



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:57 PM UTC

PDB ID : 4M11 / pdb_00004m11
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

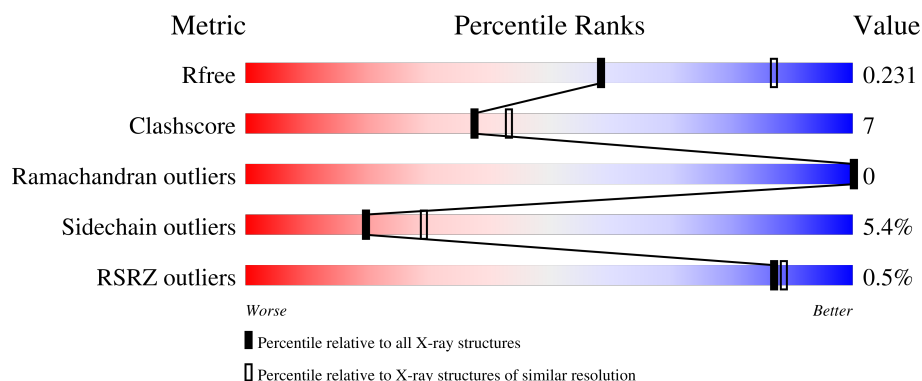
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	552	 81% 17% .
1	B	552	 82% 16% .
1	C	552	 83% 15% .
1	D	552	 86% 12% .
2	E	2	 50% 50%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MXM	C	606[A]	-	X	-	-

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



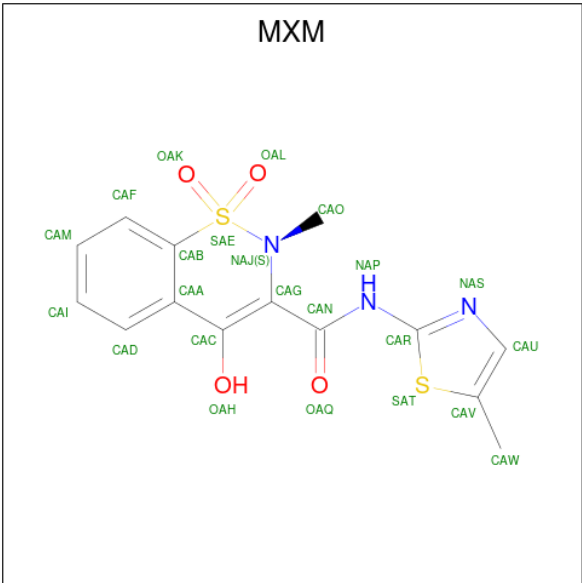
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

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



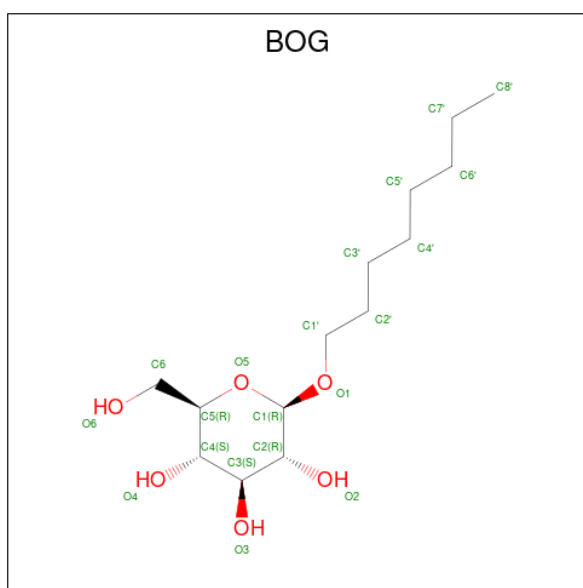
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 4-hydroxy-2-methyl-N-(5-methyl-1,3-thiazol-2-yl)-2H-1,2-benzothiazine-3-carb oxamide 1,1-dioxide (CCD ID: MXM) (formula: C₁₄H₁₃N₃O₄S₂).



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 (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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		

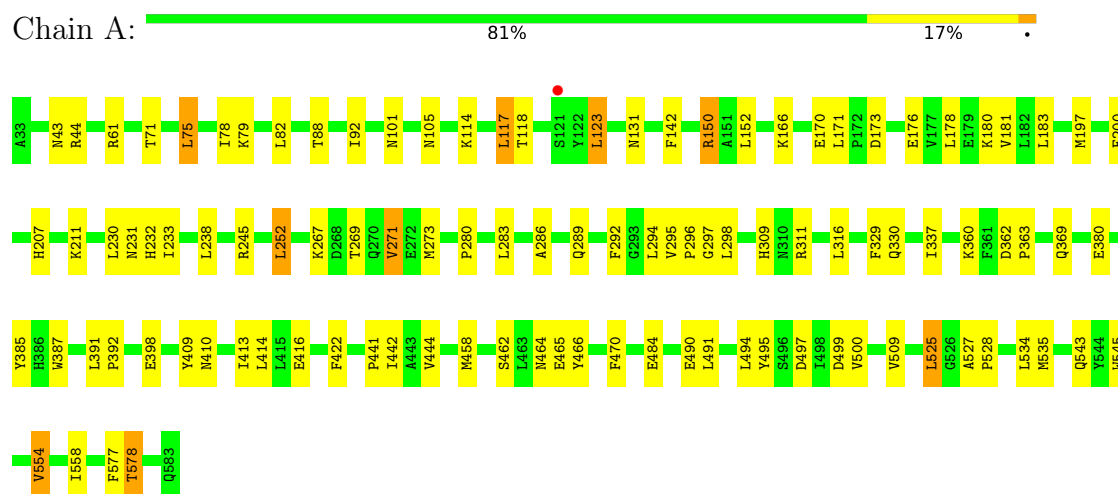
- Molecule 7 is water.

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		

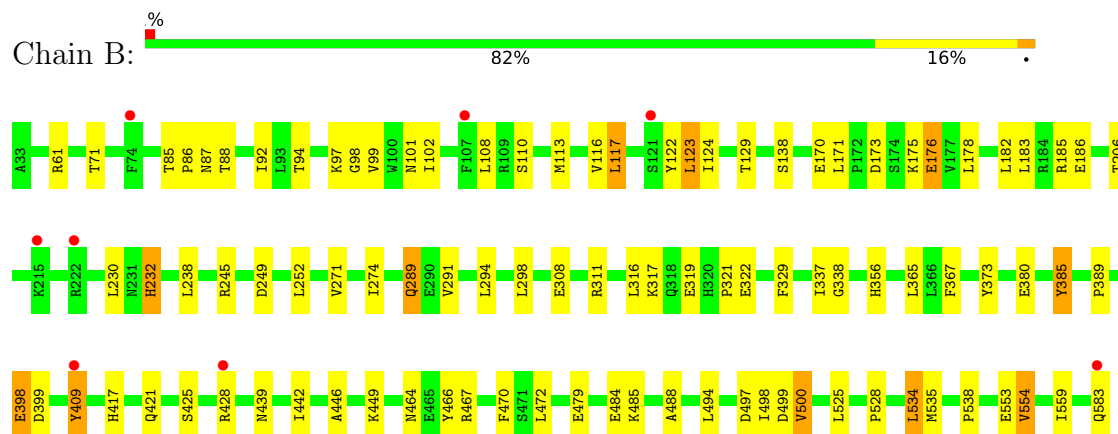
3 Residue-property plots

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.

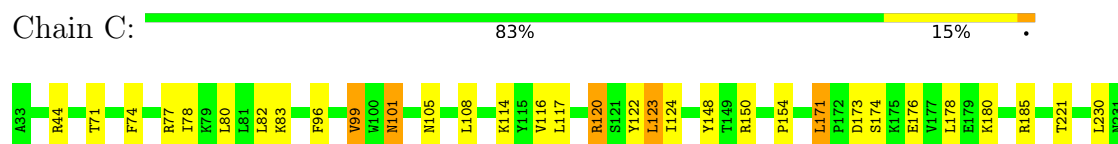
• Molecule 1: Prostaglandin G/H synthase 2

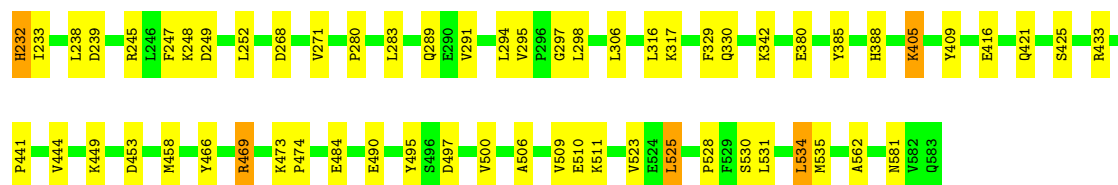


• Molecule 1: Prostaglandin G/H synthase 2

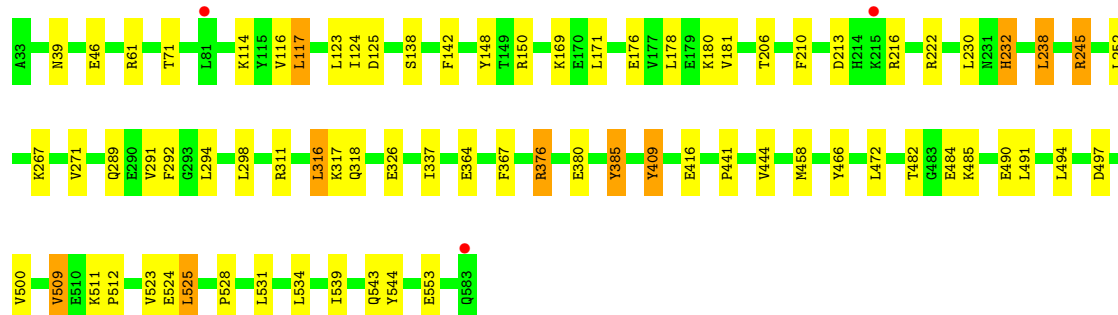
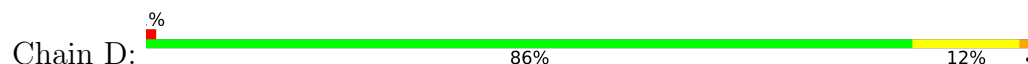


• Molecule 1: Prostaglandin G/H synthase 2





- 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)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.202 , 0.231 0.202 , 0.231	Depositor DCC
R_{free} test set	5338 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtrriage
Anisotropy	0.539	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19520	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, HEM, MXM, 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	0.52	3/4601 (0.1%)	0.78	1/6239 (0.0%)
1	B	0.45	1/4601 (0.0%)	0.76	2/6239 (0.0%)
1	C	0.41	0/4601	0.78	2/6239 (0.0%)
1	D	0.42	0/4601	0.77	0/6239
All	All	0.45	4/18404 (0.0%)	0.77	5/24956 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	TRP	NE1-CE2	-6.26	1.30	1.37
1	A	392	PRO	N-CD	5.47	1.55	1.47
1	B	129	THR	C-O	-5.33	1.17	1.24
1	A	387	TRP	N-CA	-5.31	1.39	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	GLU	CB-CA-C	-8.22	107.09	116.54
1	B	122	TYR	N-CA-C	-6.92	103.92	114.16
1	A	391	LEU	N-CA-C	6.75	118.41	109.83
1	C	388	HIS	CA-C-N	-5.21	114.71	119.82
1	C	388	HIS	C-N-CA	-5.21	114.71	119.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4372	66	0
1	B	4474	0	4373	70	0
1	C	4474	0	4373	59	0
1	D	4474	0	4373	42	0
2	E	28	0	25	1	0
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	2	0
5	B	46	0	25	6	0
5	C	46	0	26	8	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	11	0
7	B	216	0	0	9	0
7	C	261	0	0	10	0
7	D	295	0	0	11	0
All	All	19520	0	17968	256	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 (256) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:A:892:HOH:O	2:E:2:NAG:O4	2.12	0.67
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:A:197:MET:HE2	1:A:578:THR:HG21	1.78	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:H	1:C:405:LYS:HD2	1.64	0.62
4:A:605:HEM:HBC2	4:A:605:HEM:HHD	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:VAL:HA	5:D:606[B]:MXM:H4	1.80	0.62
1:C:249:ASP:CG	1:C:317:LYS:HE3	2.25	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:HBC2	4:B:605:HEM:HHD	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
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:HBC2	4:D:605:HEM:HHD	1.84	0.58
4:B:605:HEM:HMB2	4:B:605:HEM:HBB2	1.85	0.57
1:C:96:PHE:O	1:C:99:VAL:HG13	2.04	0.57
1:C:185:ARG:NH1	6:C:607:BOG:H3'1	2.20	0.57
5:C:606[A]:MXM:NAS	5:C:606[A]:MXM:OAQ	2.35	0.57
1:A:166:LYS:HE2	1:A:499:ASP:CB	2.34	0.56
1:B:398:GLU:HG3	1:B:421:GLN:CD	2.30	0.56
5:B:606[B]:MXM:OAH	5:B:606[B]:MXM:NAP	2.25	0.56
1:C:523:VAL:HA	5:C:606[A]:MXM:H4	1.87	0.56
4:D:605:HEM:HMB1	4:D:605:HEM:HBB2	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:96:PHE:HB3	1:C:99:VAL:HG13	1.87	0.55
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.88	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:OAH	5:D:606[A]:MXM:NAP	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:PHE:HB3	1:C:99:VAL:HG11	1.88	0.53
1:C:101:ASN:O	1:C:105:ASN:ND2	2.38	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
1:D:180:LYS:HD3	1:D:490:GLU:HG3	1.92	0.52
1:D:230:LEU:HG	1:D:337:ILE:HG12	1.91	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:176:GLU:HG2	1:A:494:LEU:HD21	1.93	0.51
1:A:207:HIS:CE1	7:A:932:HOH:O	2.63	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:NAS	5:A:606[A]:MXM:OAQ	2.40	0.50
1:C:425:SER:OG	7:C:815:HOH:O	2.19	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:OAQ	5:D:606[B]:MXM:NAS	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:OAH	5:C:606[B]:MXM:NAP	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:605:HEM:HMB2	4:C:605:HEM:HBB2	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:H5'2	6:C:607:BOG:H2'1	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
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:124:ILE:HD11	1:B:528:PRO:HB2	1.95	0.47
1:B:178:LEU:HD22	1:B:449:LYS:HB2	1.97	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:B:113:MET:HE3	1:B:117:LEU:HD13	1.96	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:A:273:MET:HE3	7:A:759:HOH:O	2.17	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:HA	1:B:97:LYS:HD2	1.57	0.45
5:C:606[A]:MXM:OAQ	5:C:606[A]:MXM:H15	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OAO	5:C:606[B]:MXM:H15	2.16	0.44
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.18	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:C:247:PHE:C	1:C:248:LYS:HD2	2.43	0.43
1:B:123:LEU:HD13	1:B:123:LEU:HA	1.79	0.43
1:C:581:ASN:OD1	1:C:581:ASN:C	2.62	0.43
1:C:120:ARG:O	1:C:531:LEU:HD23	2.19	0.43
1:C:405:LYS:H	1:C:405:LYS:CD	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:HD12	1:C:123:LEU:HA	1.86	0.42
1:C:421:GLN:OE1	7:C:815:HOH:O	2.21	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:HG2	1:C:44:ARG:HH11	1.85	0.42
1:C:150:ARG:NH1	7:C:721:HOH:O	2.52	0.42
1:D:117:LEU:HD12	1:D:117:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:245:ARG:NH2	1:D:326:GLU:OE2	2.40	0.42
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.79	0.42
1:B:94:THR:C	1:B:356:HIS:NE2	2.77	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:150:ARG:NH2	1:A:458:MET:O	2.43	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: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:OAQ	5:D:606[B]:MXM:H15	2.19	0.41
1:A:43:ASN:O	1:A:44:ARG:HB2	2.21	0.41
1:B:94:THR:C	1:B:356:HIS:CD2	2.98	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:A:577:PHE:HE1	1:D:267:LYS:HD2	1.86	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:230:LEU:HD13	1:A:233:ILE:HD12	2.03	0.41
1:B:117:LEU:HD12	1:B:117:LEU:HA	1.84	0.41
1:B:322:GLU:OE2	1:B:322:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 [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	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 [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	493/493 (100%)	468 (95%)	25 (5%)	21	31
1	B	493/493 (100%)	467 (95%)	26 (5%)	20	30
1	C	493/493 (100%)	465 (94%)	28 (6%)	18	27
1	D	493/493 (100%)	466 (94%)	27 (6%)	19	28
All	All	1972/1972 (100%)	1866 (95%)	106 (5%)	20	29

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

Mol	Chain	Res	Type
1	A	71	THR
1	A	75	LEU
1	A	114	LYS
1	A	117	LEU
1	A	123	LEU
1	A	150	ARG
1	A	170	GLU
1	A	171	LEU
1	A	178	LEU
1	A	238	LEU
1	A	252	LEU
1	A	267	LYS
1	A	271	VAL
1	A	289	GLN
1	A	298	LEU
1	A	316	LEU
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	108	LEU
1	B	116	VAL
1	B	117	LEU
1	B	123	LEU
1	B	170	GLU
1	B	171	LEU

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Mol	Chain	Res	Type
1	B	176	GLU
1	B	186	GLU
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
1	B	484	GLU
1	B	498	ILE
1	B	500	VAL
1	B	534	LEU
1	B	535	MET
1	B	554	VAL
1	C	71	THR
1	C	99	VAL
1	C	101	ASN
1	C	114	LYS
1	C	116	VAL
1	C	120	ARG
1	C	123	LEU
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	271	VAL
1	C	289	GLN
1	C	291	VAL
1	C	298	LEU
1	C	306	LEU
1	C	316	LEU
1	C	385	TYR
1	C	405	LYS
1	C	416	GLU
1	C	469	ARG
1	C	484	GLU

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Mol	Chain	Res	Type
1	C	509	VAL
1	C	525	LEU
1	C	534	LEU
1	C	535	MET
1	D	71	THR
1	D	114	LYS
1	D	116	VAL
1	D	117	LEU
1	D	123	LEU
1	D	171	LEU
1	D	178	LEU
1	D	232	HIS
1	D	238	LEU
1	D	245	ARG
1	D	252	LEU
1	D	271	VAL
1	D	289	GLN
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	207	HIS
1	A	270	GLN
1	A	327	GLN
1	A	369	GLN
1	A	386	HIS
1	A	464	ASN

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Mol	Chain	Res	Type
1	A	571	ASN
1	B	39	ASN
1	B	386	HIS
1	B	421	GLN
1	B	571	ASN
1	C	270	GLN
1	C	327	GLN
1	C	445	GLN
1	C	571	ASN
1	D	105	ASN
1	D	369	GLN
1	D	374	GLN
1	D	461	GLN
1	D	571	ASN

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	2,1	14,14,15	0.59	0	17,19,21	0.46	0
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	0.57	0
2	NAG	F	1	2,1	14,14,15	0.54	0	17,19,21	0.49	0
2	NAG	F	2	2	14,14,15	0.49	0	17,19,21	0.76	0
2	NAG	G	1	2,1	14,14,15	0.43	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	2	2	14,14,15	0.22	0	17,19,21	0.62	0
2	NAG	H	1	2,1	14,14,15	0.57	0	17,19,21	0.47	0
2	NAG	H	2	2	14,14,15	0.27	0	17,19,21	0.57	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	2,1	-	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	2,1	-	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	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

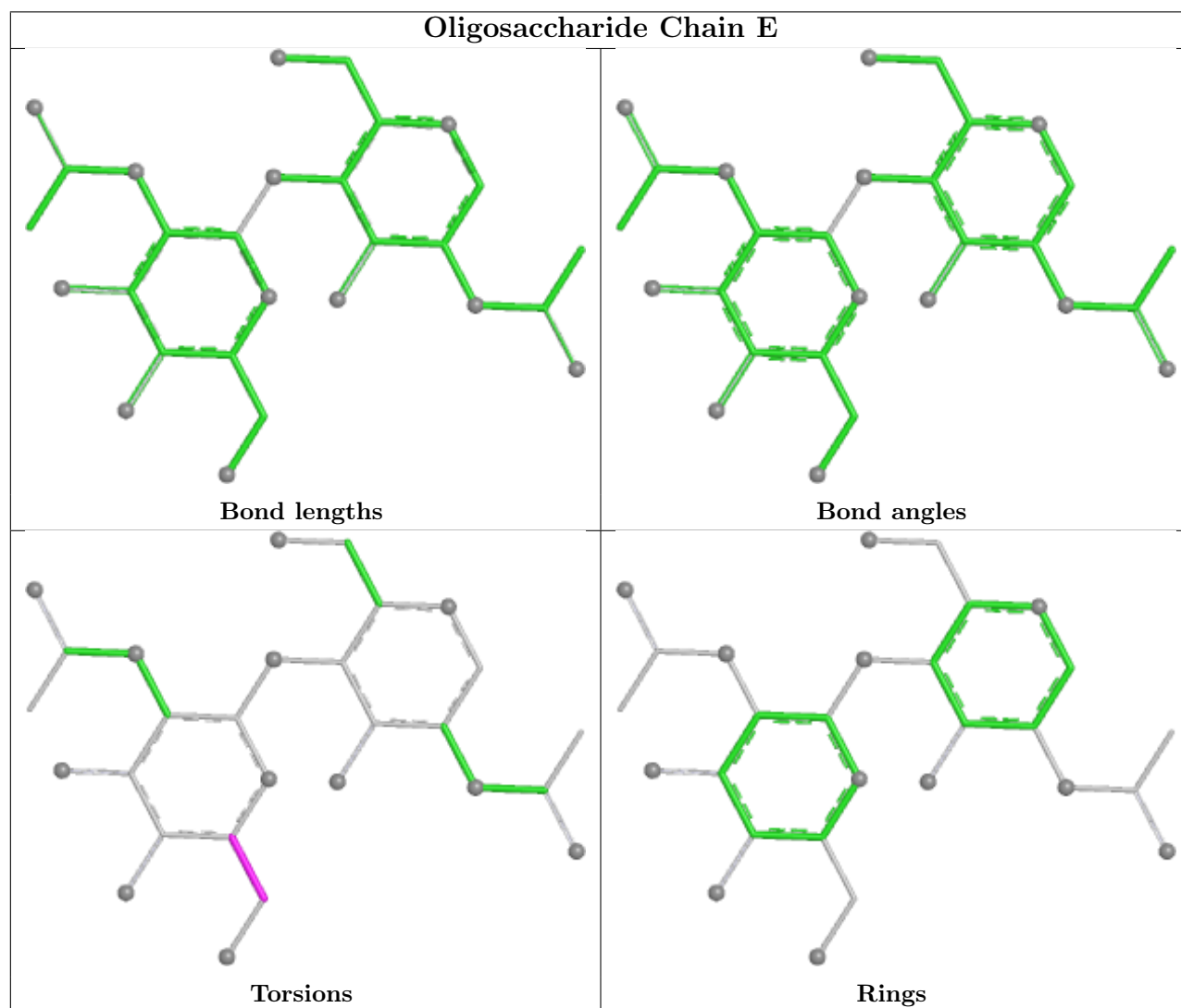
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

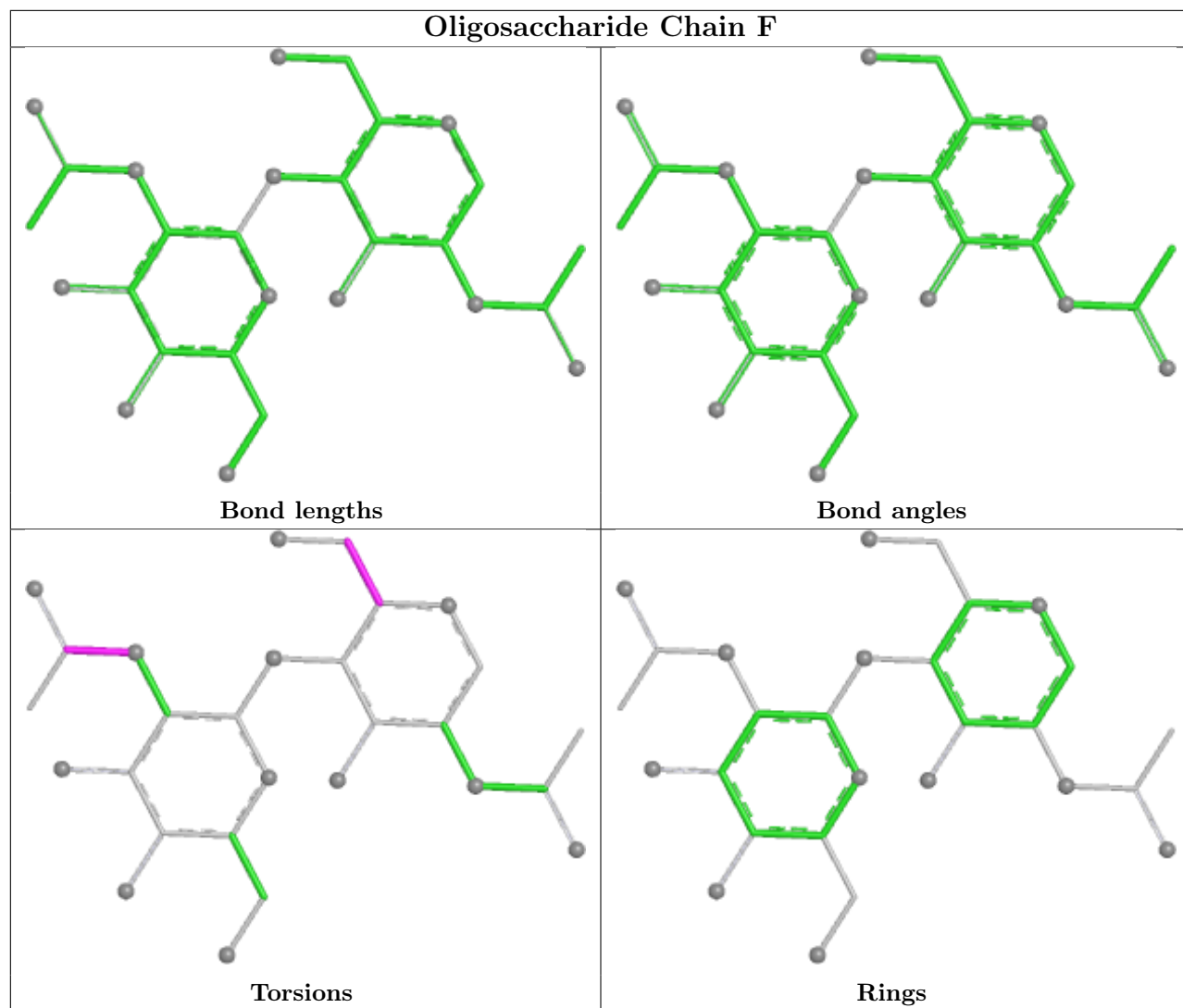
There are no ring outliers.

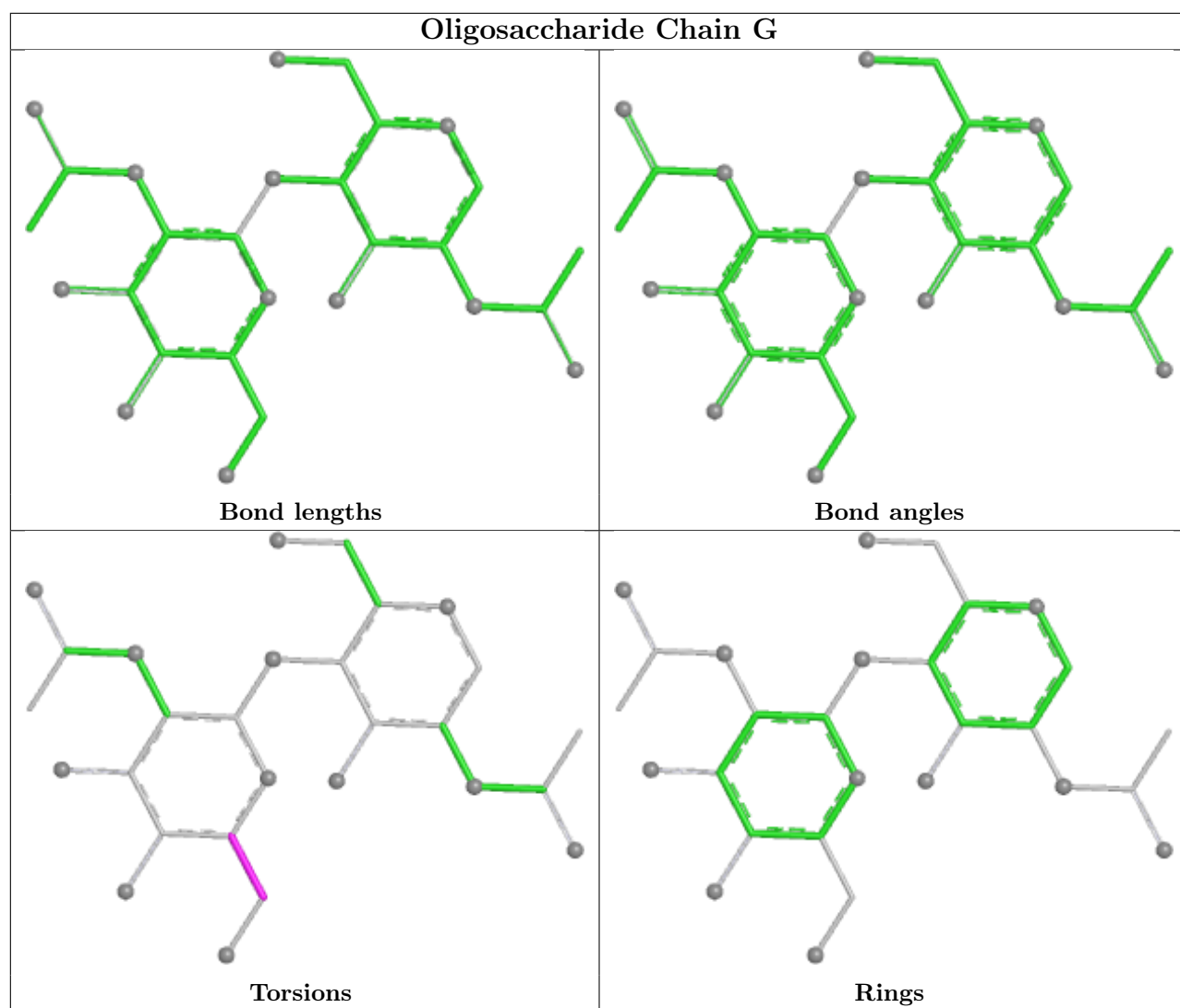
2 monomers are involved in 2 short contacts:

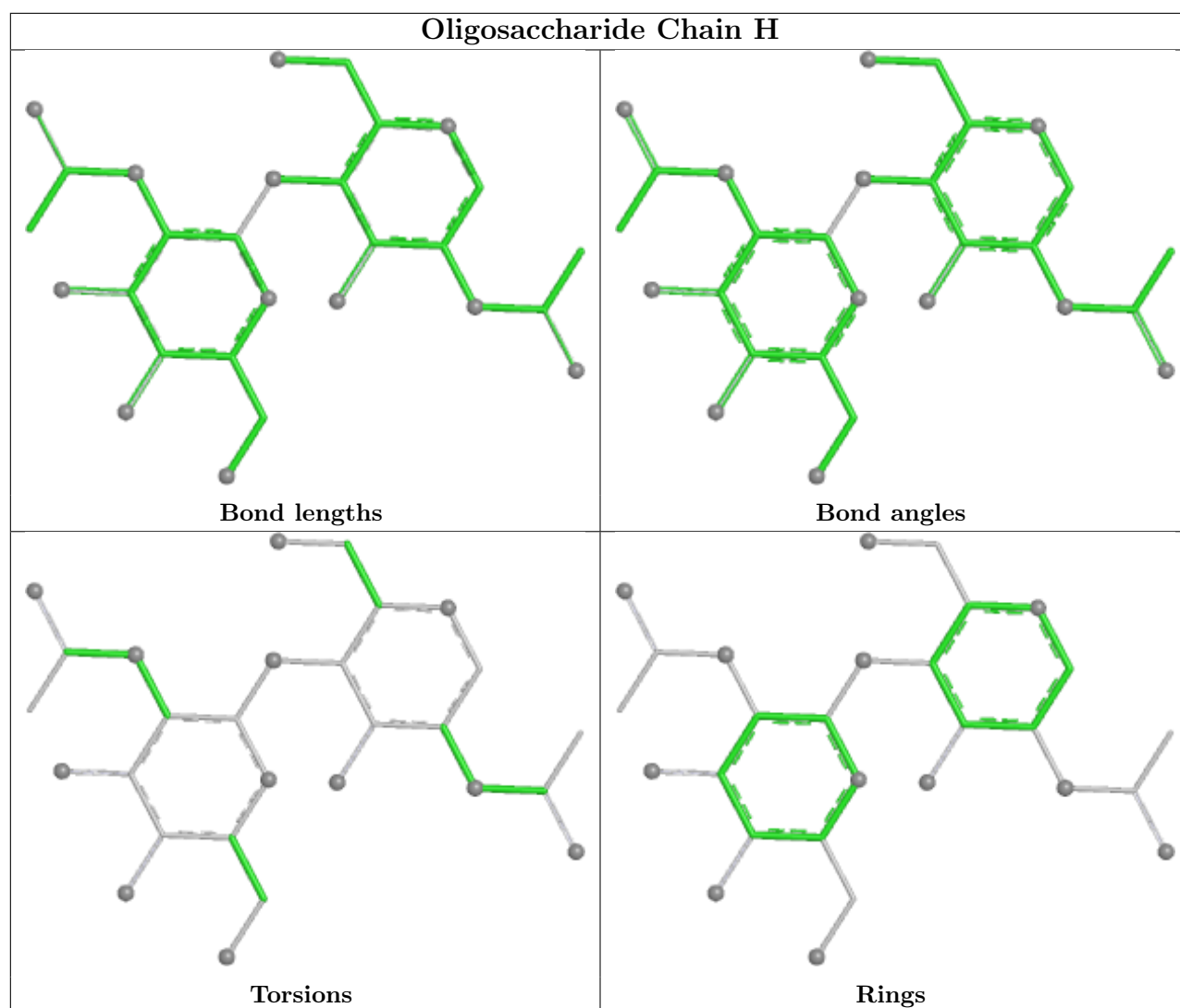
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	H	2	NAG	1	0

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 [i](#)

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	B	606[A]	-	25,25,25	5.15	12 (48%)	38,38,38	4.88	24 (63%)
5	MXM	A	606[B]	-	25,25,25	5.97	12 (48%)	38,38,38	5.16	21 (55%)
3	NAG	A	601	1	14,14,15	1.05	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	0.70	1 (7%)	17,19,21	0.50	0
3	NAG	D	601	1	14,14,15	0.91	1 (7%)	17,19,21	0.81	0
5	MXM	C	606[A]	-	25,25,25	6.28	13 (52%)	38,38,38	5.62	27 (71%)
4	HEM	B	605	7,1	50,50,50	1.95	10 (20%)	67,82,82	1.32	4 (5%)
4	HEM	D	605	7,1	50,50,50	1.93	9 (18%)	67,82,82	1.35	5 (7%)
5	MXM	D	606[B]	-	25,25,25	7.06	14 (56%)	38,38,38	5.43	23 (60%)
5	MXM	B	606[B]	-	25,25,25	5.04	13 (52%)	38,38,38	4.93	20 (52%)
6	BOG	C	607	-	20,20,20	1.58	3 (15%)	25,25,25	1.50	4 (16%)
4	HEM	A	605	7,1	50,50,50	1.86	8 (16%)	67,82,82	1.33	4 (5%)
5	MXM	A	606[A]	-	25,25,25	5.27	12 (48%)	38,38,38	4.93	24 (63%)
6	BOG	B	607	-	20,20,20	1.40	2 (10%)	25,25,25	1.65	3 (12%)
3	NAG	D	604	1	14,14,15	0.29	0	17,19,21	0.56	0
4	HEM	C	605	1	50,50,50	1.93	9 (18%)	67,82,82	1.32	6 (8%)
5	MXM	C	606[B]	-	25,25,25	6.64	12 (48%)	38,38,38	5.02	25 (65%)
3	NAG	C	604	1	14,14,15	0.87	1 (7%)	17,19,21	0.81	1 (5%)
3	NAG	C	601	1	14,14,15	0.51	0	17,19,21	0.53	0
3	NAG	B	604	1	14,14,15	0.45	0	17,19,21	0.55	0
3	NAG	A	604	1	14,14,15	0.74	1 (7%)	17,19,21	0.65	0
5	MXM	D	606[A]	-	25,25,25	6.53	13 (52%)	38,38,38	4.82	25 (65%)

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	B	606[A]	-	-	2/8/32/32	0/3/3/3
5	MXM	A	606[B]	-	-	0/8/32/32	0/3/3/3
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	D	601	1	-	0/6/23/26	0/1/1/1
5	MXM	C	606[A]	-	-	2/8/32/32	0/3/3/3
4	HEM	B	605	7,1	-	1/14/54/54	-
4	HEM	D	605	7,1	-	2/14/54/54	-
5	MXM	D	606[B]	-	-	2/8/32/32	0/3/3/3
5	MXM	B	606[B]	-	-	0/8/32/32	0/3/3/3
6	BOG	C	607	-	-	8/11/31/31	0/1/1/1
4	HEM	A	605	7,1	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MXM	A	606[A]	-	-	2/8/32/32	0/3/3/3
6	BOG	B	607	-	-	7/11/31/31	0/1/1/1
3	NAG	D	604	1	-	2/6/23/26	0/1/1/1
4	HEM	C	605	1	-	3/14/54/54	-
5	MXM	C	606[B]	-	-	0/8/32/32	0/3/3/3
3	NAG	C	604	1	-	2/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	MXM	D	606[A]	-	-	0/8/32/32	0/3/3/3

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	606[B]	MXM	SAE-NAJ	-23.54	1.33	1.64
5	D	606[A]	MXM	SAE-NAJ	-21.84	1.35	1.64
5	D	606[B]	MXM	SAE-NAJ	-21.24	1.36	1.64
5	C	606[A]	MXM	SAE-NAJ	-20.96	1.36	1.64
5	A	606[B]	MXM	SAE-NAJ	-17.73	1.40	1.64
5	B	606[A]	MXM	CAB-SAE	-16.25	1.52	1.75
5	A	606[B]	MXM	CAB-SAE	-15.45	1.53	1.75
5	A	606[A]	MXM	CAB-SAE	-15.31	1.53	1.75
5	D	606[B]	MXM	OAL-SAE	13.98	1.58	1.43
5	D	606[B]	MXM	CAB-SAE	-13.53	1.56	1.75
5	C	606[A]	MXM	OAL-SAE	13.48	1.57	1.43
5	D	606[A]	MXM	OAL-SAE	13.12	1.57	1.43
5	C	606[B]	MXM	OAL-SAE	12.84	1.57	1.43
5	A	606[A]	MXM	SAE-NAJ	-12.63	1.47	1.64
5	D	606[A]	MXM	CAB-SAE	-12.25	1.58	1.75
5	B	606[B]	MXM	CAB-SAE	-12.13	1.58	1.75
5	C	606[A]	MXM	CAB-SAE	-11.65	1.58	1.75
5	D	606[B]	MXM	CAR-SAT	-11.38	1.54	1.73
5	B	606[B]	MXM	SAE-NAJ	-10.57	1.50	1.64
5	A	606[B]	MXM	OAK-SAE	10.45	1.54	1.43
5	C	606[A]	MXM	OAK-SAE	10.41	1.54	1.43
5	A	606[A]	MXM	OAL-SAE	10.37	1.54	1.43
5	D	606[B]	MXM	OAK-SAE	10.35	1.54	1.43
5	C	606[B]	MXM	OAK-SAE	10.25	1.54	1.43
5	B	606[A]	MXM	SAE-NAJ	-10.16	1.50	1.64
5	B	606[A]	MXM	OAL-SAE	10.02	1.54	1.43
5	B	606[B]	MXM	OAL-SAE	9.97	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606[B]	MXM	OAL-SAE	9.89	1.54	1.43
5	C	606[B]	MXM	CAB-SAE	-9.87	1.61	1.75
5	D	606[A]	MXM	OAK-SAE	9.82	1.54	1.43
5	A	606[A]	MXM	OAK-SAE	9.62	1.53	1.43
5	B	606[A]	MXM	OAK-SAE	9.49	1.53	1.43
5	B	606[B]	MXM	OAK-SAE	9.41	1.53	1.43
4	B	605	HEM	C3D-C2D	7.92	1.53	1.36
4	A	605	HEM	C3D-C2D	7.90	1.53	1.36
4	D	605	HEM	C3D-C2D	7.83	1.53	1.36
4	C	605	HEM	C3D-C2D	7.82	1.53	1.36
5	B	606[B]	MXM	CAV-SAT	-7.02	1.54	1.72
5	C	606[B]	MXM	CAV-SAT	-6.61	1.55	1.72
5	B	606[B]	MXM	CAR-SAT	-6.31	1.63	1.73
5	D	606[A]	MXM	CAG-NAJ	-6.10	1.37	1.44
5	B	606[A]	MXM	CAG-CAC	5.76	1.44	1.36
5	A	606[A]	MXM	CAG-CAC	5.73	1.44	1.36
5	D	606[B]	MXM	CAR-NAP	-5.73	1.29	1.38
5	A	606[B]	MXM	CAV-SAT	-5.67	1.58	1.72
5	B	606[B]	MXM	CAG-CAC	5.56	1.43	1.36
4	C	605	HEM	FE-ND	5.46	2.11	1.94
5	A	606[B]	MXM	CAG-CAC	5.44	1.43	1.36
4	D	605	HEM	FE-ND	5.29	2.11	1.94
5	C	606[A]	MXM	CAG-CAC	5.29	1.43	1.36
5	D	606[B]	MXM	CAG-CAC	5.26	1.43	1.36
5	C	606[B]	MXM	CAG-CAC	5.22	1.43	1.36
4	B	605	HEM	FE-NB	5.15	2.10	1.94
5	C	606[B]	MXM	CAO-NAJ	5.09	1.54	1.48
5	D	606[B]	MXM	CAG-NAJ	-5.08	1.38	1.44
5	D	606[A]	MXM	CAG-CAC	5.06	1.43	1.36
4	B	605	HEM	FE-ND	4.92	2.10	1.94
5	B	606[B]	MXM	CAG-NAJ	-4.74	1.38	1.44
5	D	606[B]	MXM	CAV-SAT	-4.73	1.60	1.72
5	B	606[A]	MXM	CAG-NAJ	-4.61	1.39	1.44
5	D	606[A]	MXM	CAA-CAB	-4.46	1.35	1.40
5	D	606[A]	MXM	CAR-NAP	-4.43	1.31	1.38
5	A	606[A]	MXM	CAG-NAJ	-4.40	1.39	1.44
5	D	606[B]	MXM	CAG-CAN	-4.32	1.37	1.46
4	D	605	HEM	FE-NB	4.32	2.08	1.94
5	D	606[A]	MXM	CAG-CAN	-4.23	1.37	1.46
5	C	606[B]	MXM	CAG-NAJ	-4.20	1.39	1.44
5	D	606[B]	MXM	CAA-CAC	-4.11	1.39	1.45
4	A	605	HEM	FE-NC	4.05	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	606[B]	MXM	CAG-CAN	-4.05	1.37	1.46
5	C	606[B]	MXM	CAA-CAB	-4.01	1.36	1.40
4	A	605	HEM	FE-NB	3.94	2.07	1.94
5	D	606[A]	MXM	CAO-NAJ	3.94	1.52	1.48
6	C	607	BOG	O2-C2	-3.90	1.33	1.43
4	C	605	HEM	FE-NB	3.89	2.06	1.94
4	A	605	HEM	FE-ND	3.86	2.06	1.94
6	B	607	BOG	O2-C2	-3.80	1.33	1.43
5	C	606[A]	MXM	CAR-NAP	-3.80	1.32	1.38
5	C	606[A]	MXM	CAG-NAJ	-3.63	1.40	1.44
5	C	606[A]	MXM	CAG-CAN	-3.59	1.38	1.46
5	A	606[B]	MXM	CAG-NAJ	-3.54	1.40	1.44
4	C	605	HEM	FE-NC	3.49	2.06	1.95
4	B	605	HEM	FE-NC	3.46	2.06	1.95
5	D	606[A]	MXM	CAA-CAC	-3.44	1.40	1.45
5	A	606[B]	MXM	CAR-SAT	-3.33	1.68	1.73
3	A	601	NAG	C1-C2	3.27	1.56	1.52
5	B	606[A]	MXM	CAR-SAT	-3.26	1.68	1.73
4	D	605	HEM	FE-NA	3.25	2.05	1.95
5	C	606[B]	MXM	CAR-NAP	-3.24	1.33	1.38
5	B	606[B]	MXM	CAG-CAN	-3.23	1.39	1.46
5	C	606[B]	MXM	CAA-CAC	-3.23	1.40	1.45
5	B	606[B]	MXM	CAA-CAB	-3.22	1.37	1.40
5	C	606[A]	MXM	CAA-CAC	-3.20	1.40	1.45
5	A	606[B]	MXM	CAA-CAC	-3.17	1.40	1.45
5	A	606[B]	MXM	CAA-CAB	-3.15	1.37	1.40
4	C	605	HEM	CAB-C3B	3.15	1.55	1.47
4	C	605	HEM	CAC-C3C	3.13	1.55	1.47
5	D	606[B]	MXM	CAA-CAB	-3.12	1.37	1.40
4	A	605	HEM	CAB-C3B	3.11	1.55	1.47
4	B	605	HEM	CAB-C3B	3.11	1.55	1.47
5	B	606[B]	MXM	CAA-CAC	-3.09	1.40	1.45
4	D	605	HEM	CAB-C3B	3.09	1.55	1.47
5	D	606[B]	MXM	CAR-NAS	3.03	1.36	1.31
5	C	606[A]	MXM	CAA-CAB	-3.02	1.37	1.40
4	D	605	HEM	FE-NC	3.00	2.05	1.95
5	C	606[A]	MXM	CAR-SAT	-2.97	1.68	1.73
4	A	605	HEM	CAC-C3C	2.97	1.55	1.47
5	A	606[B]	MXM	CAG-CAN	-2.94	1.40	1.46
5	A	606[A]	MXM	CAA-CAB	-2.90	1.37	1.40
6	C	607	BOG	O3-C3	-2.89	1.35	1.43
4	B	605	HEM	CAC-C3C	2.87	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	605	HEM	CAC-C3C	2.87	1.55	1.47
5	B	606[A]	MXM	CAA-CAB	-2.83	1.37	1.40
5	D	606[A]	MXM	CAV-SAT	-2.75	1.65	1.72
4	C	605	HEM	FE-NA	2.71	2.04	1.95
5	A	606[A]	MXM	CAG-CAN	-2.68	1.40	1.46
3	C	604	NAG	O5-C1	-2.67	1.39	1.43
3	D	601	NAG	O5-C1	2.62	1.48	1.43
5	B	606[A]	MXM	CAG-CAN	-2.62	1.40	1.46
5	A	606[A]	MXM	CAA-CAC	-2.54	1.41	1.45
6	B	607	BOG	O3-C3	-2.54	1.36	1.43
4	A	605	HEM	FE-NA	2.47	2.03	1.95
5	D	606[B]	MXM	CAN-NAP	-2.43	1.32	1.37
5	A	606[B]	MXM	CAR-NAP	-2.42	1.34	1.38
3	A	604	NAG	O5-C1	-2.36	1.39	1.43
5	C	606[A]	MXM	CAR-NAS	2.35	1.35	1.31
5	B	606[A]	MXM	CAA-CAC	-2.30	1.42	1.45
5	B	606[B]	MXM	CAR-NAP	-2.29	1.34	1.38
4	B	605	HEM	FE-NA	2.29	2.02	1.95
5	A	606[A]	MXM	CAR-SAT	-2.28	1.70	1.73
5	C	606[A]	MXM	CAO-NAJ	2.24	1.50	1.48
4	C	605	HEM	CMB-C2B	2.19	1.55	1.50
5	B	606[A]	MXM	CAV-SAT	-2.19	1.67	1.72
4	D	605	HEM	CMA-C3A	2.14	1.55	1.50
3	B	601	NAG	C1-C2	2.10	1.55	1.52
5	B	606[A]	MXM	CAR-NAP	-2.10	1.35	1.38
5	A	606[A]	MXM	CAU-NAS	-2.09	1.33	1.37
5	B	606[B]	MXM	CAR-NAS	2.07	1.34	1.31
5	A	606[A]	MXM	CAR-NAP	-2.07	1.35	1.38
4	B	605	HEM	CMC-C2C	2.07	1.55	1.50
4	B	605	HEM	CMA-C3A	2.06	1.55	1.50
4	C	605	HEM	CMC-C2C	2.04	1.55	1.50
6	C	607	BOG	O4-C4	-2.04	1.37	1.43
4	B	605	HEM	CMB-C2B	2.03	1.54	1.50
5	D	606[A]	MXM	CAN-NAP	-2.01	1.33	1.37
4	A	605	HEM	CMA-C3A	2.01	1.54	1.50
4	D	605	HEM	CMB-C2B	2.00	1.54	1.50

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	606[B]	MXM	CAO-NAJ-SAE	13.48	137.78	116.91
5	C	606[A]	MXM	OAL-SAE-OAK	-12.71	102.37	118.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606[B]	MXM	CAO-NAJ-SAE	12.60	136.42	116.91
5	D	606[B]	MXM	OAL-SAE-OAK	-12.59	102.51	118.53
5	B	606[B]	MXM	CAO-NAJ-SAE	12.51	136.28	116.91
5	D	606[A]	MXM	OAL-SAE-OAK	-12.19	103.02	118.53
5	C	606[B]	MXM	OAL-SAE-OAK	-12.16	103.06	118.53
5	A	606[A]	MXM	CAO-NAJ-SAE	12.07	135.60	116.91
5	C	606[A]	MXM	CAO-NAJ-SAE	12.02	135.52	116.91
5	B	606[A]	MXM	CAO-NAJ-SAE	11.85	135.26	116.91
5	C	606[B]	MXM	CAO-NAJ-SAE	11.70	135.03	116.91
5	D	606[A]	MXM	CAO-NAJ-SAE	11.68	134.99	116.91
5	A	606[B]	MXM	CAB-SAE-NAJ	11.34	116.50	101.91
5	B	606[B]	MXM	CAV-SAT-CAR	10.93	97.37	89.32
5	A	606[B]	MXM	CAB-CAA-CAC	-10.40	114.69	120.47
5	C	606[B]	MXM	CAB-SAE-NAJ	10.24	115.09	101.91
5	D	606[A]	MXM	CAB-CAA-CAC	-9.90	114.97	120.47
5	B	606[B]	MXM	CAG-NAJ-SAE	-9.68	100.25	113.14
5	B	606[A]	MXM	CAB-SAE-NAJ	9.57	114.24	101.91
5	A	606[A]	MXM	CAB-SAE-NAJ	9.55	114.20	101.91
5	C	606[A]	MXM	SAT-CAR-NAS	-9.52	105.16	115.58
5	A	606[B]	MXM	CAG-NAJ-SAE	-9.48	100.52	113.14
5	B	606[B]	MXM	CAB-SAE-NAJ	9.44	114.06	101.91
5	D	606[A]	MXM	CAB-SAE-NAJ	9.43	114.05	101.91
5	A	606[B]	MXM	OAL-SAE-OAK	-9.43	106.54	118.53
5	B	606[A]	MXM	CAG-NAJ-SAE	-9.39	100.64	113.14
5	A	606[A]	MXM	CAG-NAJ-SAE	-9.34	100.71	113.14
5	D	606[B]	MXM	CAB-CAA-CAC	-9.31	115.30	120.47
5	B	606[B]	MXM	CAB-CAA-CAC	-9.23	115.34	120.47
5	B	606[B]	MXM	OAL-SAE-OAK	-9.19	106.84	118.53
5	C	606[A]	MXM	CAB-SAE-NAJ	9.18	113.73	101.91
5	D	606[B]	MXM	CAV-SAT-CAR	9.12	96.03	89.32
5	A	606[B]	MXM	CAV-SAT-CAR	8.94	95.90	89.32
5	B	606[A]	MXM	OAL-SAE-OAK	-8.93	107.18	118.53
5	A	606[A]	MXM	OAL-SAE-OAK	-8.90	107.20	118.53
5	C	606[B]	MXM	CAB-CAA-CAC	-8.82	115.57	120.47
5	D	606[B]	MXM	CAV-CAU-NAS	-8.45	108.39	117.12
5	A	606[A]	MXM	SAT-CAR-NAS	-8.41	106.37	115.58
5	B	606[A]	MXM	SAT-CAR-NAS	-8.41	106.38	115.58
5	D	606[B]	MXM	CAB-SAE-NAJ	8.31	112.61	101.91
5	D	606[B]	MXM	CAG-NAJ-SAE	-8.13	102.32	113.14
5	C	606[B]	MXM	SAT-CAR-NAS	-8.06	106.75	115.58
5	C	606[B]	MXM	CAV-SAT-CAR	8.01	95.22	89.32
5	A	606[B]	MXM	SAT-CAR-NAS	-7.84	107.00	115.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	606[A]	MXM	CAU-NAS-CAR	7.76	118.57	109.66
5	A	606[A]	MXM	CAW-CAV-CAU	-7.76	121.63	129.10
5	C	606[A]	MXM	OAL-SAE-NAJ	7.54	113.62	108.14
5	D	606[B]	MXM	OAL-SAE-NAJ	7.52	113.61	108.14
5	C	606[A]	MXM	CAB-CAA-CAC	-7.52	116.30	120.47
5	A	606[A]	MXM	CAB-CAA-CAC	-7.51	116.30	120.47
5	B	606[A]	MXM	CAB-CAA-CAC	-7.51	116.30	120.47
5	C	606[A]	MXM	CAW-CAV-CAU	-7.45	121.92	129.10
5	C	606[A]	MXM	OAK-SAE-NAJ	-7.37	102.78	108.14
5	B	606[B]	MXM	SAT-CAR-NAS	-7.35	107.53	115.58
5	A	606[B]	MXM	OAK-SAE-NAJ	-7.34	102.80	108.14
5	C	606[B]	MXM	CAO-NAJ-CAG	-7.33	105.16	115.07
5	D	606[A]	MXM	CAO-NAJ-CAG	-7.16	105.38	115.07
5	C	606[A]	MXM	CAG-NAJ-SAE	-6.95	103.88	113.14
5	D	606[B]	MXM	SAT-CAR-NAS	-6.94	107.98	115.58
5	B	606[A]	MXM	CAW-CAV-CAU	-6.71	122.63	129.10
5	A	606[B]	MXM	CAO-NAJ-CAG	-6.71	105.99	115.07
5	D	606[A]	MXM	CAG-NAJ-SAE	-6.70	104.22	113.14
5	C	606[B]	MXM	CAG-NAJ-SAE	-6.66	104.28	113.14
5	D	606[B]	MXM	OAK-SAE-NAJ	-6.66	103.30	108.14
5	A	606[A]	MXM	CAU-NAS-CAR	6.58	117.21	109.66
5	B	606[A]	MXM	CAV-SAT-CAR	6.48	94.09	89.32
5	B	606[B]	MXM	CAO-NAJ-CAG	-6.48	106.30	115.07
5	C	606[A]	MXM	CAV-SAT-CAR	6.42	94.04	89.32
5	C	606[A]	MXM	CAV-CAU-NAS	-6.38	110.53	117.12
5	B	606[A]	MXM	CAU-NAS-CAR	6.34	116.94	109.66
5	A	606[A]	MXM	CAA-CAB-SAE	-6.32	109.47	117.29
5	C	606[A]	MXM	CAA-CAB-SAE	-6.31	109.49	117.29
5	B	606[A]	MXM	CAA-CAB-SAE	-6.26	109.54	117.29
5	C	606[B]	MXM	OAK-SAE-NAJ	-6.24	103.59	108.14
5	C	606[A]	MXM	CAC-CAG-NAJ	-6.17	116.07	120.87
5	D	606[A]	MXM	CAW-CAV-CAU	-6.15	123.17	129.10
5	D	606[B]	MXM	CAO-NAJ-CAG	-6.11	106.81	115.07
5	B	606[B]	MXM	OAH-CAC-CAG	-6.06	117.25	122.66
5	C	606[B]	MXM	CAA-CAB-SAE	-5.98	109.89	117.29
5	D	606[A]	MXM	SAT-CAR-NAS	-5.95	109.07	115.58
5	C	606[A]	MXM	CAO-NAJ-CAG	-5.91	107.08	115.07
5	B	606[A]	MXM	OAH-CAC-CAG	-5.83	117.46	122.66
5	D	606[A]	MXM	OAL-SAE-CAB	5.78	117.02	109.10
5	C	606[A]	MXM	CAR-NAP-CAN	-5.76	115.19	123.78
5	A	606[B]	MXM	OAL-SAE-NAJ	5.69	112.28	108.14
4	B	605	HEM	C4D-ND-C1D	5.68	111.94	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	606[A]	MXM	SAT-CAR-NAP	5.68	131.33	123.72
4	A	605	HEM	C4D-ND-C1D	5.67	111.92	105.21
4	D	605	HEM	C4D-ND-C1D	5.66	111.91	105.21
5	B	606[B]	MXM	CAA-CAB-SAE	-5.60	110.36	117.29
4	C	605	HEM	C4D-ND-C1D	5.49	111.71	105.21
5	D	606[B]	MXM	CAR-NAP-CAN	-5.48	115.61	123.78
5	D	606[A]	MXM	SAT-CAR-NAP	5.48	131.05	123.72
5	D	606[B]	MXM	OAL-SAE-CAB	5.41	116.51	109.10
5	A	606[B]	MXM	CAA-CAB-SAE	-5.40	110.61	117.29
5	A	606[A]	MXM	CAV-SAT-CAR	5.39	93.29	89.32
5	D	606[B]	MXM	CAW-CAV-CAU	-5.26	124.03	129.10
5	A	606[A]	MXM	OAH-CAC-CAG	-5.22	118.00	122.66
5	B	606[B]	MXM	CAA-CAC-CAG	5.01	125.85	122.65
5	A	606[B]	MXM	OAH-CAC-CAG	-4.97	118.23	122.66
5	D	606[A]	MXM	CAA-CAB-SAE	-4.93	111.19	117.29
5	A	606[A]	MXM	CAC-CAG-NAJ	-4.91	117.05	120.87
5	D	606[B]	MXM	CAA-CAB-SAE	-4.90	111.22	117.29
5	C	606[B]	MXM	OAL-SAE-CAB	4.88	115.79	109.10
5	B	606[A]	MXM	CAC-CAG-NAJ	-4.85	117.09	120.87
5	C	606[A]	MXM	CAC-CAG-CAN	4.79	125.10	120.84
5	A	606[A]	MXM	SAT-CAR-NAP	4.70	130.02	123.72
5	A	606[A]	MXM	CAO-NAJ-CAG	-4.59	108.87	115.07
5	B	606[A]	MXM	CAO-NAJ-CAG	-4.57	108.89	115.07
5	C	606[A]	MXM	OAL-SAE-CAB	4.56	115.34	109.10
6	B	607	BOG	C1'-O1-C1	4.55	121.45	113.68
5	D	606[B]	MXM	CAU-NAS-CAR	4.54	114.87	109.66
5	D	606[B]	MXM	CAC-CAG-NAJ	-4.51	117.36	120.87
5	C	606[B]	MXM	OAH-CAC-CAG	-4.48	118.66	122.66
5	D	606[A]	MXM	OAK-SAE-NAJ	-4.47	104.89	108.14
5	A	606[A]	MXM	CAR-NAP-CAN	-4.44	117.16	123.78
5	B	606[A]	MXM	CAV-CAU-NAS	-4.42	112.56	117.12
5	A	606[A]	MXM	CAV-CAU-NAS	-4.40	112.58	117.12
5	B	606[A]	MXM	SAT-CAR-NAP	4.18	129.31	123.72
5	B	606[A]	MXM	CAR-NAP-CAN	-4.16	117.58	123.78
5	A	606[A]	MXM	OAL-SAE-NAJ	4.15	111.16	108.14
5	D	606[A]	MXM	CAU-NAS-CAR	4.05	114.30	109.66
5	C	606[B]	MXM	CAW-CAV-CAU	-4.00	125.24	129.10
5	B	606[A]	MXM	OAL-SAE-NAJ	3.95	111.01	108.14
5	B	606[B]	MXM	CAV-CAU-NAS	-3.91	113.08	117.12
5	B	606[B]	MXM	OAK-SAE-NAJ	-3.91	105.30	108.14
5	D	606[A]	MXM	OAH-CAC-CAG	-3.89	119.19	122.66
5	B	606[A]	MXM	CAA-CAC-CAG	3.82	125.09	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	606[A]	MXM	OAH-CAC-CAG	-3.82	119.25	122.66
5	B	606[B]	MXM	OAL-SAE-NAJ	3.80	110.90	108.14
5	D	606[A]	MXM	CAV-CAU-NAS	-3.75	113.25	117.12
5	C	606[B]	MXM	CAC-CAG-NAJ	-3.70	117.99	120.87
5	C	606[B]	MXM	SAT-CAR-NAP	3.68	128.65	123.72
5	A	606[B]	MXM	OAK-SAE-CAB	-3.64	104.12	109.10
5	C	606[B]	MXM	OAL-SAE-NAJ	3.60	110.76	108.14
5	C	606[A]	MXM	OAQ-CAN-CAG	-3.57	115.01	121.96
5	C	606[B]	MXM	CAR-NAP-CAN	-3.48	118.59	123.78
5	D	606[A]	MXM	CAV-SAT-CAR	3.45	91.86	89.32
5	A	606[B]	MXM	SAT-CAR-NAP	3.44	128.33	123.72
5	A	606[A]	MXM	CAW-CAV-SAT	3.43	128.10	121.03
5	D	606[B]	MXM	OAH-CAC-CAG	-3.42	119.61	122.66
5	A	606[B]	MXM	CAV-CAU-NAS	-3.41	113.60	117.12
6	B	607	BOG	O5-C5-C4	3.40	115.83	109.70
5	D	606[A]	MXM	CAC-CAG-NAJ	-3.33	118.28	120.87
5	A	606[B]	MXM	CAW-CAV-CAU	-3.32	125.90	129.10
5	C	606[A]	MXM	CAF-CAB-SAE	3.28	125.79	120.45
5	B	606[B]	MXM	SAT-CAR-NAP	3.23	128.05	123.72
5	A	606[B]	MXM	CAU-NAS-CAR	3.23	113.36	109.66
5	A	606[A]	MXM	CAA-CAC-CAG	3.22	124.71	122.65
5	D	606[A]	MXM	OAL-SAE-NAJ	3.22	110.48	108.14
5	B	606[A]	MXM	CAW-CAV-SAT	3.17	127.56	121.03
6	C	607	BOG	C1'-O1-C1	3.16	119.08	113.68
5	A	606[A]	MXM	CAC-CAG-CAN	3.13	123.63	120.84
5	A	606[A]	MXM	OAK-SAE-NAJ	-3.11	105.87	108.14
6	B	607	BOG	O1-C1-C2	-3.02	103.68	108.27
4	A	605	HEM	CBD-CAD-C3D	-3.02	104.18	112.53
5	C	606[B]	MXM	CAV-CAU-NAS	-3.02	114.00	117.12
5	C	606[A]	MXM	CAA-CAC-CAG	3.01	124.58	122.65
5	C	606[B]	MXM	CAD-CAA-CAB	2.99	121.23	118.01
5	C	606[A]	MXM	CAW-CAV-SAT	2.98	127.17	121.03
5	A	606[B]	MXM	OAL-SAE-CAB	2.95	113.14	109.10
6	C	607	BOG	C1-O5-C5	2.89	119.37	113.72
5	C	606[B]	MXM	CAA-CAC-CAG	2.88	124.49	122.65
5	A	606[B]	MXM	CAA-CAC-CAG	2.87	124.48	122.65
5	B	606[A]	MXM	CAC-CAG-CAN	2.85	123.38	120.84
5	D	606[B]	MXM	CAU-CAV-SAT	2.85	111.55	108.95
5	C	606[B]	MXM	OAQ-CAN-CAG	-2.83	116.44	121.96
4	D	605	HEM	CBD-CAD-C3D	-2.81	104.76	112.53
5	D	606[B]	MXM	CAC-CAG-CAN	2.80	123.33	120.84
5	B	606[B]	MXM	CAF-CAB-SAE	2.72	124.89	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	606[B]	MXM	CAU-NAS-CAR	2.68	112.73	109.66
5	D	606[A]	MXM	CAU-CAV-SAT	2.64	111.37	108.95
5	A	606[B]	MXM	CAR-NAP-CAN	-2.64	119.84	123.78
4	C	605	HEM	CBD-CAD-C3D	-2.63	105.27	112.53
5	B	606[B]	MXM	CAW-CAV-CAU	-2.56	126.63	129.10
5	A	606[A]	MXM	OAQ-CAN-CAG	-2.53	117.03	121.96
5	D	606[A]	MXM	CAD-CAA-CAB	2.50	120.70	118.01
6	C	607	BOG	O5-C5-C4	2.49	114.19	109.70
4	B	605	HEM	CHC-C1C-NC	2.48	127.15	124.45
4	C	605	HEM	C1B-NB-C4B	2.46	108.12	105.21
4	D	605	HEM	CHC-C1C-NC	2.46	127.13	124.45
5	A	606[B]	MXM	CAC-CAG-NAJ	-2.45	118.97	120.87
5	C	606[B]	MXM	CAU-CAV-SAT	2.43	111.17	108.95
5	C	606[B]	MXM	CAF-CAB-SAE	2.41	124.38	120.45
5	D	606[A]	MXM	OAK-SAE-CAB	-2.36	105.88	109.10
5	B	606[A]	MXM	OAQ-CAN-CAG	-2.35	117.38	121.96
4	A	605	HEM	CHC-C1C-NC	2.30	126.95	124.45
6	C	607	BOG	O2-C2-C3	-2.28	104.99	110.38
5	D	606[B]	MXM	OAQ-CAN-NAP	2.28	126.96	122.88
5	D	606[B]	MXM	CAD-CAA-CAB	2.27	120.45	118.01
5	A	606[A]	MXM	CAF-CAB-SAE	2.26	124.14	120.45
4	C	605	HEM	CBA-CAA-C2A	-2.22	106.40	112.53
5	C	606[A]	MXM	CAD-CAA-CAB	2.21	120.39	118.01
4	B	605	HEM	C2A-C1A-NA	-2.19	107.72	110.15
5	B	606[B]	MXM	OAL-SAE-CAB	2.19	112.09	109.10
5	D	606[A]	MXM	CAI-CAD-CAA	-2.18	115.85	119.80
4	B	605	HEM	CBD-CAD-C3D	-2.16	106.56	112.53
5	C	606[A]	MXM	CAG-CAN-NAP	2.16	119.51	116.31
5	B	606[A]	MXM	CAF-CAB-SAE	2.15	123.96	120.45
5	B	606[A]	MXM	OAK-SAE-NAJ	-2.15	106.57	108.14
5	C	606[A]	MXM	CAU-CAV-SAT	2.15	110.91	108.95
5	D	606[A]	MXM	CAN-CAG-NAJ	2.14	120.98	116.31
4	D	605	HEM	C2A-C1A-NA	-2.13	107.79	110.15
5	A	606[A]	MXM	CAG-CAN-NAP	2.12	119.45	116.31
4	C	605	HEM	CHC-C1C-NC	2.10	126.73	124.45
4	D	605	HEM	C1B-NB-C4B	2.09	107.69	105.21
5	D	606[B]	MXM	CAI-CAD-CAA	-2.09	116.02	119.80
5	D	606[A]	MXM	CAW-CAV-SAT	2.09	125.33	121.03
5	B	606[B]	MXM	CAU-NAS-CAR	2.08	112.04	109.66
5	B	606[B]	MXM	CAR-NAP-CAN	-2.08	120.69	123.78
5	C	606[B]	MXM	CAI-CAD-CAA	-2.07	116.05	119.80
3	C	604	NAG	C1-C2-N2	-2.06	107.18	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	606[A]	MXM	CAA-CAC-CAG	2.06	123.97	122.65
4	C	605	HEM	CAC-C3C-C4C	2.02	129.66	124.82
4	A	605	HEM	CAC-C3C-C4C	2.01	129.61	124.82
5	B	606[A]	MXM	CAG-CAN-NAP	2.00	119.28	116.31

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	606[A]	MXM	SAT-CAR-NAP-CAN
5	A	606[A]	MXM	NAS-CAR-NAP-CAN
5	B	606[A]	MXM	SAT-CAR-NAP-CAN
5	B	606[A]	MXM	NAS-CAR-NAP-CAN
5	C	606[A]	MXM	SAT-CAR-NAP-CAN
5	C	606[A]	MXM	NAS-CAR-NAP-CAN
5	D	606[B]	MXM	SAT-CAR-NAP-CAN
5	D	606[B]	MXM	NAS-CAR-NAP-CAN
6	C	607	BOG	C4-C5-C6-O6
6	B	607	BOG	C4-C5-C6-O6
6	B	607	BOG	O5-C5-C6-O6
3	D	604	NAG	O5-C5-C6-O6
6	C	607	BOG	O5-C5-C6-O6
3	D	604	NAG	C4-C5-C6-O6
3	A	604	NAG	O5-C5-C6-O6
3	C	604	NAG	O5-C5-C6-O6
6	C	607	BOG	C2'-C3'-C4'-C5'
6	B	607	BOG	C3'-C4'-C5'-C6'
6	B	607	BOG	C4'-C5'-C6'-C7'
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	C3'-C4'-C5'-C6'
4	B	605	HEM	C4C-C3C-CAC-CBC
6	C	607	BOG	C1'-C2'-C3'-C4'
3	C	604	NAG	C4-C5-C6-O6
6	B	607	BOG	C2'-C1'-O1-C1
6	C	607	BOG	C2'-C1'-O1-C1
4	A	605	HEM	C4C-C3C-CAC-CBC
4	C	605	HEM	C4C-C3C-CAC-CBC
4	D	605	HEM	C4C-C3C-CAC-CBC
6	C	607	BOG	C5'-C6'-C7'-C8'
4	C	605	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	B	607	BOG	C2'-C3'-C4'-C5'
4	C	605	HEM	CAA-CBA-CGA-O1A
4	D	605	HEM	CAA-CBA-CGA-O2A

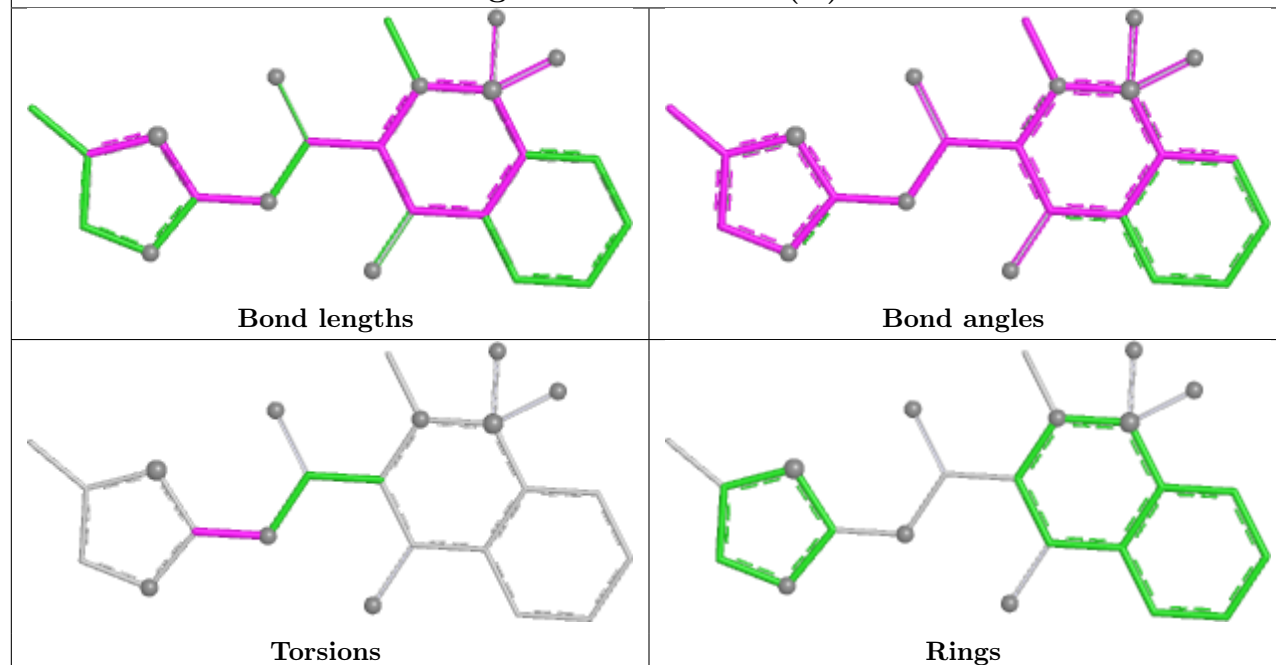
There are no ring outliers.

16 monomers are involved in 34 short contacts:

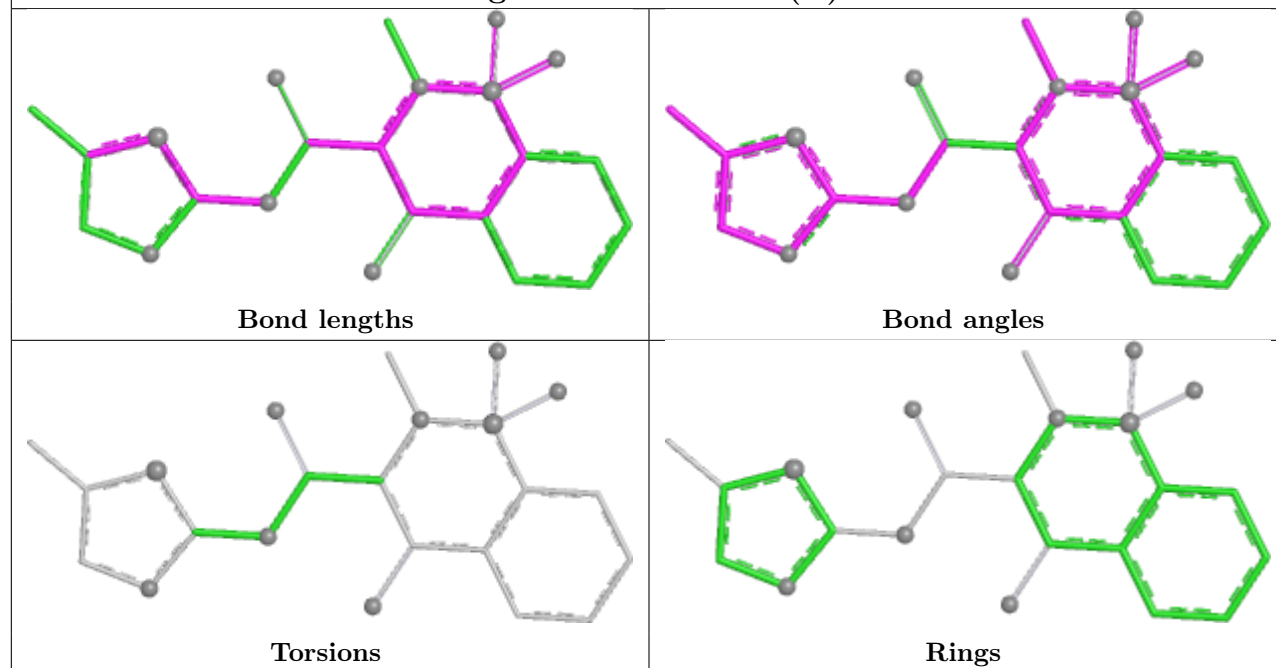
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606[A]	MXM	3	0
5	A	606[B]	MXM	1	0
3	D	601	NAG	1	0
5	C	606[A]	MXM	4	0
4	B	605	HEM	2	0
4	D	605	HEM	2	0
5	D	606[B]	MXM	4	0
5	B	606[B]	MXM	3	0
6	C	607	BOG	2	0
4	A	605	HEM	2	0
5	A	606[A]	MXM	1	0
6	B	607	BOG	1	0
4	C	605	HEM	2	0
5	C	606[B]	MXM	4	0
3	A	604	NAG	1	0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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

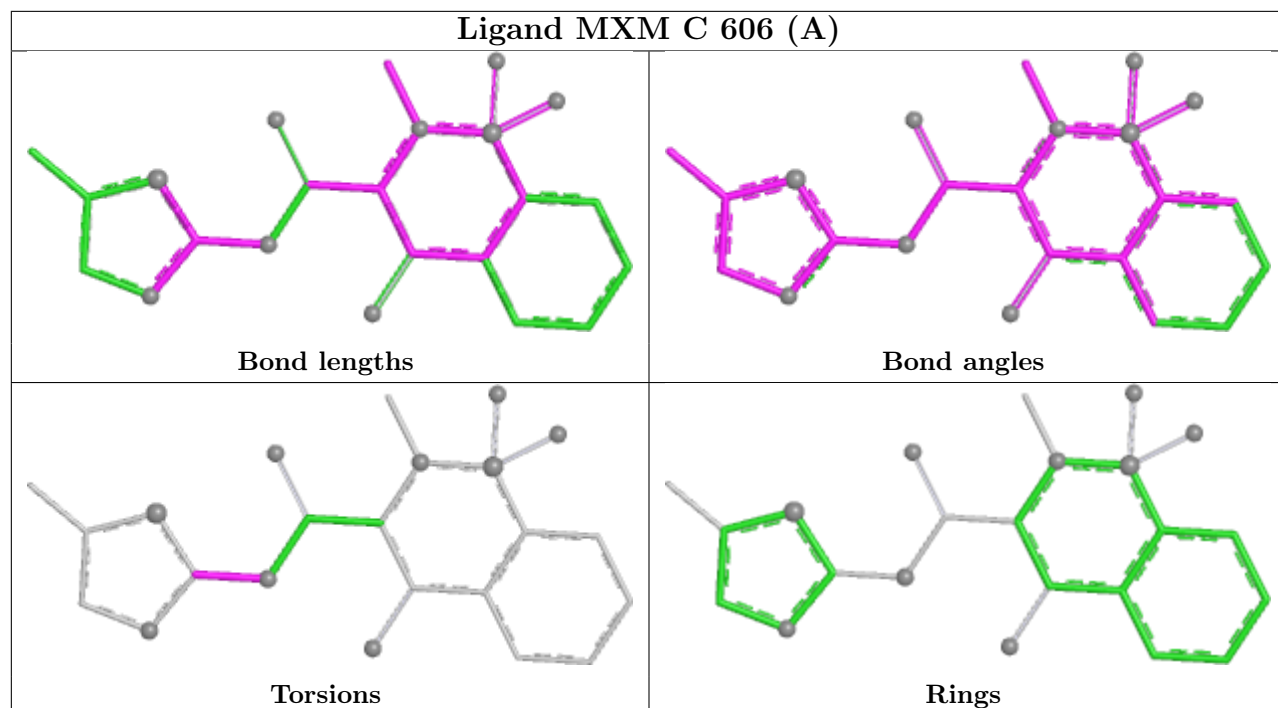
Ligand MXM B 606 (A)



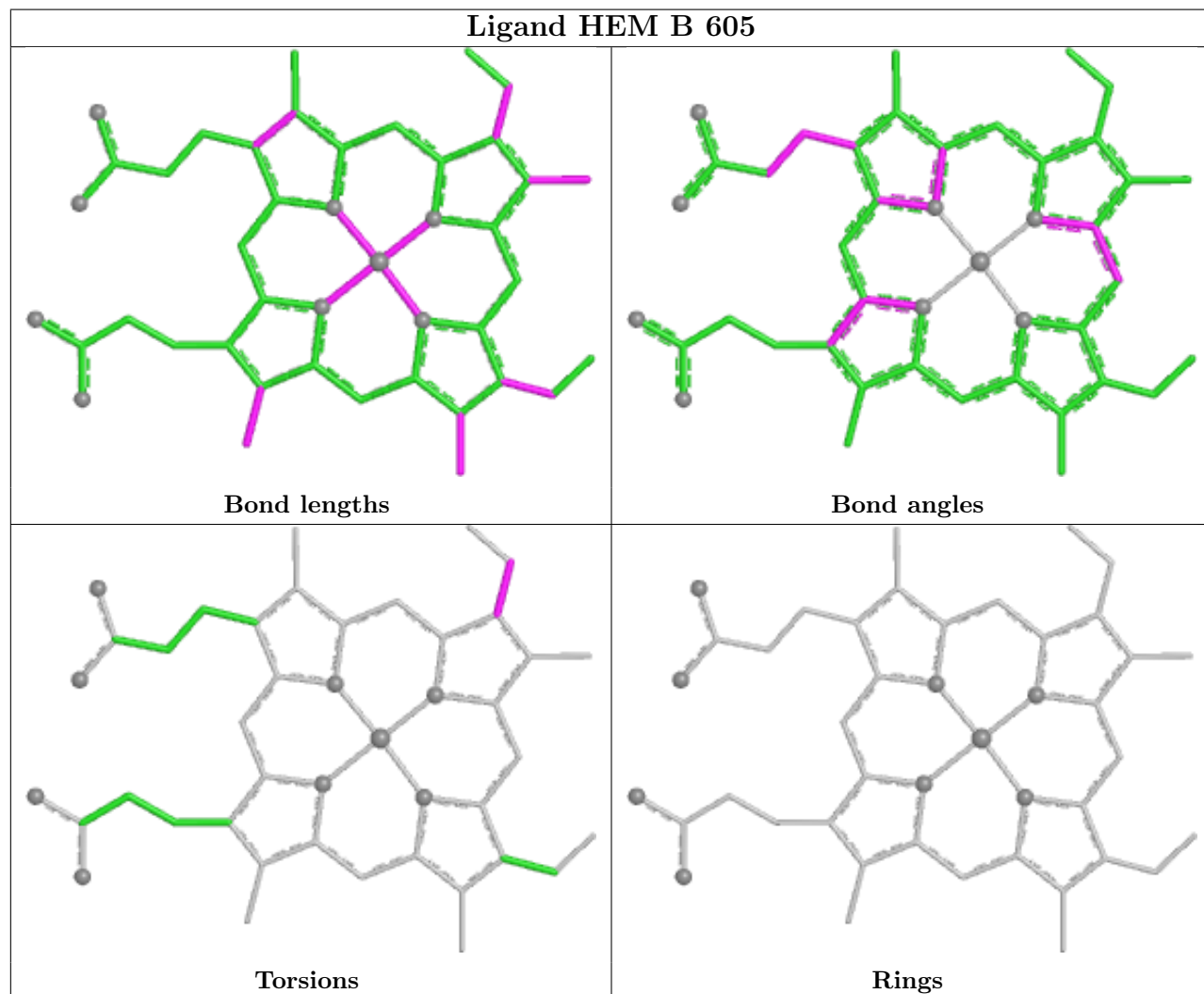
Ligand MXM A 606 (B)

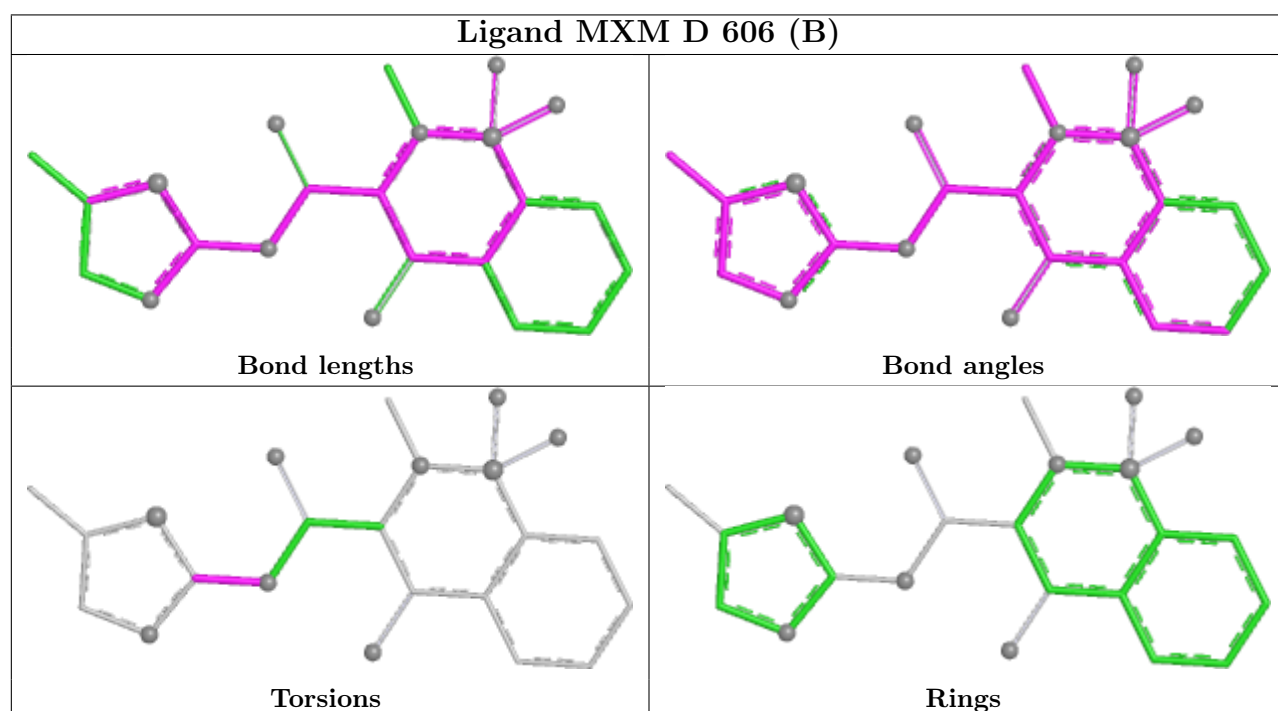
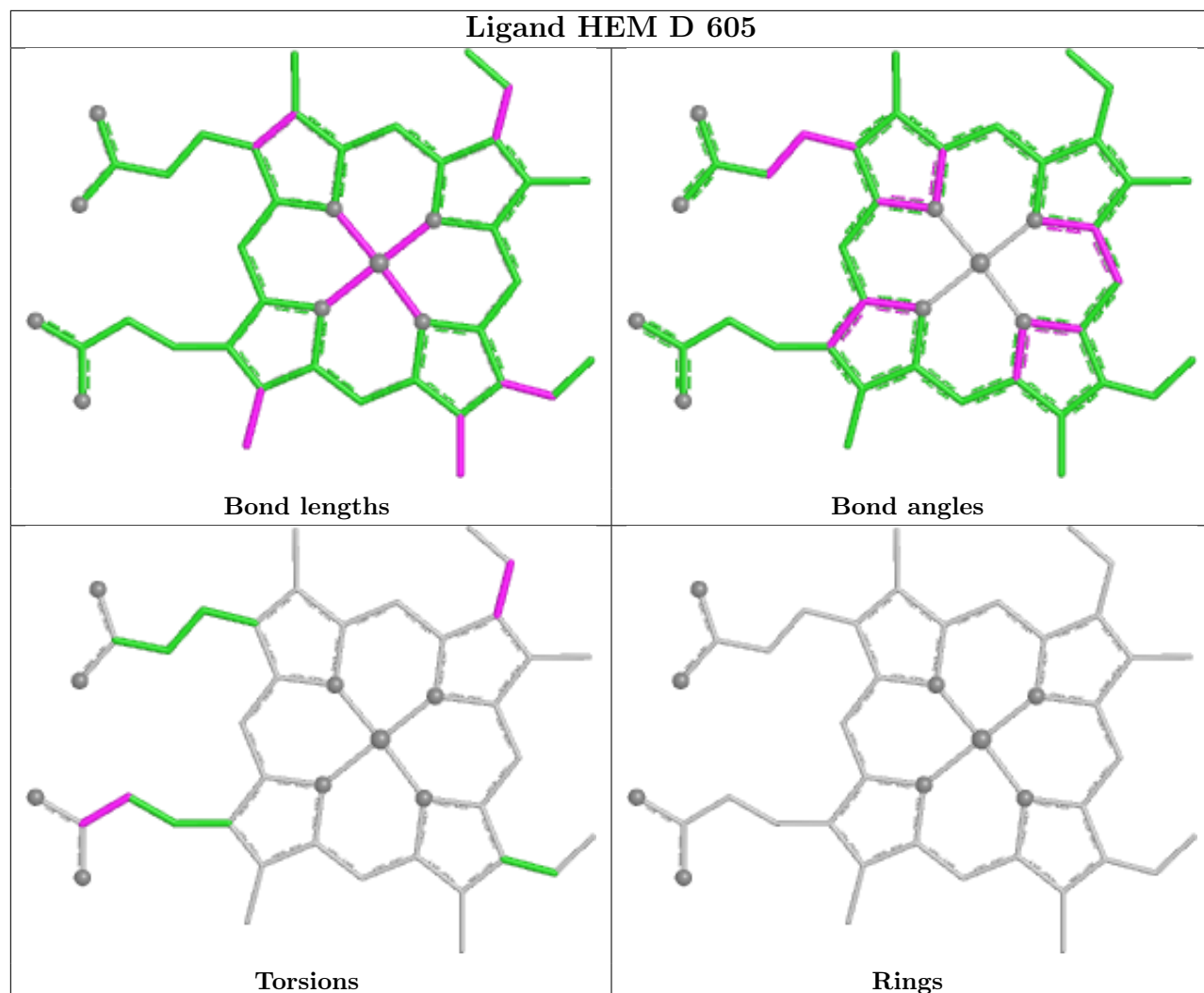


Ligand MXM C 606 (A)

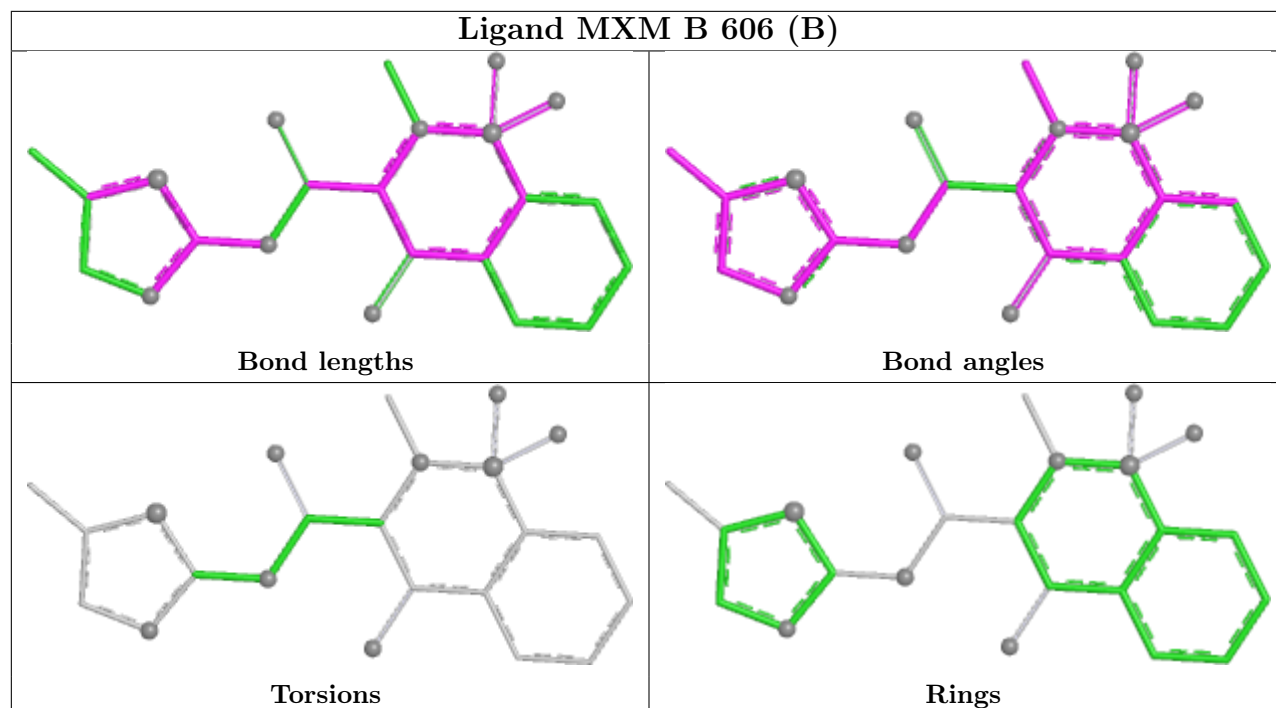


Ligand HEM B 605

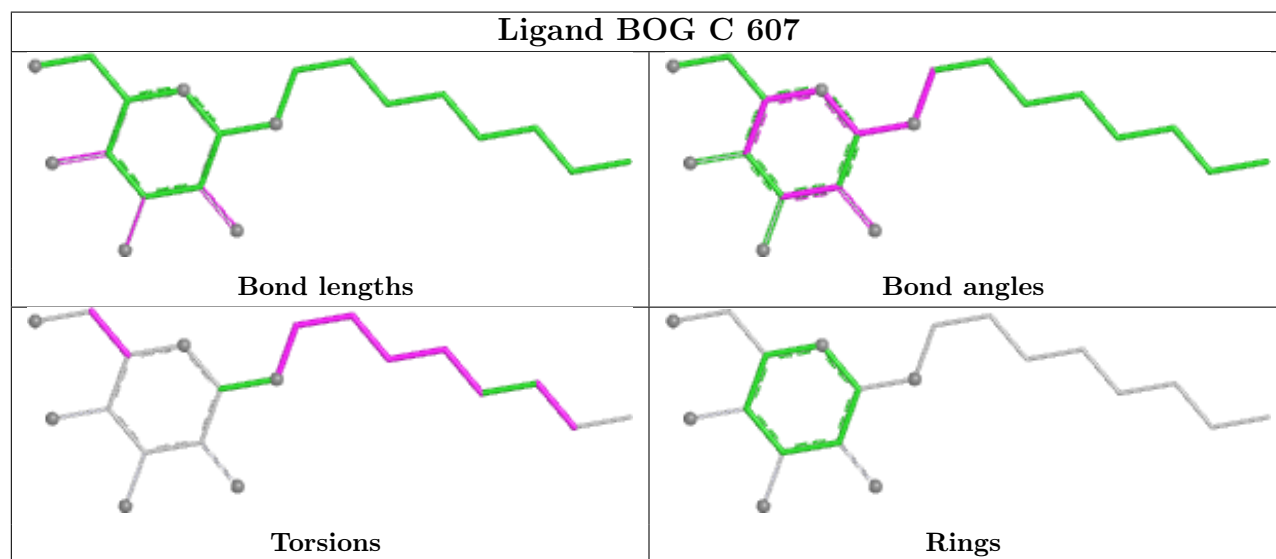


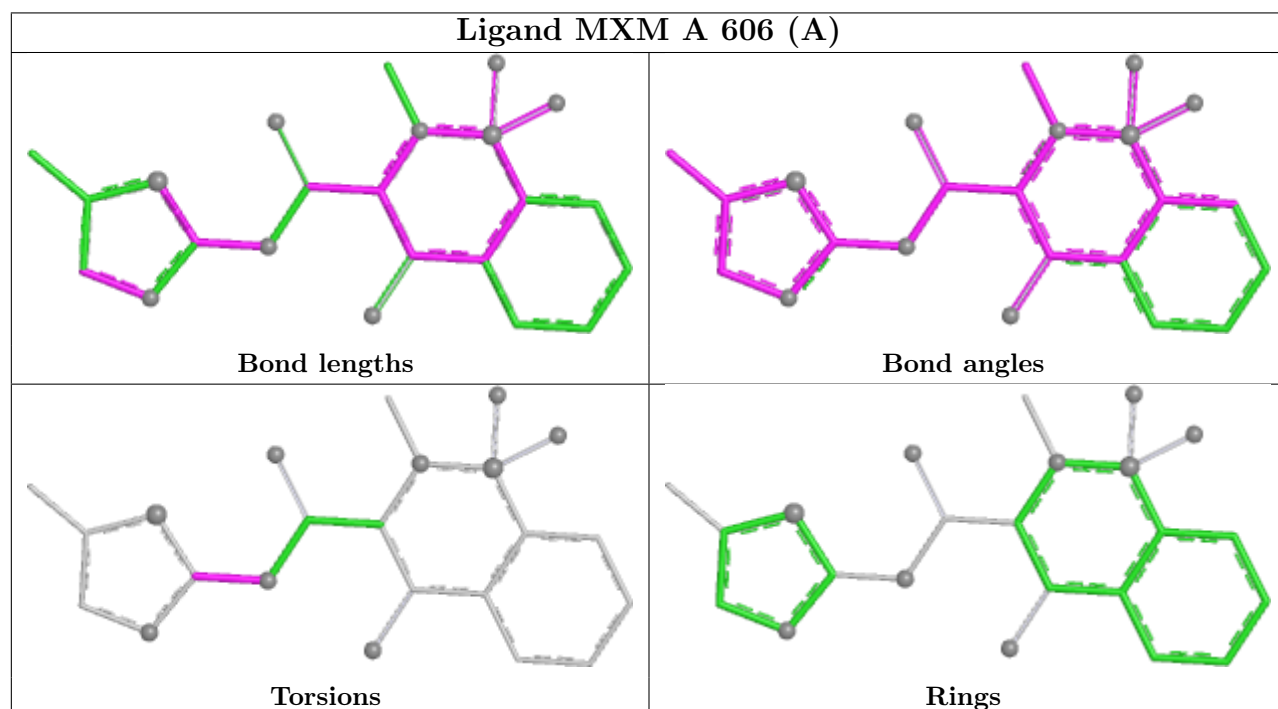
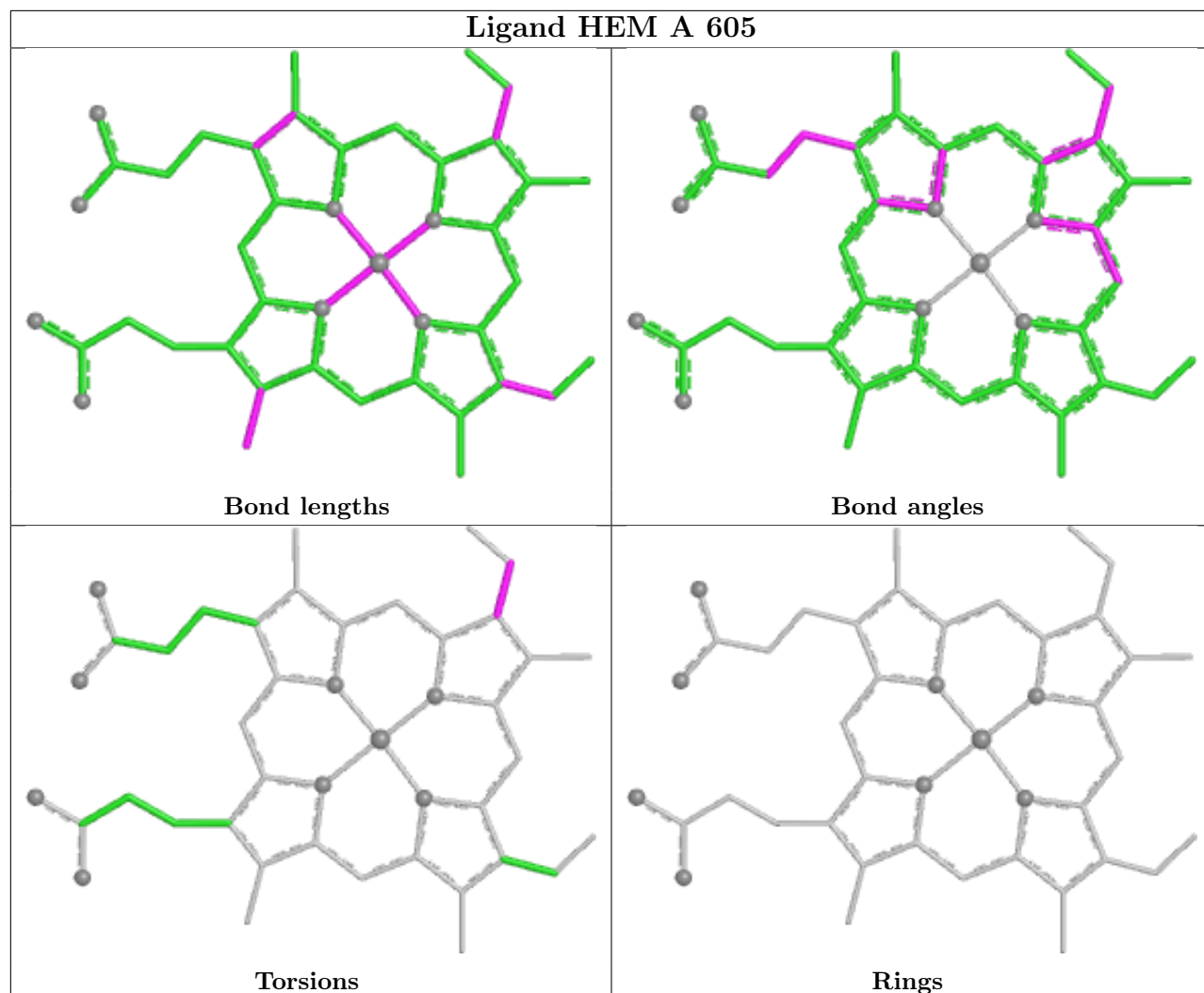


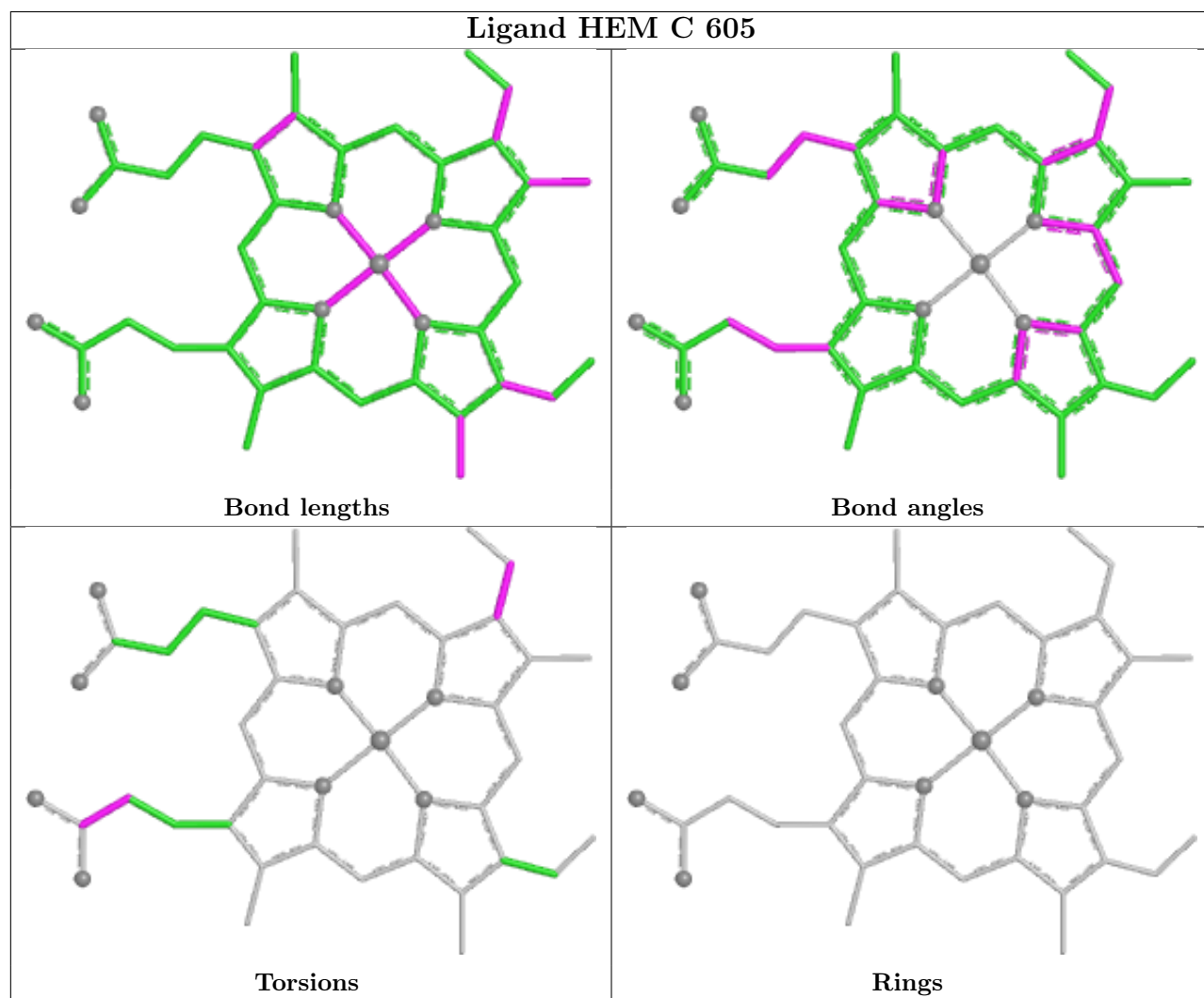
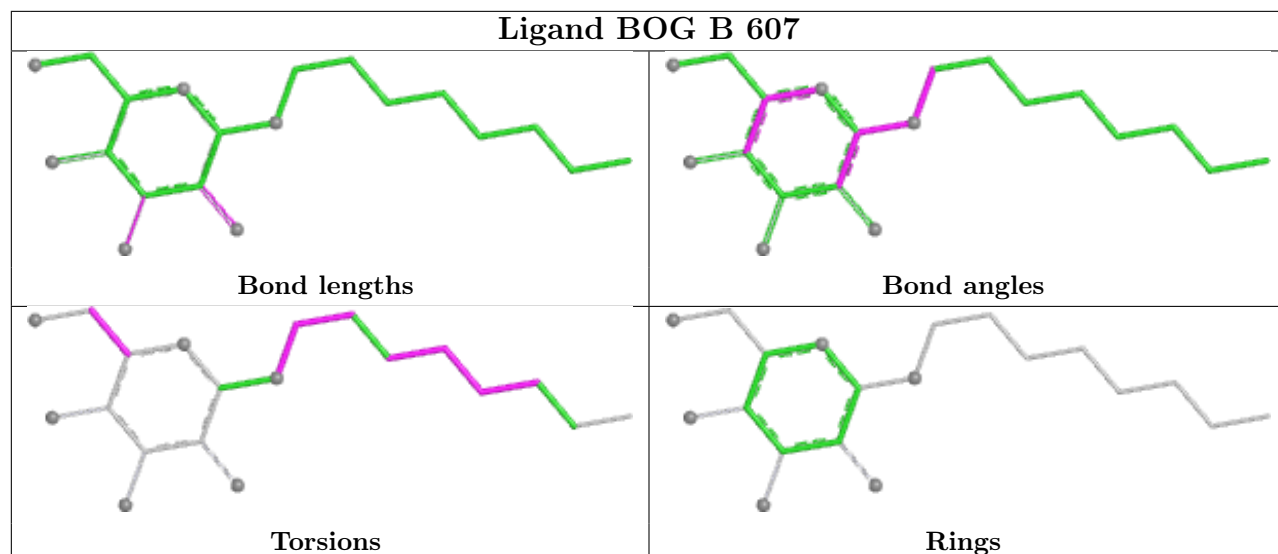
Ligand MXM B 606 (B)

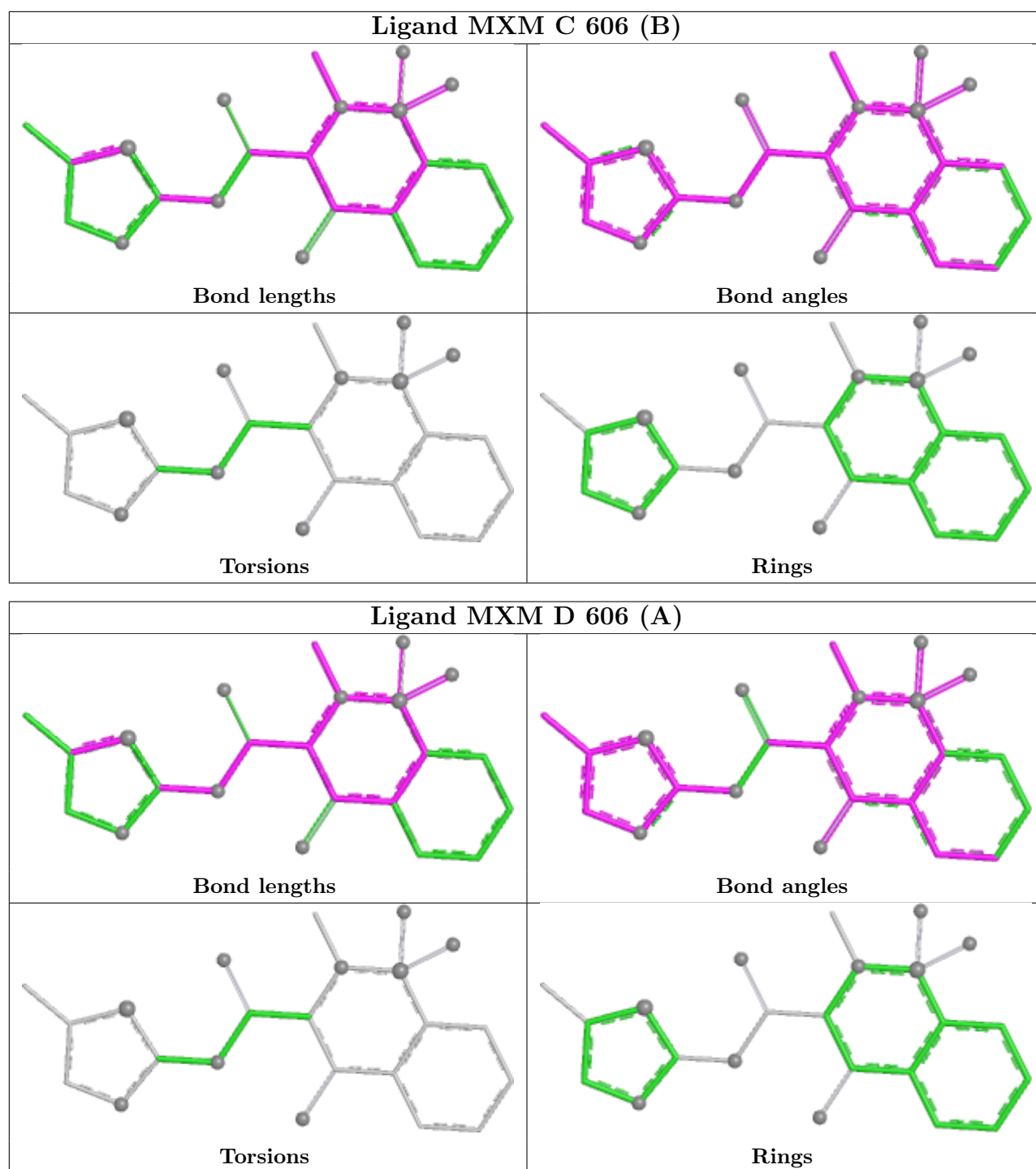


Ligand BOG C 607









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.14	1 (0%) 91 92	16, 33, 57, 75	0
1	B	552/552 (100%)	-0.04	8 (1%) 73 75	18, 37, 65, 96	0
1	C	552/552 (100%)	-0.33	0 100 100	16, 28, 53, 69	0
1	D	552/552 (100%)	-0.28	3 (0%) 87 88	17, 29, 51, 83	0
All	All	2208/2208 (100%)	-0.20	12 (0%) 87 88	16, 31, 58, 96	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	TYR	4.9
1	B	583	GLN	3.6
1	D	81	LEU	2.6
1	D	583	GLN	2.4
1	B	121	SER	2.3
1	B	428	ARG	2.3
1	D	215	LYS	2.3
1	B	222	ARG	2.2
1	B	107	PHE	2.2
1	B	74	PHE	2.1
1	A	121	SER	2.1
1	B	215	LYS	2.1

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

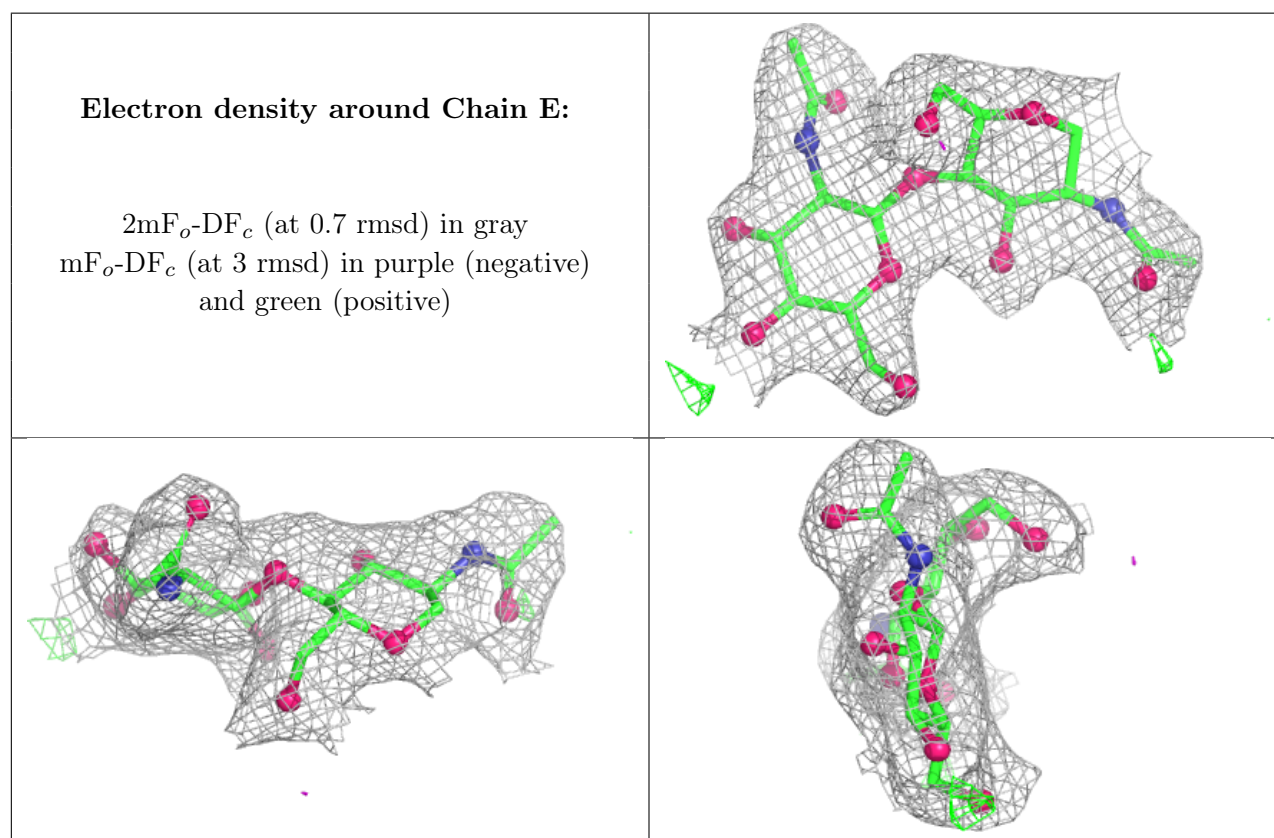
There are no non-standard protein/DNA/RNA residues in this entry.

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.

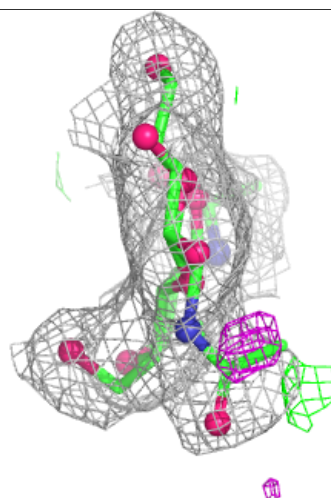
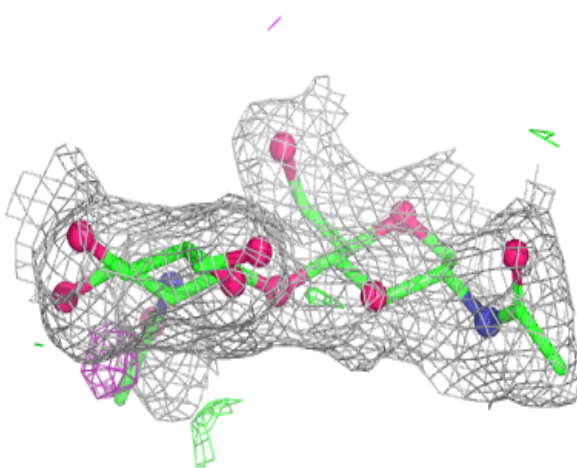
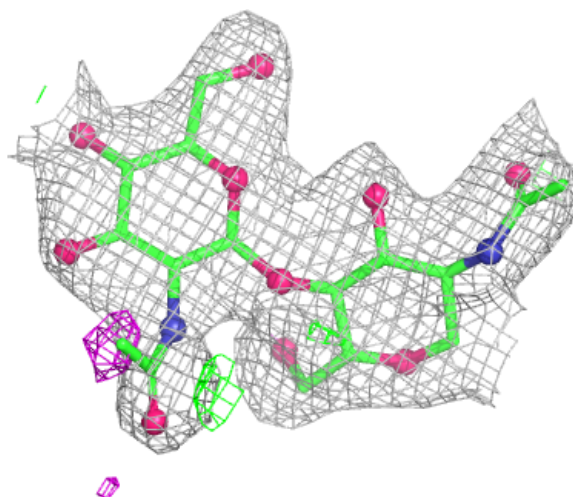
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.84	0.11	40,43,45,45	0
2	NAG	F	2	14/15	0.86	0.11	42,46,49,51	0
2	NAG	E	2	14/15	0.87	0.10	40,42,45,46	0
2	NAG	G	2	14/15	0.91	0.08	39,43,45,46	0
2	NAG	E	1	14/15	0.92	0.08	24,30,32,37	0
2	NAG	G	1	14/15	0.93	0.08	21,28,32,35	0
2	NAG	F	1	14/15	0.94	0.07	25,29,34,38	0
2	NAG	H	1	14/15	0.95	0.07	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.



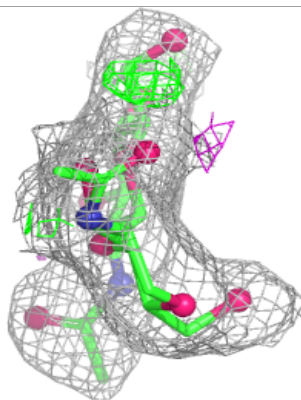
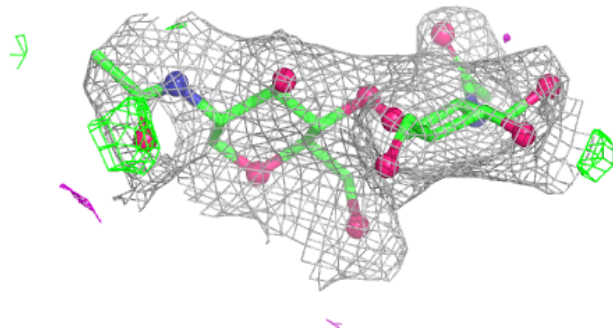
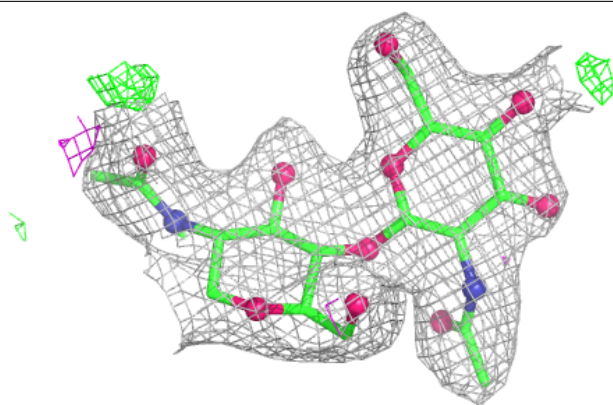
Electron density around Chain F:

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

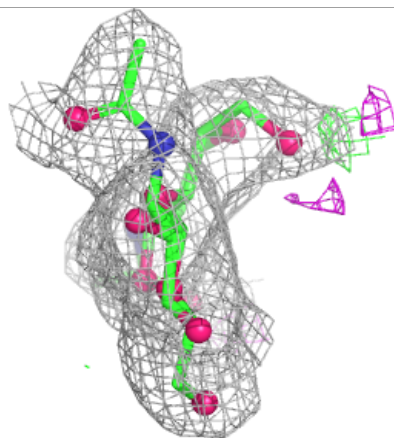
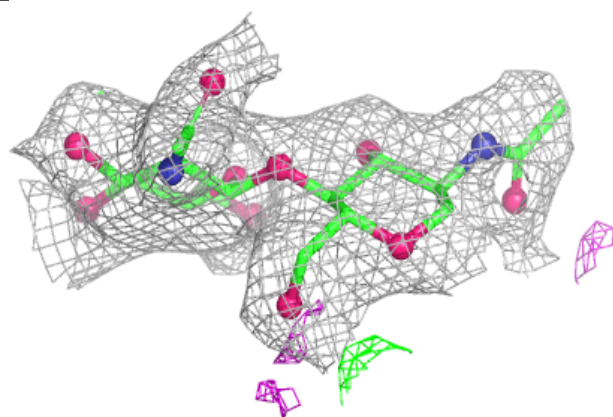
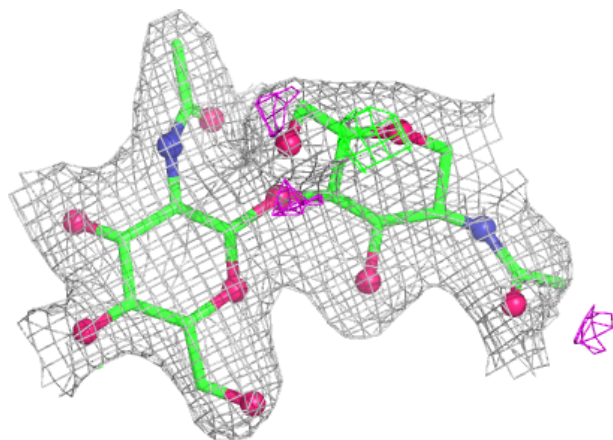


Electron density around Chain G:

$2mF_o-DF_c$ (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 ⓘ

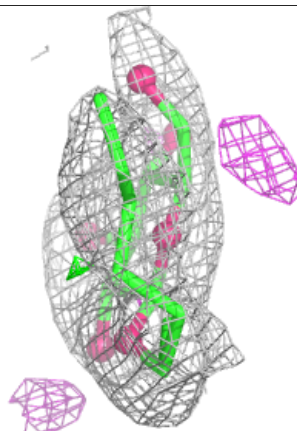
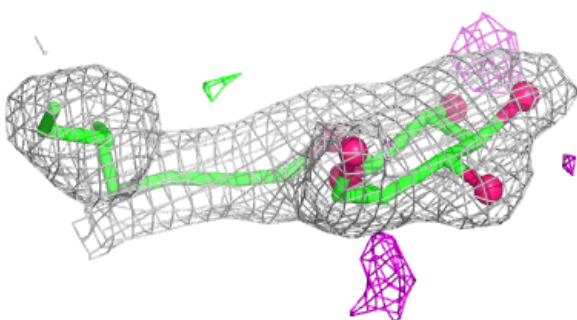
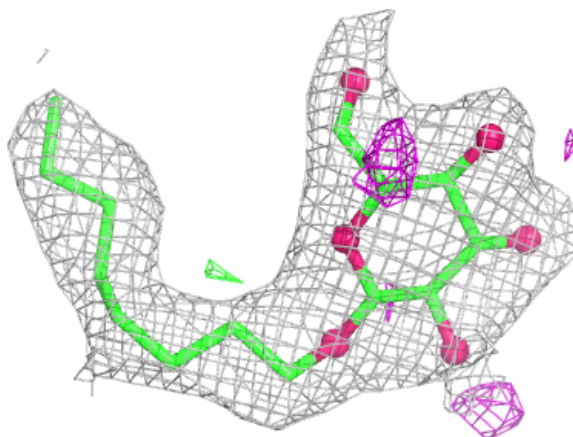
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.74	0.14	38,53,56,56	0
3	NAG	C	601	14/15	0.74	0.13	43,47,49,50	0
3	NAG	D	601	14/15	0.75	0.12	38,44,45,47	0
3	NAG	B	604	14/15	0.77	0.12	37,42,43,45	0
3	NAG	B	601	14/15	0.79	0.11	41,48,50,50	0
3	NAG	D	604	14/15	0.81	0.12	42,46,48,49	0
3	NAG	C	604	14/15	0.85	0.11	35,40,43,43	0
6	BOG	B	607	20/20	0.86	0.10	37,43,45,46	0
3	NAG	A	604	14/15	0.89	0.09	34,40,42,43	0
6	BOG	C	607	20/20	0.89	0.10	36,40,42,42	0
5	MXM	D	606[A]	23/23	0.91	0.10	20,25,26,26	23
5	MXM	D	606[B]	23/23	0.91	0.10	20,24,26,26	23
5	MXM	B	606[A]	23/23	0.92	0.10	29,31,32,33	23
5	MXM	B	606[B]	23/23	0.92	0.10	29,31,32,33	23
5	MXM	A	606[A]	23/23	0.93	0.11	27,32,33,34	23
5	MXM	A	606[B]	23/23	0.93	0.11	27,32,33,34	23
5	MXM	C	606[A]	23/23	0.94	0.09	23,27,28,29	23
5	MXM	C	606[B]	23/23	0.94	0.09	22,27,28,29	23
4	HEM	D	605	43/43	0.96	0.09	20,25,44,52	0
4	HEM	C	605	43/43	0.97	0.08	17,22,36,44	0
4	HEM	A	605	43/43	0.97	0.08	23,26,42,46	0
4	HEM	B	605	43/43	0.97	0.08	26,30,44,51	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.

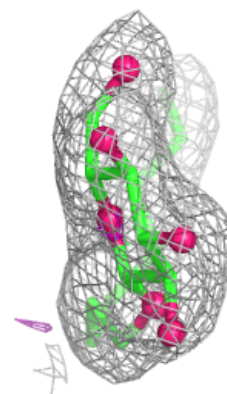
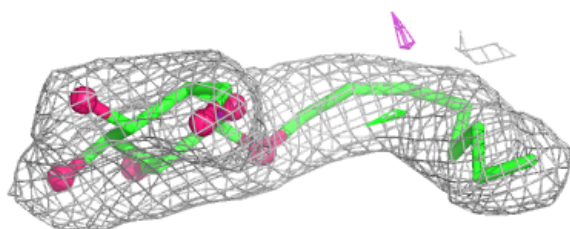
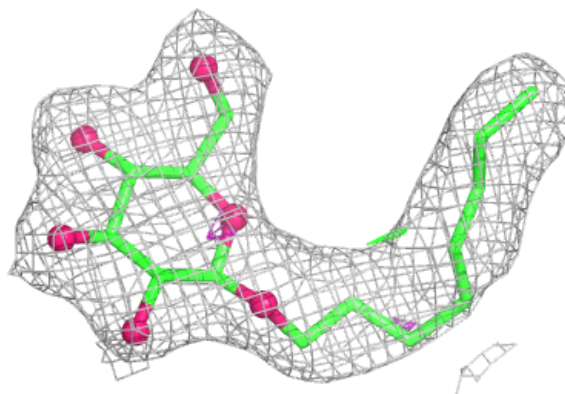
Electron density around BOG B 607:

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

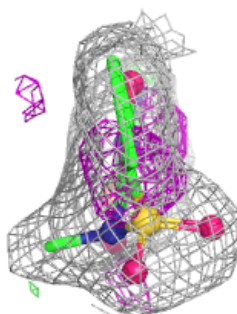
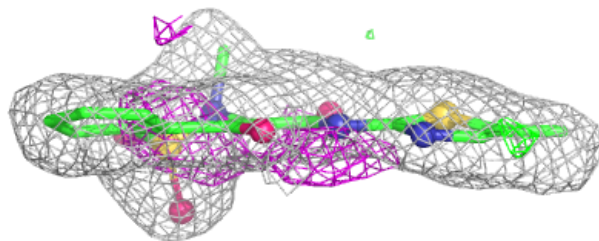
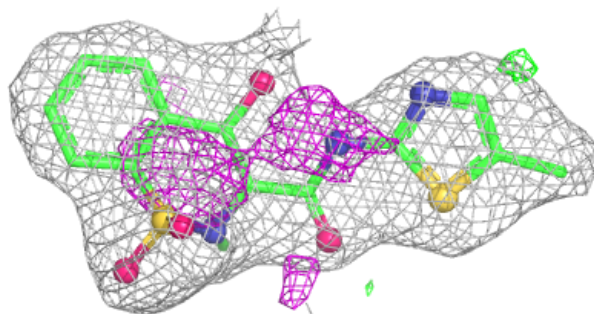


Electron density around BOG C 607:

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

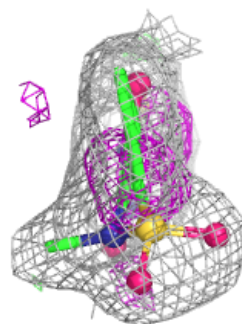
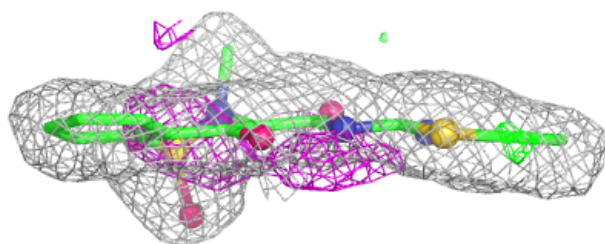
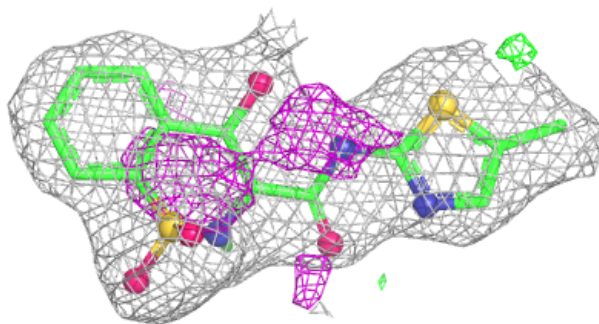
**Electron density around MXM D 606 (A):**

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

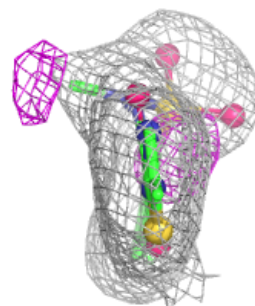
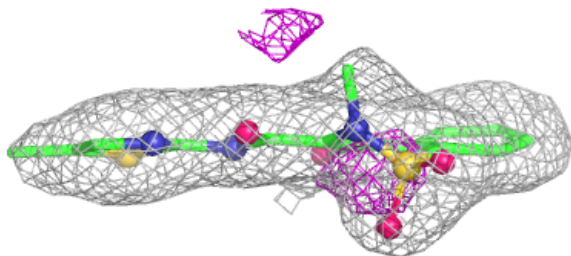
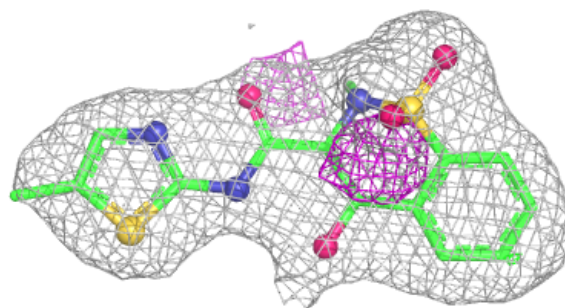


Electron density around MXM D 606 (B):

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

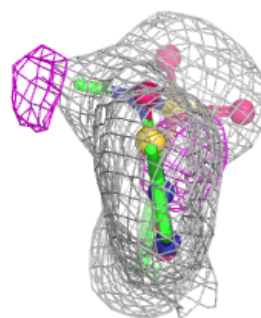
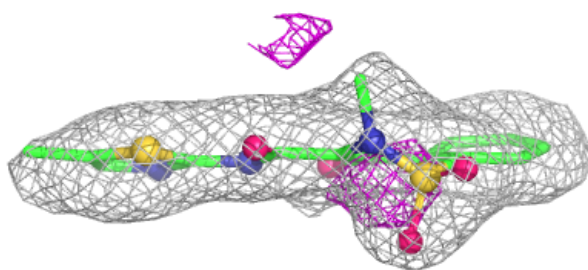
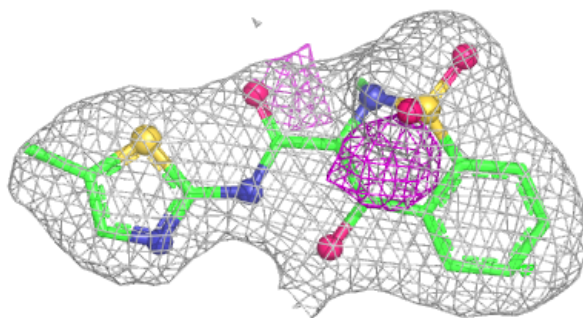
**Electron density around MXM B 606 (A):**

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

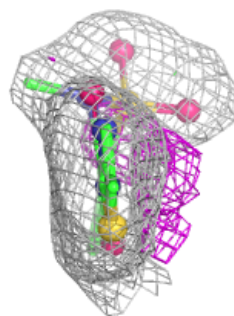
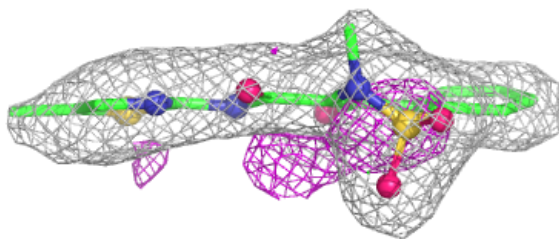
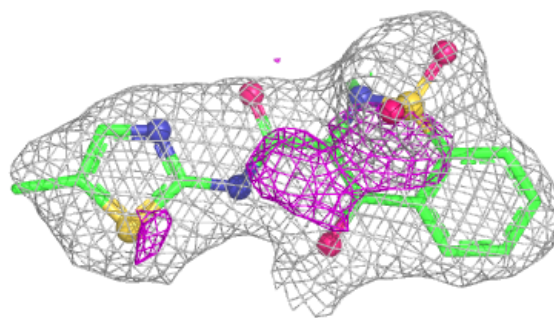


Electron density around MXM B 606 (B):

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

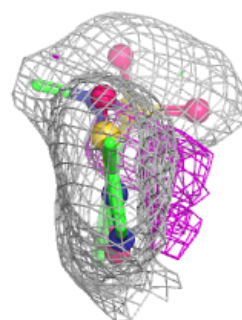
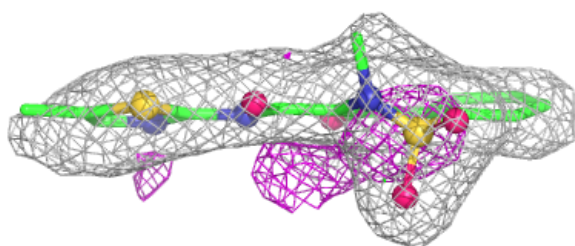
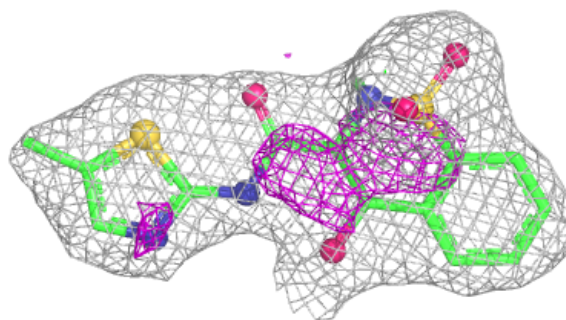
**Electron density around MXM A 606 (A):**

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

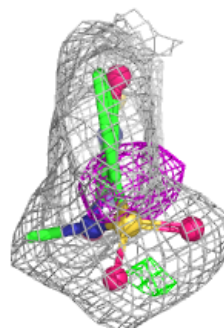
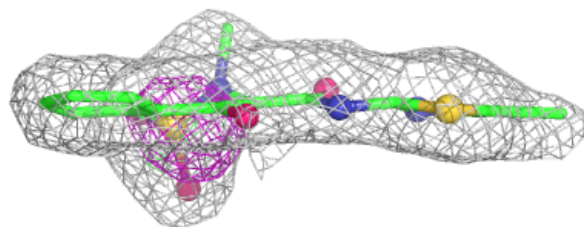
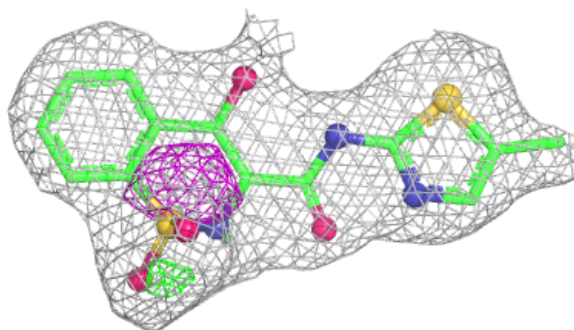


Electron density around MXM A 606 (B):

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and green (positive)

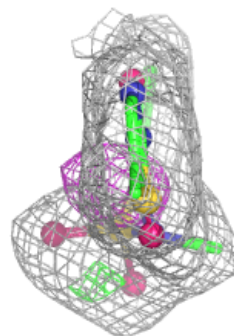
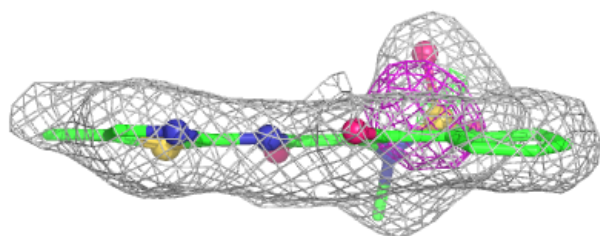
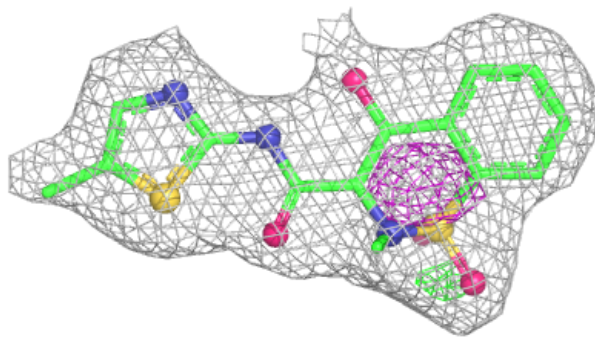
**Electron density around MXM C 606 (A):**

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and green (positive)



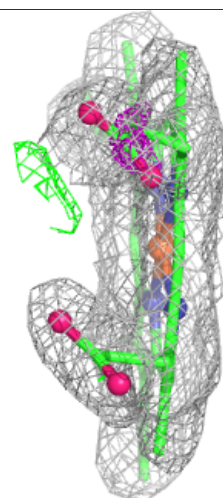
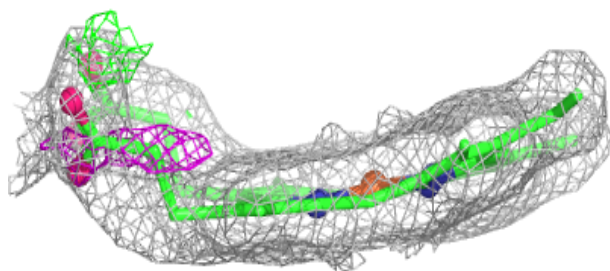
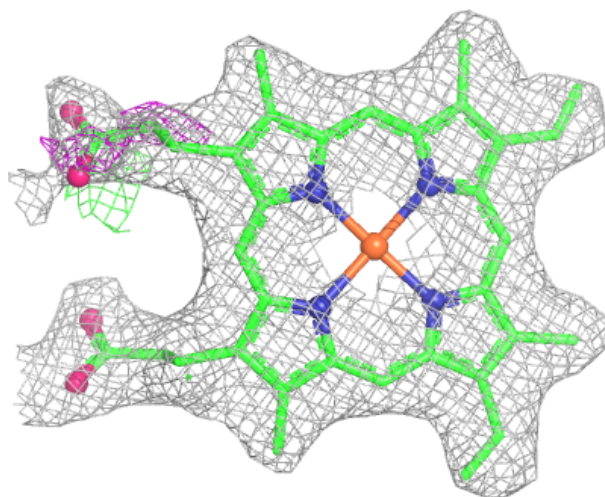
Electron density around MXM C 606 (B):

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



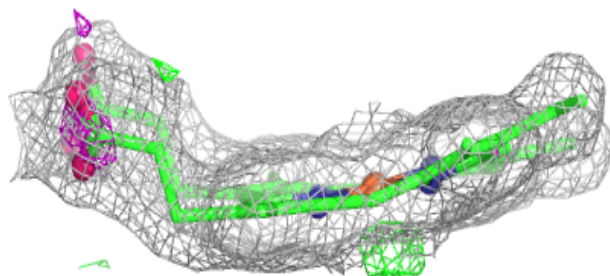
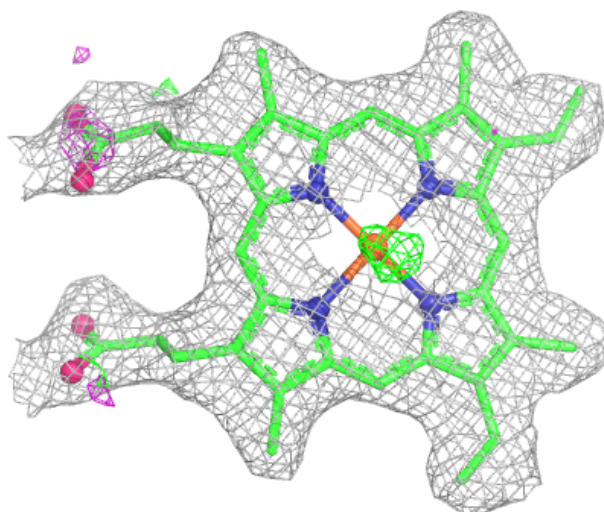
Electron density around HEM D 605:

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



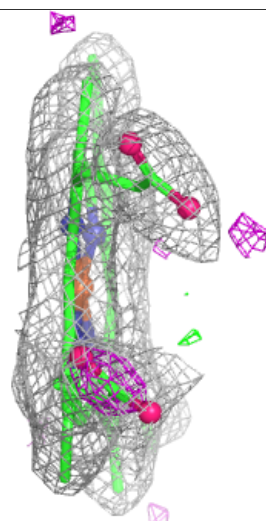
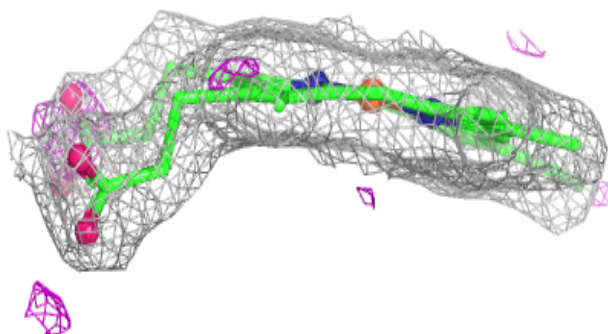
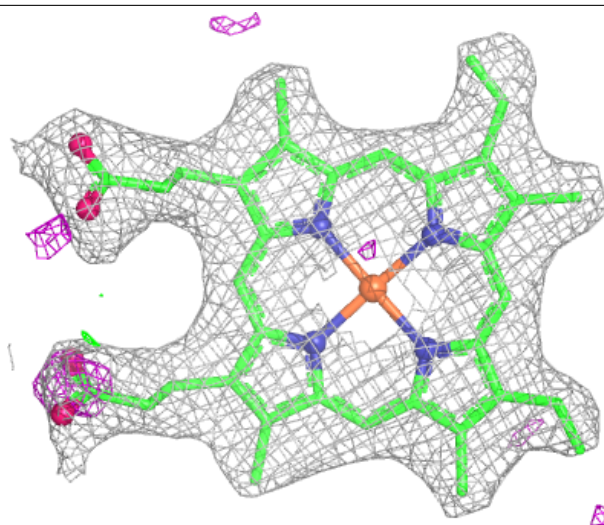
Electron density around HEM C 605:

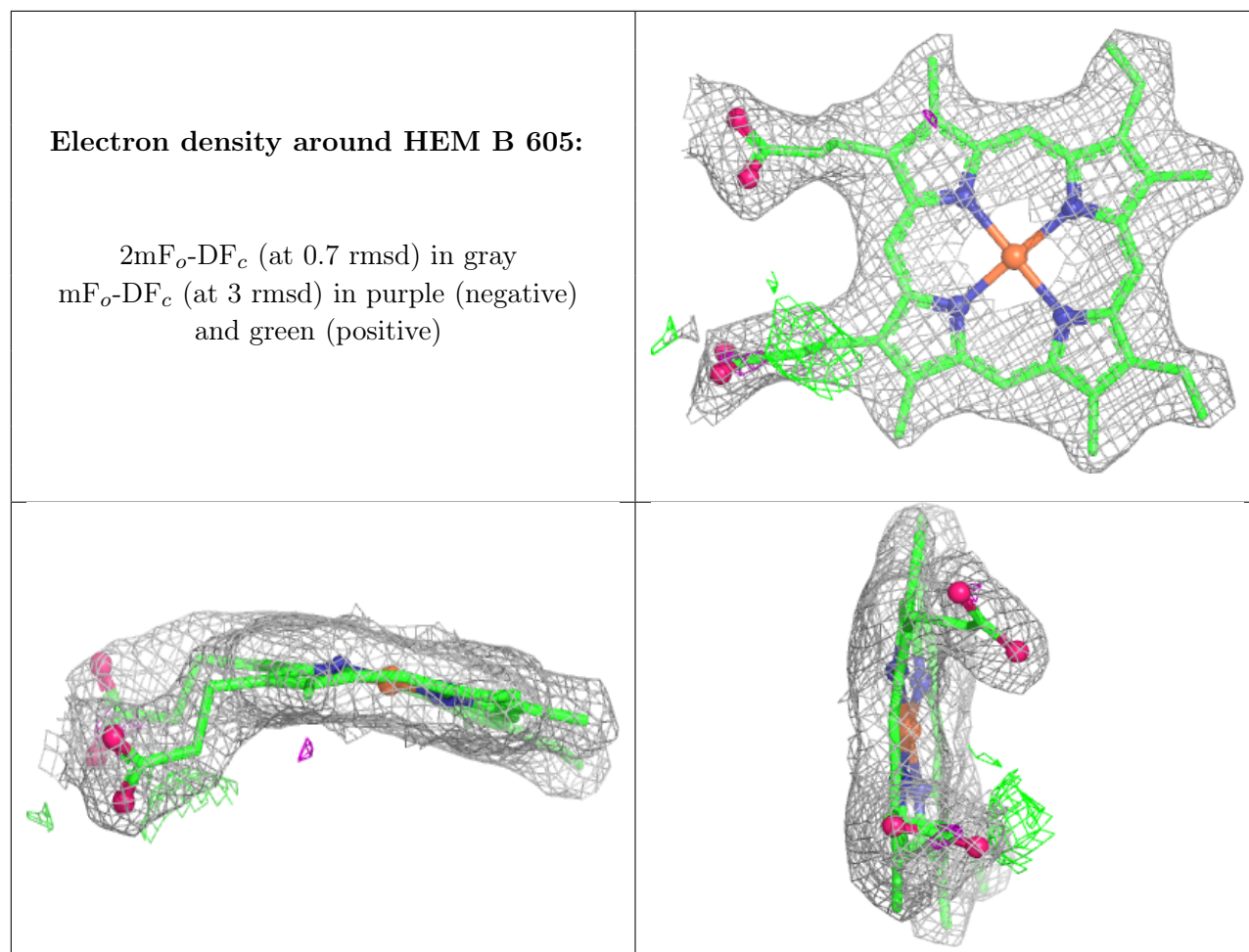
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.