



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:12 PM UTC

PDB ID : 4O1Z / pdb_00004o1z
Title : Crystal Structure of Ovine Cyclooxygenase-1 Complex with Meloxicam
Authors : Xu, S.; Hermanson, D.J.; Banerjee, S.; Ghebreselasie, K.; Clayton, G.M.; Garavito, R.M.; Marnett, L.J.
Deposited on : 2013-12-16
Resolution : 2.40 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

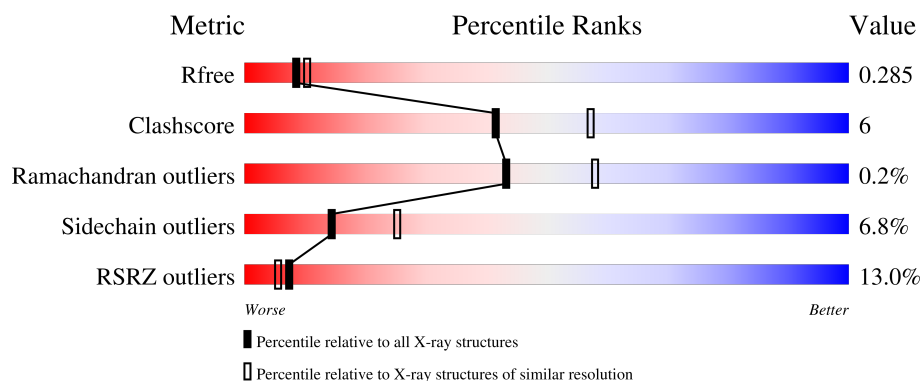
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	569	14% 79% 16% ..
1	B	569	11% 79% 17% ..
2	C	2	50% 50%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9615 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4492	2912	760	792	28			
1	B	553	Total	C	N	O	S	0	0	0
			4492	2912	760	792	28			

There are 2 discrepancies between the modelled and reference sequences:

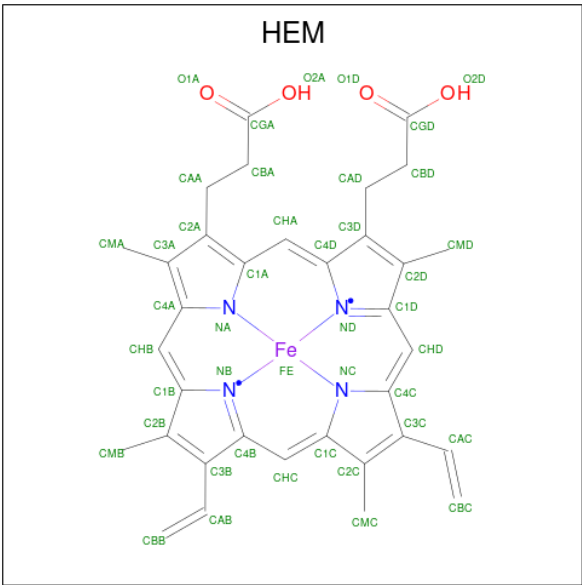
Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	SEE REMARK 999	UNP P05979
B	92	LEU	MET	SEE REMARK 999	UNP P05979

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



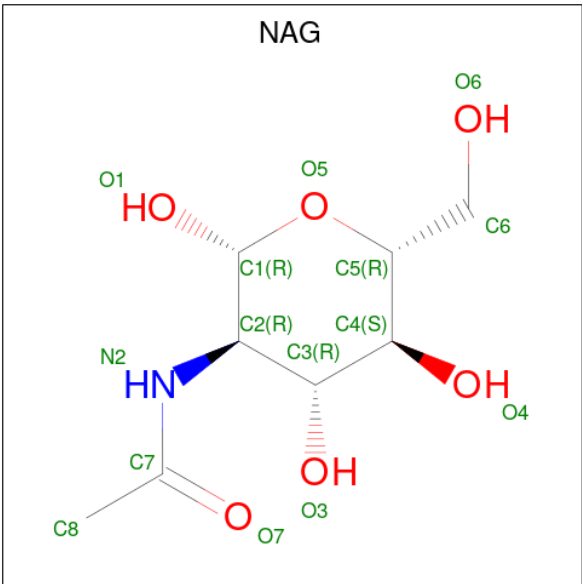
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



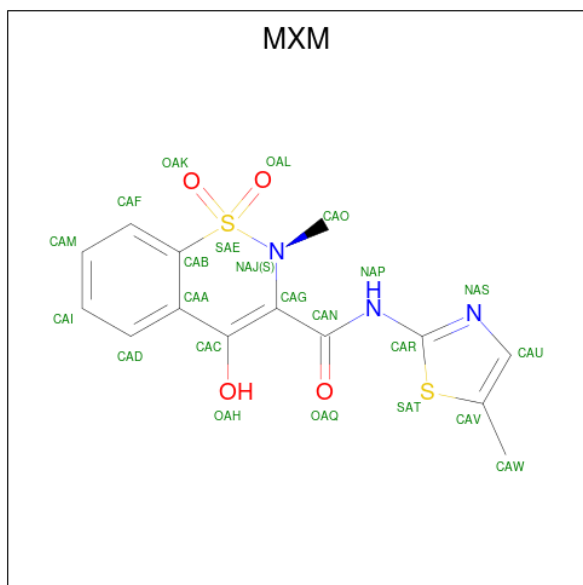
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 4-hydroxy-2-methyl-N-(5-methyl-1,3-thiazol-2-yl)-2H-1,2-benzothiazine-3-carboxamide 1,1-dioxide (CCD ID: 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		

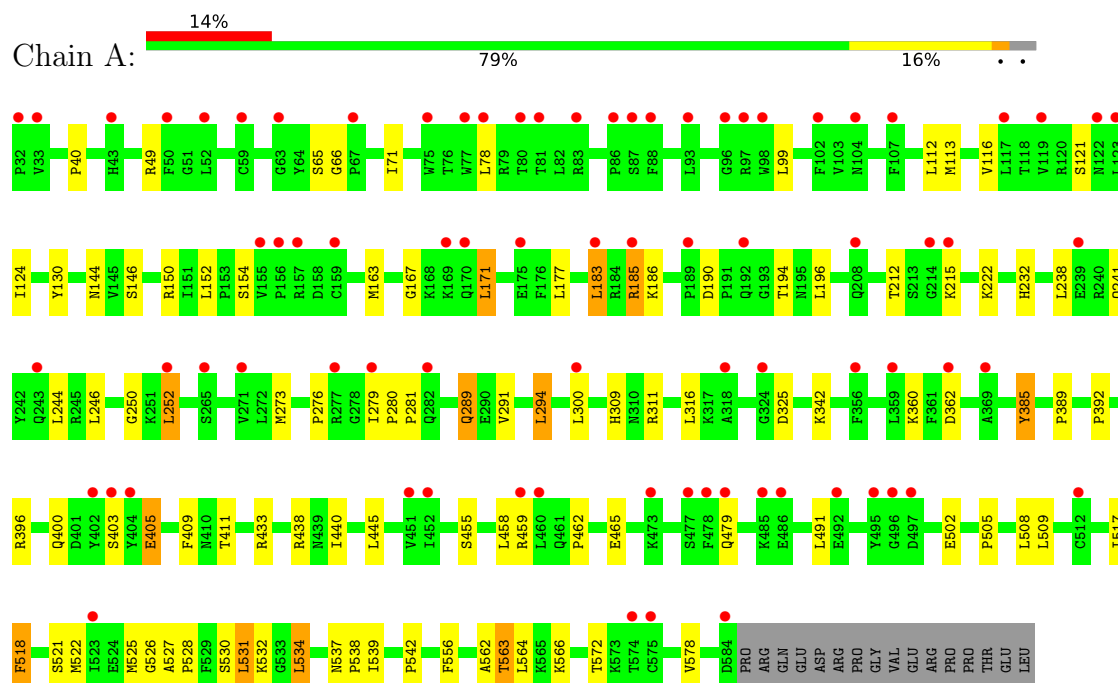
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total	O	0	0
			161	161		
6	B	152	Total	O	0	0
			152	152		

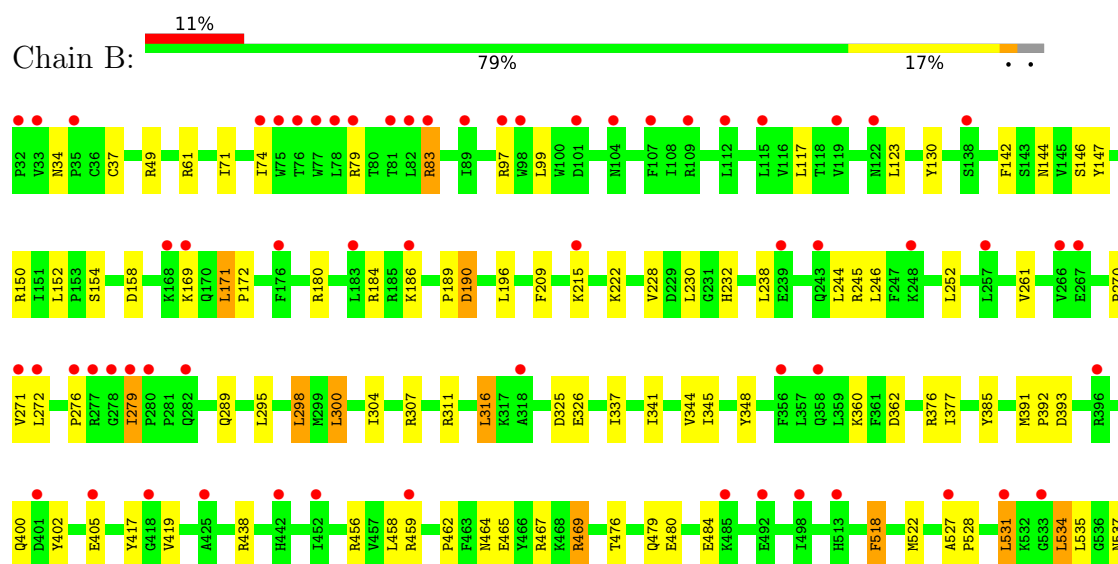
3 Residue-property plots

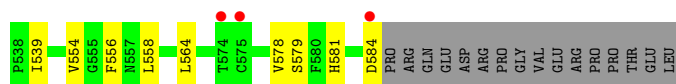
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1



• Molecule 1: Prostaglandin G/H synthase 1





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

Chain C: 50% 50%



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

Chain D: 100%



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

Chain E: 50% 50%



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

Chain F: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	181.33Å 181.33Å 103.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.55 – 2.40 43.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.55-2.40) 99.6 (43.55-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.150 , 0.173 0.269 , 0.285	Depositor DCC
R_{free} test set	3013 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.436 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9615	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/4631	0.77	2/6286 (0.0%)
1	B	0.44	0/4631	0.78	4/6286 (0.1%)
All	All	0.42	0/9262	0.77	6/12572 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ILE	CA-C-N	6.11	124.06	119.66
1	B	279	ILE	C-N-CA	6.11	124.06	119.66
1	A	66	GLY	CA-C-N	5.34	124.98	119.05
1	A	66	GLY	C-N-CA	5.34	124.98	119.05
1	B	71	ILE	CA-C-N	5.17	125.38	120.31
1	B	71	ILE	C-N-CA	5.17	125.38	120.31

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	4492	0	4395	55	0
1	B	4492	0	4395	55	0
2	C	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	1	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
3	A	43	0	30	3	0
3	B	43	0	30	3	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
5	A	46	0	24	1	0
5	B	46	0	24	2	0
6	A	161	0	0	16	0
6	B	152	0	0	8	0
All	All	9615	0	9024	117	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 6.

All (117) 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:123:LEU:O	1:B:469:ARG:NH2	2.21	0.74
6:A:1052:HOH:O	2:D:2:NAG:O4	2.06	0.73
3:A:801:HEM:HBC2	3:A:801:HEM:HHD	1.72	0.71
1:A:521:SER:O	6:A:1056:HOH:O	2.07	0.70
1:A:532:LYS:NZ	6:A:903:HOH:O	2.22	0.70
1:B:189:PRO:O	6:B:1049:HOH:O	2.11	0.69
1:A:525:MET:N	6:A:1056:HOH:O	2.22	0.69
1:A:563:THR:HG22	1:A:566:LYS:H	1.56	0.69
1:A:572:THR:O	6:A:969:HOH:O	2.09	0.69
1:B:79:ARG:HH11	1:B:83:ARG:NH2	1.93	0.66
1:B:180:ARG:O	1:B:438:ARG:NH1	2.28	0.66
5:B:807[B]:MXM:OAH	5:B:807[B]:MXM:NAP	2.22	0.65
5:A:807[B]:MXM:OAH	5:A:807[B]:MXM:NAP	2.21	0.65
1:B:79:ARG:HH11	1:B:83:ARG:HH21	1.46	0.64
3:B:801:HEM:HHD	3:B:801:HEM:HBC2	1.80	0.62
1:A:311:ARG:NH2	6:A:909:HOH:O	2.33	0.62
6:A:1031:HOH:O	2:C:2:NAG:O4	2.16	0.61
1:B:459:ARG:NH2	6:B:956:HOH:O	2.34	0.61
1:A:185:ARG:HE	1:A:438:ARG:HH11	1.49	0.60
1:B:196:LEU:HD21	1:B:392:PRO:HD3	1.83	0.60
1:B:245:ARG:NH2	1:B:325:ASP:OD2	2.35	0.59
1:B:97:ARG:NH2	6:B:994:HOH:O	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:SER:HG	1:B:581:HIS:HD1	1.51	0.58
1:A:522:MET:O	6:A:1056:HOH:O	2.17	0.58
1:B:150:ARG:HD3	1:B:152:LEU:O	2.04	0.58
1:B:196:LEU:HD11	1:B:392:PRO:HG3	1.86	0.58
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.87	0.57
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.87	0.57
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.45	0.56
1:A:522:MET:C	6:A:1056:HOH:O	2.48	0.56
3:A:801:HEM:HMB2	3:A:801:HEM:HBB2	1.87	0.56
1:A:196:LEU:HD11	1:A:392:PRO:HG3	1.87	0.56
1:B:345:ILE:HG13	1:B:534:LEU:HD12	1.86	0.56
1:A:563:THR:HB	1:A:566:LYS:HD3	1.88	0.55
1:A:385:TYR:OH	6:A:1017:HOH:O	2.18	0.55
1:B:190:ASP:O	6:B:911:HOH:O	2.17	0.54
1:A:130:TYR:HB2	1:A:150:ARG:HG3	1.88	0.54
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.91	0.53
1:A:150:ARG:HD3	1:A:152:LEU:O	2.08	0.53
1:A:526:GLY:N	6:A:1056:HOH:O	2.13	0.53
1:A:360:LYS:HE2	1:A:362:ASP:HB2	1.89	0.53
1:A:542:PRO:O	1:B:61:ARG:NH1	2.41	0.53
1:B:579:SER:OG	1:B:581:HIS:ND1	2.37	0.53
1:A:250:GLY:N	1:A:325:ASP:OD1	2.33	0.52
6:B:1038:HOH:O	2:E:2:NAG:O4	2.18	0.52
1:B:184:ARG:NH1	1:B:393:ASP:OD1	2.40	0.51
1:B:391:MET:HE2	3:B:801:HEM:HAB	1.92	0.51
1:B:469:ARG:O	1:B:469:ARG:NE	2.37	0.50
1:A:185:ARG:HH21	1:A:438:ARG:NH1	2.08	0.50
1:B:400:GLN:NE2	2:F:2:NAG:O4	2.44	0.50
1:A:212:THR:OG1	3:A:801:HEM:O1D	2.30	0.50
1:B:479:GLN:HG3	6:B:1023:HOH:O	2.12	0.50
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.94	0.49
1:A:163:MET:HE3	1:A:171:LEU:HD21	1.94	0.49
1:B:154:SER:HB2	1:B:459:ARG:HB2	1.93	0.49
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.95	0.49
1:A:154:SER:HB2	1:A:459:ARG:HB2	1.94	0.49
1:B:245:ARG:NH1	1:B:326:GLU:OE2	2.36	0.49
3:B:801:HEM:HBB2	3:B:801:HEM:HMB2	1.95	0.48
1:A:183:LEU:HG	1:A:445:LEU:HD22	1.95	0.48
1:B:295:LEU:HB2	1:B:298:LEU:HD22	1.95	0.48
1:B:402:TYR:OH	1:B:417:TYR:OH	2.19	0.48
1:B:341:ILE:HG23	1:B:534:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.48	0.47
1:B:360:LYS:HE2	1:B:362:ASP:HB2	1.97	0.47
1:B:311:ARG:NH2	6:B:1033:HOH:O	2.47	0.47
1:B:537:ASN:OD1	1:B:539:ILE:HG12	2.14	0.47
1:A:40:PRO:HB3	4:A:802:NAG:H62	1.97	0.47
1:A:241:GLN:OE1	6:A:968:HOH:O	2.21	0.46
1:A:294:LEU:HD12	1:A:409:PHE:HD1	1.81	0.45
1:A:491:LEU:HD11	1:A:509:LEU:HD13	1.99	0.45
1:A:65:SER:N	1:A:71:ILE:O	2.48	0.45
1:B:222:LYS:HB3	1:B:222:LYS:HE2	1.71	0.45
1:B:230:LEU:HD13	1:B:337:ILE:HG12	1.99	0.45
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.52	0.44
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.99	0.44
1:B:476:THR:OG1	1:B:480:GLU:OE2	2.26	0.44
1:A:144:ASN:OD1	1:A:146:SER:HB2	2.16	0.44
1:B:300:LEU:HD21	1:B:419:VAL:HG13	2.00	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
1:B:531:LEU:HD23	5:B:807[B]:MXM:OAL	2.17	0.44
1:A:403:SER:OG	1:A:405:GLU:HG2	2.17	0.44
1:A:538:PRO:HG3	1:B:142:PHE:CE2	2.53	0.44
1:A:167:GLY:O	6:A:948:HOH:O	2.21	0.44
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.99	0.43
1:A:537:ASN:OD1	1:A:539:ILE:HG12	2.18	0.43
1:A:49:ARG:HG3	6:A:964:HOH:O	2.19	0.43
1:B:79:ARG:NH1	1:B:83:ARG:HH21	2.16	0.43
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.87	0.42
1:B:172:PRO:O	1:B:456:ARG:NH2	2.44	0.42
1:A:252:LEU:HD22	1:A:309:HIS:CD2	2.55	0.42
1:B:464:ASN:HA	1:B:467:ARG:HG3	2.01	0.42
1:A:289:GLN:OE1	1:A:291:VAL:HG22	2.19	0.42
1:A:113:MET:HE2	1:A:360:LYS:H	1.85	0.42
1:A:273:MET:O	6:A:912:HOH:O	2.22	0.42
1:A:279:ILE:HD13	1:A:411:THR:HG21	2.02	0.42
1:A:502:GLU:HB2	1:A:505:PRO:HG2	2.02	0.41
1:B:209:PHE:HB2	1:B:377:ILE:HG13	2.02	0.41
1:A:163:MET:HE1	6:A:1011:HOH:O	2.18	0.41
1:A:433:ARG:HG3	1:A:517:ILE:HA	2.02	0.41
1:B:34:ASN:HB2	1:B:158:ASP:OD2	2.20	0.41
1:A:121:SER:HB3	1:A:531:LEU:HD11	2.03	0.41
1:B:130:TYR:HB2	1:B:150:ARG:HG3	2.03	0.41
1:B:276:PRO:HD2	1:B:279:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:VAL:O	1:B:307:ARG:NH1	2.54	0.41
1:B:144:ASN:OD1	1:B:146:SER:HB2	2.21	0.41
1:B:300:LEU:O	1:B:304:ILE:HG13	2.20	0.41
1:B:316:LEU:HD12	1:B:316:LEU:HA	1.86	0.41
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.83	0.41
1:A:530:SER:O	1:A:534:LEU:HD22	2.21	0.41
1:B:169:LYS:HD3	1:B:169:LYS:HA	1.90	0.41
1:A:124:ILE:HD11	1:A:528:PRO:HB2	2.02	0.40
1:A:396:ARG:HG3	1:A:400:GLN:O	2.22	0.40
1:B:558:LEU:HA	1:B:558:LEU:HD23	1.88	0.40
1:A:190:ASP:OD2	1:A:194:THR:OG1	2.37	0.40
1:B:147:TYR:HB2	6:B:974:HOH:O	2.20	0.40
1:B:344:VAL:O	1:B:348:TYR:HB3	2.21	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	551/569 (97%)	529 (96%)	22 (4%)	0	100	100
1	B	551/569 (97%)	523 (95%)	26 (5%)	2 (0%)	30	43
All	All	1102/1138 (97%)	1052 (96%)	48 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	PRO
1	B	74	ILE

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	488/503 (97%)	457 (94%)	31 (6%)	16	28
1	B	488/503 (97%)	453 (93%)	35 (7%)	13	23
All	All	976/1006 (97%)	910 (93%)	66 (7%)	14	25

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	99	LEU
1	A	171	LEU
1	A	177	LEU
1	A	183	LEU
1	A	185	ARG
1	A	186	LYS
1	A	215	LYS
1	A	222	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	289	GLN
1	A	294	LEU
1	A	300	LEU
1	A	316	LEU
1	A	385	TYR
1	A	405	GLU
1	A	455	SER
1	A	458	LEU
1	A	479	GLN
1	A	508	LEU
1	A	518	PHE
1	A	531	LEU
1	A	534	LEU

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Mol	Chain	Res	Type
1	A	556	PHE
1	A	563	THR
1	A	564	LEU
1	A	578	VAL
1	B	49	ARG
1	B	83	ARG
1	B	99	LEU
1	B	117	LEU
1	B	171	LEU
1	B	186	LYS
1	B	190	ASP
1	B	215	LYS
1	B	228	VAL
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	271	VAL
1	B	272	LEU
1	B	289	GLN
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	376	ARG
1	B	385	TYR
1	B	405	GLU
1	B	458	LEU
1	B	469	ARG
1	B	484	GLU
1	B	518	PHE
1	B	531	LEU
1	B	534	LEU
1	B	535	LEU
1	B	554	VAL
1	B	556	PHE
1	B	564	LEU
1	B	578	VAL
1	B	584	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	90	HIS
1	A	386	HIS
1	A	388	HIS
1	B	400	GLN
1	B	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	C	1	1,2	14,14,15	0.41	0	17,19,21	0.67	0
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	0.49	0
2	NAG	D	1	1,2	14,14,15	0.98	2 (14%)	17,19,21	0.63	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.57	0
2	NAG	E	1	1,2	14,14,15	0.83	1 (7%)	17,19,21	1.05	0
2	NAG	E	2	2	14,14,15	1.03	0	17,19,21	1.40	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.98	2 (14%)	17,19,21	0.63	0
2	NAG	F	2	2	14,14,15	0.49	0	17,19,21	1.84	3 (17%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
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	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C1-C2	2.82	1.56	1.52
2	F	1	NAG	O5-C1	-2.69	1.39	1.43
2	D	1	NAG	O5-C1	-2.67	1.39	1.43
2	D	1	NAG	C1-C2	2.25	1.55	1.52
2	F	1	NAG	C1-C2	2.24	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	6.20	120.49	112.19
2	F	2	NAG	C4-C3-C2	3.01	115.43	111.02
2	E	2	NAG	O5-C1-C2	-2.94	106.74	111.29
2	E	2	NAG	O5-C5-C6	2.19	111.93	107.66
2	F	2	NAG	O5-C1-C2	2.02	114.42	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6

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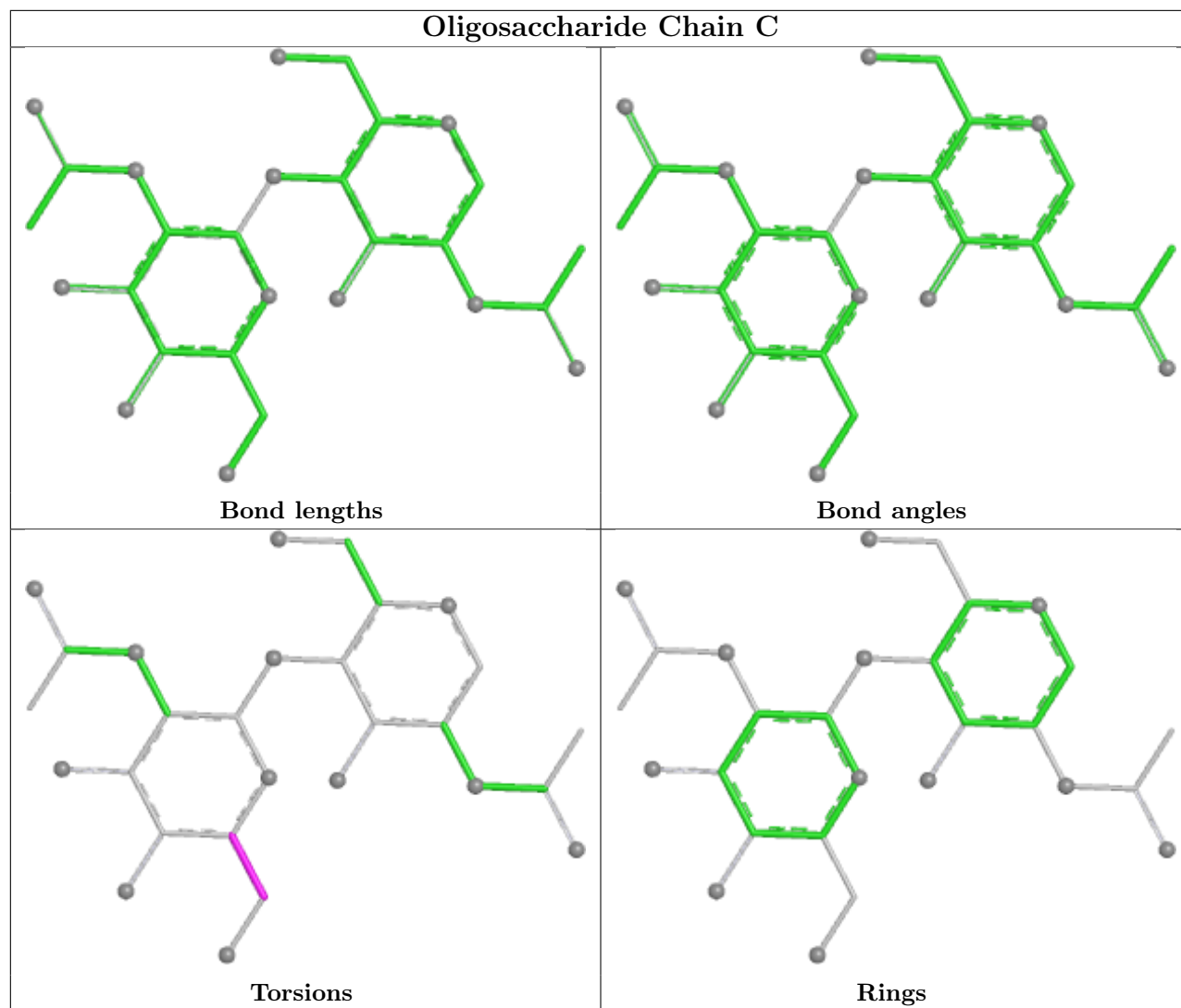
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6

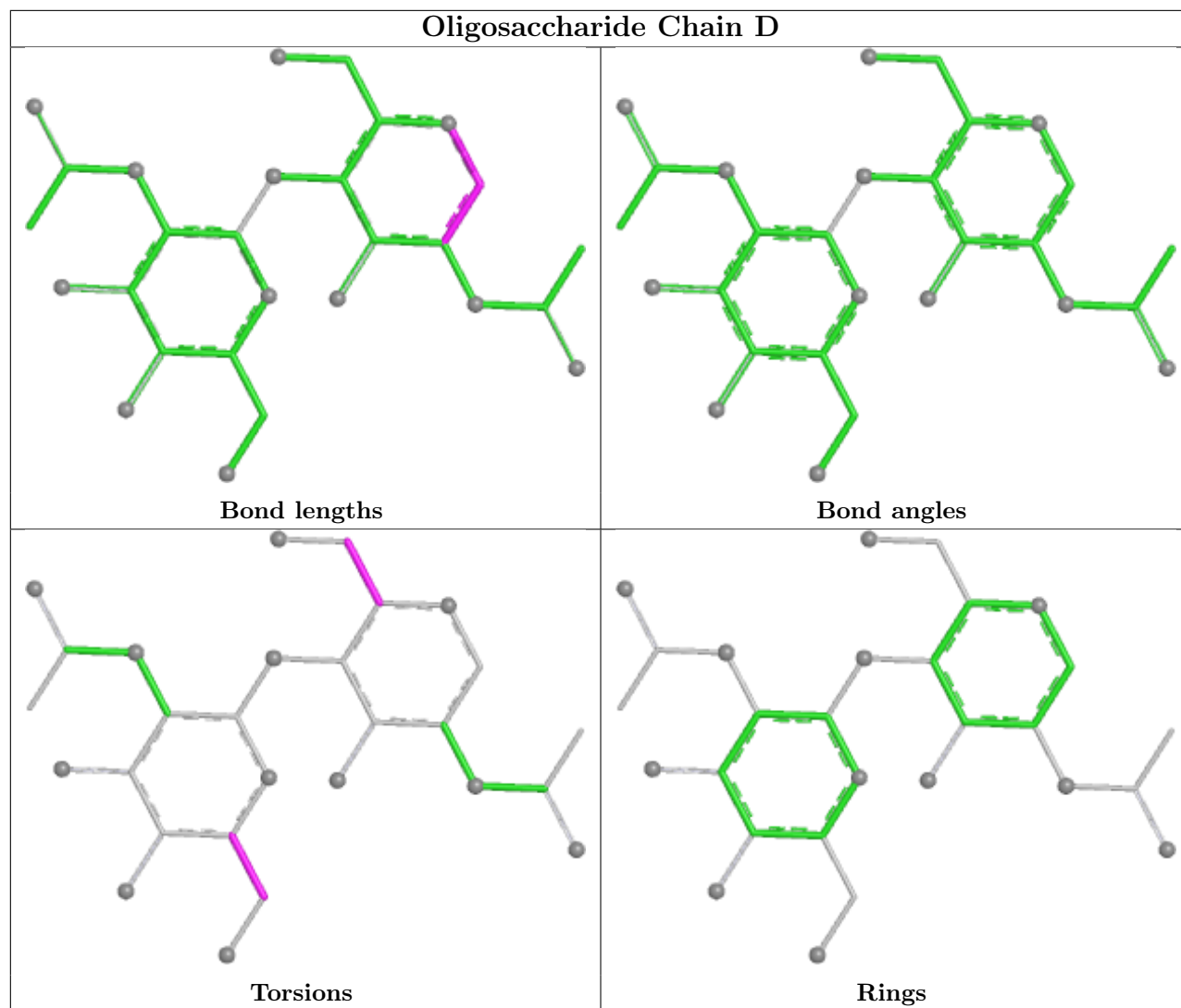
There are no ring outliers.

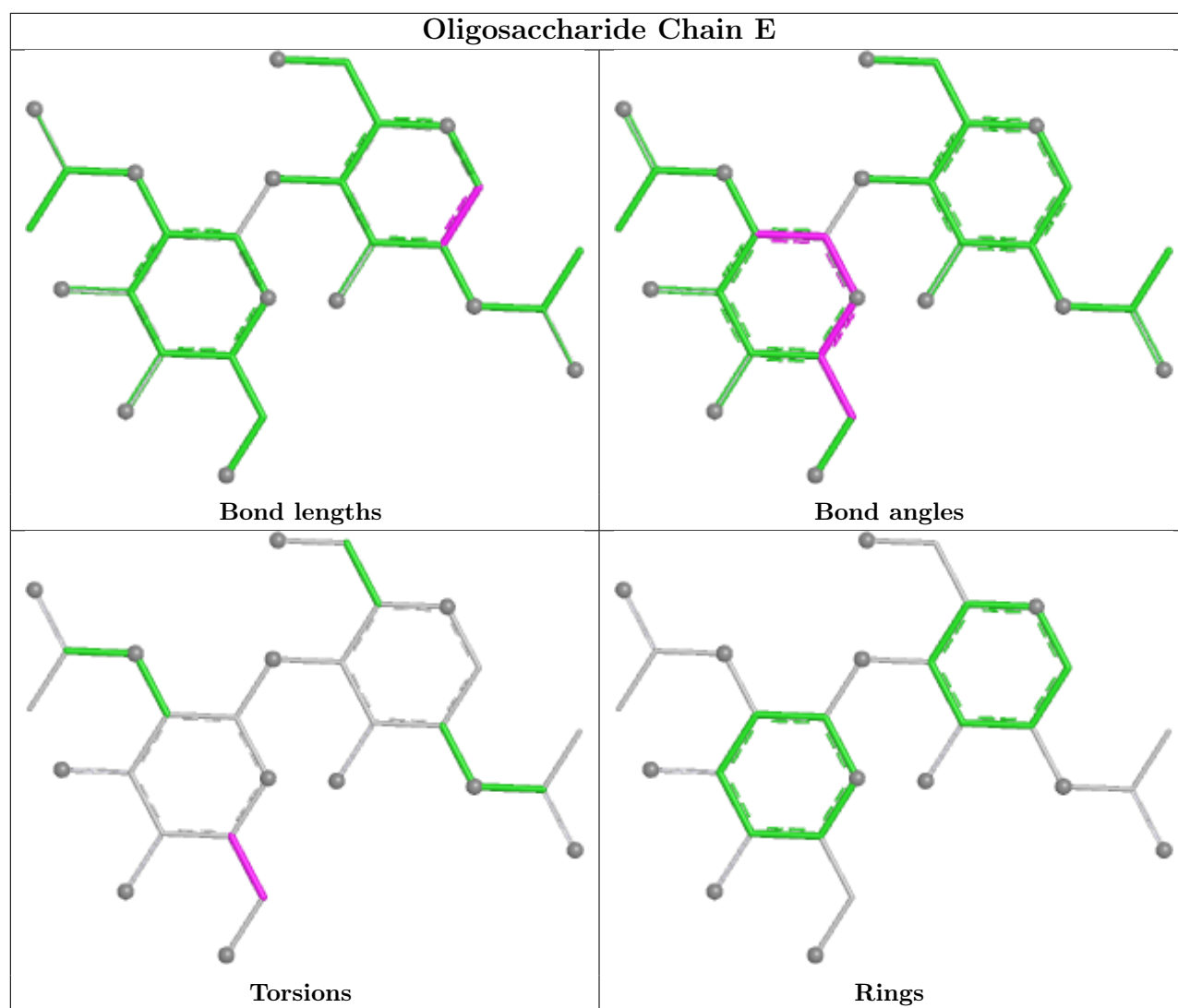
4 monomers are involved in 4 short contacts:

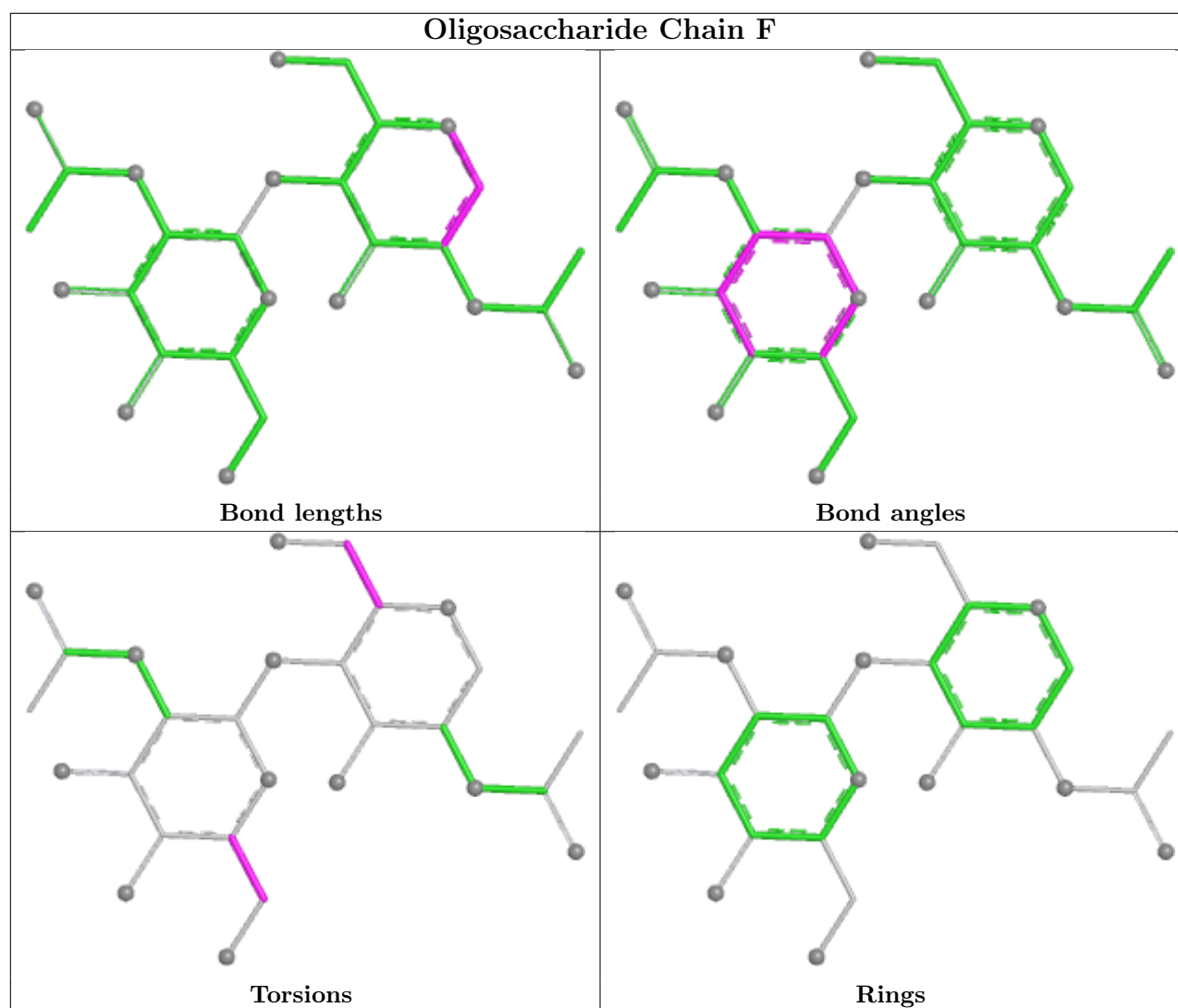
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	1	0
2	E	2	NAG	1	0
2	D	2	NAG	1	0
2	C	2	NAG	1	0

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](#)

8 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	A	807[B]	-	25,25,25	4.90	12 (48%)	38,38,38	4.79	20 (52%)
5	MXM	A	807[A]	-	25,25,25	5.59	12 (48%)	38,38,38	4.73	22 (57%)
3	HEM	B	801	1	50,50,50	1.85	8 (16%)	67,82,82	1.18	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	801	1	50,50,50	1.94	9 (18%)	67,82,82	1.23	4 (5%)
4	NAG	A	802	1	14,14,15	0.21	0	17,19,21	0.52	0
5	MXM	B	807[B]	-	25,25,25	4.86	12 (48%)	38,38,38	4.97	20 (52%)
5	MXM	B	807[A]	-	25,25,25	5.78	12 (48%)	38,38,38	4.86	20 (52%)
4	NAG	B	802	1	14,14,15	0.16	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
5	MXM	A	807[B]	-	-	0/8/32/32	0/3/3/3
5	MXM	A	807[A]	-	-	3/8/32/32	0/3/3/3
3	HEM	B	801	1	-	1/14/54/54	-
3	HEM	A	801	1	-	1/14/54/54	-
4	NAG	A	802	1	-	0/6/23/26	0/1/1/1
5	MXM	B	807[B]	-	-	0/8/32/32	0/3/3/3
5	MXM	B	807[A]	-	-	3/8/32/32	0/3/3/3
4	NAG	B	802	1	-	2/6/23/26	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	807[A]	MXM	CAB-SAE	-17.24	1.50	1.75
5	B	807[A]	MXM	SAE-NAJ	-17.09	1.41	1.64
5	B	807[A]	MXM	CAB-SAE	-14.34	1.54	1.75
5	A	807[B]	MXM	CAB-SAE	-13.33	1.56	1.75
5	A	807[A]	MXM	SAE-NAJ	-12.13	1.48	1.64
5	B	807[B]	MXM	CAB-SAE	-11.76	1.58	1.75
5	B	807[B]	MXM	SAE-NAJ	-11.64	1.48	1.64
5	B	807[A]	MXM	OAL-SAE	10.30	1.54	1.43
5	A	807[B]	MXM	OAL-SAE	10.24	1.54	1.43
5	A	807[A]	MXM	OAL-SAE	10.03	1.54	1.43
5	B	807[B]	MXM	OAL-SAE	9.93	1.54	1.43
5	A	807[B]	MXM	SAE-NAJ	-9.50	1.51	1.64
5	A	807[A]	MXM	OAK-SAE	9.26	1.53	1.43
5	A	807[B]	MXM	OAK-SAE	8.94	1.53	1.43
5	B	807[B]	MXM	OAK-SAE	8.34	1.52	1.43
5	B	807[A]	MXM	OAK-SAE	7.89	1.51	1.43
3	B	801	HEM	C3D-C2D	7.84	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3D-C2D	7.75	1.53	1.36
5	B	807[A]	MXM	CAG-NAJ	-6.62	1.36	1.44
5	B	807[A]	MXM	CAR-SAT	-5.92	1.64	1.73
5	A	807[A]	MXM	CAG-NAJ	-5.77	1.37	1.44
5	B	807[B]	MXM	CAG-CAC	5.60	1.43	1.36
5	A	807[A]	MXM	CAR-SAT	-5.48	1.64	1.73
5	B	807[B]	MXM	CAV-SAT	-5.33	1.59	1.72
5	A	807[B]	MXM	CAG-CAC	5.31	1.43	1.36
5	B	807[A]	MXM	CAG-CAC	5.21	1.43	1.36
3	A	801	HEM	FE-NA	5.12	2.12	1.95
5	A	807[B]	MXM	CAV-SAT	-5.10	1.59	1.72
5	A	807[A]	MXM	CAG-CAC	5.08	1.43	1.36
5	B	807[B]	MXM	CAR-SAT	-5.08	1.65	1.73
5	A	807[B]	MXM	CAR-SAT	-4.99	1.65	1.73
5	A	807[B]	MXM	CAG-NAJ	-4.84	1.38	1.44
3	A	801	HEM	FE-ND	4.80	2.09	1.94
5	B	807[B]	MXM	CAG-NAJ	-4.75	1.38	1.44
3	B	801	HEM	FE-NA	4.55	2.10	1.95
3	A	801	HEM	FE-NB	4.30	2.08	1.94
3	B	801	HEM	FE-ND	3.85	2.06	1.94
5	B	807[A]	MXM	CAA-CAB	-3.63	1.36	1.40
5	A	807[A]	MXM	CAA-CAB	-3.50	1.36	1.40
5	B	807[A]	MXM	CAG-CAN	-3.46	1.39	1.46
5	A	807[B]	MXM	CAA-CAB	-3.37	1.36	1.40
5	A	807[A]	MXM	CAG-CAN	-3.31	1.39	1.46
5	B	807[B]	MXM	CAA-CAB	-3.24	1.37	1.40
5	A	807[B]	MXM	CAG-CAN	-3.21	1.39	1.46
3	A	801	HEM	CAB-C3B	3.08	1.55	1.47
3	A	801	HEM	CAC-C3C	3.07	1.55	1.47
5	A	807[A]	MXM	CAA-CAC	-3.06	1.40	1.45
5	B	807[A]	MXM	CAV-SAT	-3.05	1.65	1.72
3	B	801	HEM	CAB-C3B	3.05	1.55	1.47
5	A	807[A]	MXM	CAV-SAT	-3.04	1.65	1.72
3	B	801	HEM	FE-NB	3.04	2.04	1.94
5	B	807[A]	MXM	CAR-NAP	-2.97	1.33	1.38
5	B	807[A]	MXM	CAA-CAC	-2.96	1.41	1.45
5	A	807[A]	MXM	CAR-NAP	-2.92	1.33	1.38
3	B	801	HEM	CAC-C3C	2.92	1.55	1.47
5	B	807[B]	MXM	CAG-CAN	-2.86	1.40	1.46
5	A	807[B]	MXM	CAA-CAC	-2.86	1.41	1.45
5	B	807[B]	MXM	CAA-CAC	-2.63	1.41	1.45
5	B	807[B]	MXM	CAR-NAP	-2.58	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	807[B]	MXM	CAR-NAP	-2.45	1.34	1.38
3	B	801	HEM	CMB-C2B	2.09	1.55	1.50
3	A	801	HEM	C2A-C3A	-2.05	1.33	1.38
3	B	801	HEM	CMA-C3A	2.03	1.54	1.50
3	A	801	HEM	CMC-C2C	2.03	1.54	1.50
3	A	801	HEM	CMB-C2B	2.02	1.54	1.50

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	807[A]	MXM	CAO-NAJ-SAE	11.80	135.17	116.91
5	B	807[B]	MXM	CAO-NAJ-SAE	11.69	135.01	116.91
5	A	807[A]	MXM	CAO-NAJ-SAE	11.55	134.80	116.91
5	A	807[B]	MXM	CAO-NAJ-SAE	11.55	134.80	116.91
5	B	807[B]	MXM	CAB-SAE-NAJ	11.12	116.23	101.91
5	B	807[A]	MXM	CAB-SAE-NAJ	11.00	116.07	101.91
5	B	807[A]	MXM	CAG-NAJ-SAE	-10.93	98.59	113.14
5	B	807[B]	MXM	CAG-NAJ-SAE	-10.73	98.86	113.14
5	A	807[A]	MXM	CAB-SAE-NAJ	10.58	115.53	101.91
5	A	807[A]	MXM	CAG-NAJ-SAE	-10.57	99.07	113.14
5	A	807[B]	MXM	CAG-NAJ-SAE	-10.49	99.17	113.14
5	A	807[B]	MXM	CAB-SAE-NAJ	10.14	114.97	101.91
5	B	807[A]	MXM	CAB-CAA-CAC	-9.46	115.22	120.47
5	B	807[B]	MXM	CAB-CAA-CAC	-8.83	115.57	120.47
5	B	807[A]	MXM	OAL-SAE-OAK	-8.60	107.59	118.53
5	A	807[B]	MXM	CAB-CAA-CAC	-8.52	115.74	120.47
5	A	807[A]	MXM	OAL-SAE-OAK	-8.41	107.83	118.53
5	B	807[B]	MXM	OAL-SAE-OAK	-8.39	107.86	118.53
5	A	807[A]	MXM	CAB-CAA-CAC	-8.37	115.82	120.47
5	A	807[B]	MXM	OAL-SAE-OAK	-8.30	107.97	118.53
5	B	807[B]	MXM	CAV-SAT-CAR	8.06	95.26	89.32
5	A	807[B]	MXM	CAV-SAT-CAR	8.00	95.21	89.32
5	B	807[B]	MXM	CAA-CAB-SAE	-7.19	108.40	117.29
5	B	807[A]	MXM	CAA-CAB-SAE	-7.02	108.61	117.29
5	B	807[B]	MXM	SAT-CAR-NAS	-6.97	107.95	115.58
5	A	807[A]	MXM	CAW-CAV-CAU	-6.92	122.43	129.10
5	A	807[B]	MXM	OAH-CAC-CAG	-6.83	116.57	122.66
5	A	807[B]	MXM	SAT-CAR-NAS	-6.75	108.19	115.58
5	B	807[B]	MXM	OAH-CAC-CAG	-6.72	116.67	122.66
5	A	807[A]	MXM	CAA-CAB-SAE	-6.49	109.26	117.29
5	A	807[B]	MXM	CAA-CAB-SAE	-6.45	109.31	117.29
5	B	807[A]	MXM	CAW-CAV-CAU	-6.21	123.11	129.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	807[A]	MXM	SAT-CAR-NAS	-6.20	108.80	115.58
5	B	807[A]	MXM	OAH-CAC-CAG	-6.16	117.17	122.66
5	B	807[A]	MXM	SAT-CAR-NAS	-6.10	108.90	115.58
5	A	807[A]	MXM	OAH-CAC-CAG	-6.01	117.30	122.66
5	B	807[B]	MXM	CAA-CAC-CAG	6.01	126.49	122.65
5	B	807[A]	MXM	CAV-SAT-CAR	5.84	93.62	89.32
5	A	807[A]	MXM	CAV-SAT-CAR	5.57	93.42	89.32
5	A	807[B]	MXM	CAA-CAC-CAG	5.47	126.14	122.65
5	B	807[B]	MXM	OAK-SAE-NAJ	-5.43	104.19	108.14
3	A	801	HEM	C4D-ND-C1D	5.14	111.29	105.21
5	B	807[A]	MXM	CAV-CAU-NAS	-5.06	111.90	117.12
3	B	801	HEM	C4D-ND-C1D	4.97	111.09	105.21
5	A	807[B]	MXM	OAL-SAE-NAJ	4.92	111.72	108.14
5	A	807[A]	MXM	CAV-CAU-NAS	-4.90	112.07	117.12
5	A	807[A]	MXM	CAU-NAS-CAR	4.62	114.95	109.66
5	B	807[A]	MXM	CAU-NAS-CAR	4.60	114.94	109.66
5	B	807[B]	MXM	CAV-CAU-NAS	-4.53	112.44	117.12
5	B	807[A]	MXM	CAC-CAG-NAJ	-4.46	117.40	120.87
5	A	807[B]	MXM	CAO-NAJ-CAG	-4.36	109.17	115.07
5	B	807[B]	MXM	CAW-CAV-CAU	-4.33	124.93	129.10
5	B	807[B]	MXM	CAO-NAJ-CAG	-4.27	109.29	115.07
5	B	807[A]	MXM	OAK-SAE-NAJ	-4.26	105.04	108.14
5	A	807[B]	MXM	CAW-CAV-CAU	-4.16	125.09	129.10
5	A	807[B]	MXM	CAV-CAU-NAS	-4.02	112.97	117.12
5	A	807[B]	MXM	OAK-SAE-NAJ	-3.91	105.30	108.14
5	B	807[A]	MXM	CAR-NAP-CAN	-3.68	118.30	123.78
5	A	807[A]	MXM	OAL-SAE-NAJ	3.65	110.80	108.14
5	A	807[A]	MXM	CAR-NAP-CAN	-3.62	118.38	123.78
5	B	807[B]	MXM	CAF-CAB-SAE	3.58	126.29	120.45
5	A	807[A]	MXM	CAC-CAG-NAJ	-3.56	118.11	120.87
5	A	807[A]	MXM	CAO-NAJ-CAG	-3.52	110.31	115.07
5	B	807[B]	MXM	SAT-CAR-NAP	3.50	128.40	123.72
5	B	807[B]	MXM	CAU-NAS-CAR	3.48	113.66	109.66
5	A	807[B]	MXM	SAT-CAR-NAP	3.48	128.38	123.72
5	B	807[A]	MXM	CAF-CAB-SAE	3.35	125.92	120.45
5	B	807[A]	MXM	CAA-CAC-CAG	3.29	124.75	122.65
5	A	807[A]	MXM	CAA-CAC-CAG	3.16	124.67	122.65
5	A	807[B]	MXM	CAF-CAB-SAE	3.09	125.48	120.45
5	A	807[B]	MXM	CAU-NAS-CAR	3.05	113.16	109.66
5	B	807[B]	MXM	OAL-SAE-NAJ	3.04	110.35	108.14
5	A	807[A]	MXM	CAW-CAV-SAT	2.81	126.81	121.03
5	A	807[A]	MXM	OAK-SAE-NAJ	-2.73	106.16	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	807[A]	MXM	CAF-CAB-SAE	2.58	124.65	120.45
5	B	807[A]	MXM	CAW-CAV-SAT	2.54	126.26	121.03
5	A	807[B]	MXM	CAC-CAG-CAN	-2.49	118.63	120.84
5	A	807[A]	MXM	OAK-SAE-CAB	-2.34	105.90	109.10
5	B	807[B]	MXM	CAC-CAG-NAJ	-2.34	119.05	120.87
5	A	807[B]	MXM	CAC-CAG-NAJ	-2.34	119.05	120.87
3	A	801	HEM	C3B-C2B-C1B	2.21	108.07	106.41
3	A	801	HEM	CAD-C3D-C4D	2.18	128.50	124.70
5	B	807[A]	MXM	NAP-CAR-NAS	2.17	125.31	121.19
3	B	801	HEM	CHC-C1C-NC	2.14	126.78	124.45
5	B	807[B]	MXM	CAC-CAG-CAN	-2.11	118.96	120.84
3	A	801	HEM	CHC-C1C-NC	2.09	126.73	124.45
5	A	807[A]	MXM	NAP-CAR-NAS	2.08	125.12	121.19
5	B	807[A]	MXM	CAO-NAJ-CAG	-2.06	112.29	115.07
3	B	801	HEM	C3B-C2B-C1B	2.02	107.93	106.41

There are no chirality outliers.

All (10) torsion outliers are listed below:

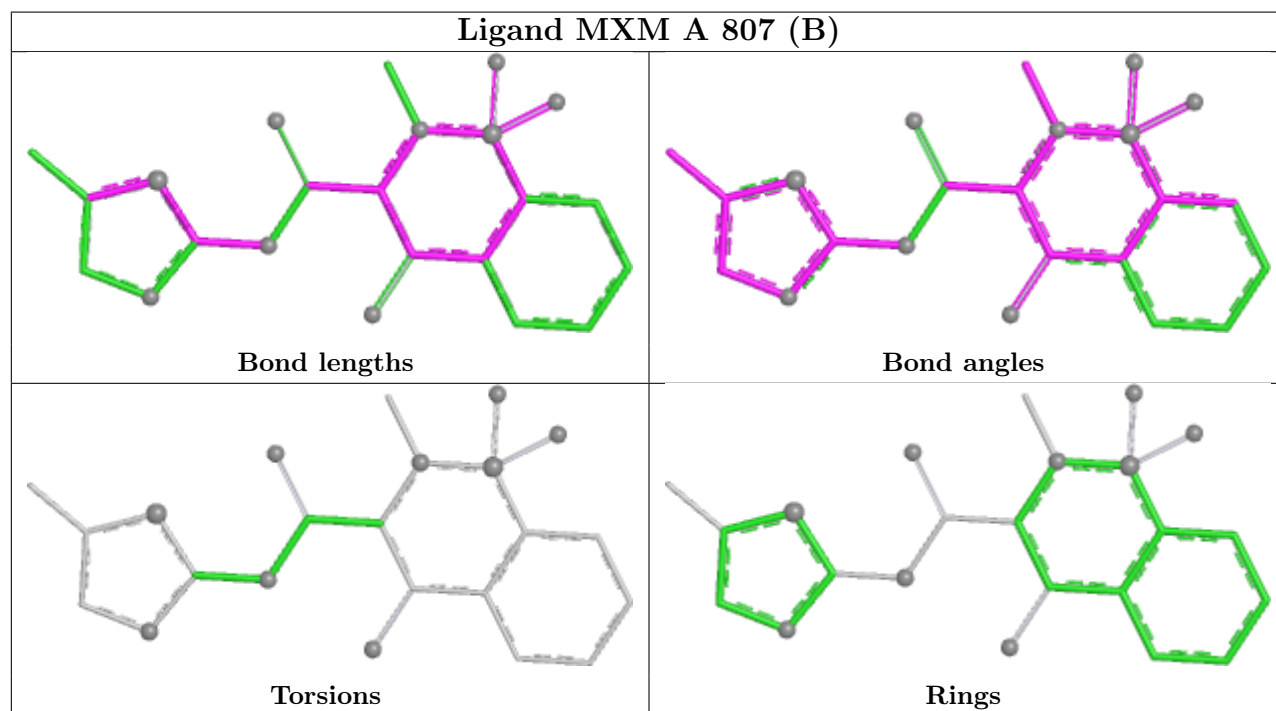
Mol	Chain	Res	Type	Atoms
5	A	807[A]	MXM	SAT-CAR-NAP-CAN
5	A	807[A]	MXM	NAS-CAR-NAP-CAN
5	A	807[A]	MXM	CAC-CAG-CAN-NAP
5	B	807[A]	MXM	SAT-CAR-NAP-CAN
5	B	807[A]	MXM	NAS-CAR-NAP-CAN
5	B	807[A]	MXM	CAC-CAG-CAN-NAP
3	A	801	HEM	C4C-C3C-CAC-CBC
3	B	801	HEM	C4C-C3C-CAC-CBC
4	B	802	NAG	C4-C5-C6-O6
4	B	802	NAG	O5-C5-C6-O6

There are no ring outliers.

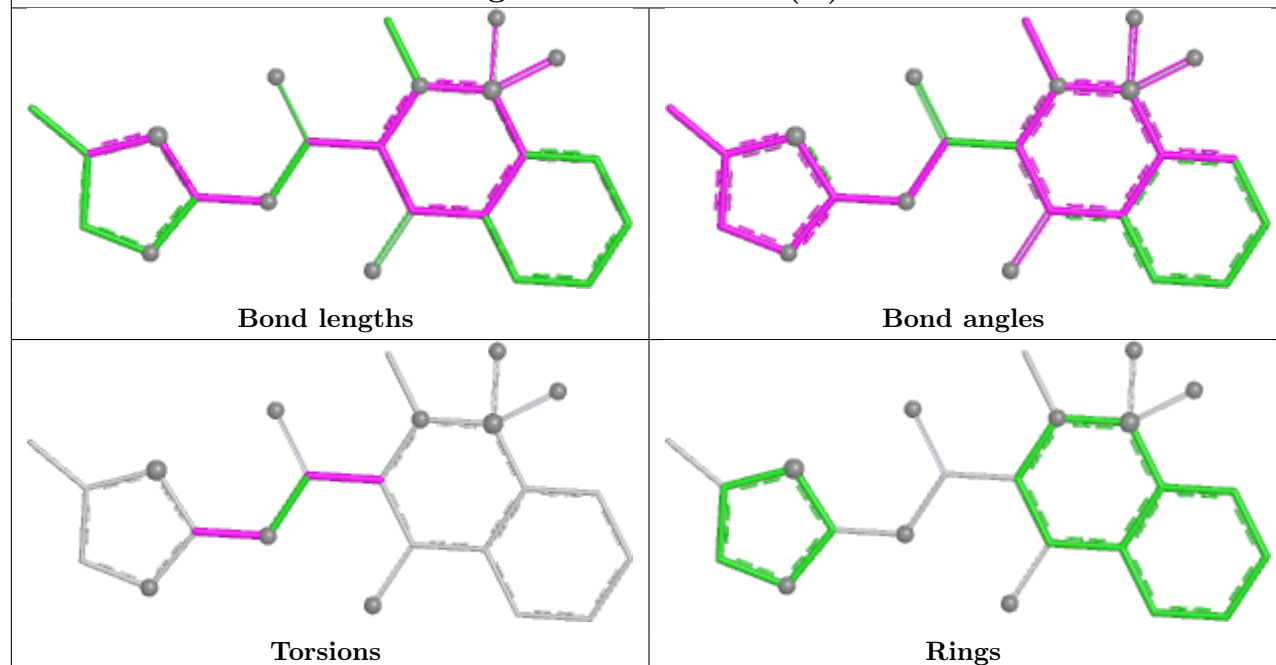
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	807[B]	MXM	1	0
3	B	801	HEM	3	0
3	A	801	HEM	3	0
4	A	802	NAG	1	0
5	B	807[B]	MXM	2	0

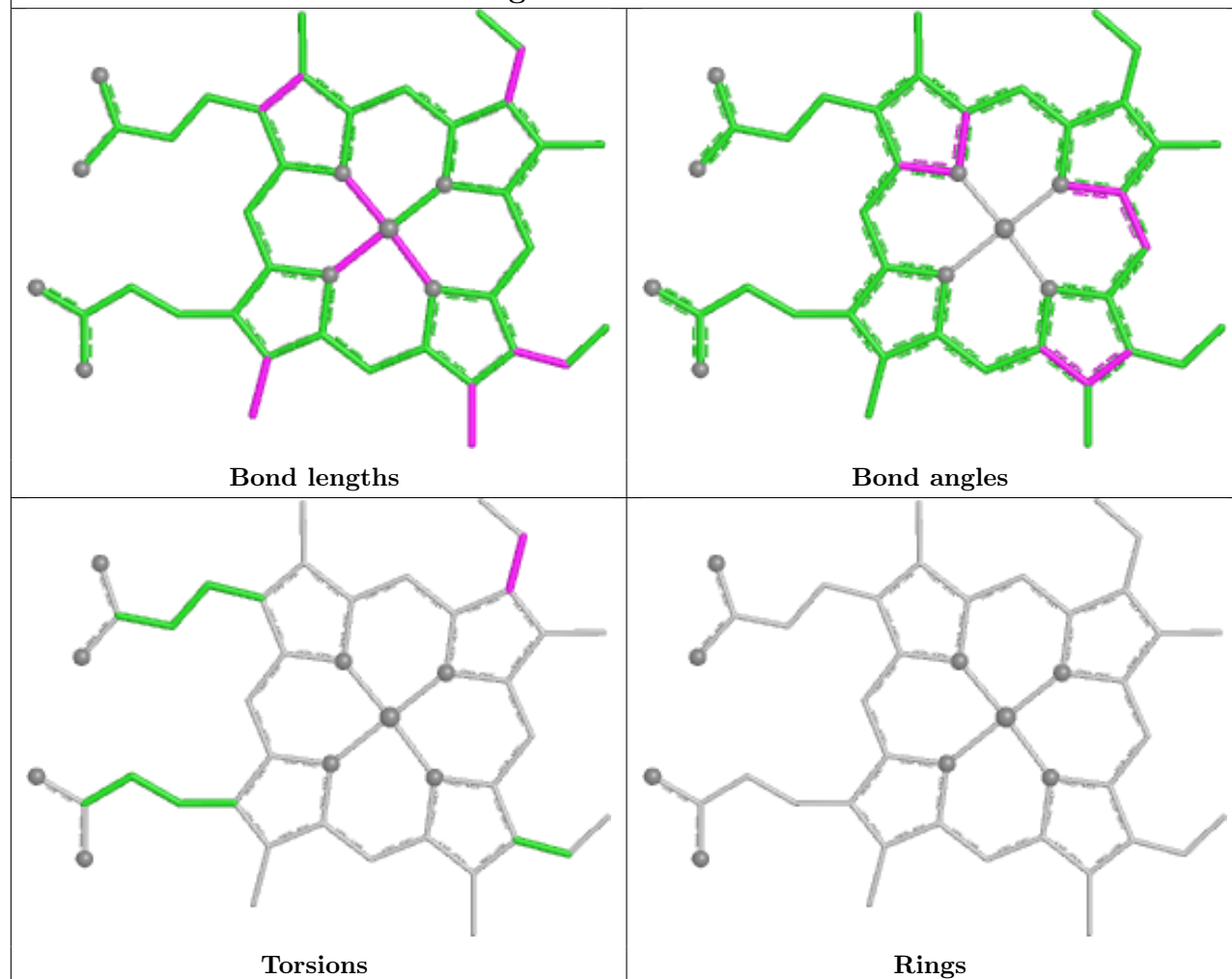
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

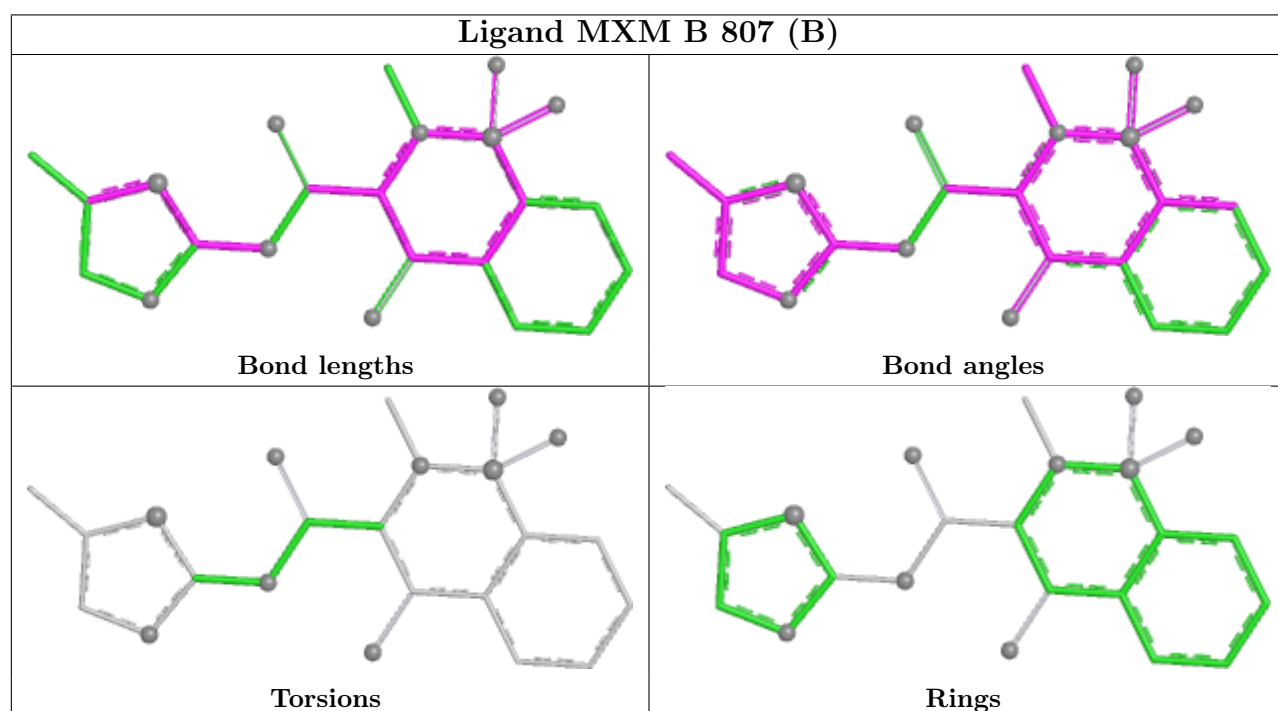
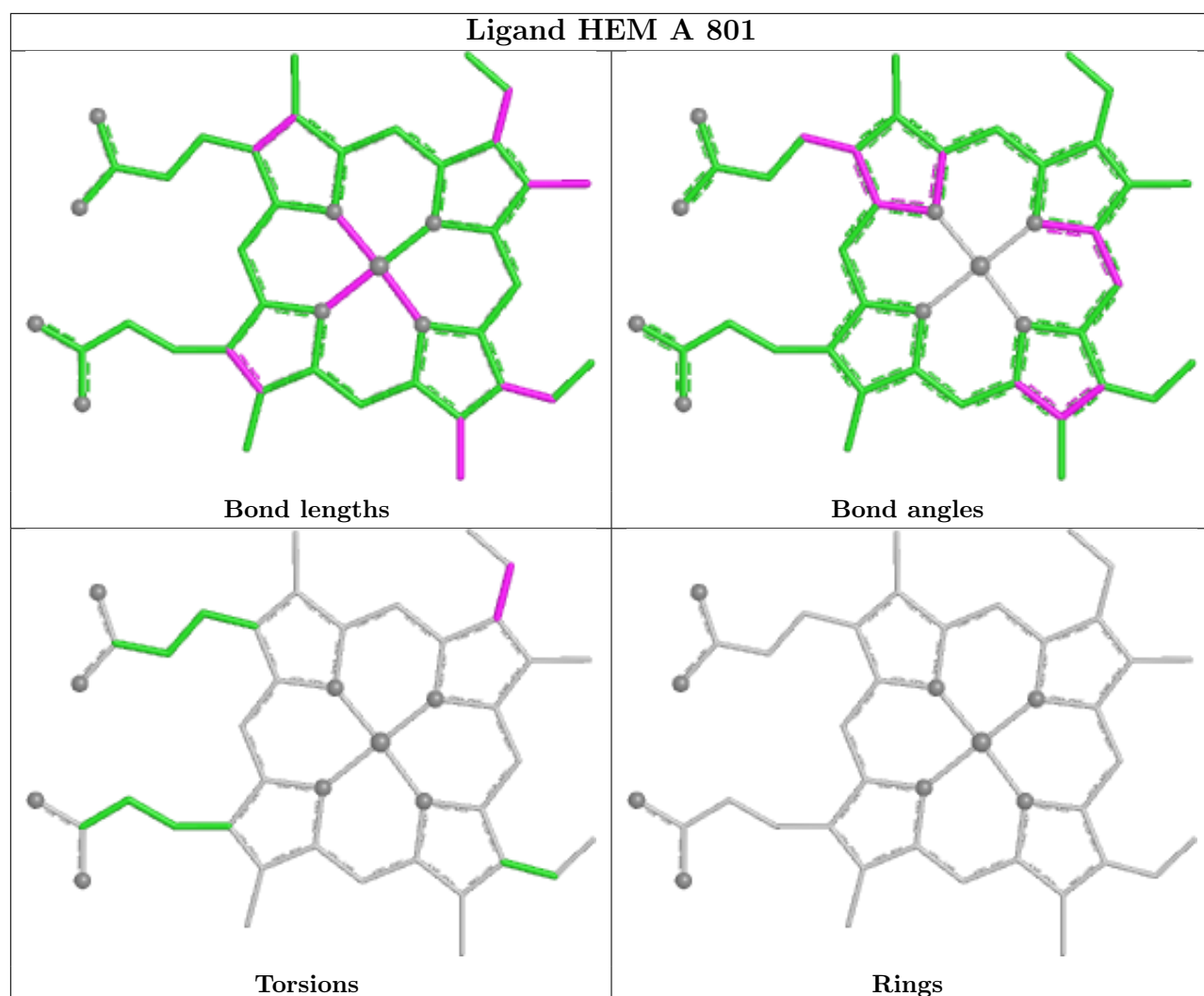


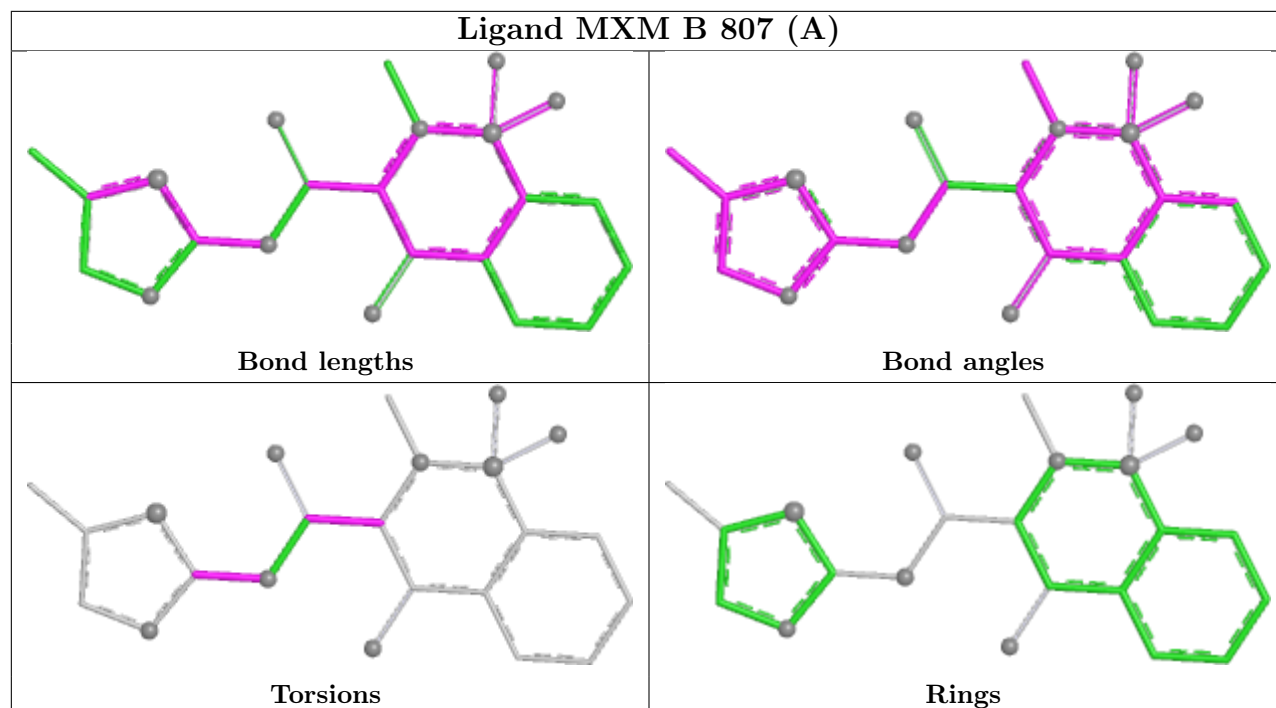
Ligand MXM A 807 (A)



Ligand HEM B 801







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	553/569 (97%)	1.11	79 (14%) 6 5	30, 47, 69, 100	0
1	B	553/569 (97%)	1.00	65 (11%) 9 6	31, 45, 72, 92	0
All	All	1106/1138 (97%)	1.05	144 (13%) 7 5	30, 46, 71, 100	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	PRO	4.9
1	A	75	TRP	4.8
1	B	75	TRP	4.5
1	A	83	ARG	4.4
1	B	282	GLN	4.2
1	B	280	PRO	4.2
1	A	175	GLU	4.0
1	A	452	ILE	3.8
1	A	122	ASN	3.8
1	B	33	VAL	3.7
1	A	77	TRP	3.7
1	A	107	PHE	3.6
1	B	81	THR	3.6
1	B	318	ALA	3.6
1	B	107	PHE	3.5
1	A	478	PHE	3.4
1	A	185	ARG	3.4
1	B	176	PHE	3.4
1	B	77	TRP	3.4
1	B	101	ASP	3.2
1	A	67	PRO	3.2
1	A	318	ALA	3.1
1	A	59	CYS	3.1
1	A	486	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	3.1
1	A	359	LEU	3.1
1	A	356	PHE	3.0
1	A	119	VAL	3.0
1	A	239	GLU	3.0
1	B	485	LYS	3.0
1	A	324	GLY	3.0
1	A	479	GLN	3.0
1	A	32	PRO	2.9
1	B	183	LEU	2.9
1	A	104	ASN	2.9
1	B	277	ARG	2.9
1	B	82	LEU	2.9
1	B	267	GLU	2.9
1	B	257	LEU	2.9
1	B	83	ARG	2.8
1	B	76	THR	2.8
1	A	170	GLN	2.8
1	A	88	PHE	2.8
1	B	109	ARG	2.8
1	A	265	SER	2.8
1	B	239	GLU	2.8
1	B	35	PRO	2.8
1	B	215	LYS	2.8
1	A	33	VAL	2.7
1	B	168	LYS	2.7
1	A	97	ARG	2.7
1	A	52	LEU	2.7
1	B	119	VAL	2.7
1	A	574	THR	2.7
1	B	248	LYS	2.6
1	A	403	SER	2.6
1	A	98	TRP	2.6
1	A	215	LYS	2.6
1	A	485	LYS	2.6
1	A	512	CYS	2.6
1	A	155	VAL	2.6
1	A	477	SER	2.6
1	A	459	ARG	2.6
1	B	278	GLY	2.6
1	B	396	ARG	2.6
1	A	102	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	78	LEU	2.5
1	B	358	GLN	2.5
1	B	575	CYS	2.5
1	A	80	THR	2.5
1	A	189	PRO	2.5
1	A	214	GLY	2.5
1	A	50	PHE	2.5
1	B	112	LEU	2.5
1	A	523	ILE	2.5
1	B	584	ASP	2.5
1	B	356	PHE	2.5
1	A	575	CYS	2.4
1	A	63	GLY	2.4
1	A	300	LEU	2.4
1	A	81	THR	2.4
1	B	574	THR	2.4
1	A	402	TYR	2.4
1	B	122	ASN	2.4
1	A	473	LYS	2.4
1	B	513	HIS	2.4
1	B	425	ALA	2.4
1	B	276	PRO	2.3
1	B	401	ASP	2.3
1	A	404	TYR	2.3
1	B	271	VAL	2.3
1	A	277	ARG	2.3
1	B	97	ARG	2.3
1	B	533	GLY	2.3
1	B	442	HIS	2.3
1	B	104	ASN	2.3
1	B	527	ALA	2.3
1	A	279	ILE	2.3
1	B	115	LEU	2.3
1	B	531	LEU	2.3
1	A	362	ASP	2.3
1	A	271	VAL	2.3
1	A	86	PRO	2.3
1	A	157	ARG	2.3
1	A	496	GLY	2.2
1	B	74	ILE	2.2
1	B	79	ARG	2.2
1	A	369	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	GLN	2.2
1	B	492	GLU	2.2
1	A	169	LYS	2.2
1	A	208	GLN	2.2
1	A	243	GLN	2.2
1	A	282	GLN	2.2
1	A	495	TYR	2.2
1	B	272	LEU	2.2
1	B	78	LEU	2.1
1	B	89	ILE	2.1
1	B	279	ILE	2.1
1	B	452	ILE	2.1
1	B	405	GLU	2.1
1	B	498	ILE	2.1
1	B	459	ARG	2.1
1	A	87	SER	2.1
1	A	96	GLY	2.1
1	A	117	LEU	2.1
1	B	418	GLY	2.1
1	A	584	ASP	2.1
1	B	138	SER	2.1
1	A	451	VAL	2.1
1	B	266	VAL	2.1
1	A	123	LEU	2.1
1	A	460	LEU	2.1
1	B	98	TRP	2.1
1	B	186	LYS	2.1
1	A	497	ASP	2.1
1	A	159	CYS	2.1
1	A	43	HIS	2.1
1	A	156	PRO	2.0
1	B	243	GLN	2.0
1	A	93	LEU	2.0
1	A	252	LEU	2.0
1	A	492	GLU	2.0
1	B	169	LYS	2.0

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

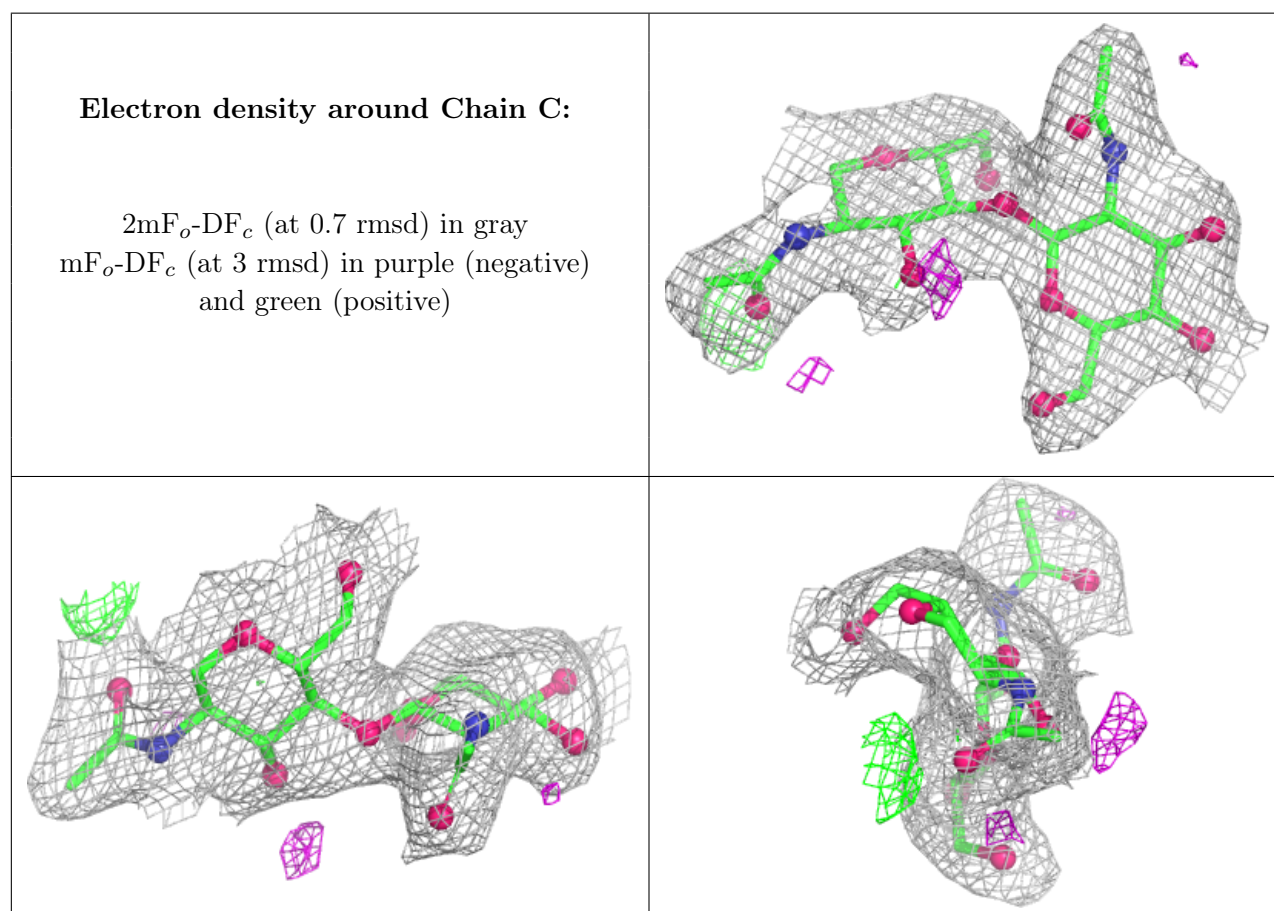
There are no non-standard protein/DNA/RNA residues in this entry.

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.

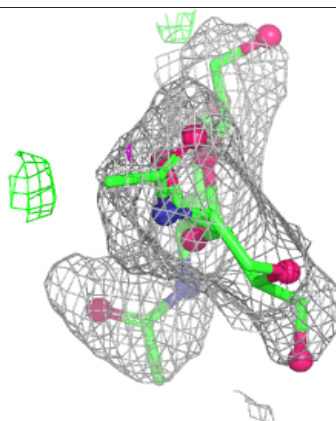
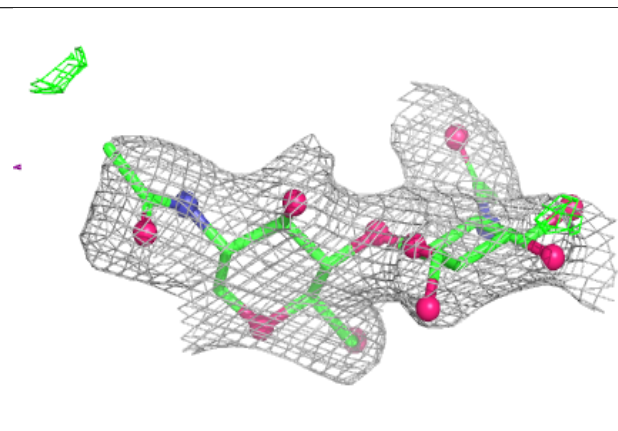
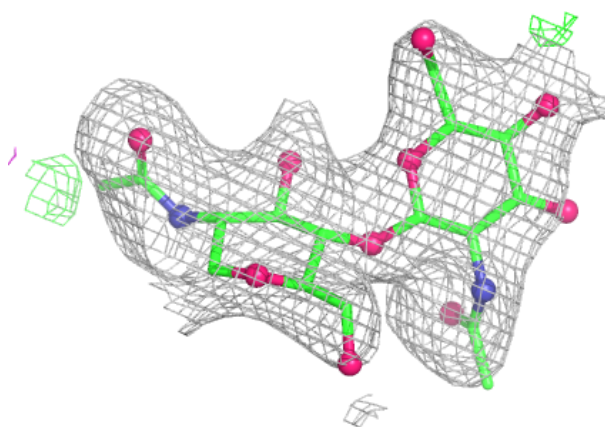
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.75	0.21	53,74,99,106	0
2	NAG	F	1	14/15	0.82	0.18	51,60,68,71	0
2	NAG	D	1	14/15	0.86	0.15	51,60,68,71	0
2	NAG	E	2	14/15	0.86	0.11	39,48,62,69	0
2	NAG	D	2	14/15	0.87	0.13	55,67,77,87	0
2	NAG	C	2	14/15	0.89	0.11	39,48,62,69	0
2	NAG	C	1	14/15	0.89	0.09	20,37,44,47	0
2	NAG	E	1	14/15	0.92	0.09	26,41,48,59	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.



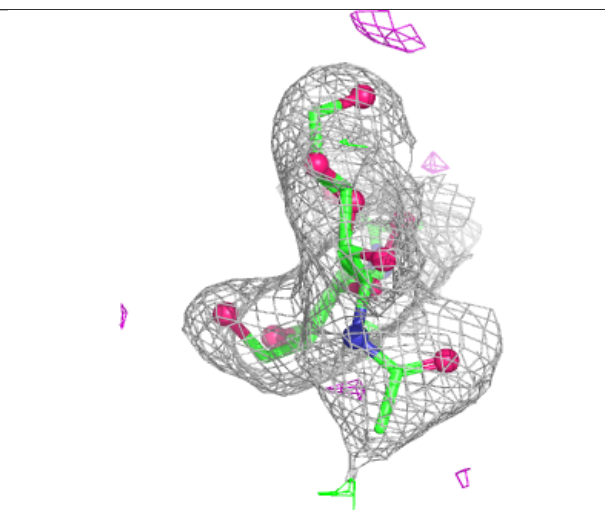
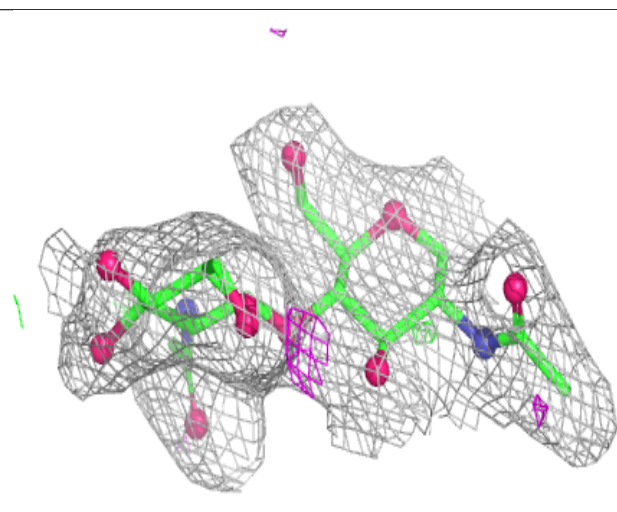
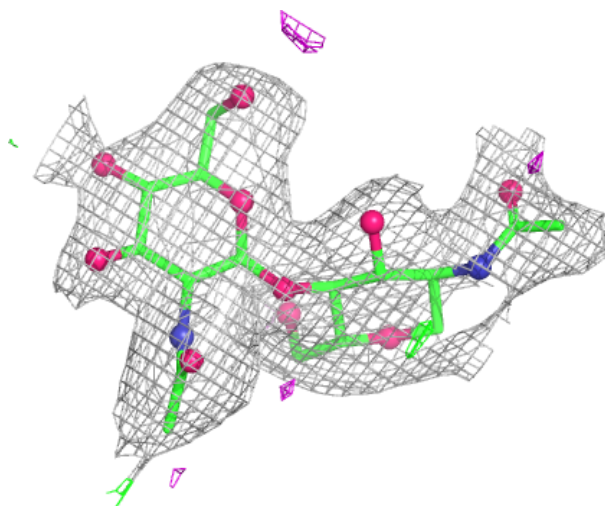
Electron density around Chain D:

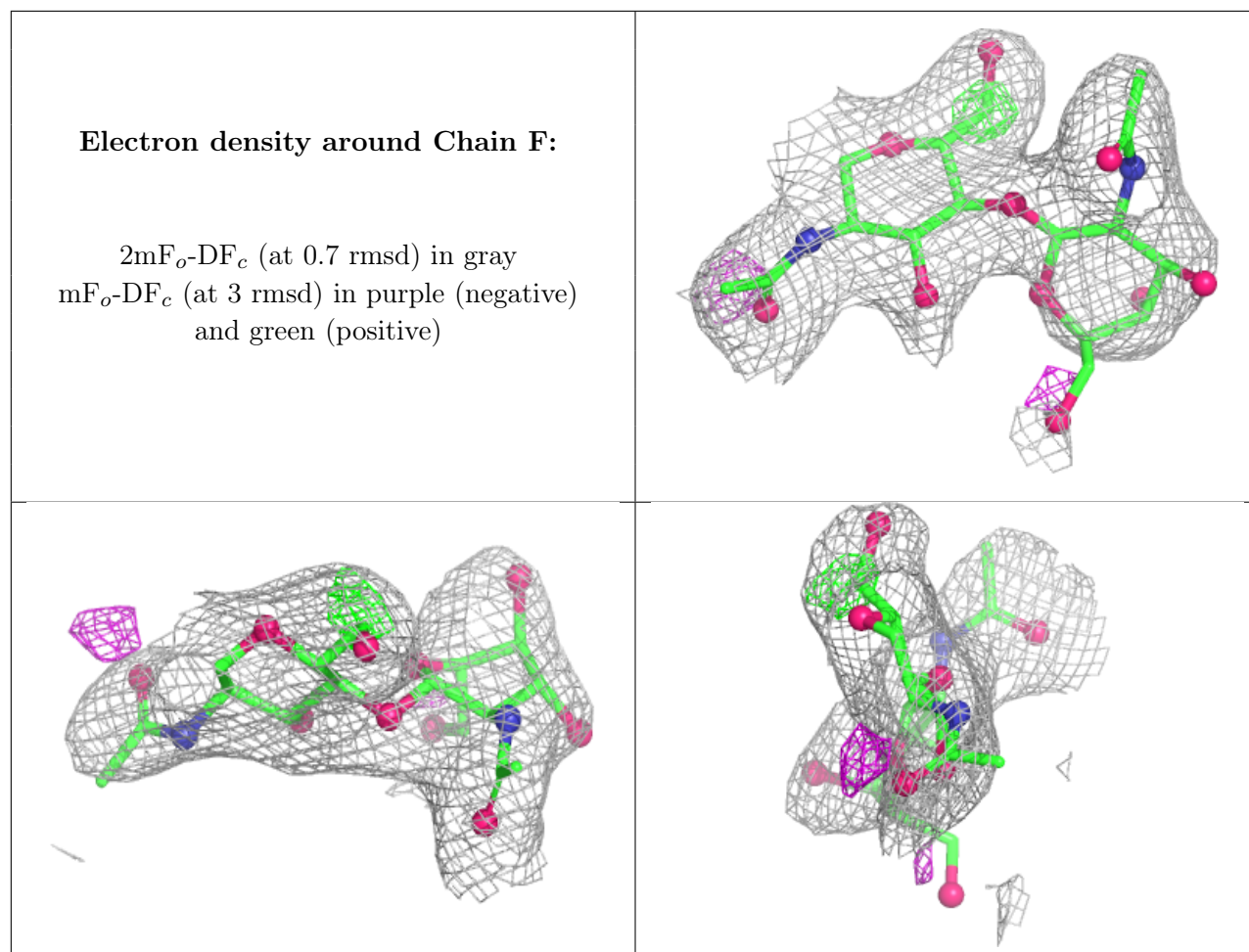
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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

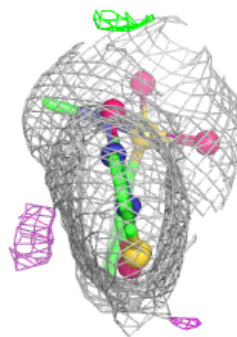
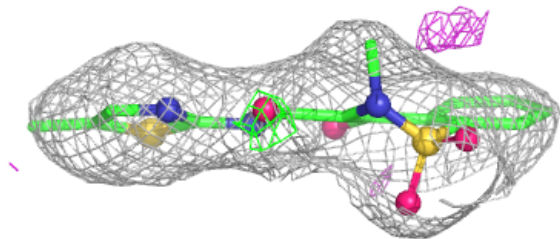
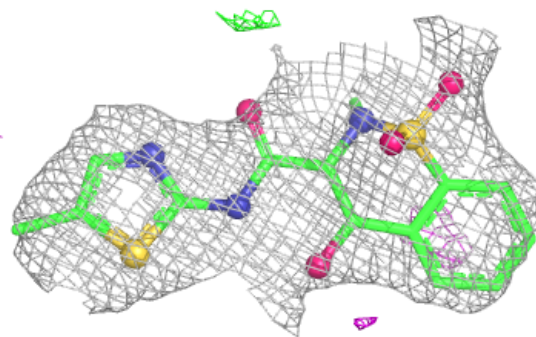
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	802	14/15	0.79	0.18	57,70,91,104	0
4	NAG	B	802	14/15	0.83	0.18	53,67,91,97	0
5	MXM	A	807[A]	23/23	0.83	0.26	51,63,72,77	23
5	MXM	A	807[B]	23/23	0.83	0.26	50,63,74,84	0
5	MXM	B	807[A]	23/23	0.84	0.27	48,63,70,74	23
5	MXM	B	807[B]	23/23	0.84	0.27	47,65,71,78	0
3	HEM	B	801	43/43	0.92	0.14	32,48,64,101	0
3	HEM	A	801	43/43	0.94	0.13	30,46,56,118	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.

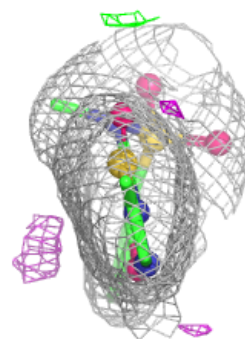
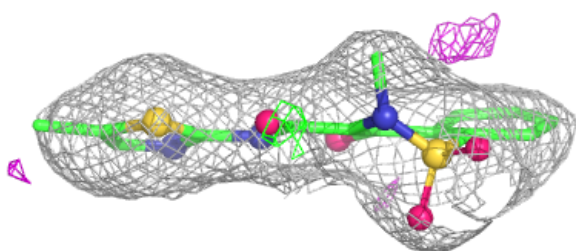
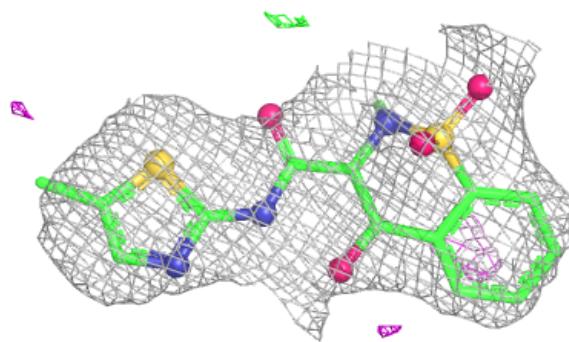
Electron density around MXM A 807 (A):

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

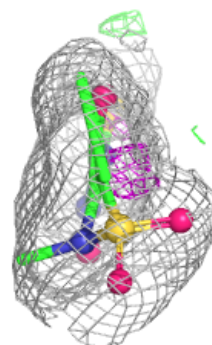
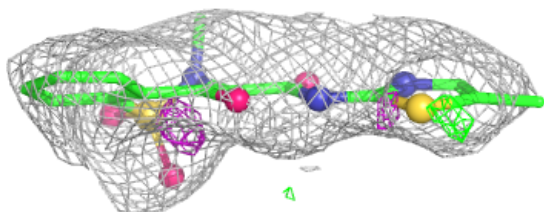
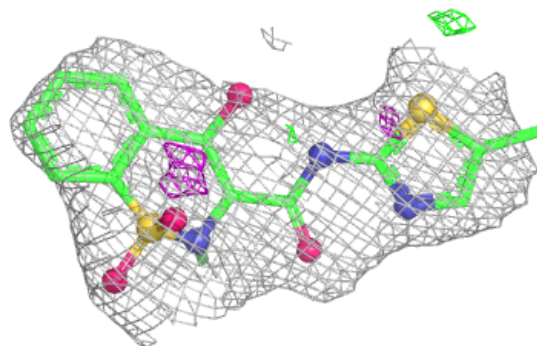


Electron density around MXM A 807 (B):

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

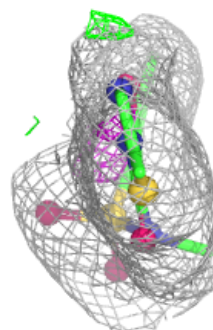
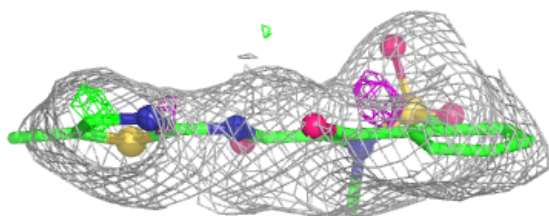
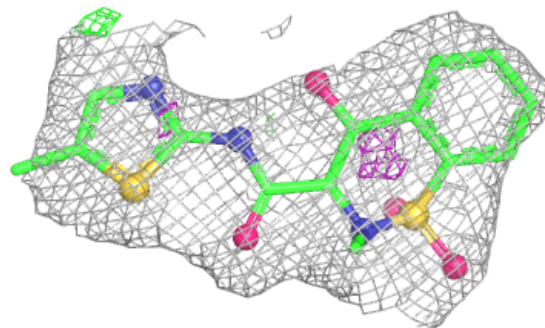
**Electron density around MXM B 807 (A):**

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



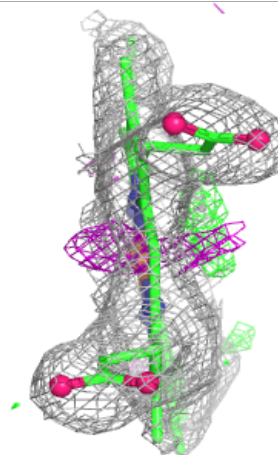
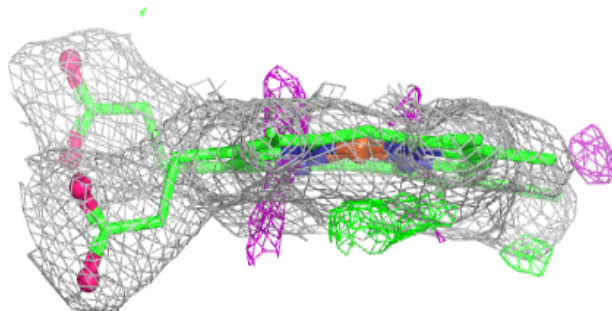
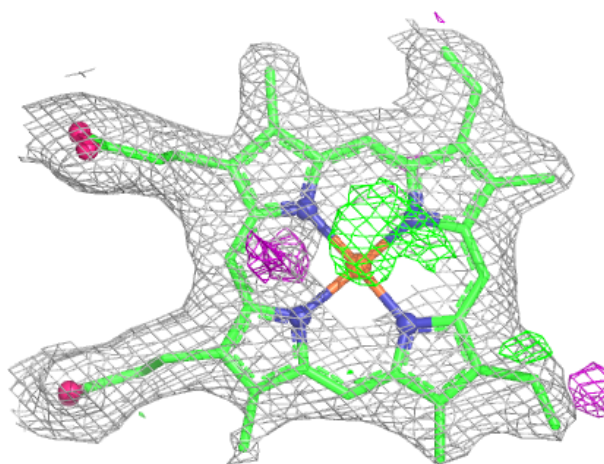
Electron density around MXM B 807 (B):

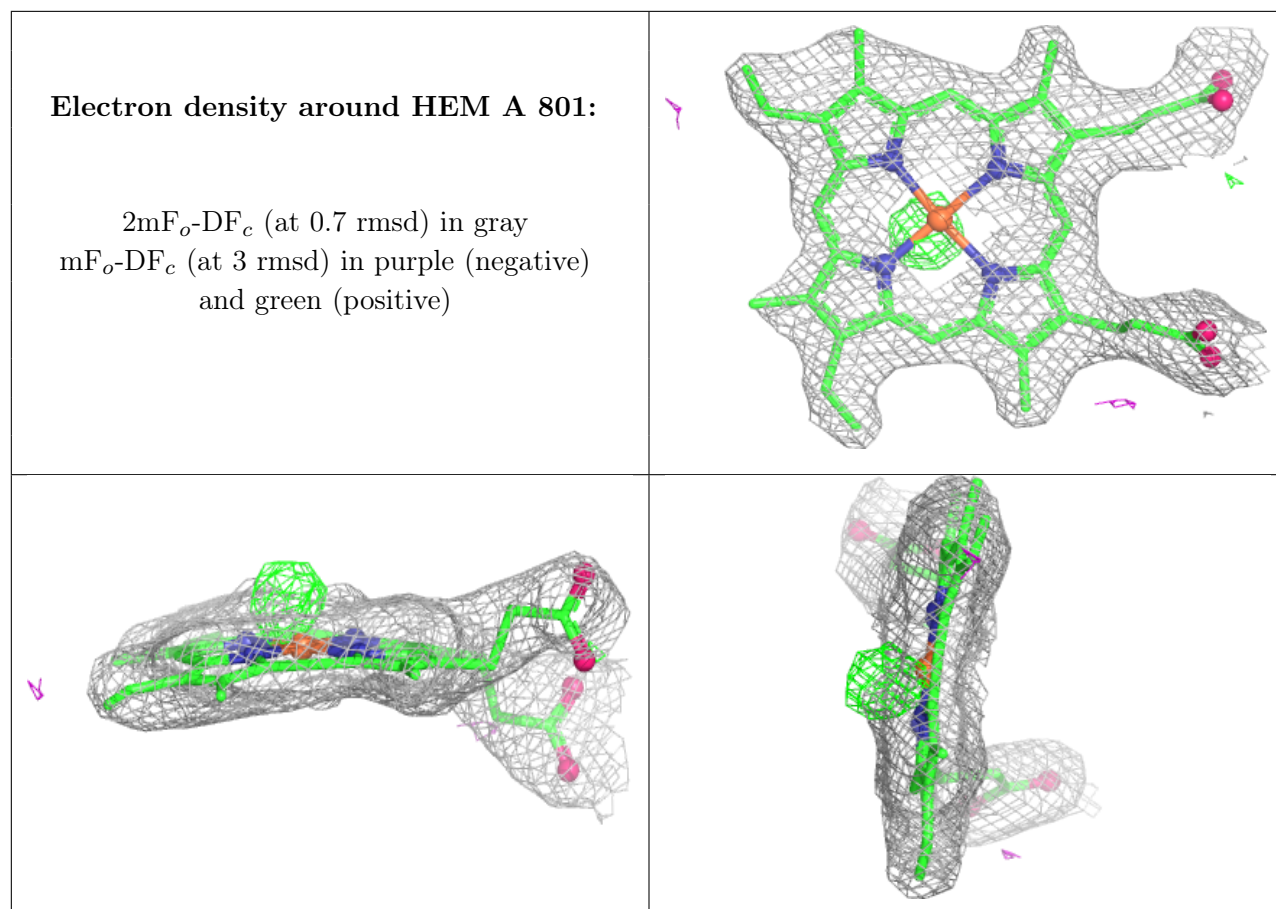
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 801:

$2mF_o-DF_c$ (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.