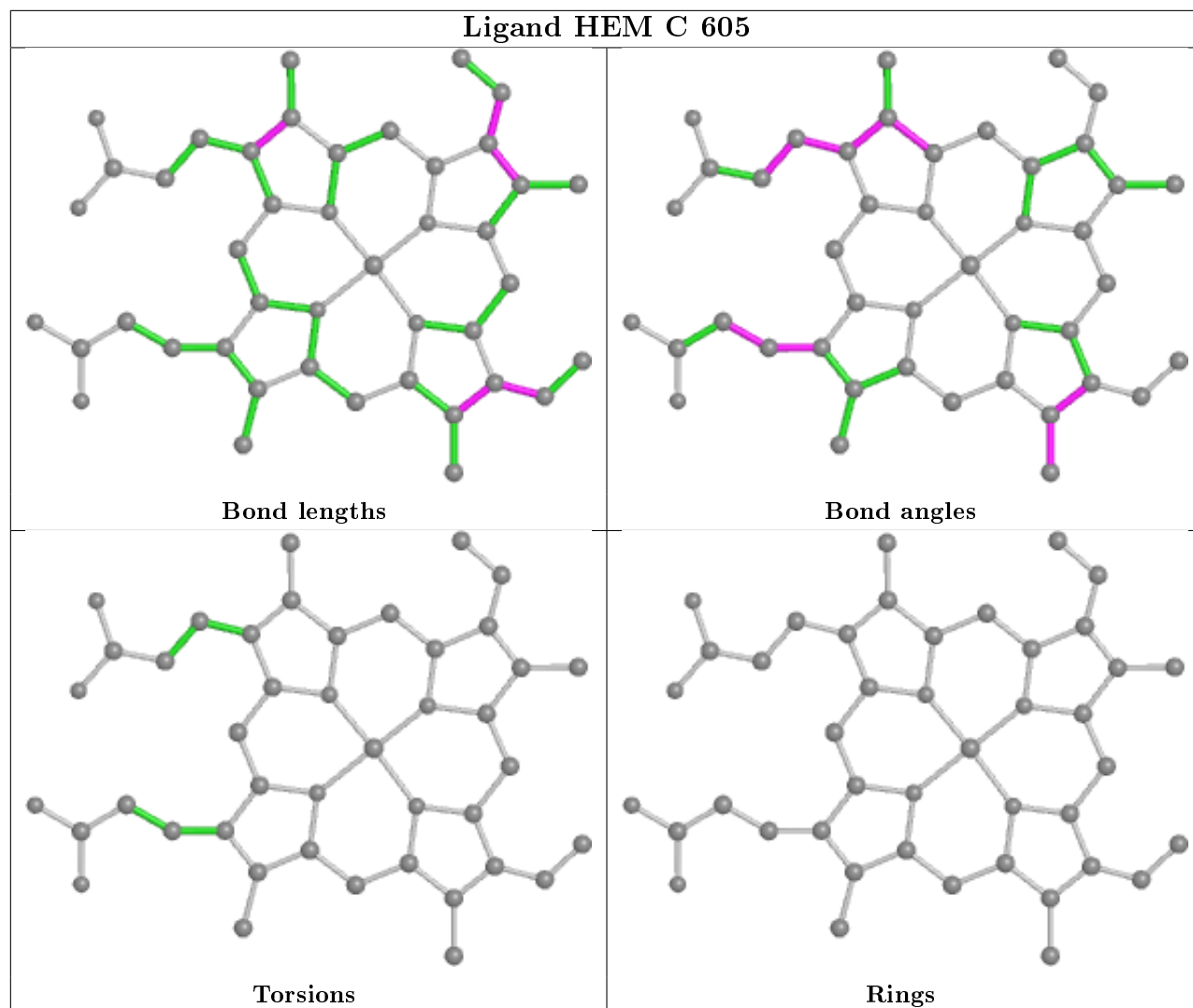
Ligand HEM A 605



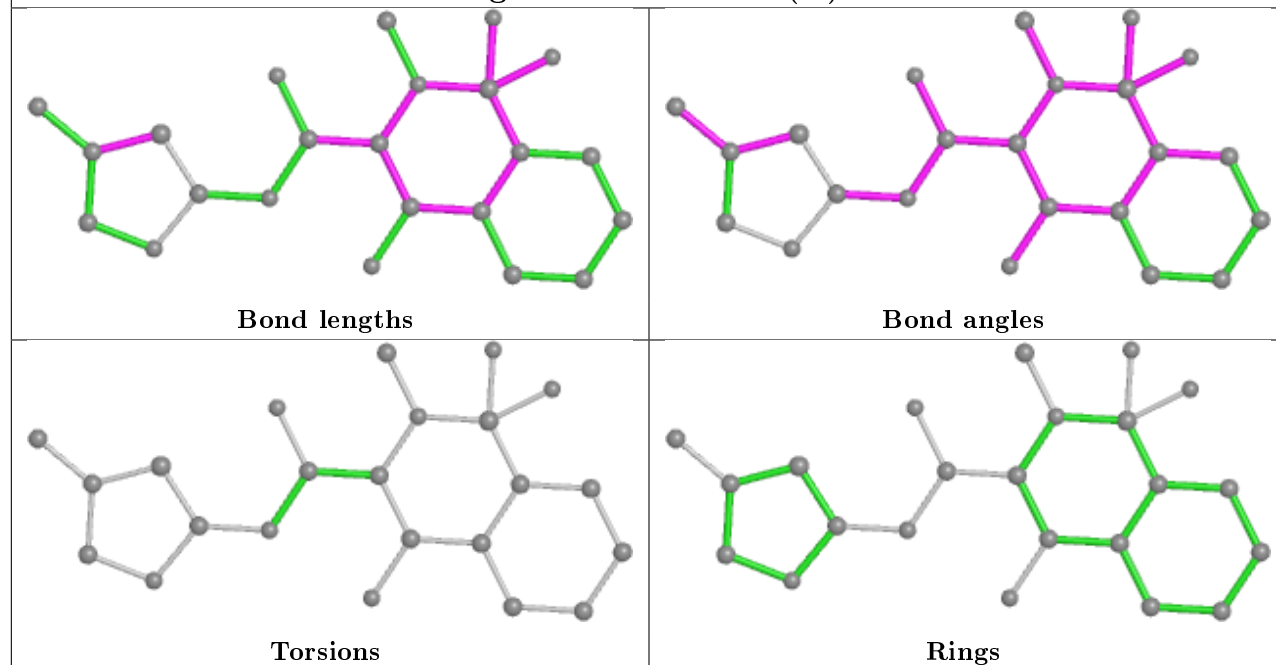




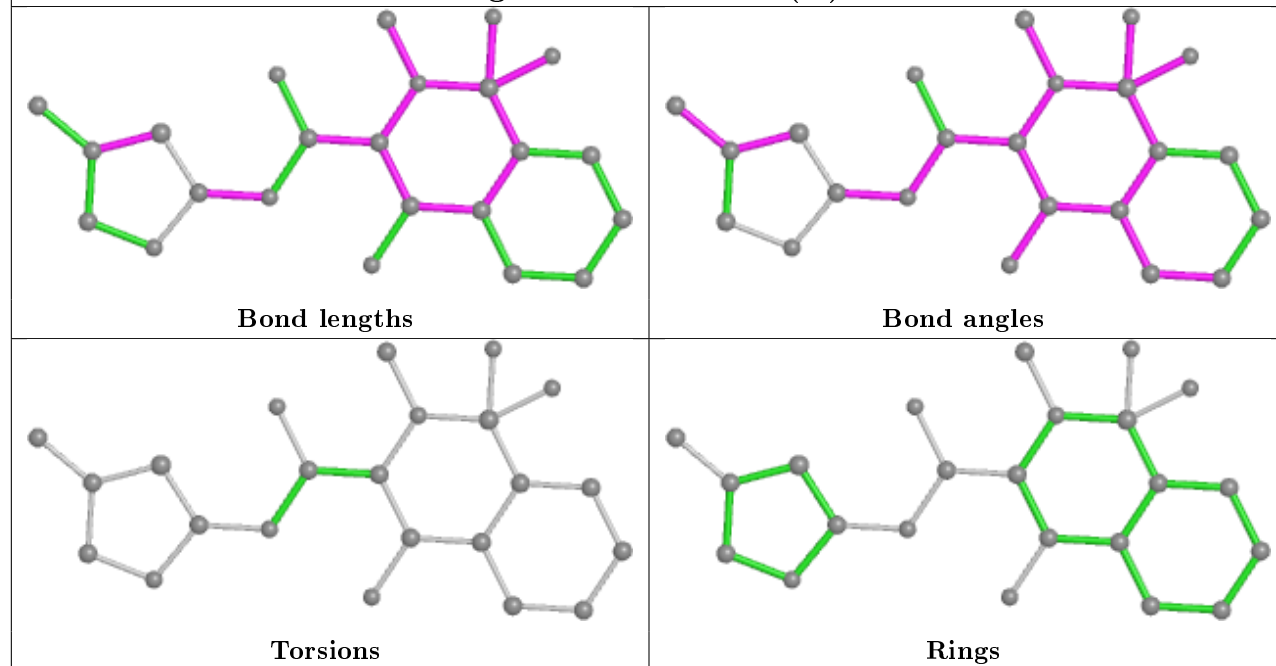


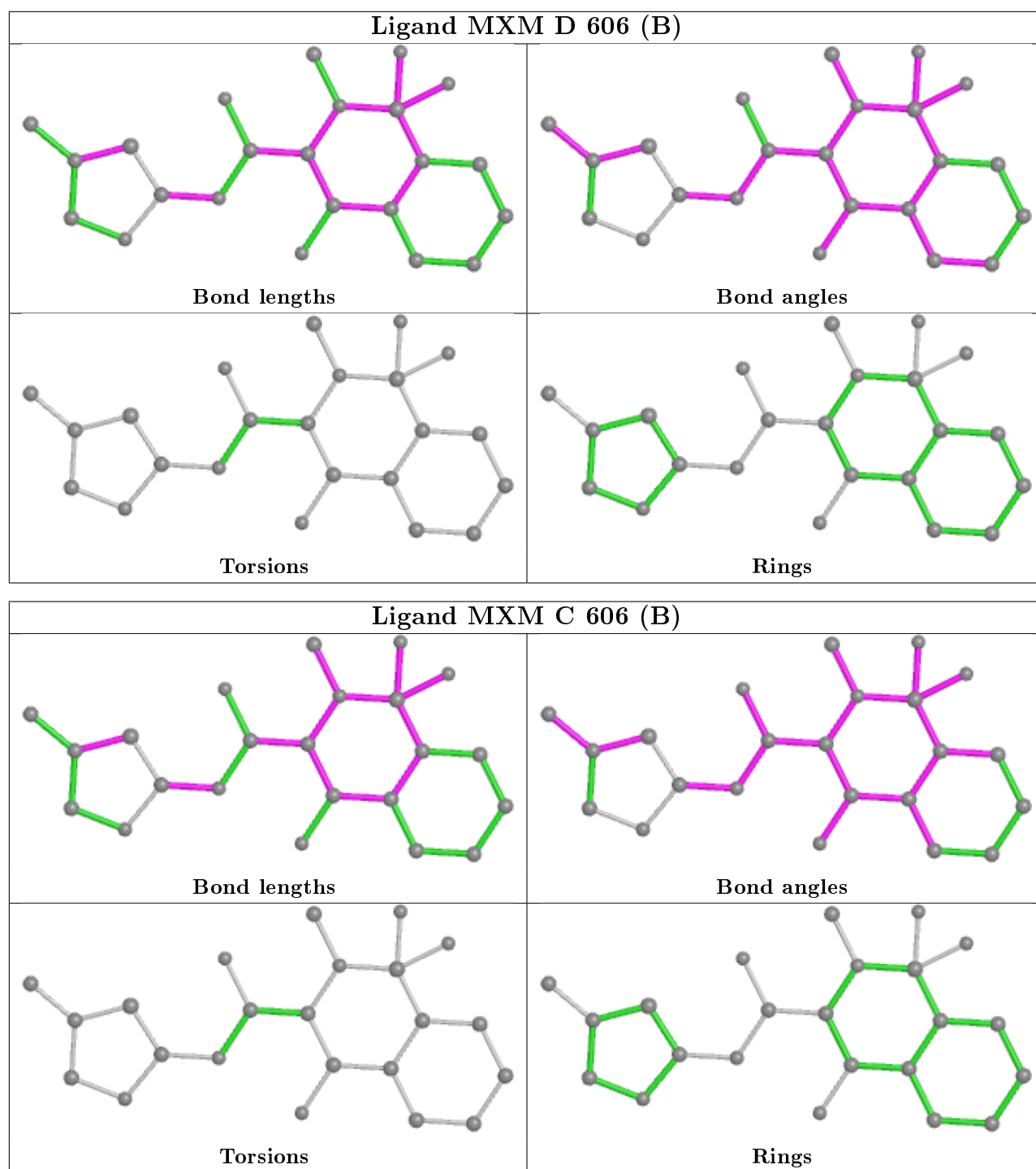


Ligand MXM B 606 (A)



Ligand MXM D 606 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/552 (100%)	-0.09	7 (1%) 77 76	16, 33, 57, 75	0
1	B	552/552 (100%)	-0.09	19 (3%) 45 41	18, 37, 65, 96	0
1	C	552/552 (100%)	-0.18	10 (1%) 68 65	16, 28, 53, 69	0
1	D	552/552 (100%)	-0.23	10 (1%) 68 65	17, 29, 51, 83	0
All	All	2208/2208 (100%)	-0.15	46 (2%) 63 60	16, 31, 58, 96	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	7.5
1	D	82	LEU	6.2
1	B	74	PHE	5.6
1	A	82	LEU	5.3
1	D	81	LEU	5.1
1	C	82	LEU	5.1
1	B	583	GLN	4.7
1	A	74	PHE	4.3
1	B	70	THR	3.4
1	C	74	PHE	3.4
1	B	409	TYR	3.3
1	D	215	LYS	3.3
1	B	81	LEU	3.2
1	C	53	ASP	3.0
1	D	79	LYS	3.0
1	B	80	LEU	2.9
1	D	80	LEU	2.9
1	B	52	PHE	2.8
1	D	74	PHE	2.8
1	B	75	LEU	2.7
1	D	583	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	79	LYS	2.7
1	B	215	LYS	2.7
1	B	77	ARG	2.6
1	D	75	LEU	2.6
1	A	53	ASP	2.4
1	A	239	ASP	2.4
1	C	33	ALA	2.4
1	D	77	ARG	2.3
1	A	96	PHE	2.3
1	C	115	TYR	2.3
1	C	81	LEU	2.3
1	C	52	PHE	2.3
1	B	485	LYS	2.2
1	B	428	ARG	2.2
1	B	33	ALA	2.2
1	A	78	ILE	2.2
1	B	399	ASP	2.1
1	B	105(A)	ILE	2.1
1	B	398	GLU	2.1
1	C	77	ARG	2.1
1	D	536	GLY	2.1
1	C	105	ASN	2.1
1	A	248	LYS	2.0
1	C	70	THR	2.0
1	B	108	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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

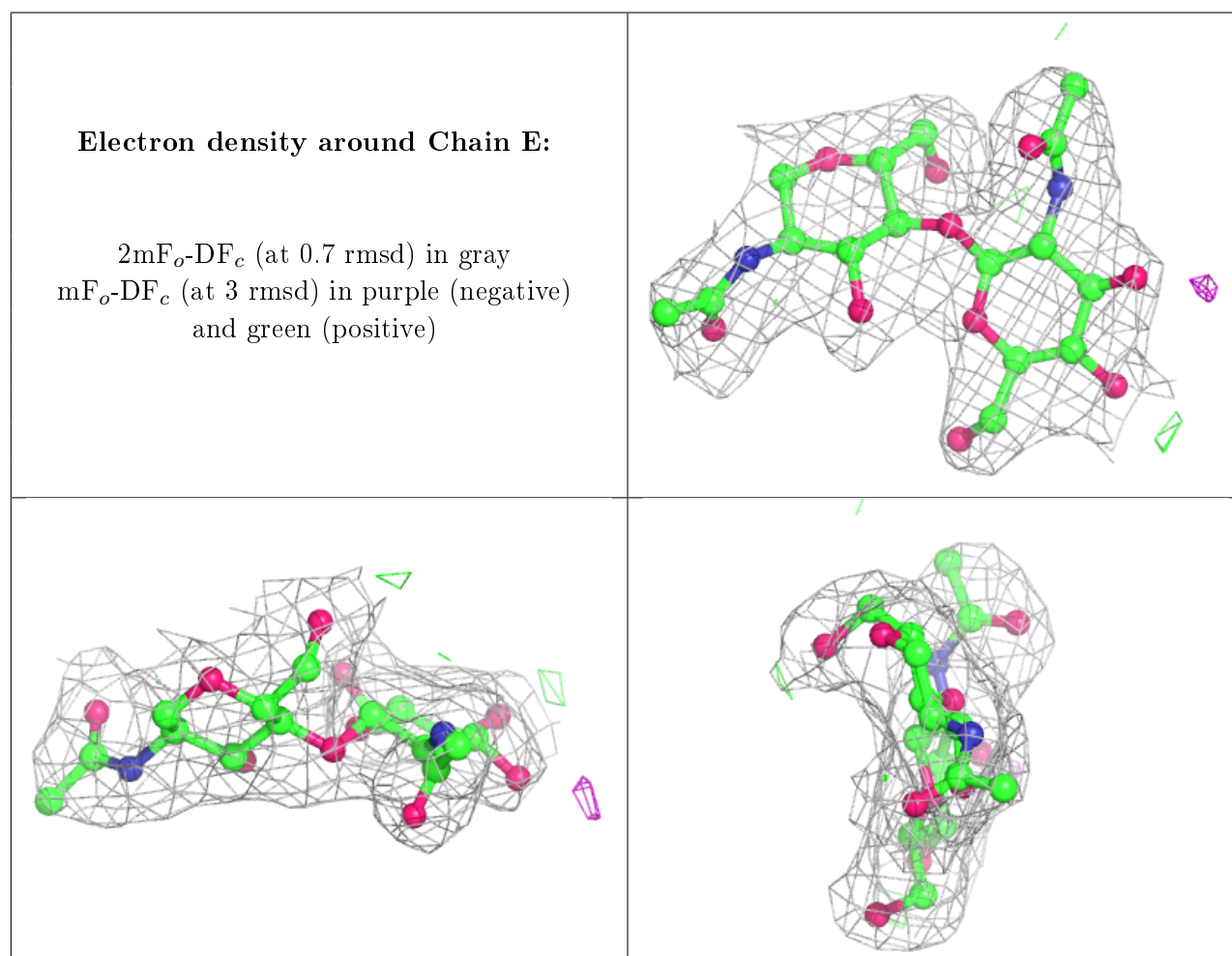
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	H	2	14/15	0.86	0.23	40,43,45,45	0
2	NAG	F	2	14/15	0.87	0.22	42,46,49,51	0
2	NAG	E	2	14/15	0.92	0.14	40,42,45,46	0

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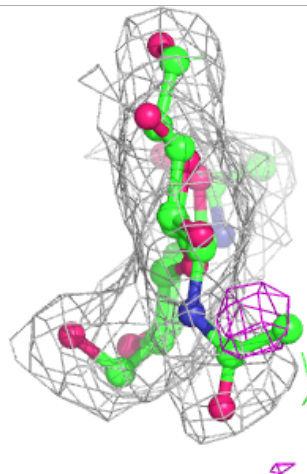
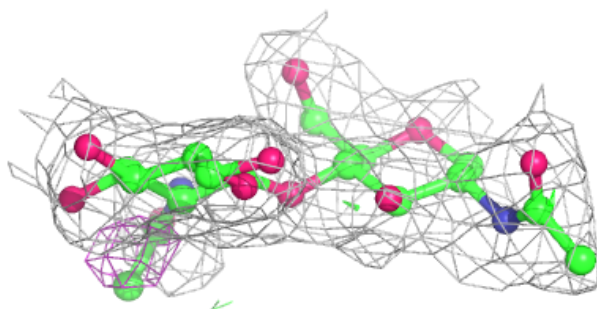
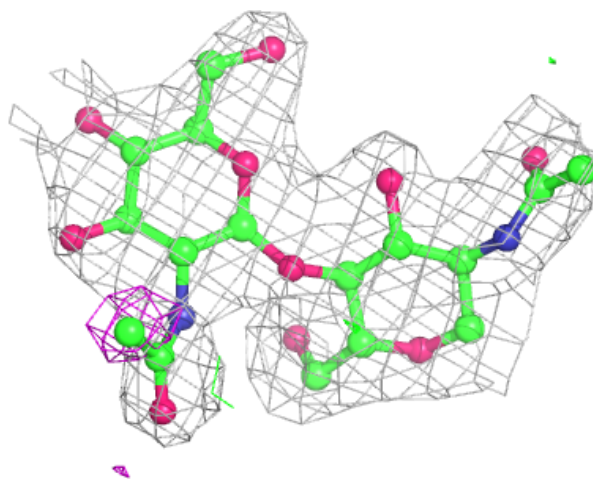
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	G	2	14/15	0.94	0.14	39,43,45,46	0
2	NAG	E	1	14/15	0.94	0.12	24,30,32,37	0
2	NAG	F	1	14/15	0.94	0.11	25,29,34,38	0
2	NAG	G	1	14/15	0.95	0.12	21,28,32,35	0
2	NAG	H	1	14/15	0.96	0.11	25,27,30,35	0

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.



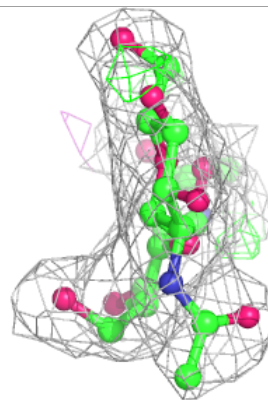
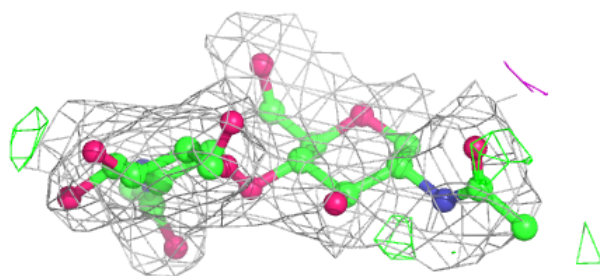
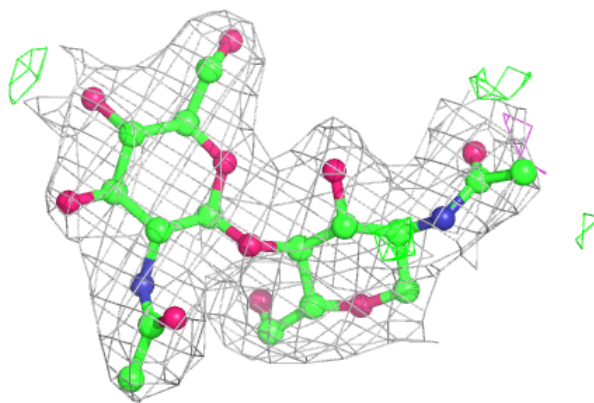
Electron density around Chain F:

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

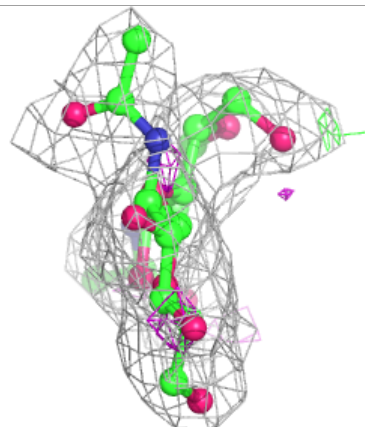
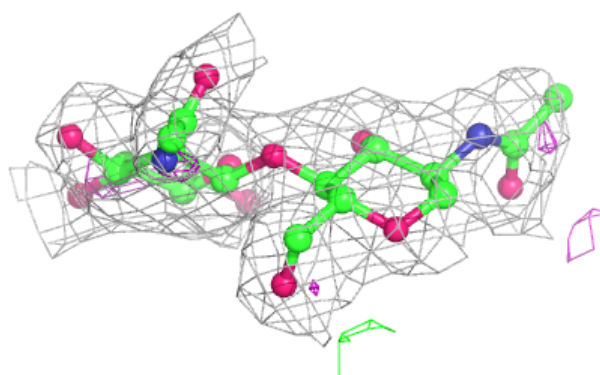
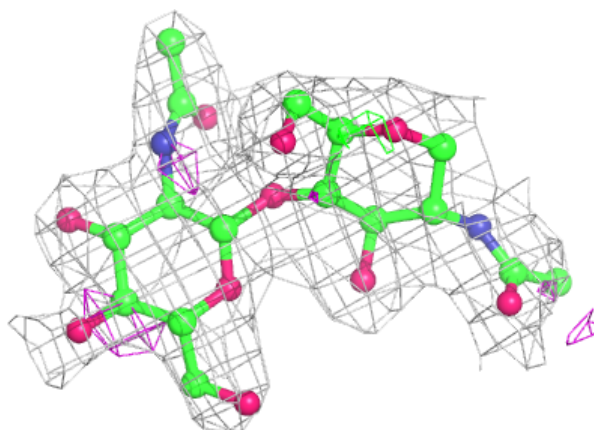


Electron density around Chain G:

$2mF_o-DF_c$ (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 ⓘ

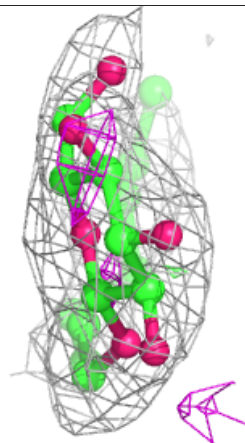
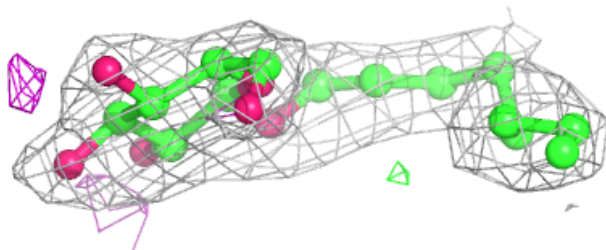
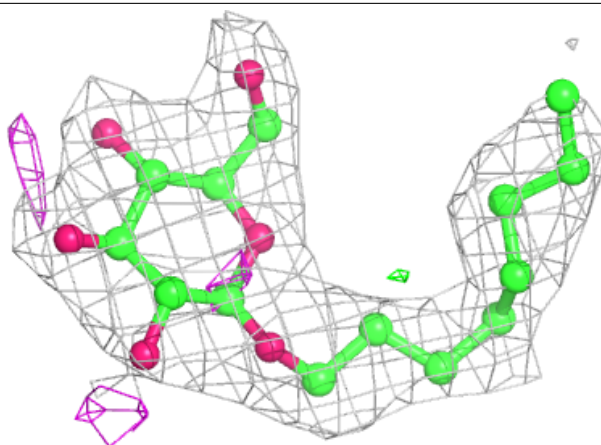
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	601	14/15	0.78	0.20	38,53,56,56	0
3	NAG	B	601	14/15	0.82	0.25	41,48,50,50	0
3	NAG	C	601	14/15	0.83	0.26	43,47,49,50	0
3	NAG	D	601	14/15	0.83	0.23	38,44,45,47	0
3	NAG	B	604	14/15	0.87	0.23	37,42,43,45	0
3	NAG	C	604	14/15	0.88	0.18	35,40,43,43	0
6	BOG	B	607	20/20	0.88	0.24	37,43,45,46	0
6	BOG	C	607	20/20	0.90	0.15	36,40,42,42	0
3	NAG	D	604	14/15	0.91	0.22	42,46,48,49	0
5	MXM	A	606[B]	23/23	0.93	0.16	27,32,33,34	23
5	MXM	A	606[A]	23/23	0.93	0.16	27,32,33,34	23
5	MXM	D	606[A]	23/23	0.93	0.14	20,25,26,26	23
3	NAG	A	604	14/15	0.93	0.16	34,40,42,43	0
5	MXM	D	606[B]	23/23	0.93	0.14	20,24,26,26	23
5	MXM	B	606[A]	23/23	0.94	0.16	29,31,32,33	23
5	MXM	B	606[B]	23/23	0.94	0.16	29,31,32,33	23
5	MXM	C	606[A]	23/23	0.95	0.15	23,27,28,29	23
4	HEM	D	605	43/43	0.95	0.14	20,25,44,52	0
5	MXM	C	606[B]	23/23	0.95	0.15	22,27,28,29	23
4	HEM	B	605	43/43	0.96	0.13	26,30,44,51	0
4	HEM	A	605	43/43	0.96	0.14	23,26,42,46	0
4	HEM	C	605	43/43	0.96	0.14	17,22,36,44	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.

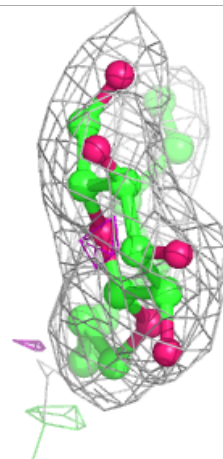
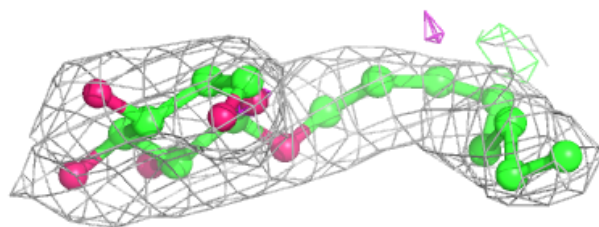
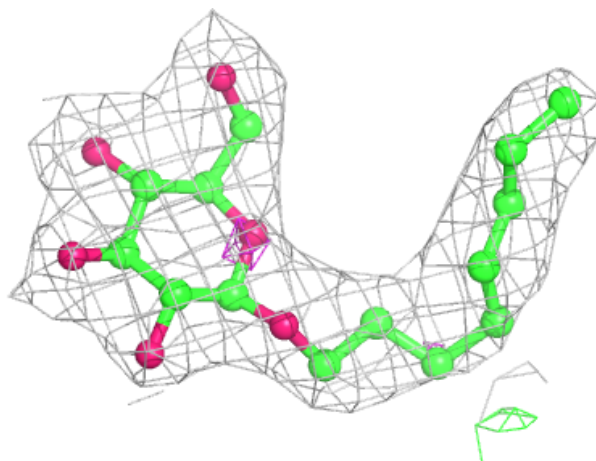
Electron density around BOG B 607:

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



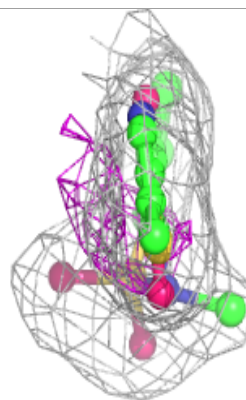
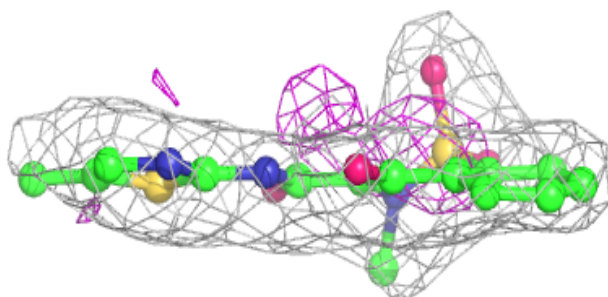
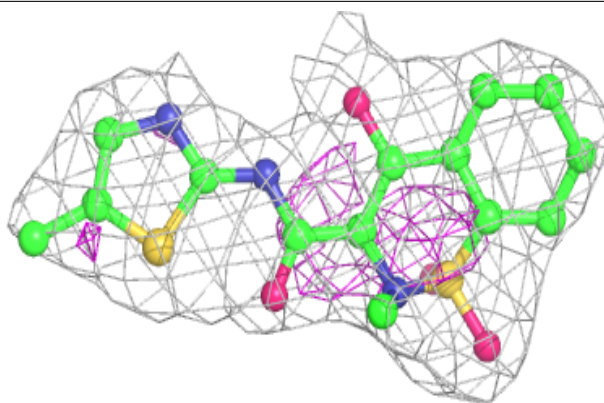
Electron density around BOG C 607:

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

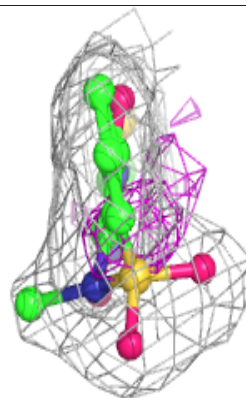
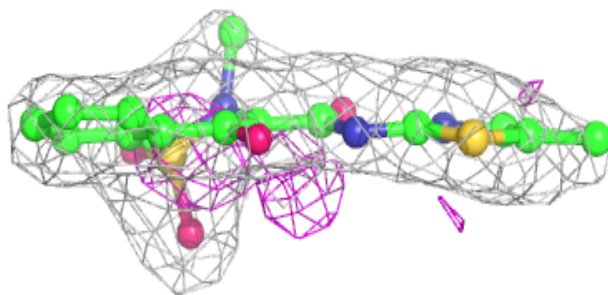
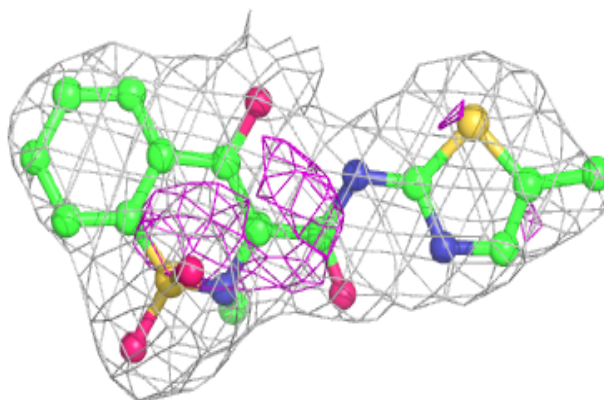


Electron density around MXM A 606 (B):

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

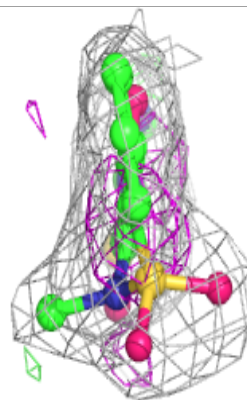
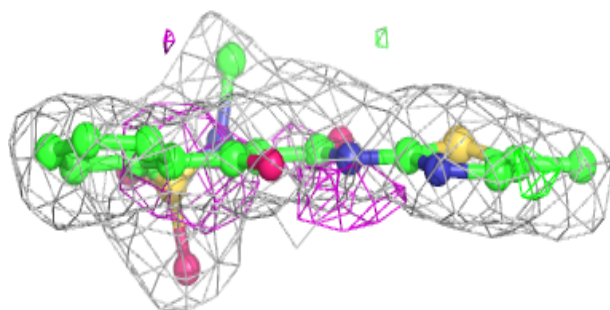
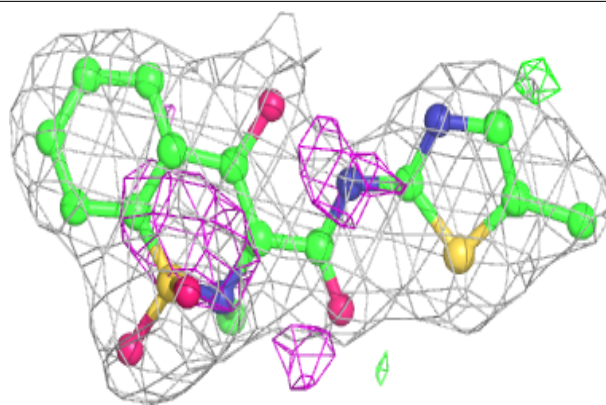
**Electron density around MXM A 606 (A):**

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

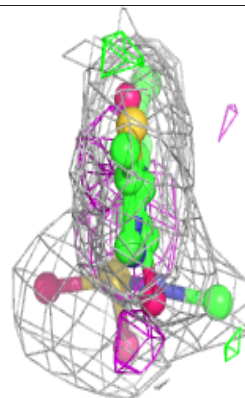
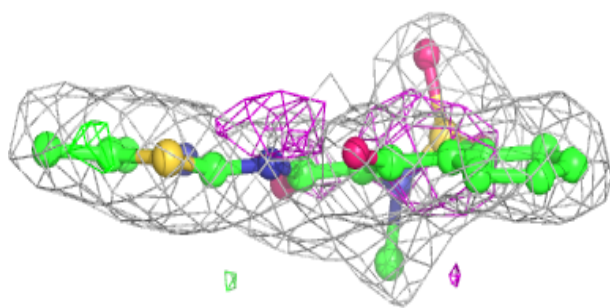
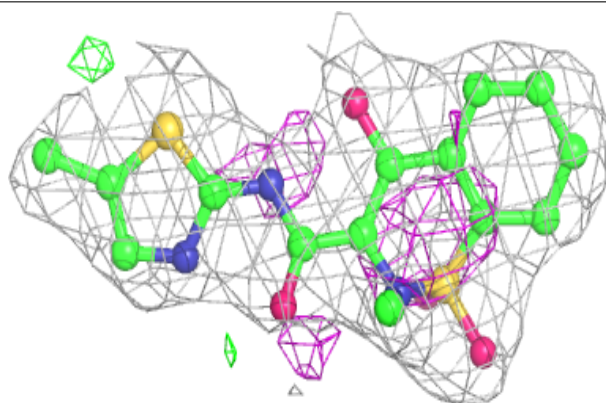


Electron density around MXM D 606 (A):

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

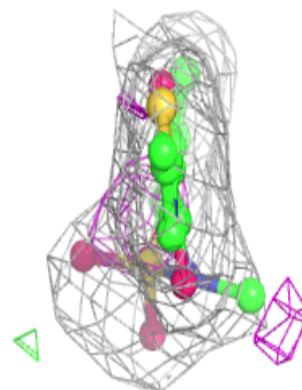
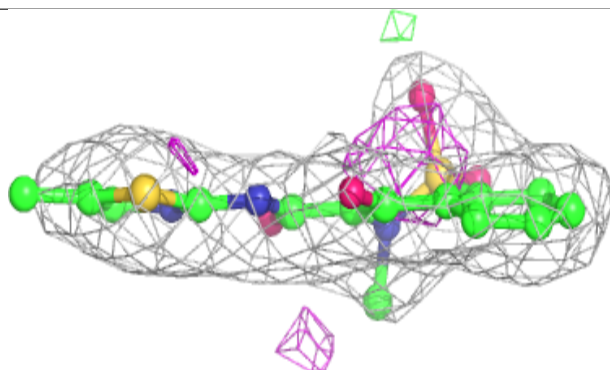
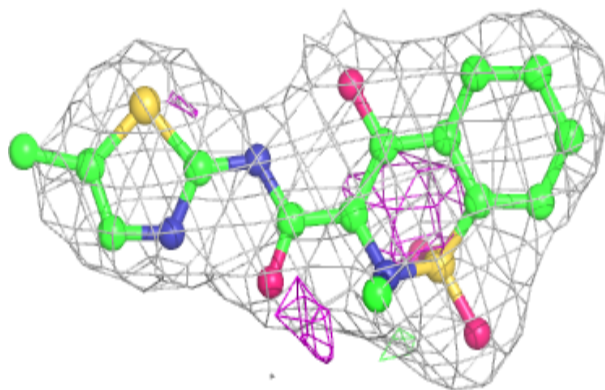
**Electron density around MXM D 606 (B):**

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

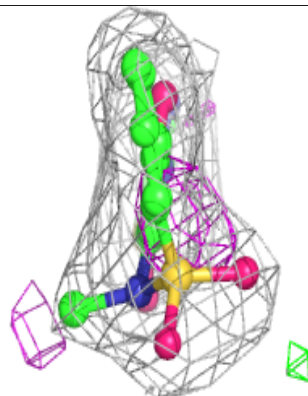
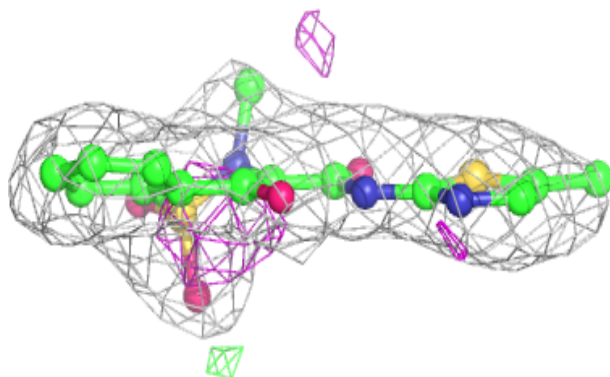
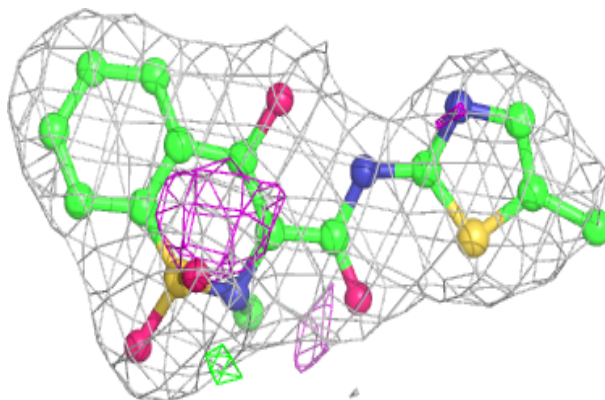


Electron density around MXM B 606 (A):

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

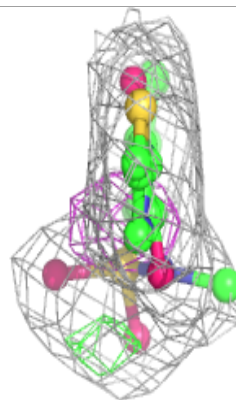
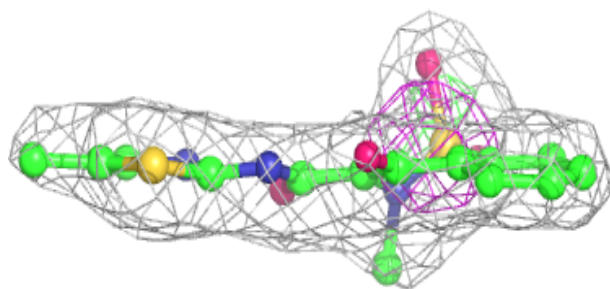
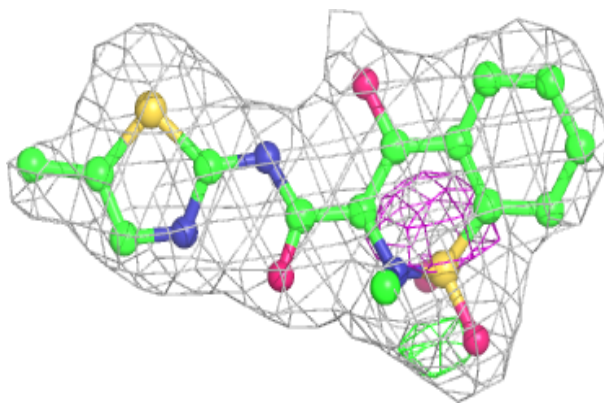
**Electron density around MXM B 606 (B):**

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



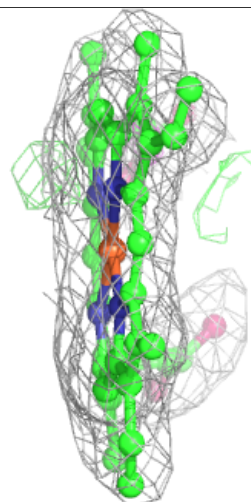
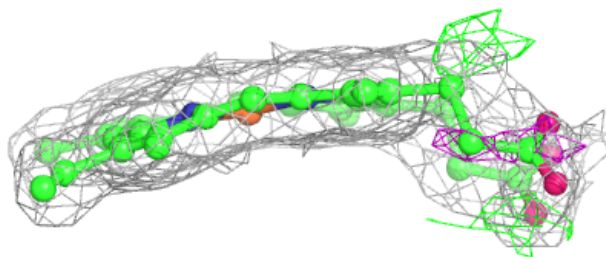
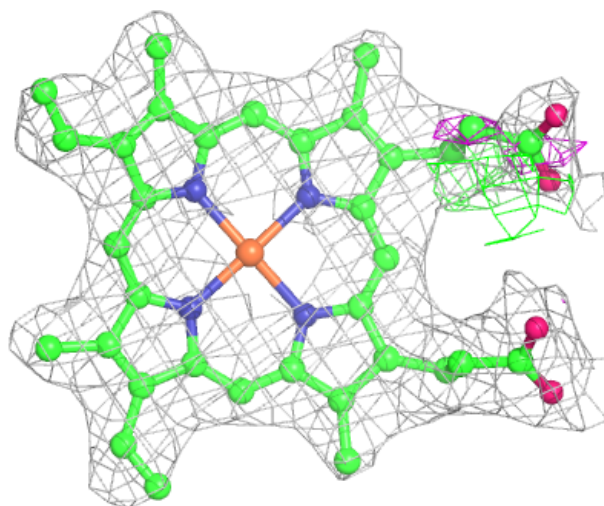
Electron density around MXM C 606 (A):

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



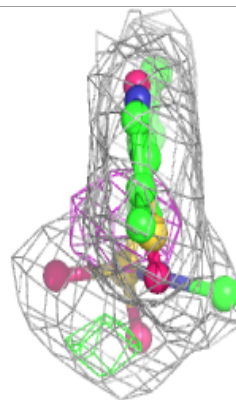
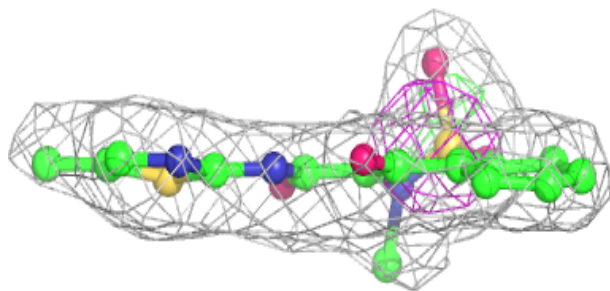
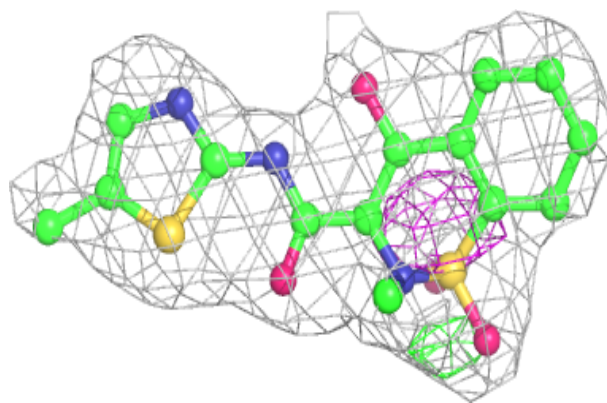
Electron density around HEM D 605:

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



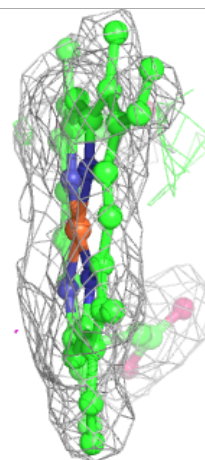
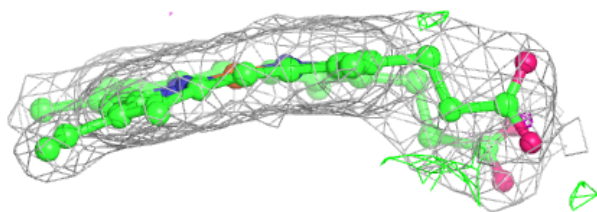
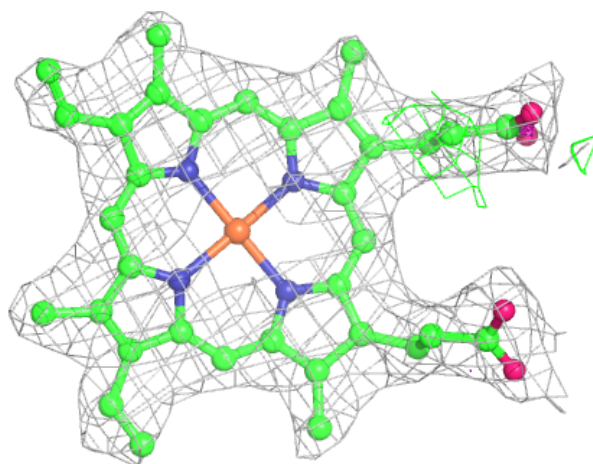
Electron density around MXM C 606 (B):

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



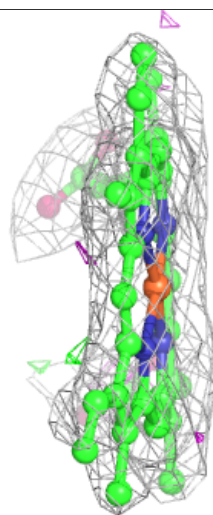
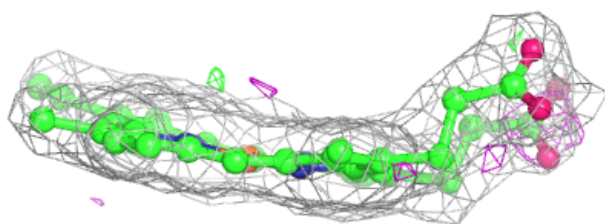
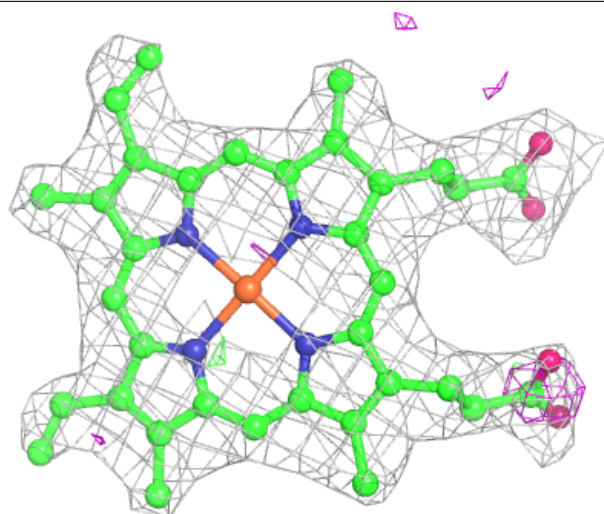
Electron density around HEM B 605:

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



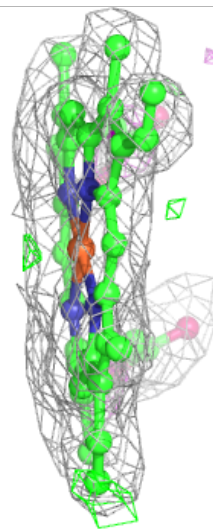
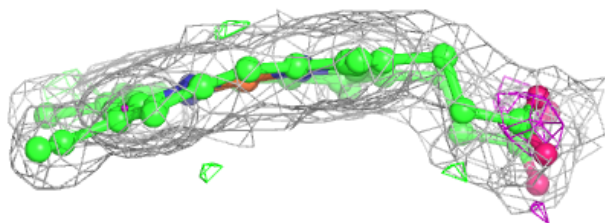
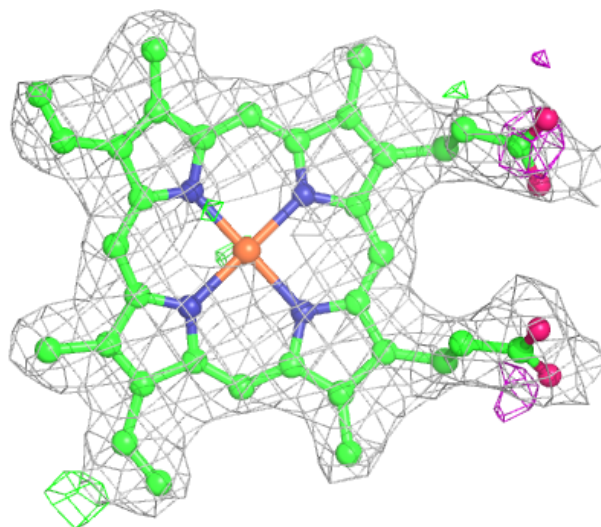
Electron density around HEM A 605:

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



Electron density around HEM C 605:

$2mF_o-DF_c$ (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.