Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2025 – 03:19 pm GMT

PDB ID	:	9HE7
Title	:	Unspecific peroxygenase from Psathyrella aberdarensis (PabUPO-II) in complex with myristic acid
Authors	:	Fernandez-Garcia, A.; Sanz-Aparicio, J.
Deposited on	:	2024-11-13
Resolution	:	2.00 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:

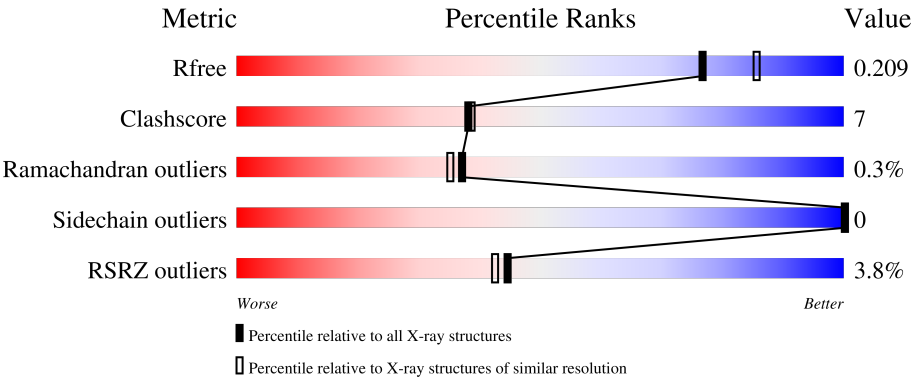
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	335	3% 92% 8%
1	B	335	3% 93% 7%
1	C	335	5% 93% 7%
2	G	5	100%
3	I	7	71% 29%

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Mol	Chain	Length	Quality of chain
4	Z	4	50% 50%
4	q	4	100%
5	a	6	33% 67%
6	s	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MYR	C	401	-	-	X	-
8	GOL	A	402	-	-	X	-
8	GOL	B	403	-	-	X	-

2 Entry composition

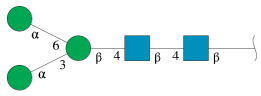
There are 13 unique types of molecules in this entry. The entry contains 9489 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heme-thiolate peroxidase.

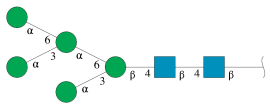
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	10	0
			2646	1682	456	501	7			
1	B	335	Total	C	N	O	S	0	8	0
			2637	1676	455	499	7			
1	C	335	Total	C	N	O	S	0	8	0
			2635	1675	454	499	7			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

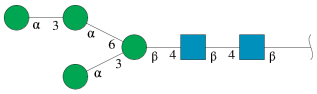


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

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

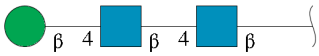
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Z	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



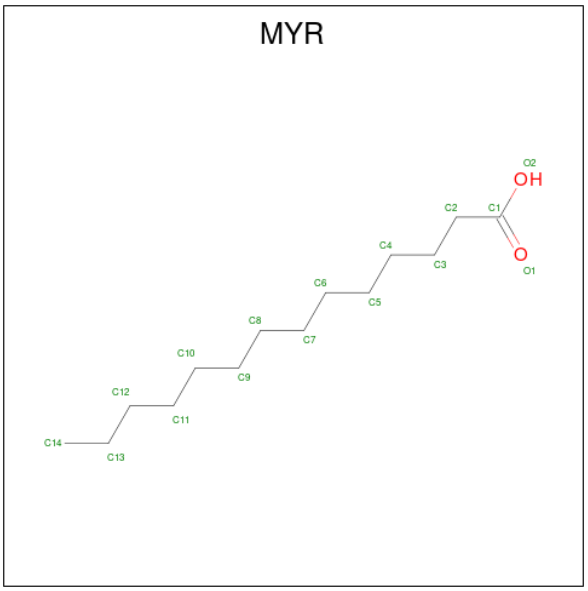
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	a	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



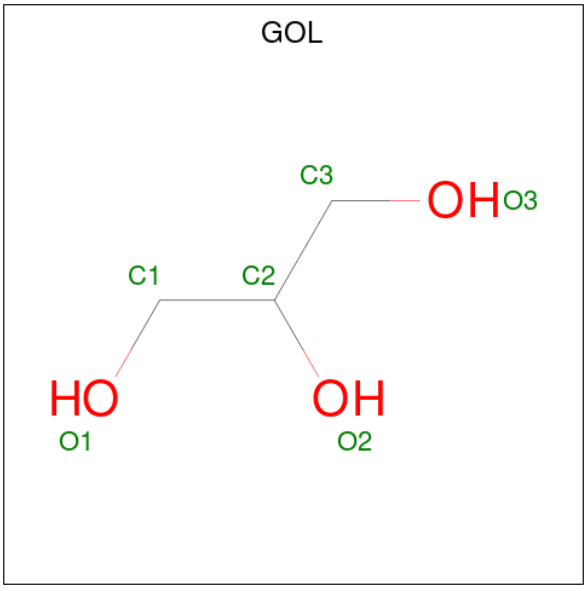
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	s	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 32 28 4	0	1
7	B	1	Total C O 32 28 4	0	1
7	C	1	Total C O 16 14 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

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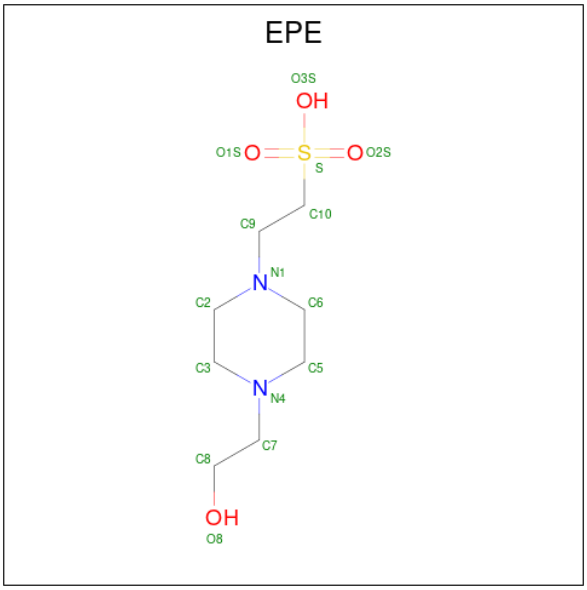
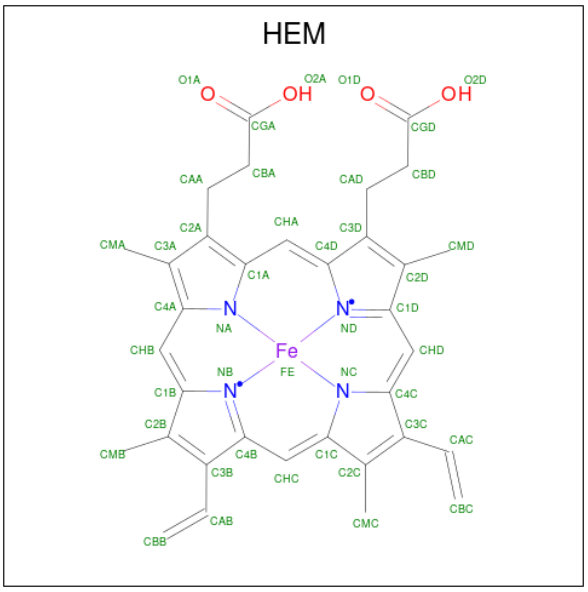
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



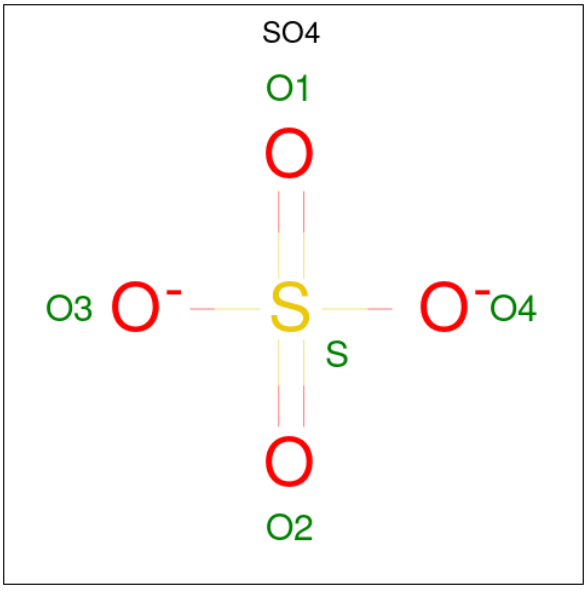
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O S 15 8 2 4 1	0	0
9	B	1	Total C N O S 15 8 2 4 1	0	0
9	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O S 5 4 1	0	0
11	A	1	Total O S 5 4 1	0	0
11	A	1	Total O S 5 4 1	0	0
11	B	1	Total O S 5 4 1	0	0
11	C	1	Total O S 5 4 1	0	0
11	C	1	Total O S 5 4 1	0	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Mg 1 1	0	0
12	B	1	Total Mg 1 1	0	0
12	C	1	Total Mg 1 1	0	0

- Molecule 13 is water.

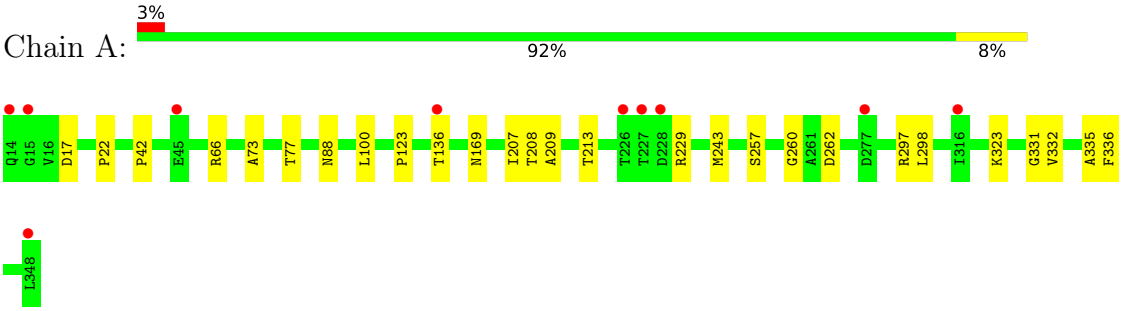
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	363	Total O 363 363	0	0
13	B	287	Total O 287 287	0	0
13	C	238	Total O 238 238	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

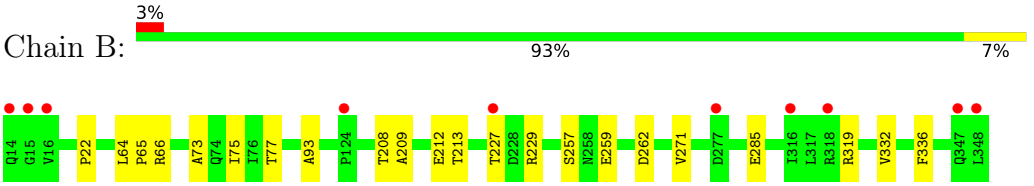
• Molecule 1: Heme-thiolate peroxidase

Chain A:



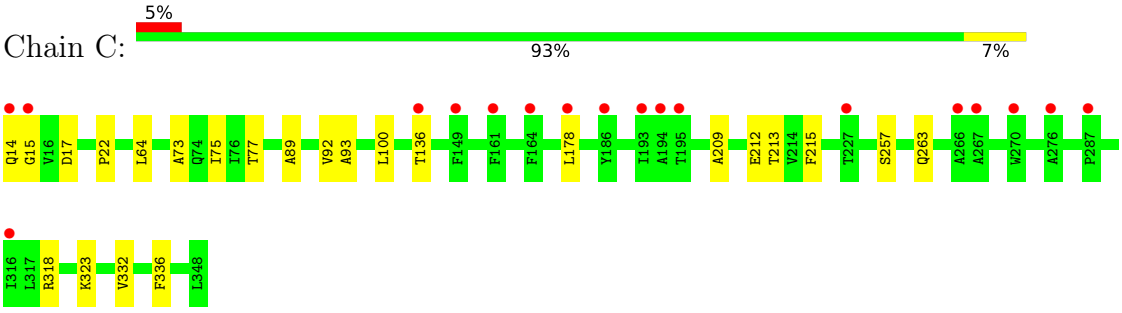
• Molecule 1: Heme-thiolate peroxidase

Chain B:



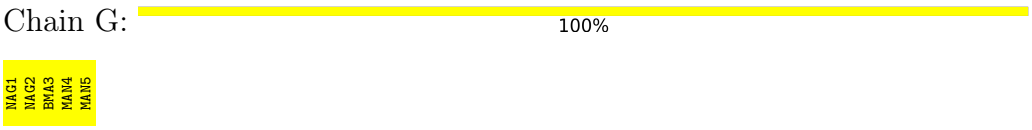
• Molecule 1: Heme-thiolate peroxidase

Chain C:



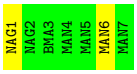
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

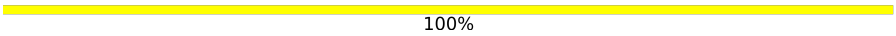


• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

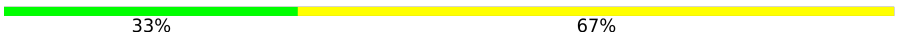
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



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

Chain s:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	271.96Å 74.86Å 105.83Å 90.00° 111.81° 90.00°	Depositor
Resolution (Å)	49.18 – 2.00 49.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.18-2.00) 99.9 (49.18-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.177 , 0.196 0.190 , 0.209	Depositor DCC
R_{free} test set	6670 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9489	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, EPE, MG, SO4, BMA, MYR, NAG, MAN, HEM

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	0.39	0/2757	0.68	0/3767
1	B	0.37	0/2742	0.67	0/3746
1	C	0.38	0/2740	0.68	0/3744
All	All	0.38	0/8239	0.68	0/11257

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2646	0	2506	37	0
1	B	2637	0	2493	28	0
1	C	2635	0	2492	27	0
2	G	61	0	52	0	0
3	I	83	0	70	0	0
4	Z	50	0	43	0	0
4	q	50	0	43	0	0
5	a	72	0	61	0	0
6	s	39	0	34	0	0
7	A	32	0	54	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	32	0	54	15	0
7	C	16	0	27	13	0
8	A	18	0	24	9	0
8	B	12	0	16	9	0
8	C	6	0	8	0	0
9	A	15	0	18	4	0
9	B	30	0	36	4	0
10	A	43	0	30	1	0
10	B	43	0	30	1	0
10	C	43	0	30	3	0
11	A	20	0	0	0	0
11	B	5	0	0	0	0
11	C	10	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
13	A	363	0	0	17	0
13	B	287	0	0	13	0
13	C	238	0	0	7	0
All	All	9489	0	8121	113	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 (113) 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:212[A]:GLU:OE2	7:B:401[A]:MYR:C14	1.79	1.28
1:B:212[A]:GLU:OE2	7:B:401[A]:MYR:H141	1.34	1.13
1:C:212[A]:GLU:OE2	7:C:401:MYR:C14	2.00	1.09
1:A:243[B]:MET:CE	13:A:812:HOH:O	2.00	1.07
1:A:243[B]:MET:HE1	13:A:812:HOH:O	1.57	1.03
1:C:212[A]:GLU:OE2	7:C:401:MYR:H141	1.60	0.97
7:B:401[B]:MYR:H22	13:B:680:HOH:O	1.65	0.96
1:A:260:GLY:H	8:A:405:GOL:H32	1.33	0.92
1:B:212[A]:GLU:OE2	7:B:401[A]:MYR:H142	1.67	0.91
1:A:262:ASP:CG	8:A:405:GOL:H2	1.92	0.90
1:A:207:ILE:HD12	1:A:298:LEU:HD12	1.53	0.87
1:C:73:ALA:O	1:C:77[B]:THR:HG22	1.78	0.83
8:A:402:GOL:H32	13:A:713:HOH:O	1.79	0.80
1:A:66:ARG:H	8:A:402:GOL:H31	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212[A]:GLU:OE2	7:C:401:MYR:H142	1.84	0.74
1:C:77[B]:THR:HG21	13:C:689:HOH:O	1.87	0.74
1:A:243[B]:MET:HE2	13:A:812:HOH:O	1.71	0.74
1:A:169:ASN:O	1:C:318[B]:ARG:NH2	2.20	0.74
1:A:100:LEU:HD13	1:A:136[B]:THR:HG23	1.68	0.73
1:C:14:GLN:HG2	1:C:15:GLY:H	1.54	0.73
1:A:136[A]:THR:HG23	13:A:562:HOH:O	1.89	0.72
9:B:402:EPE:H62	13:B:749:HOH:O	1.90	0.71
1:C:77[A]:THR:HG22	13:C:692:HOH:O	1.89	0.71
1:A:136[A]:THR:HG21	13:A:780:HOH:O	1.90	0.70
1:A:136[A]:THR:HG22	13:A:785:HOH:O	1.92	0.69
1:A:262:ASP:OD1	8:A:405:GOL:H2	1.92	0.69
7:B:401[B]:MYR:C2	13:B:680:HOH:O	2.30	0.68
1:A:207:ILE:HD12	1:A:298:LEU:CD1	2.26	0.66
1:B:208:THR:HG22	7:B:401[B]:MYR:H62	1.77	0.66
1:B:66:ARG:H	8:B:403:GOL:C3	2.09	0.65
1:A:229:ARG:NH2	13:A:501:HOH:O	2.19	0.65
1:A:73:ALA:O	1:A:77[B]:THR:HG22	1.99	0.63
7:B:401[B]:MYR:H143	13:B:508:HOH:O	1.97	0.63
1:A:77[B]:THR:HG23	13:A:568:HOH:O	1.99	0.62
10:C:403:HEM:HBB2	10:C:403:HEM:HHC	1.81	0.62
1:B:212[A]:GLU:CD	7:B:401[A]:MYR:H141	2.17	0.62
1:B:77[A]:THR:HG22	13:B:724:HOH:O	1.99	0.62
1:B:66:ARG:N	8:B:403:GOL:H32	2.15	0.61
8:A:404:GOL:H11	13:A:605:HOH:O	2.01	0.60
1:C:92:VAL:HB	7:C:401:MYR:H72	1.83	0.60
1:A:88[B]:ASN:ND2	1:A:331:GLY:O	2.34	0.59
8:A:404:GOL:C1	13:A:605:HOH:O	2.50	0.58
1:C:22:PRO:HG2	1:C:77[A]:THR:HG23	1.86	0.58
1:B:66:ARG:H	8:B:403:GOL:H32	1.68	0.57
1:A:77[B]:THR:HG21	13:A:759:HOH:O	2.04	0.57
1:A:22:PRO:HG2	1:A:77[A]:THR:HG23	1.87	0.56
7:B:401[A]:MYR:C6	13:B:761:HOH:O	2.52	0.56
1:B:22:PRO:HG2	1:B:77[A]:THR:HG23	1.86	0.56
1:A:17:ASP:OD1	1:A:323:LYS:NZ	2.39	0.55
1:B:229:ARG:NH2	13:B:501:HOH:O	2.30	0.55
7:B:401[A]:MYR:H62	13:B:761:HOH:O	2.05	0.54
1:C:17:ASP:OD1	1:C:323:LYS:NZ	2.40	0.54
1:C:93:ALA:HB2	7:C:401:MYR:H102	1.89	0.54
7:B:401[B]:MYR:H81	13:B:758:HOH:O	2.07	0.54
1:A:66:ARG:N	8:A:402:GOL:H31	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:401[B]:MYR:H22	13:A:753:HOH:O	2.09	0.53
1:A:77[A]:THR:HG21	13:A:759:HOH:O	2.10	0.52
1:A:123:PRO:HD3	13:A:633:HOH:O	2.09	0.52
1:B:66:ARG:HB2	8:B:403:GOL:H31	1.92	0.52
1:B:271:VAL:HG11	1:B:285[B]:GLU:CD	2.31	0.51
1:C:136[A]:THR:HG21	13:C:683:HOH:O	2.09	0.51
10:B:406:HEM:HHC	10:B:406:HEM:HBB2	1.93	0.51
1:A:42:PRO:CB	9:B:402:EPE:H101	2.40	0.51
1:A:208:THR:HG22	7:A:401[B]:MYR:H51	1.94	0.50
1:C:89:ALA:HA	7:C:401:MYR:H61	1.93	0.50
1:B:259:GLU:HA	8:B:405:GOL:H2	1.94	0.50
1:C:77[A]:THR:HG21	13:C:689:HOH:O	2.12	0.50
1:C:100:LEU:HD13	1:C:136[B]:THR:HG23	1.94	0.50
1:B:262:ASP:CG	8:B:405:GOL:H31	2.33	0.49
1:A:136[B]:THR:HG22	13:A:510:HOH:O	2.11	0.49
1:B:73:ALA:O	1:B:77[B]:THR:HG22	2.13	0.49
7:C:401:MYR:H62	13:C:716:HOH:O	2.13	0.49
7:C:401:MYR:H82	13:C:716:HOH:O	2.12	0.48
1:A:66:ARG:H	8:A:402:GOL:C3	2.21	0.48
1:B:66:ARG:N	8:B:403:GOL:C3	2.74	0.47
1:C:178:LEU:HD21	1:C:263:GLN:OE1	2.14	0.47
1:A:209:ALA:O	1:A:213:THR:HG23	2.13	0.47
1:C:136[B]:THR:HG21	13:C:683:HOH:O	2.13	0.47
1:B:212[A]:GLU:CD	7:B:401[A]:MYR:C14	2.76	0.47
1:C:92:VAL:HG11	7:C:401:MYR:H51	1.96	0.47
1:B:227:THR:HG22	13:B:707:HOH:O	2.15	0.47
1:B:77[B]:THR:HG23	13:B:590:HOH:O	2.15	0.46
1:B:209:ALA:O	1:B:213:THR:HG23	2.15	0.46
1:A:297:ARG:NH2	9:A:403:EPE:H81	2.31	0.46
1:B:93:ALA:HB2	7:B:401[B]:MYR:H41	1.97	0.46
1:C:209:ALA:O	1:C:213:THR:HG23	2.16	0.46
10:C:403:HEM:HBC2	10:C:403:HEM:CMC	2.45	0.46
1:A:88[B]:ASN:HD22	1:A:335:ALA:HB2	1.82	0.45
10:A:406:HEM:HBB2	10:A:406:HEM:HHC	1.99	0.45
1:A:297:ARG:HE	9:A:403:EPE:H32	1.81	0.45
1:A:297:ARG:CG	9:A:403:EPE:H22	2.46	0.45
1:C:93:ALA:HB2	7:C:401:MYR:H81	1.98	0.45
7:A:401[A]:MYR:H122	13:A:753:HOH:O	2.16	0.45
1:C:22:PRO:HG2	1:C:77[A]:THR:CG2	2.46	0.44
1:C:64:LEU:HD21	1:C:75:ILE:HA	1.99	0.44
1:B:66:ARG:H	8:B:403:GOL:H31	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:HB3	9:B:402:EPE:H101	2.01	0.43
1:B:64:LEU:HD21	1:B:75:ILE:HA	2.00	0.43
1:A:42:PRO:HB2	9:B:402:EPE:H101	2.00	0.43
1:C:212[A]:GLU:CD	7:C:401:MYR:H141	2.33	0.42
1:C:215:PHE:HE2	7:C:401:MYR:H132	1.84	0.42
1:B:65:PRO:HA	8:B:403:GOL:H12	2.01	0.42
1:A:332:VAL:HG13	1:A:336:PHE:CD2	2.55	0.42
1:C:332:VAL:HG13	1:C:336:PHE:CD2	2.54	0.42
7:A:401[A]:MYR:H22	7:A:401[A]:MYR:H51	1.66	0.42
1:B:208:THR:HG22	7:B:401[B]:MYR:C6	2.47	0.42
1:B:319:ARG:HD3	13:B:679:HOH:O	2.19	0.42
10:C:403:HEM:HHC	10:C:403:HEM:CBB	2.47	0.42
7:A:401[A]:MYR:H91	7:A:401[A]:MYR:H61	1.79	0.41
1:A:297:ARG:HH21	9:A:403:EPE:H81	1.85	0.41
7:B:401[B]:MYR:H72	13:B:761:HOH:O	2.21	0.41
1:B:332:VAL:HG13	1:B:336:PHE:CD2	2.57	0.40
1:C:92:VAL:HB	7:C:401:MYR:C7	2.50	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	343/335 (102%)	335 (98%)	7 (2%)	1 (0%)	37	35
1	B	341/335 (102%)	333 (98%)	7 (2%)	1 (0%)	37	35
1	C	341/335 (102%)	332 (97%)	8 (2%)	1 (0%)	37	35
All	All	1025/1005 (102%)	1000 (98%)	22 (2%)	3 (0%)	37	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	SER
1	B	257	SER
1	C	257	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/274 (104%)	284 (100%)	0	100	100
1	B	282/274 (103%)	282 (100%)	0	100	100
1	C	282/274 (103%)	282 (100%)	0	100	100
All	All	848/822 (103%)	848 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

29 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	G	1	1,2	14,14,15	0.69	0	17,19,21	1.42	2 (11%)
2	NAG	G	2	2	14,14,15	0.32	0	17,19,21	0.87	1 (5%)
2	BMA	G	3	2	11,11,12	0.40	0	15,15,17	0.98	1 (6%)
2	MAN	G	4	2	11,11,12	1.03	1 (9%)	15,15,17	1.03	1 (6%)
2	MAN	G	5	2	11,11,12	0.74	0	15,15,17	1.15	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
3	NAG	I	2	3	14,14,15	0.36	0	17,19,21	0.66	0
3	BMA	I	3	3	11,11,12	0.35	0	15,15,17	0.72	0
3	MAN	I	4	3	11,11,12	0.55	0	15,15,17	0.96	0
3	MAN	I	5	3	11,11,12	0.55	0	15,15,17	0.59	0
3	MAN	I	6	3	11,11,12	0.50	0	15,15,17	0.92	1 (6%)
3	MAN	I	7	3	11,11,12	0.56	0	15,15,17	0.96	0
4	NAG	Z	1	1,4	14,14,15	0.42	0	17,19,21	2.07	5 (29%)
4	NAG	Z	2	4	14,14,15	0.31	0	17,19,21	0.72	0
4	BMA	Z	3	4	11,11,12	0.61	0	15,15,17	0.62	0
4	MAN	Z	4	4	11,11,12	1.22	2 (18%)	15,15,17	0.92	1 (6%)
5	NAG	a	1	1,5	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
5	NAG	a	2	5	14,14,15	0.32	0	17,19,21	0.54	0
5	BMA	a	3	5	11,11,12	0.46	0	15,15,17	1.15	2 (13%)
5	MAN	a	4	5	11,11,12	0.65	0	15,15,17	1.45	2 (13%)
5	MAN	a	5	5	11,11,12	0.49	0	15,15,17	0.72	0
5	MAN	a	6	5	11,11,12	0.71	0	15,15,17	1.44	2 (13%)
4	NAG	q	1	1,4	14,14,15	0.31	0	17,19,21	1.47	2 (11%)
4	NAG	q	2	4	14,14,15	0.36	0	17,19,21	1.15	2 (11%)
4	BMA	q	3	4	11,11,12	0.37	0	15,15,17	1.04	1 (6%)
4	MAN	q	4	4	11,11,12	0.60	0	15,15,17	0.88	1 (6%)
6	NAG	s	1	6,1	14,14,15	0.31	0	17,19,21	0.56	0
6	NAG	s	2	6	14,14,15	0.35	0	17,19,21	1.25	3 (17%)
6	BMA	s	3	6	11,11,12	0.40	0	15,15,17	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	MAN	I	5	3	-	1/2/19/22	0/1/1/1
3	MAN	I	6	3	-	2/2/19/22	0/1/1/1
3	MAN	I	7	3	-	2/2/19/22	0/1/1/1
4	NAG	Z	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Z	4	4	-	0/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	MAN	a	4	5	-	2/2/19/22	0/1/1/1
5	MAN	a	5	5	-	1/2/19/22	0/1/1/1
5	MAN	a	6	5	-	2/2/19/22	0/1/1/1
4	NAG	q	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	q	2	4	-	2/6/23/26	0/1/1/1
4	BMA	q	3	4	-	0/2/19/22	0/1/1/1
4	MAN	q	4	4	-	2/2/19/22	0/1/1/1
6	NAG	s	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	s	2	6	-	2/6/23/26	0/1/1/1
6	BMA	s	3	6	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	4	MAN	C2-C3	2.76	1.56	1.52
2	G	4	MAN	C2-C3	2.71	1.56	1.52
4	Z	4	MAN	O5-C5	2.70	1.48	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	q	1	NAG	C1-C2-N2	5.08	119.17	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	1	NAG	C1-C2-N2	5.04	119.10	110.49
5	a	6	MAN	C1-C2-C3	4.65	115.38	109.67
4	Z	1	NAG	O5-C1-C2	-4.47	104.23	111.29
2	G	1	NAG	C2-N2-C7	3.69	128.15	122.90
2	G	5	MAN	C1-O5-C5	3.65	117.13	112.19
2	G	1	NAG	C1-C2-N2	3.33	116.18	110.49
2	G	4	MAN	O2-C2-C3	3.27	116.69	110.14
5	a	4	MAN	C3-C4-C5	3.12	115.80	110.24
4	q	3	BMA	C1-C2-C3	3.01	113.36	109.67
4	Z	1	NAG	C1-O5-C5	2.91	116.14	112.19
4	Z	1	NAG	C4-C3-C2	-2.85	106.84	111.02
4	q	2	NAG	C1-C2-N2	2.83	115.31	110.49
5	a	4	MAN	C1-O5-C5	2.81	116.00	112.19
5	a	3	BMA	O2-C2-C3	2.72	115.58	110.14
2	G	2	NAG	C1-C2-N2	2.65	115.01	110.49
3	I	6	MAN	C1-C2-C3	2.63	112.90	109.67
2	G	3	BMA	C1-O5-C5	2.59	115.70	112.19
6	s	2	NAG	O5-C5-C4	-2.58	104.54	110.83
3	I	1	NAG	C1-C2-N2	2.53	114.81	110.49
4	Z	4	MAN	C1-O5-C5	2.49	115.56	112.19
4	q	4	MAN	C1-O5-C5	2.38	115.42	112.19
6	s	2	NAG	C2-N2-C7	2.23	126.07	122.90
5	a	1	NAG	C1-C2-N2	2.19	114.23	110.49
2	G	5	MAN	C1-C2-C3	2.18	112.34	109.67
4	q	2	NAG	C1-O5-C5	2.14	115.09	112.19
6	s	2	NAG	C4-C3-C2	2.12	114.13	111.02
4	q	1	NAG	O5-C1-C2	-2.12	107.94	111.29
4	Z	1	NAG	O3-C3-C2	2.09	113.79	109.47
5	a	6	MAN	C1-O5-C5	2.03	114.95	112.19
5	a	3	BMA	O3-C3-C4	2.02	115.03	110.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O7-C7-N2-C2
3	I	7	MAN	O5-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
5	a	6	MAN	O5-C5-C6-O6
4	q	4	MAN	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
6	s	1	NAG	C8-C7-N2-C2

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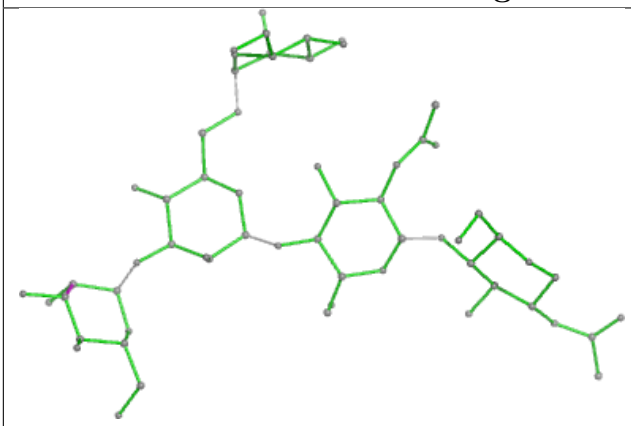
Mol	Chain	Res	Type	Atoms
6	s	1	NAG	O7-C7-N2-C2
5	a	4	MAN	O5-C5-C6-O6
6	s	2	NAG	C4-C5-C6-O6
3	I	7	MAN	C4-C5-C6-O6
5	a	6	MAN	C4-C5-C6-O6
4	q	4	MAN	O5-C5-C6-O6
4	q	2	NAG	C8-C7-N2-C2
2	G	1	NAG	C1-C2-N2-C7
3	I	6	MAN	C4-C5-C6-O6
4	q	2	NAG	O7-C7-N2-C2
5	a	4	MAN	C4-C5-C6-O6
3	I	6	MAN	O5-C5-C6-O6
6	s	3	BMA	O5-C5-C6-O6
4	Z	1	NAG	C1-C2-N2-C7
5	a	5	MAN	C4-C5-C6-O6
3	I	5	MAN	C4-C5-C6-O6
4	q	1	NAG	C3-C2-N2-C7

There are no ring outliers.

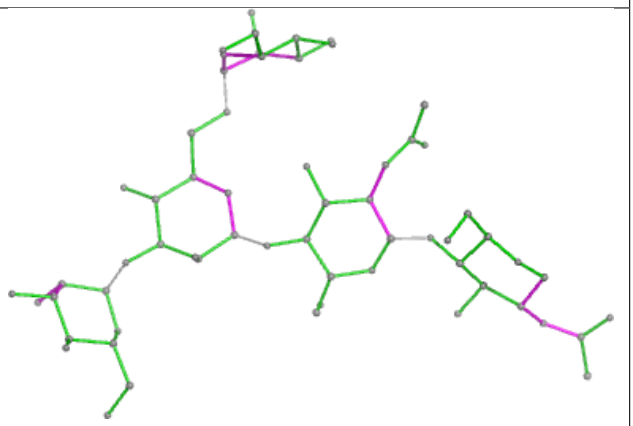
No monomer is involved in short contacts.

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

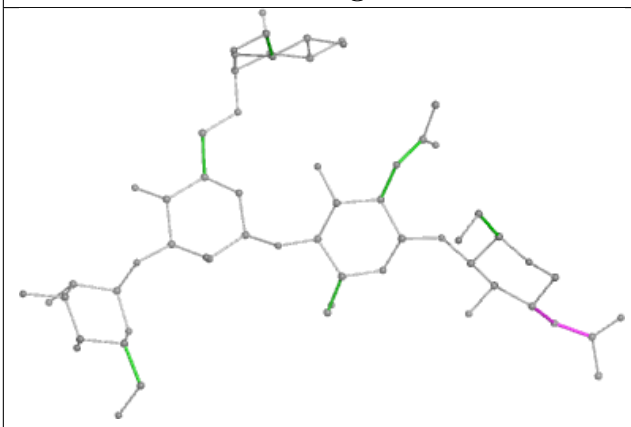
Oligosaccharide Chain G



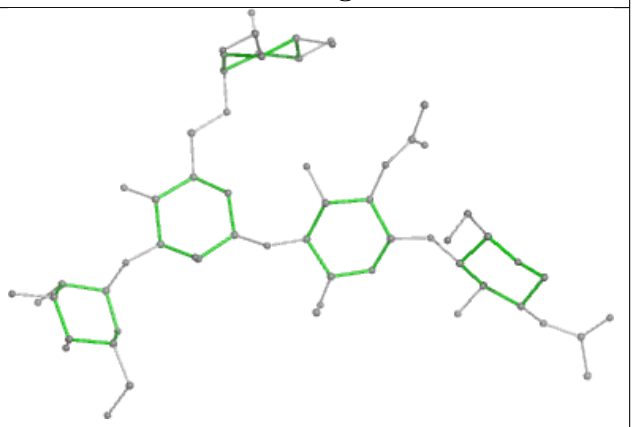
Bond lengths



Bond angles

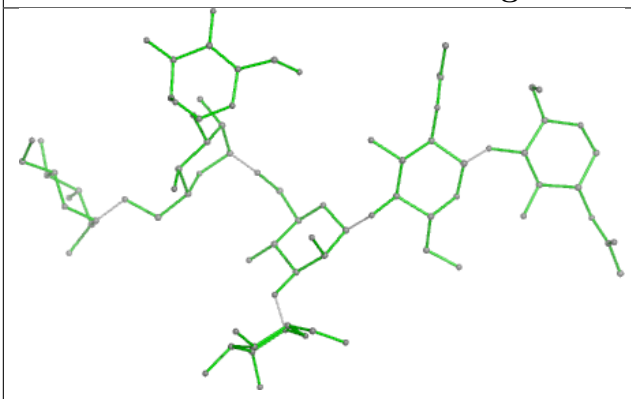


Torsions

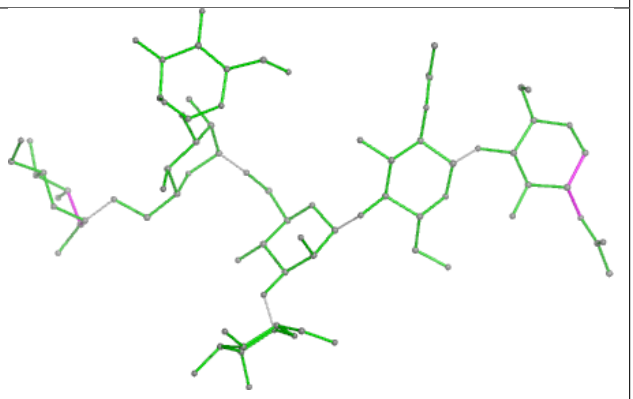


Rings

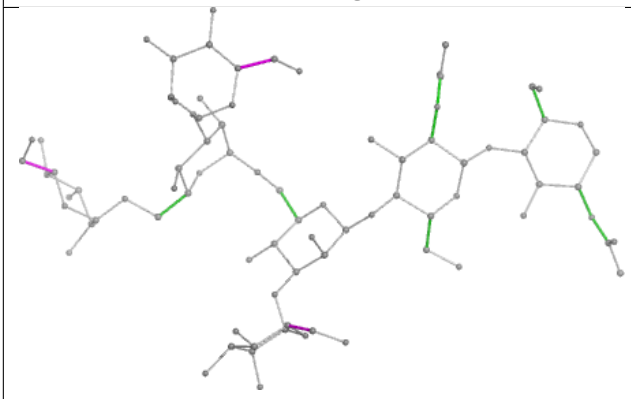
Oligosaccharide Chain I



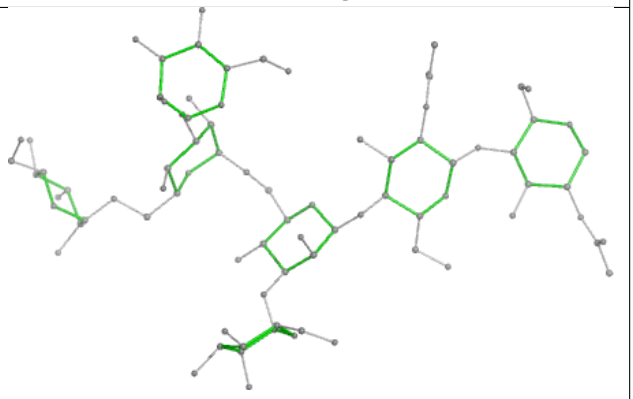
Bond lengths



Bond angles

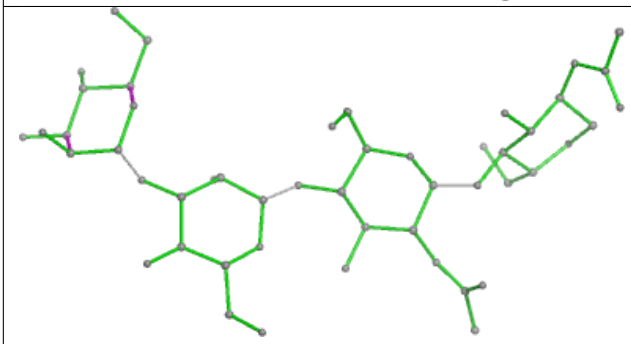


Torsions

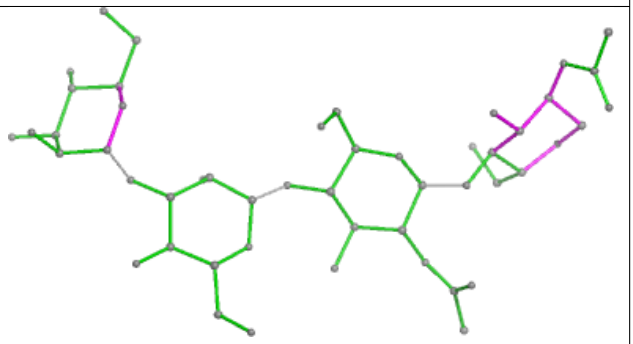


Rings

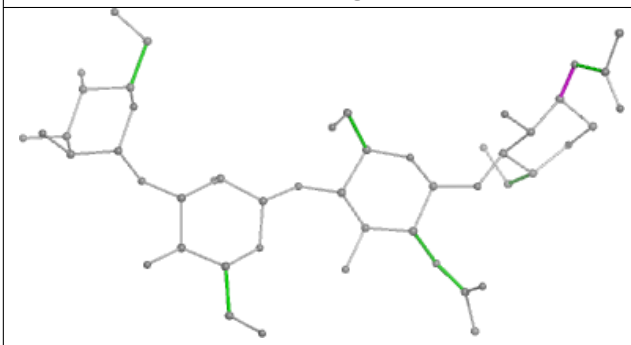
Oligosaccharide Chain Z



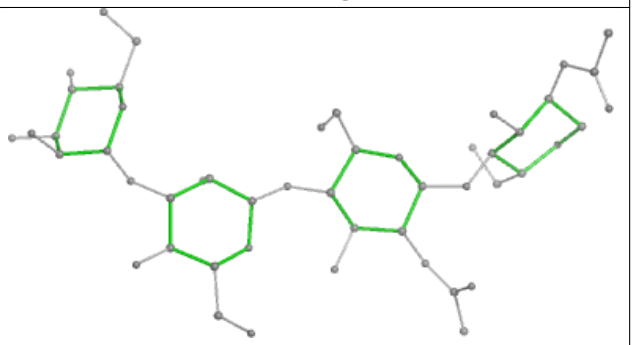
Bond lengths



Bond angles

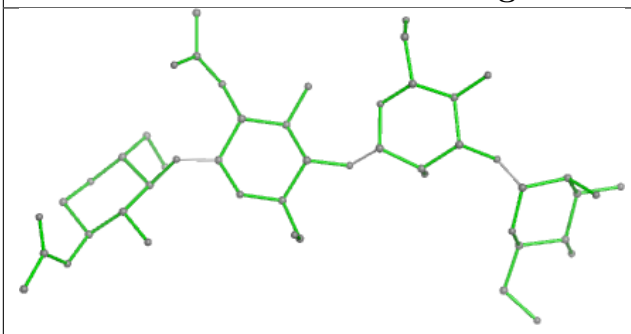


Torsions

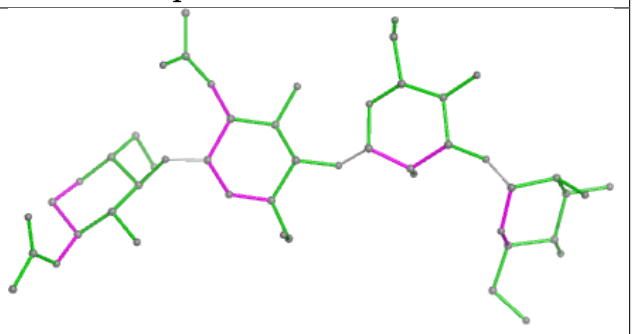


Rings

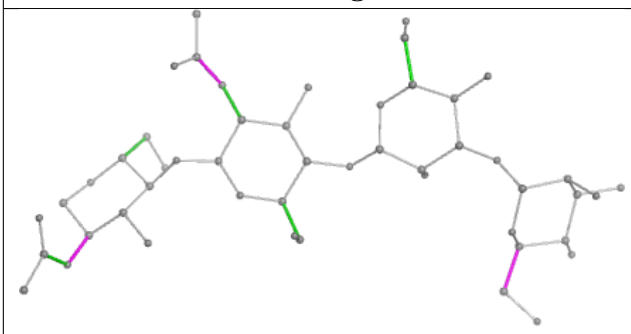
Oligosaccharide Chain q



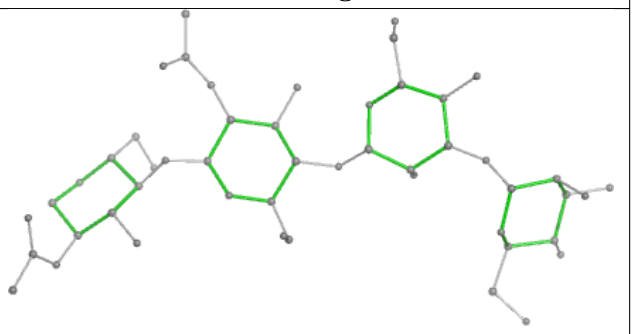
Bond lengths



Bond angles

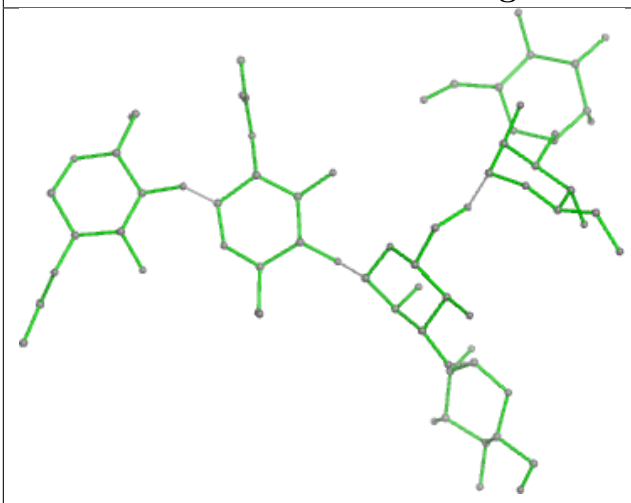


Torsions

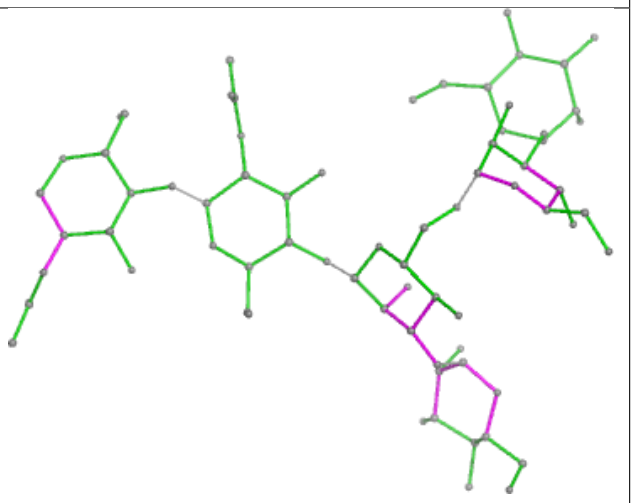


Rings

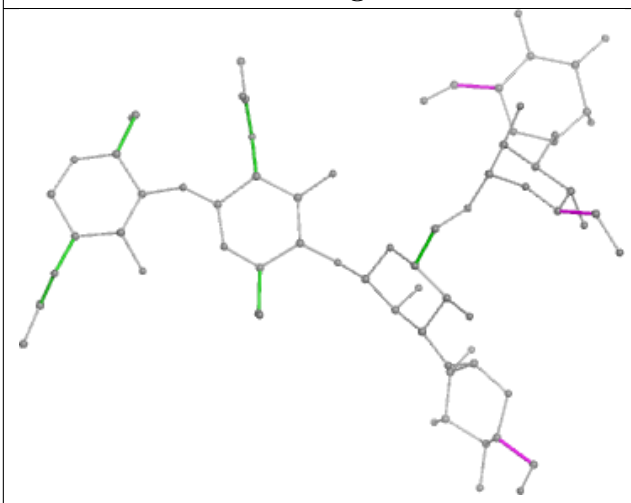
Oligosaccharide Chain a



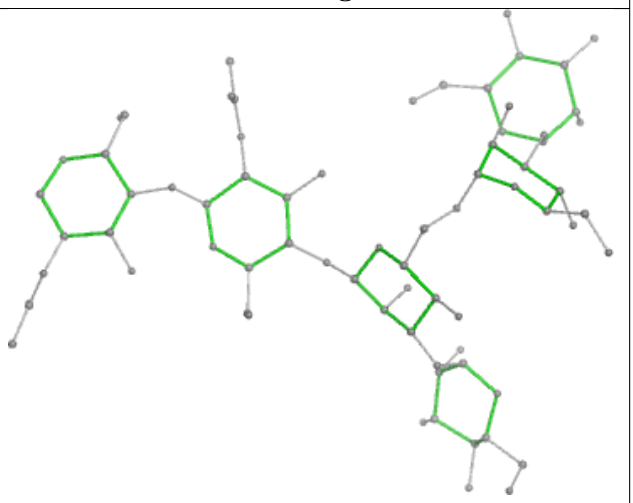
Bond lengths



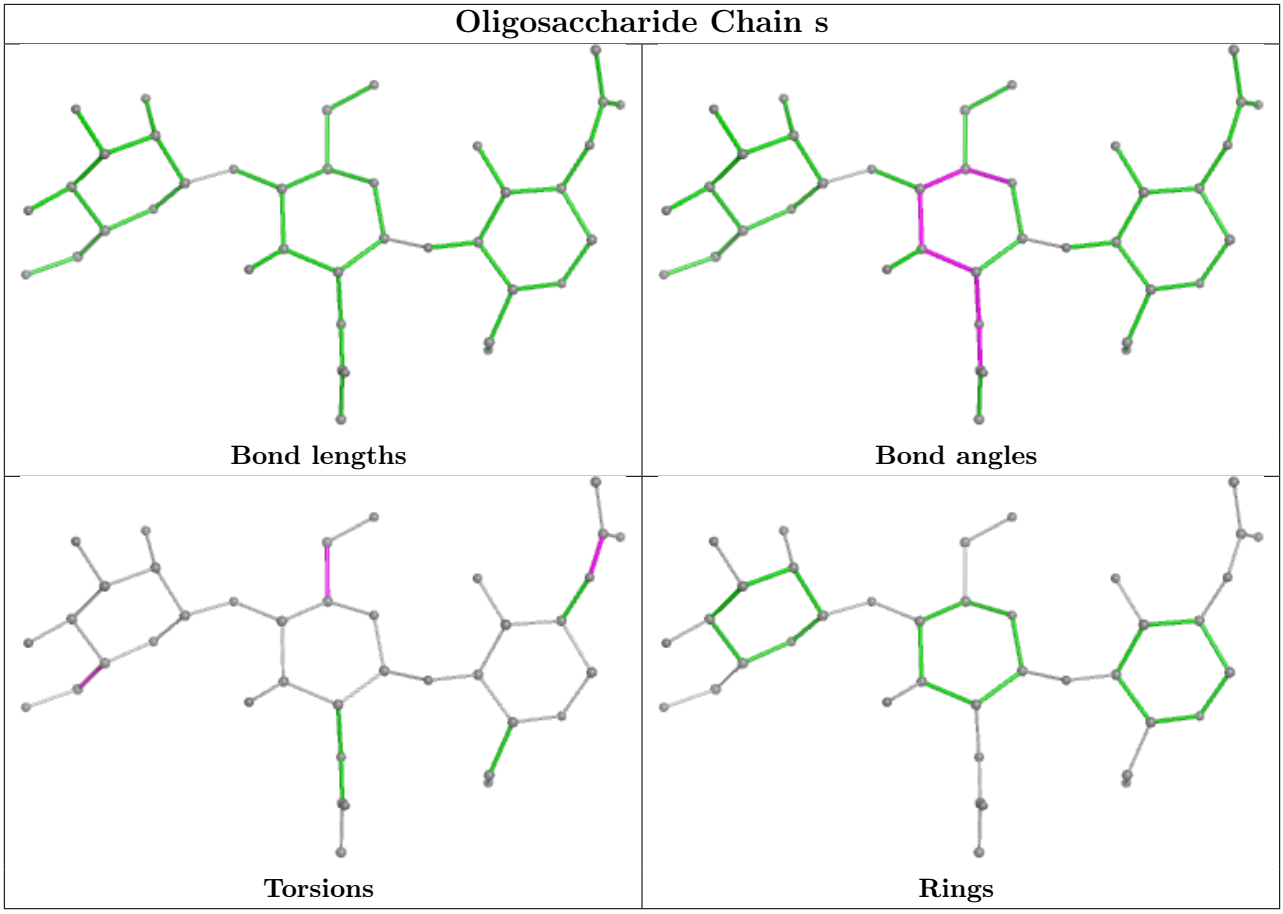
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	SO4	B	407	-	4,4,4	0.29	0	6,6,6	0.22	0
11	SO4	C	405	-	4,4,4	0.28	0	6,6,6	0.08	0
7	MYR	A	401[B]	10	15,15,15	0.52	0	15,15,15	0.61	0
8	GOL	A	402	-	5,5,5	0.12	0	5,5,5	0.44	0
8	GOL	B	403	-	5,5,5	0.09	0	5,5,5	0.49	0
11	SO4	C	404	-	4,4,4	0.32	0	6,6,6	0.09	0
11	SO4	A	408	-	4,4,4	0.45	0	6,6,6	0.33	0
8	GOL	B	405	-	5,5,5	0.15	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MYR	B	401[B]	-	15,15,15	0.55	0	15,15,15	0.63	0
8	GOL	C	402	-	5,5,5	0.16	0	5,5,5	0.37	0
10	HEM	C	403	12,1	41,50,50	1.18	4 (9%)	45,82,82	1.90	12 (26%)
11	SO4	A	409	-	4,4,4	0.31	0	6,6,6	0.21	0
10	HEM	B	406	12,1	41,50,50	1.32	6 (14%)	45,82,82	2.05	15 (33%)
8	GOL	A	405	-	5,5,5	0.11	0	5,5,5	0.48	0
11	SO4	A	410	-	4,4,4	0.30	0	6,6,6	0.15	0
7	MYR	A	401[A]	-	15,15,15	0.58	0	15,15,15	0.54	0
9	EPE	B	402	-	15,15,15	1.25	1 (6%)	18,20,20	1.85	2 (11%)
9	EPE	B	404	-	15,15,15	0.87	1 (6%)	18,20,20	0.90	0
8	GOL	A	404	-	5,5,5	0.16	0	5,5,5	0.57	0
9	EPE	A	403	-	15,15,15	0.91	1 (6%)	18,20,20	1.04	1 (5%)
11	SO4	A	407	-	4,4,4	0.29	0	6,6,6	0.05	0
7	MYR	C	401	-	15,15,15	0.58	0	15,15,15	0.50	0
7	MYR	B	401[A]	-	15,15,15	0.54	0	15,15,15	0.51	0
10	HEM	A	406	7,12,1	41,50,50	1.23	2 (4%)	45,82,82	2.11	20 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	B	406	12,1	-	0/12/54/54	-
7	MYR	A	401[A]	-	-	5/13/13/13	-
7	MYR	C	401	-	-	10/13/13/13	-
7	MYR	B	401[A]	-	-	6/13/13/13	-
10	HEM	A	406	7,12,1	-	0/12/54/54	-
8	GOL	B	403	-	-	1/4/4/4	-
7	MYR	A	401[B]	10	-	10/13/13/13	-
8	GOL	B	405	-	-	2/4/4/4	-
7	MYR	B	401[B]	-	-	4/13/13/13	-
8	GOL	C	402	-	-	1/4/4/4	-
9	EPE	B	402	-	-	5/9/19/19	0/1/1/1
9	EPE	B	404	-	-	3/9/19/19	0/1/1/1
8	GOL	A	404	-	-	4/4/4/4	-
10	HEM	C	403	12,1	-	0/12/54/54	-
8	GOL	A	402	-	-	4/4/4/4	-
8	GOL	A	405	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EPE	A	403	-	-	1/9/19/19	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	402	EPE	O3S-S	4.49	1.63	1.47
10	A	406	HEM	C1B-NB	-3.57	1.34	1.40
10	B	406	HEM	C4D-ND	-3.10	1.35	1.40
9	A	403	EPE	O3S-S	2.98	1.58	1.47
10	B	406	HEM	C1B-NB	-2.76	1.35	1.40
10	B	406	HEM	C1D-ND	-2.73	1.33	1.38
10	C	403	HEM	C4D-ND	-2.73	1.35	1.40
9	B	404	EPE	O3S-S	2.67	1.57	1.47
10	B	406	HEM	O1A-CGA	2.50	1.30	1.22
10	A	406	HEM	C4D-ND	-2.46	1.36	1.40
10	C	403	HEM	C1B-NB	-2.44	1.36	1.40
10	B	406	HEM	FE-NB	2.15	2.07	1.96
10	B	406	HEM	O2D-CGD	-2.10	1.23	1.30
10	C	403	HEM	FE-NB	2.09	2.07	1.96
10	C	403	HEM	CHB-C1B	2.06	1.40	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	402	EPE	O3S-S-C10	6.41	116.13	105.77
10	B	406	HEM	CHC-C4B-NB	5.65	130.57	124.43
10	C	403	HEM	CHC-C4B-NB	4.86	129.71	124.43
10	A	406	HEM	CHC-C4B-NB	4.58	129.41	124.43
10	B	406	HEM	C1B-NB-C4B	4.54	109.76	105.07
10	A	406	HEM	C1B-NB-C4B	4.07	109.28	105.07
10	C	403	HEM	CHB-C1B-NB	3.90	129.20	124.38
10	C	403	HEM	C1B-NB-C4B	3.73	108.93	105.07
10	A	406	HEM	O2A-CGA-CBA	3.68	125.86	114.03
10	A	406	HEM	CMB-C2B-C1B	3.48	130.34	125.04
10	A	406	HEM	C2C-C3C-C4C	3.47	109.32	106.90
10	C	403	HEM	CHD-C1D-ND	3.39	128.11	124.43
10	B	406	HEM	O2A-CGA-CBA	3.38	124.89	114.03
10	C	403	HEM	CBA-CAA-C2A	-3.33	106.94	112.62
10	B	406	HEM	O2D-CGD-O1D	-3.30	115.07	123.30
10	B	406	HEM	CHB-C1B-NB	3.25	128.39	124.38
10	B	406	HEM	CHA-C4D-ND	3.22	128.36	124.38
10	A	406	HEM	CHB-C1B-NB	3.18	128.31	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	403	EPE	O3S-S-C10	-3.15	100.67	105.77
10	B	406	HEM	CMB-C2B-C1B	3.14	129.83	125.04
10	B	406	HEM	CHD-C1D-ND	3.06	127.75	124.43
10	A	406	HEM	CBA-CAA-C2A	-2.98	107.54	112.62
10	B	406	HEM	CBA-CAA-C2A	-2.97	107.55	112.62
10	C	403	HEM	CHA-C4D-ND	2.96	128.04	124.38
10	C	403	HEM	CAD-CBD-CGD	-2.86	107.45	113.60
9	B	402	EPE	O1S-S-C10	-2.74	103.61	106.92
10	B	406	HEM	CHA-C4D-C3D	-2.71	120.23	125.33
10	A	406	HEM	CHD-C1D-ND	2.67	127.33	124.43
10	A	406	HEM	CHD-C1D-C2D	-2.66	120.83	124.98
10	A	406	HEM	CHA-C4D-ND	2.63	127.63	124.38
10	C	403	HEM	CHD-C1D-C2D	-2.53	121.03	124.98
10	A	406	HEM	O2D-CGD-O1D	-2.50	117.07	123.30
10	C	403	HEM	O2A-CGA-O1A	-2.49	117.09	123.30
10	B	406	HEM	CAD-CBD-CGD	-2.47	108.29	113.60
10	C	403	HEM	CHA-C4D-C3D	-2.46	120.71	125.33
10	A	406	HEM	CMB-C2B-C3B	-2.41	122.40	128.30
10	A	406	HEM	CMA-C3A-C4A	-2.39	124.78	128.46
10	A	406	HEM	O2A-CGA-O1A	-2.31	117.55	123.30
10	A	406	HEM	CHA-C4D-C3D	-2.28	121.04	125.33
10	A	406	HEM	CAD-C3D-C4D	2.27	128.62	124.66
10	B	406	HEM	CHD-C1D-C2D	-2.26	121.46	124.98
10	C	403	HEM	CHB-C1B-C2B	-2.22	120.57	126.72
10	A	406	HEM	CMD-C2D-C1D	2.19	128.37	125.04
10	A	406	HEM	CAB-C3B-C2B	-2.17	121.47	128.60
10	A	406	HEM	CMC-C2C-C3C	2.15	128.70	124.68
10	B	406	HEM	O1A-CGA-CBA	-2.12	116.26	123.08
10	B	406	HEM	CMB-C2B-C3B	-2.09	123.17	128.30
10	C	403	HEM	C2C-C3C-C4C	2.06	108.34	106.90
10	A	406	HEM	O1A-CGA-CBA	-2.03	116.57	123.08
10	B	406	HEM	CAD-C3D-C4D	2.01	128.18	124.66

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	402	GOL	O1-C1-C2-O2
8	A	402	GOL	O1-C1-C2-C3
8	B	405	GOL	C1-C2-C3-O3
9	A	403	EPE	C8-C7-N4-C5
9	B	402	EPE	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
9	B	402	EPE	S-C10-C9-N1
9	B	402	EPE	C9-C10-S-O2S
9	B	402	EPE	C9-C10-S-O3S
9	B	404	EPE	C8-C7-N4-C5
9	B	404	EPE	S-C10-C9-N1
7	A	401[A]	MYR	C6-C7-C8-C9
7	A	401[B]	MYR	C10-C11-C12-C13
7	B	401[A]	MYR	C7-C8-C9-C10
7	A	401[A]	MYR	C1-C2-C3-C4
7	B	401[B]	MYR	C4-C5-C6-C7
7	C	401	MYR	C11-C10-C9-C8
7	B	401[A]	MYR	C6-C7-C8-C9
7	A	401[A]	MYR	C2-C3-C4-C5
7	C	401	MYR	C11-C12-C13-C14
8	A	404	GOL	O1-C1-C2-C3
8	A	404	GOL	C1-C2-C3-O3
8	A	405	GOL	O1-C1-C2-C3
8	A	405	GOL	C1-C2-C3-O3
7	A	401[B]	MYR	C1-C2-C3-C4
7	B	401[B]	MYR	C2-C3-C4-C5
7	C	401	MYR	C2-C3-C4-C5
7	C	401	MYR	C5-C6-C7-C8
7	A	401[B]	MYR	C3-C4-C5-C6
8	A	404	GOL	O2-C2-C3-O3
7	B	401[A]	MYR	C11-C12-C13-C14
7	A	401[B]	MYR	C6-C7-C8-C9
7	B	401[A]	MYR	C10-C11-C12-C13
7	C	401	MYR	C7-C8-C9-C10
7	C	401	MYR	C6-C7-C8-C9
7	A	401[B]	MYR	C2-C3-C4-C5
8	A	404	GOL	O1-C1-C2-O2
7	A	401[B]	MYR	C11-C12-C13-C14
7	C	401	MYR	C3-C4-C5-C6
7	B	401[A]	MYR	C2-C3-C4-C5
7	A	401[A]	MYR	C11-C10-C9-C8
7	A	401[A]	MYR	C10-C11-C12-C13
8	A	402	GOL	O2-C2-C3-O3
8	A	405	GOL	O2-C2-C3-O3
7	B	401[A]	MYR	C9-C10-C11-C12
8	B	403	GOL	O1-C1-C2-O2
9	B	402	EPE	C9-C10-S-O1S
7	A	401[B]	MYR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
8	B	405	GOL	O2-C2-C3-O3
7	C	401	MYR	C1-C2-C3-C4
7	C	401	MYR	O1-C1-C2-C3
7	B	401[B]	MYR	O1-C1-C2-C3
7	C	401	MYR	O2-C1-C2-C3
7	B	401[B]	MYR	O2-C1-C2-C3
8	A	402	GOL	C1-C2-C3-O3
7	A	401[B]	MYR	O1-C1-C2-C3
7	A	401[B]	MYR	O2-C1-C2-C3
8	C	402	GOL	O1-C1-C2-C3
9	B	404	EPE	C9-C10-S-O2S
7	A	401[B]	MYR	C7-C8-C9-C10

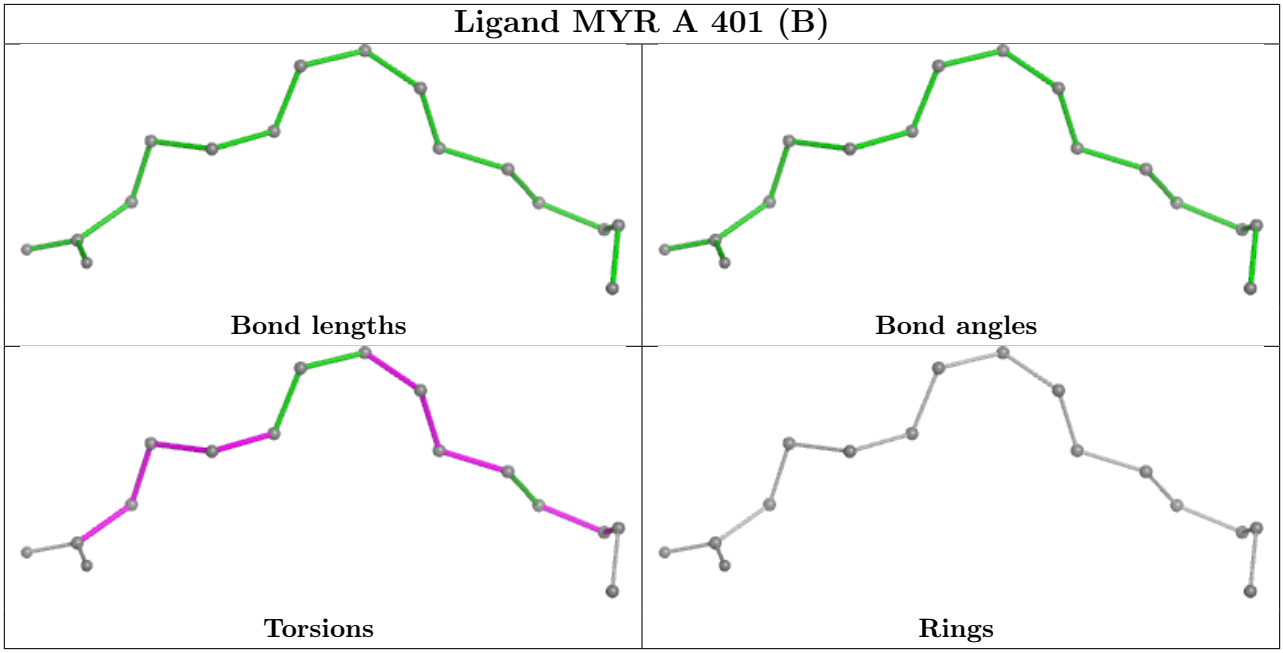
There are no ring outliers.

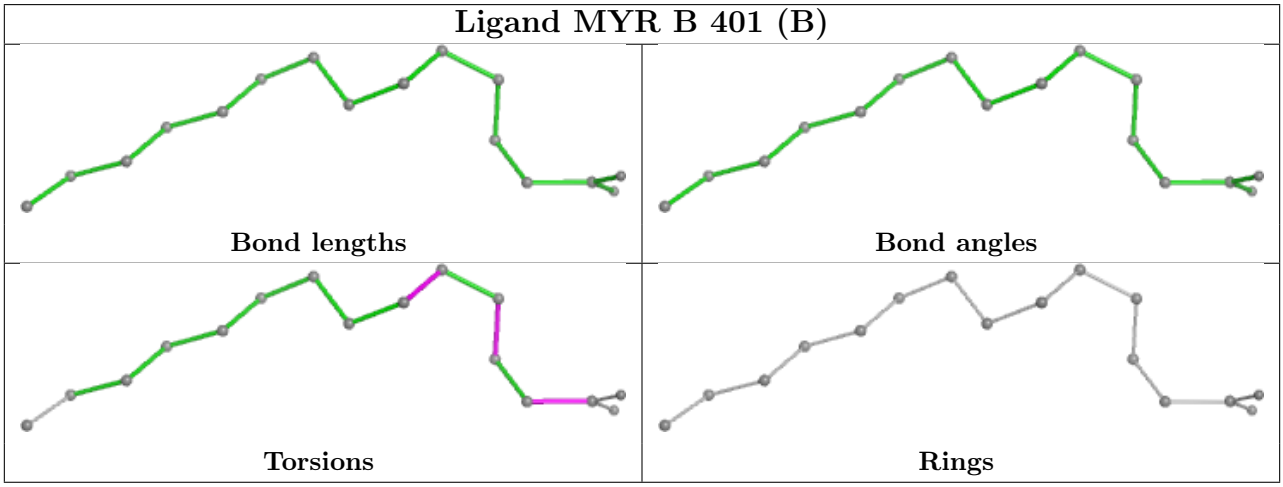
15 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401[B]	MYR	2	0
8	A	402	GOL	4	0
8	B	403	GOL	7	0
8	B	405	GOL	2	0
7	B	401[B]	MYR	8	0
10	C	403	HEM	3	0
10	B	406	HEM	1	0
8	A	405	GOL	3	0
7	A	401[A]	MYR	3	0
9	B	402	EPE	4	0
8	A	404	GOL	2	0
9	A	403	EPE	4	0
7	C	401	MYR	13	0
7	B	401[A]	MYR	7	0
10	A	406	HEM	1	0

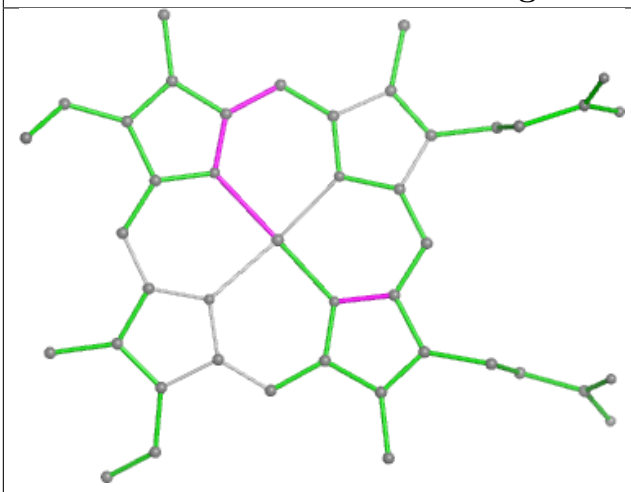
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

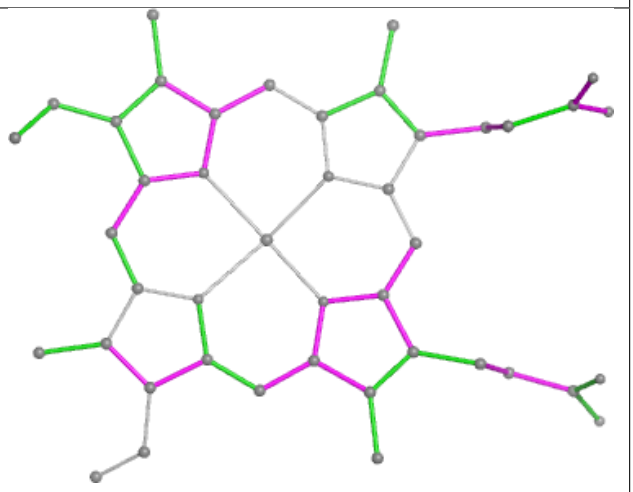




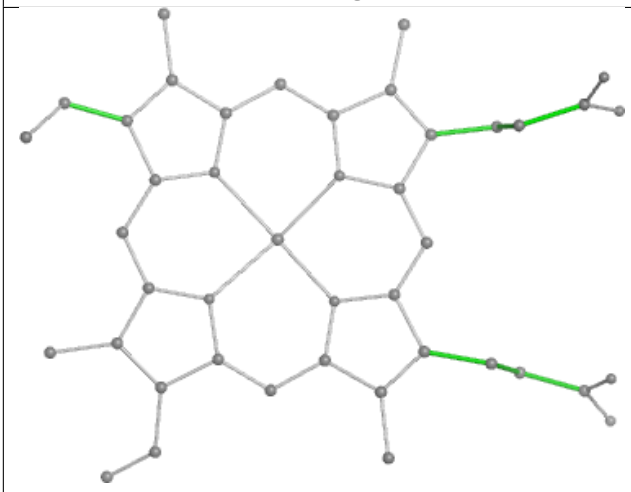
Ligand HEM C 403



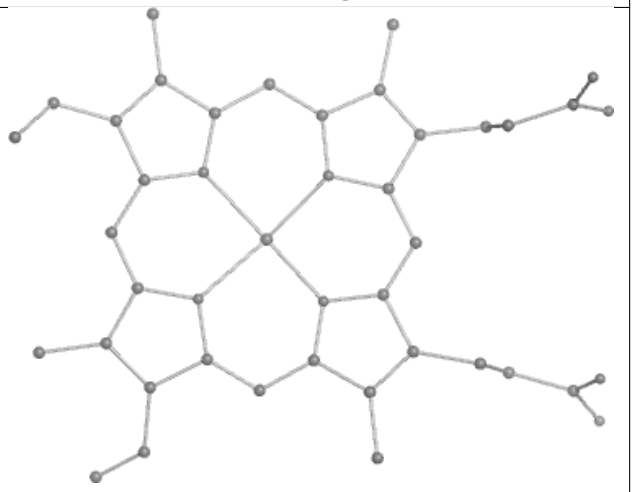
Bond lengths



Bond angles

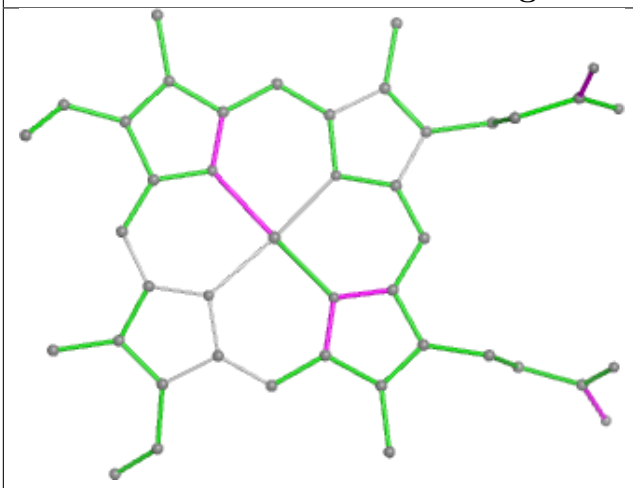


Torsions

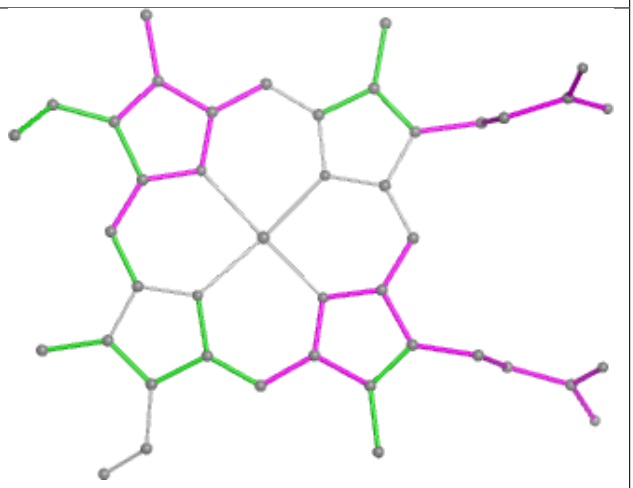


Rings

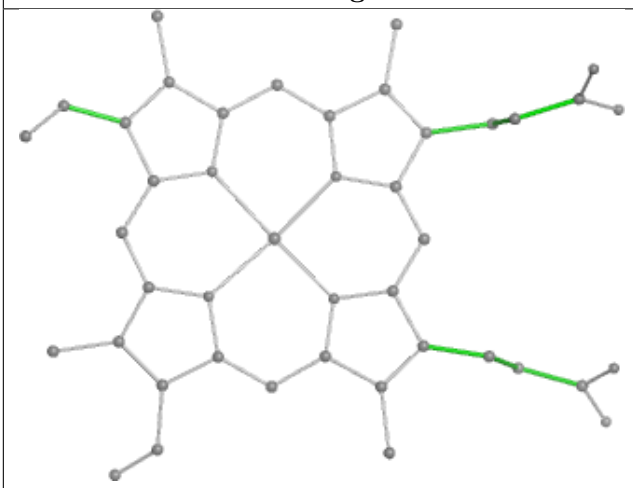
Ligand HEM B 406



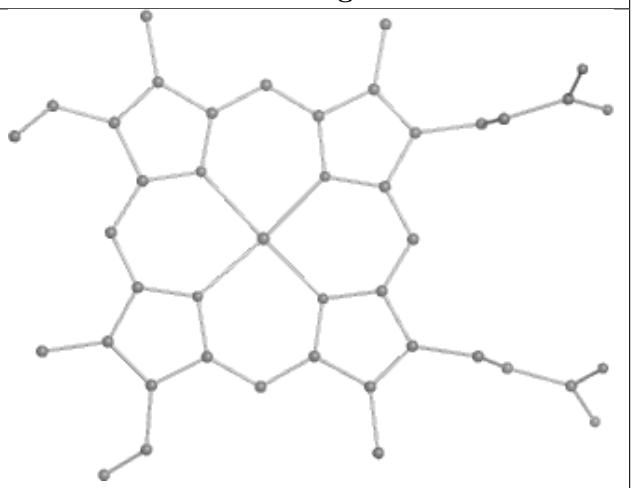
Bond lengths



Bond angles

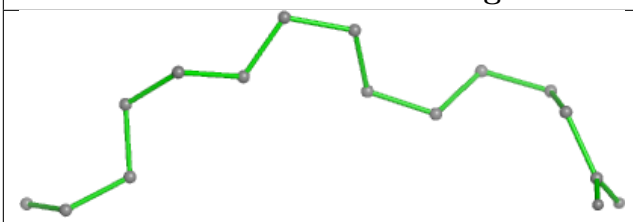


Torsions

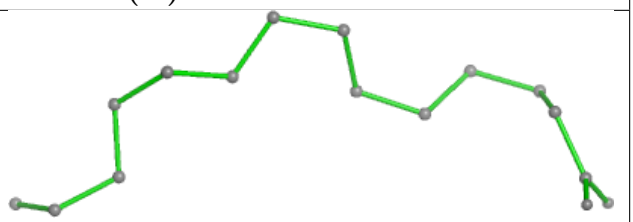


Rings

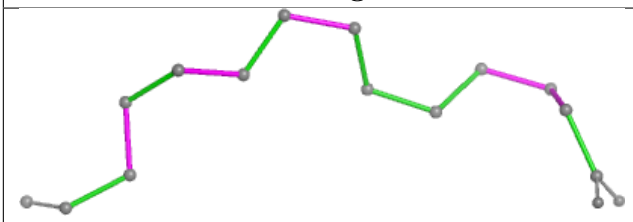
Ligand MYR A 401 (A)



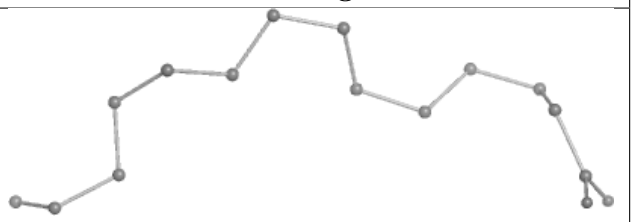
Bond lengths



Bond angles

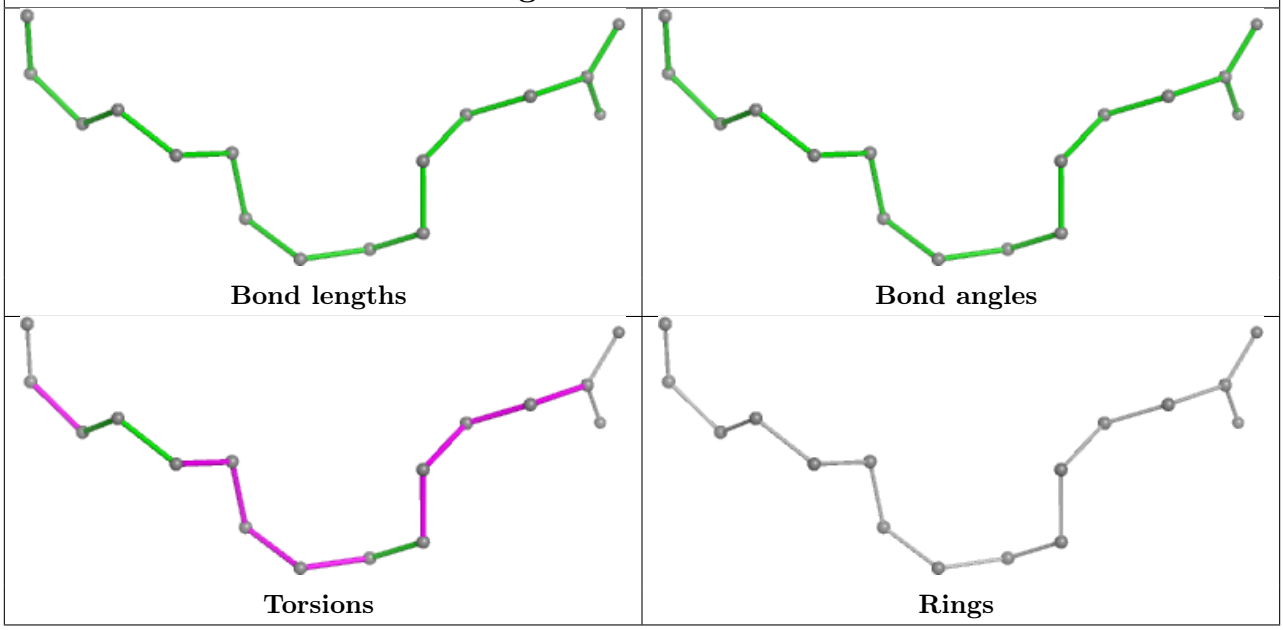


Torsions

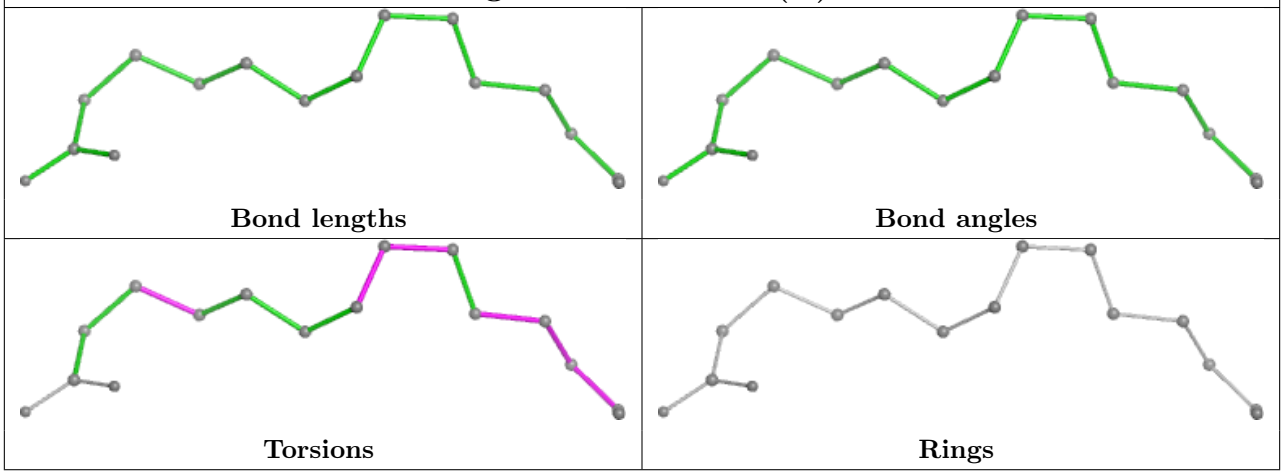


Rings

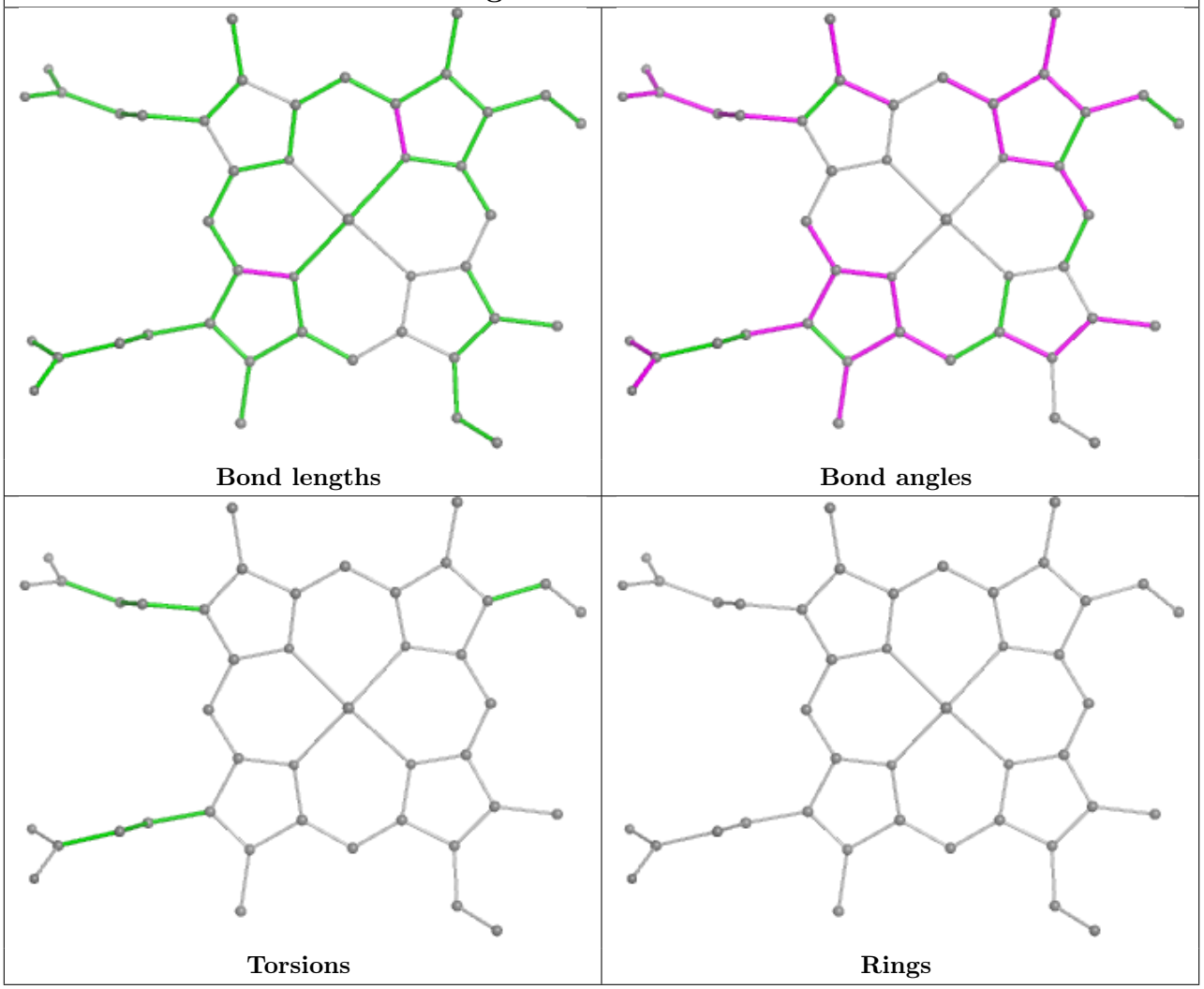
Ligand MYR C 401



Ligand MYR B 401 (A)



Ligand HEM A 406



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, 95^{th} 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	335/335 (100%)	-0.20	10 (2%)	52	51	17, 33, 51, 114	10 (2%)
1	B	335/335 (100%)	0.11	10 (2%)	52	51	18, 39, 61, 129	8 (2%)
1	C	335/335 (100%)	0.43	18 (5%)	32	30	17, 44, 71, 134	8 (2%)
All	All	1005/1005 (100%)	0.11	38 (3%)	44	42	17, 38, 66, 134	26 (2%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	GLY	5.4
1	B	316	ILE	4.2
1	B	16	VAL	3.9
1	C	227	THR	3.9
1	C	14	GLN	3.8
1	B	348	LEU	3.6
1	A	226	THR	3.4
1	B	277	ASP	3.1
1	A	227	THR	3.0
1	C	276	ALA	3.0
1	C	195	THR	2.8
1	B	347[A]	GLN	2.8
1	A	14	GLN	2.6
1	B	227	THR	2.6
1	A	316	ILE	2.6
1	C	186	TYR	2.5
1	C	164	PHE	2.5
1	B	14	GLN	2.5
1	C	178	LEU	2.5
1	C	15	GLY	2.5
1	C	149	PHE	2.4
1	C	316	ILE	2.4
1	C	270	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	124	PRO	2.3
1	C	266	ALA	2.3
1	A	136[A]	THR	2.3
1	B	318[A]	ARG	2.2
1	A	228	ASP	2.2
1	A	277	ASP	2.2
1	A	45	GLU	2.2
1	C	136[A]	THR	2.2
1	C	194	ALA	2.1
1	A	348	LEU	2.1
1	C	161	PHE	2.1
1	C	193	ILE	2.1
1	A	15	GLY	2.1
1	C	267	ALA	2.0
1	C	287	PRO	2.0

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

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

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

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, 95^{th} 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
11	SO4	C	404	5/5	0.67	0.10	104,105,117,117	0
9	EPE	A	403	15/15	0.69	0.22	77,87,95,104	0
11	SO4	A	410	5/5	0.72	0.14	78,92,111,112	0
9	EPE	B	404	15/15	0.73	0.21	85,95,105,113	0
11	SO4	A	407	5/5	0.73	0.14	82,95,103,108	0
8	GOL	A	405	6/6	0.75	0.17	58,65,72,74	0
8	GOL	B	403	6/6	0.77	0.21	63,70,80,87	0
11	SO4	A	408	5/5	0.77	0.18	38,51,66,81	0

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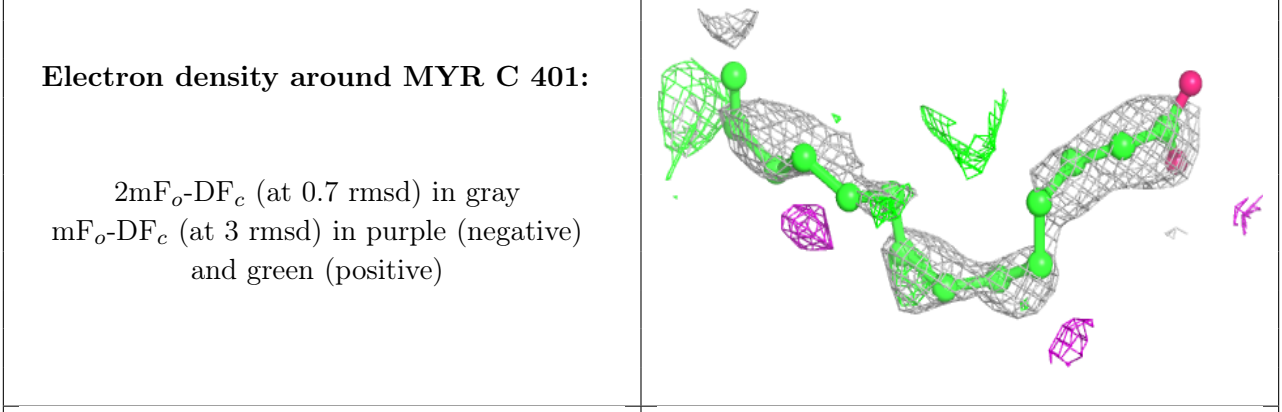
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	SO4	C	405	5/5	0.78	0.10	89,91,98,103	0
8	GOL	B	405	6/6	0.82	0.18	58,70,73,73	0
11	SO4	B	407	5/5	0.83	0.11	69,72,87,88	0
8	GOL	C	402	6/6	0.84	0.16	59,70,77,78	0
11	SO4	A	409	5/5	0.84	0.10	66,72,75,80	0
9	EPE	B	402	15/15	0.86	0.24	41,80,92,94	0
8	GOL	A	402	6/6	0.86	0.15	40,51,57,60	0
7	MYR	C	401	16/16	0.86	0.33	75,83,86,93	0
8	GOL	A	404	6/6	0.87	0.20	62,64,69,72	0
7	MYR	A	401[B]	16/16	0.89	0.31	63,76,80,81	16
7	MYR	B	401[A]	16/16	0.89	0.33	123,128,158,162	16
7	MYR	B	401[B]	16/16	0.89	0.33	40,45,48,52	16
7	MYR	A	401[A]	16/16	0.89	0.31	83,90,102,104	16
10	HEM	B	406	43/43	0.98	0.07	25,29,36,40	0
10	HEM	C	403	43/43	0.98	0.08	28,33,40,45	0
10	HEM	A	406	43/43	0.98	0.07	22,26,33,39	0
12	MG	C	406	1/1	0.98	0.05	42,42,42,42	0
12	MG	B	408	1/1	0.99	0.02	33,33,33,33	0
12	MG	A	411	1/1	1.00	0.02	33,33,33,33	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.

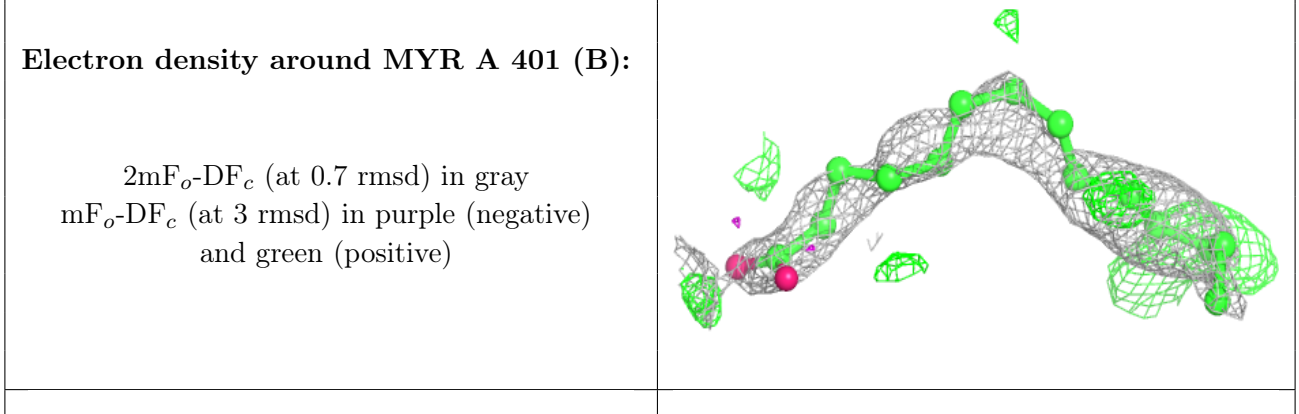
Electron density around MYR C 401:

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



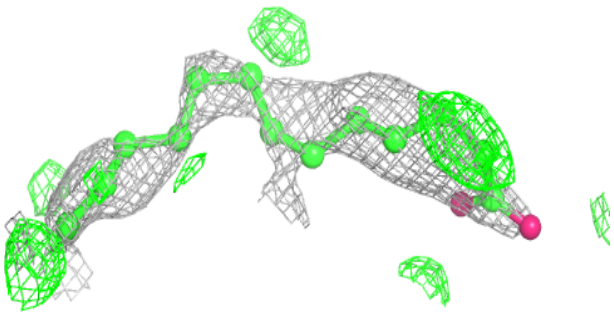
Electron density around MYR A 401 (B):

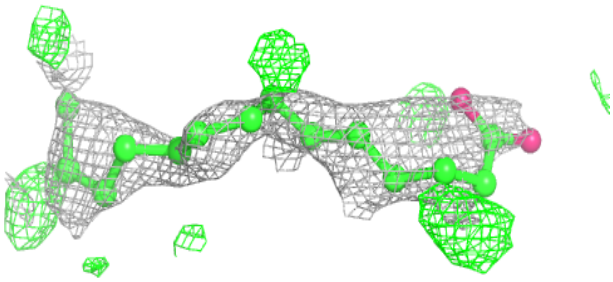
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

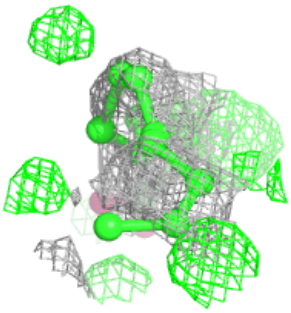


Electron density around MYR B 401 (A):

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

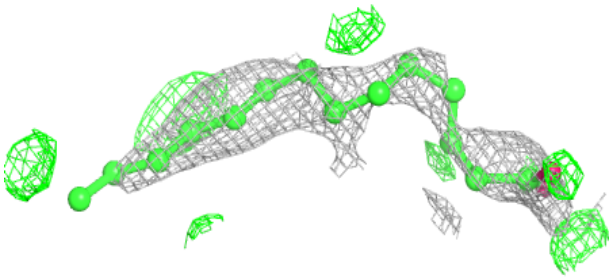


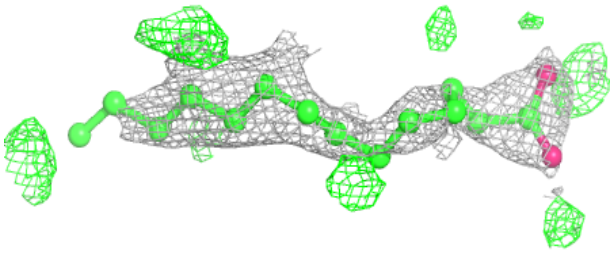


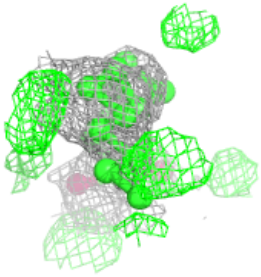


Electron density around MYR B 401 (B):

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

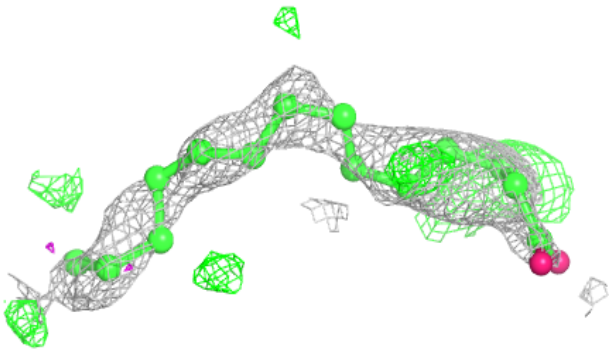


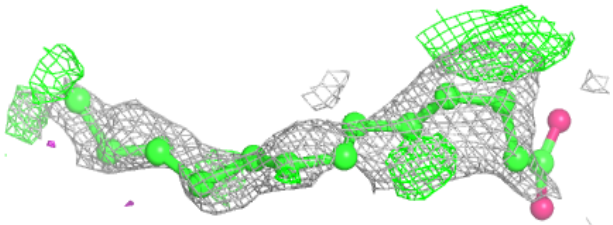


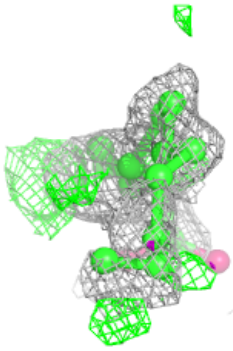


Electron density around MYR A 401 (A):

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

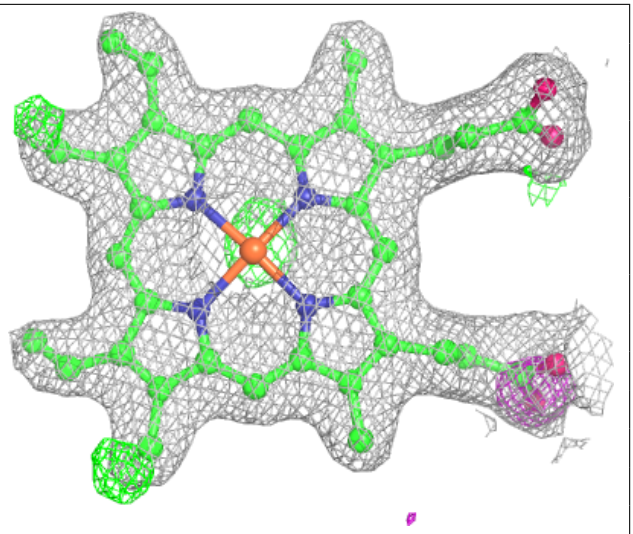


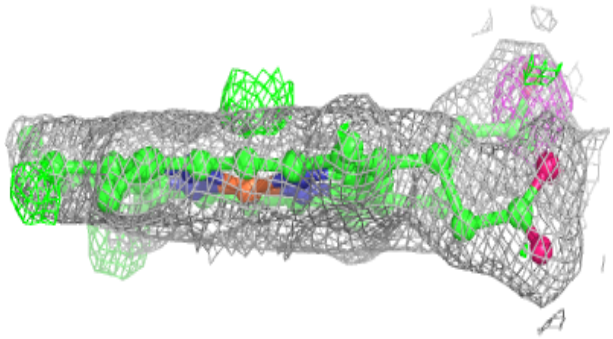


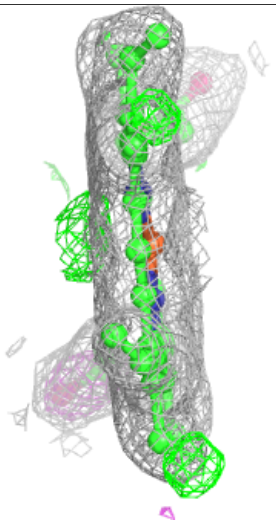


Electron density around HEM B 406:

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

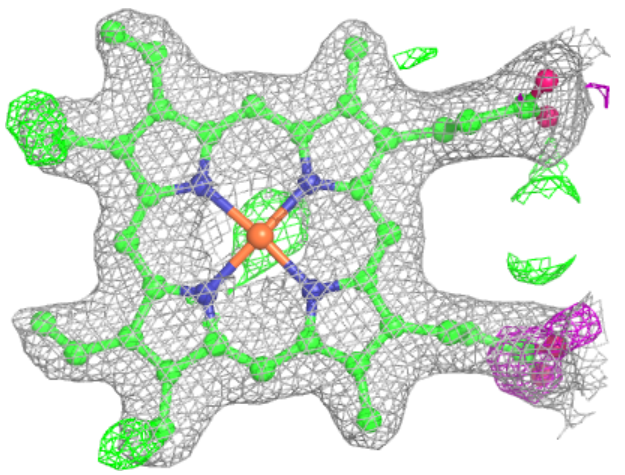


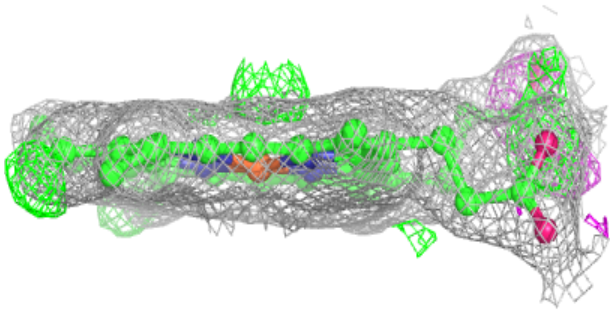


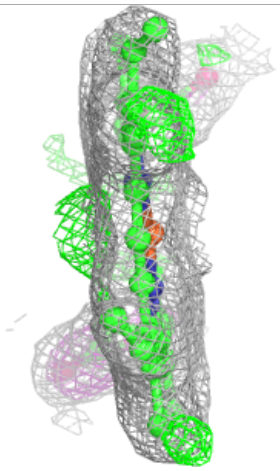


Electron density around HEM C 403:

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

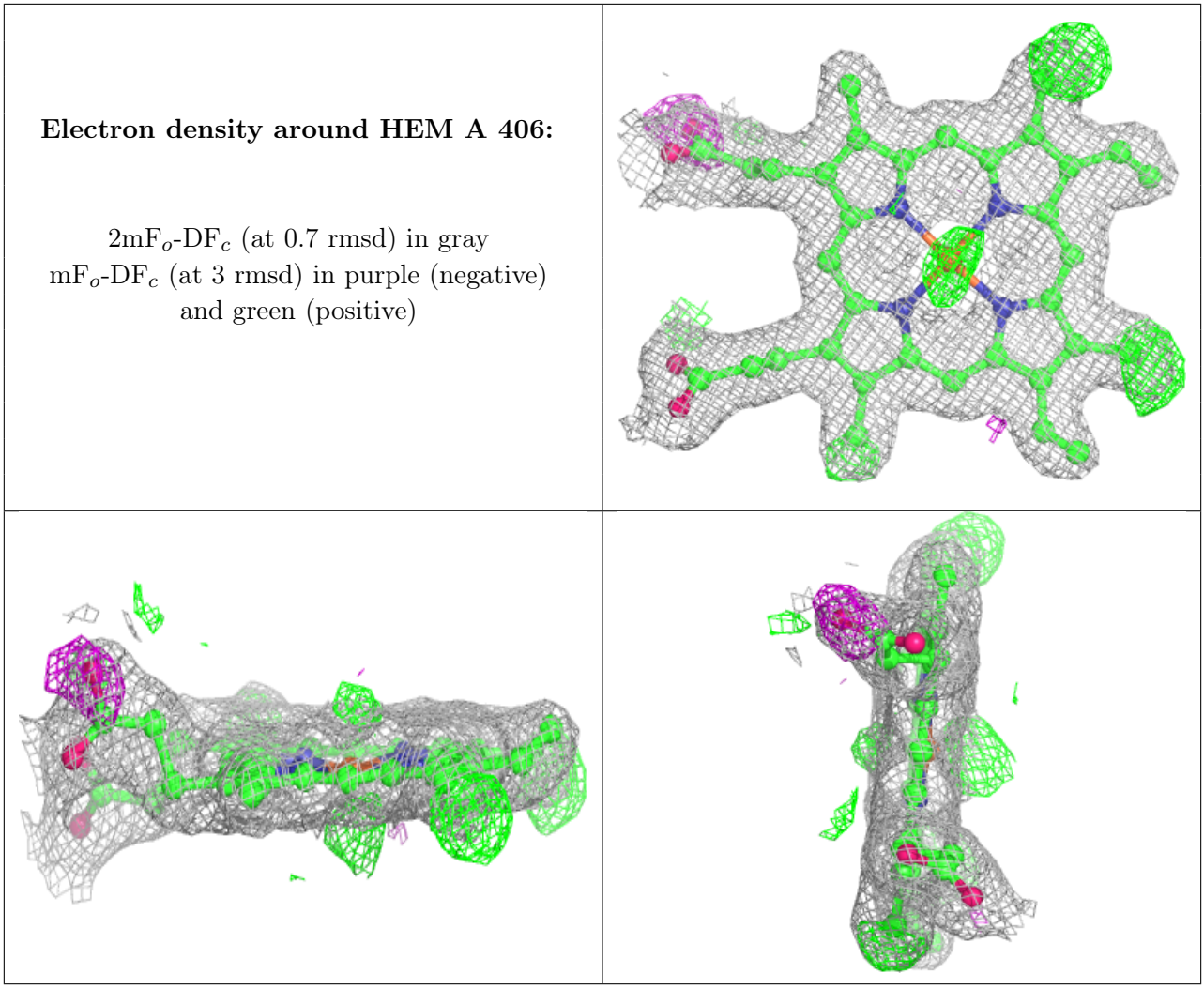






Electron density around HEM A 406:

$2mF_o$-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.