Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 07:11 pm BST

PDB ID	:	7Q6X
Title	:	OleP mutant S240Y in complex with 6DEB
Authors	:	Savino, C.; Montemiglio, L.C.; Vallone, B.; Exertier, C.; Freda, I.; Gugole, E.
Deposited on	:	2021-11-09
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

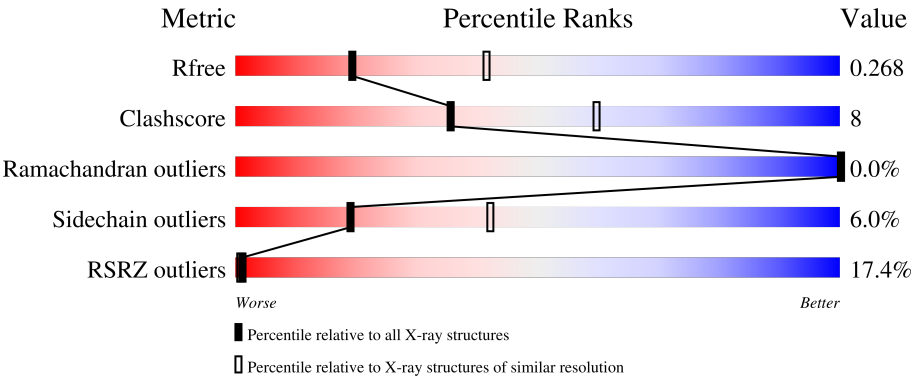
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	406	9% 76% 20%
1	B	406	9% 81% 18%
1	C	406	5% 83% 13%
1	D	406	16% 73% 23%
1	E	406	31% 76% 20%

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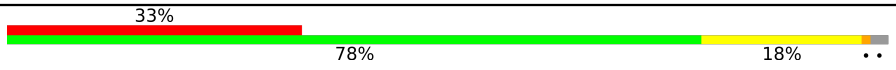
Mol	Chain	Length	Quality of chain
1	F	406	

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
4	FMT	A	504	-	-	-	X
4	FMT	E	503	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20720 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 Cytochrome P-450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	41	0
			3355	2126	598	616	15			
1	B	406	Total	C	N	O	S	0	32	0
			3361	2128	603	617	13			
1	C	399	Total	C	N	O	S	0	24	0
			3262	2060	585	604	13			
1	D	396	Total	C	N	O	S	0	48	0
			3396	2161	606	616	13			
1	E	395	Total	C	N	O	S	0	31	0
			3282	2082	587	599	14			
1	F	397	Total	C	N	O	S	0	50	0
			3402	2161	601	626	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP Q59819
A	3	ALA	-	expression tag	UNP Q59819
A	240	TYR	SER	engineered mutation	UNP Q59819
B	2	ALA	-	expression tag	UNP Q59819
B	3	ALA	-	expression tag	UNP Q59819
B	240	TYR	SER	engineered mutation	UNP Q59819
C	2	ALA	-	expression tag	UNP Q59819
C	3	ALA	-	expression tag	UNP Q59819
C	240	TYR	SER	engineered mutation	UNP Q59819
D	2	ALA	-	expression tag	UNP Q59819
D	3	ALA	-	expression tag	UNP Q59819
D	240	TYR	SER	engineered mutation	UNP Q59819
E	2	ALA	-	expression tag	UNP Q59819
E	3	ALA	-	expression tag	UNP Q59819
E	240	TYR	SER	engineered mutation	UNP Q59819
F	2	ALA	-	expression tag	UNP Q59819
F	3	ALA	-	expression tag	UNP Q59819

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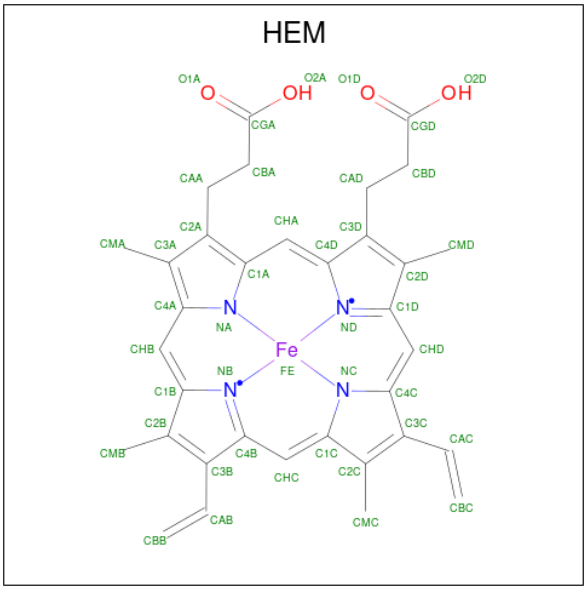
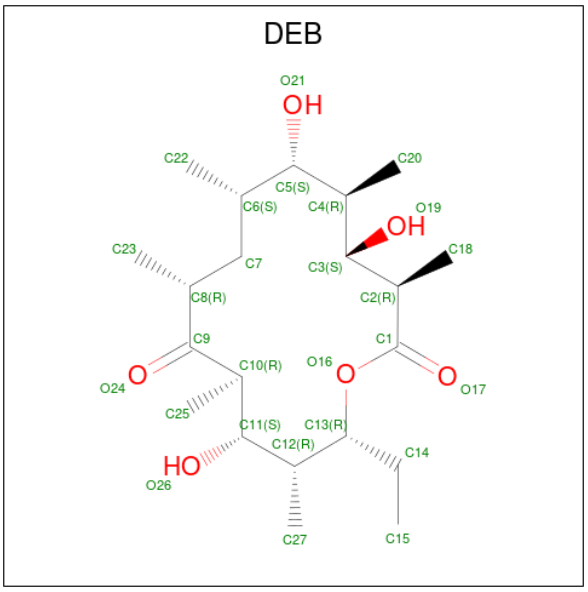
Chain	Residue	Modelled	Actual	Comment	Reference
F	240	TYR	SER	engineered mutation	UNP Q59819

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



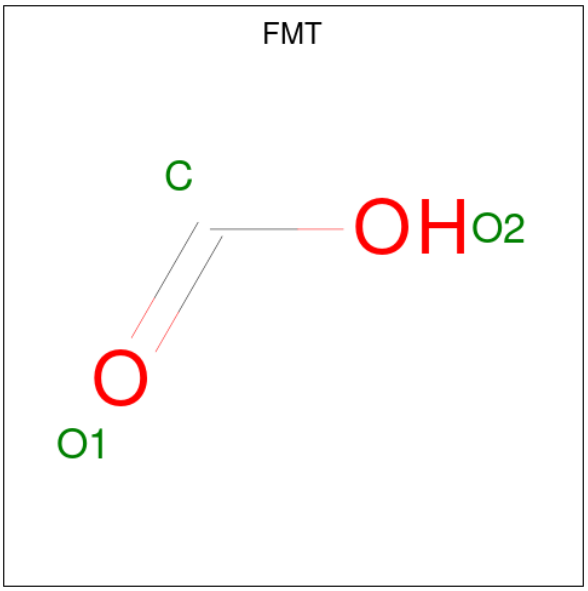
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (three-letter code: DEB) (formula: $C_{21}H_{38}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 27 21 6	0	0
3	B	1	Total C O 27 21 6	0	0
3	C	1	Total C O 27 21 6	0	0
3	D	1	Total C O 27 21 6	0	0
3	E	1	Total C O 27 21 6	0	0
3	F	1	Total C O 27 21 6	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

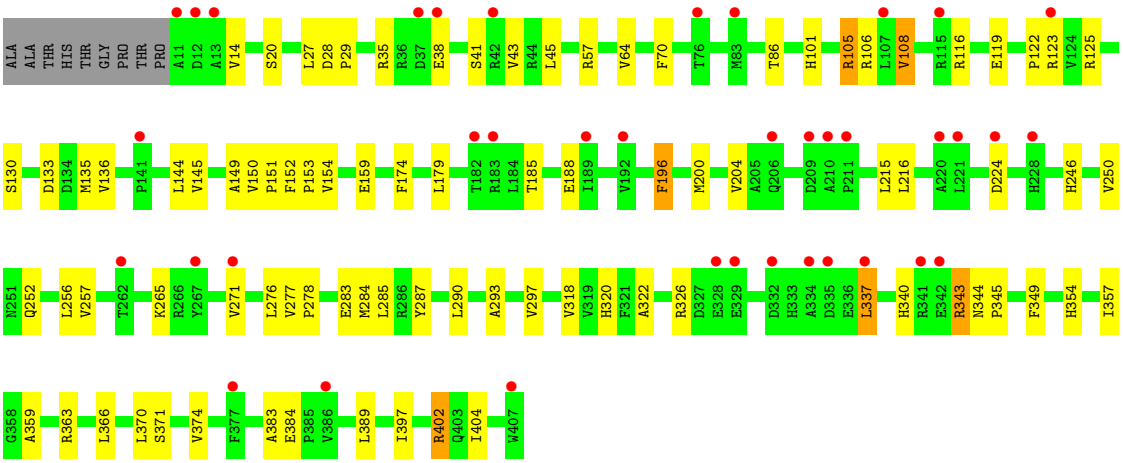
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	B	48	Total O 48 48	0	0
5	C	55	Total O 55 55	0	3
5	D	19	Total O 19 19	0	2
5	E	28	Total O 28 28	0	0
5	F	36	Total O 36 36	0	2

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.

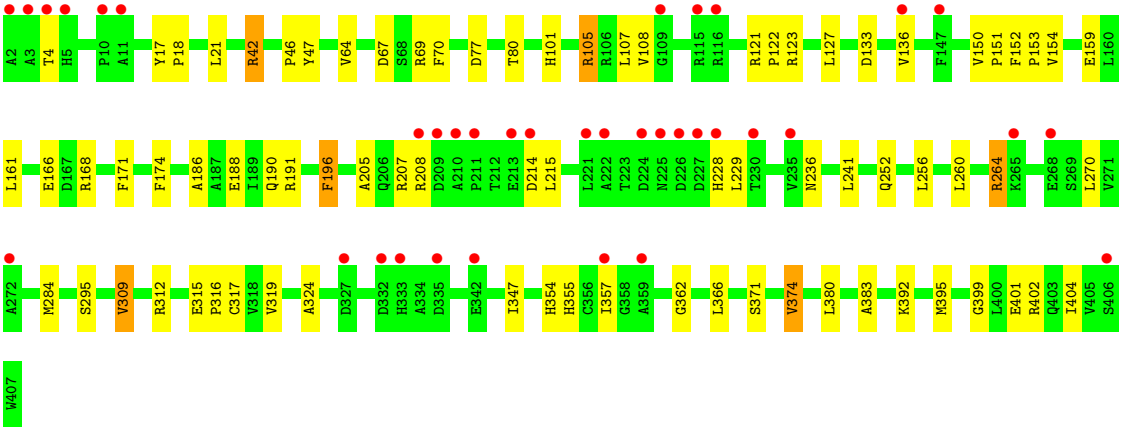
• Molecule 1: Cytochrome P-450

Chain A:



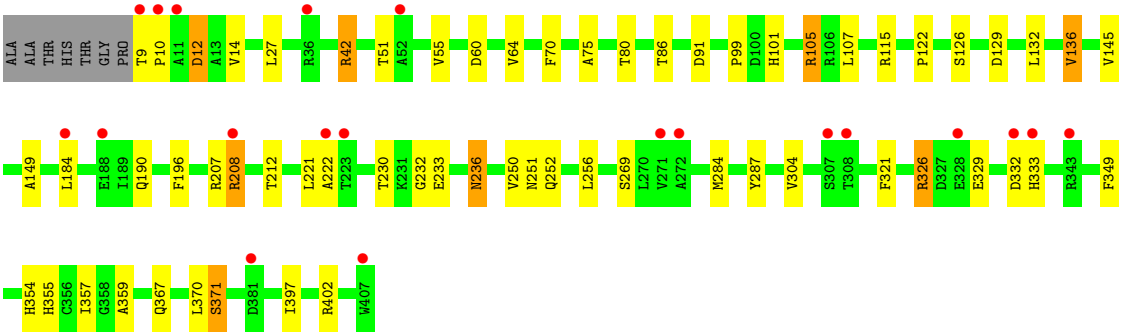
• Molecule 1: Cytochrome P-450

Chain B:



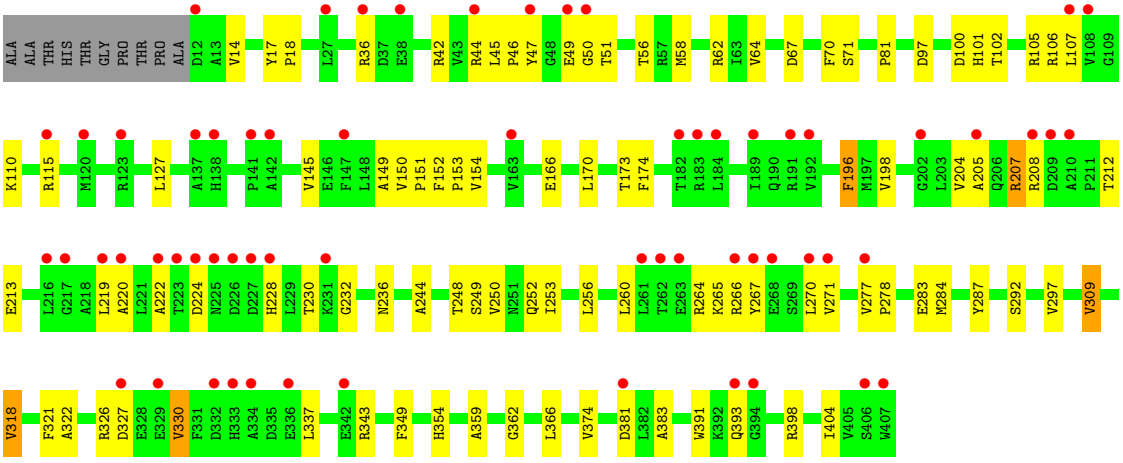
• Molecule 1: Cytochrome P-450

Chain C:



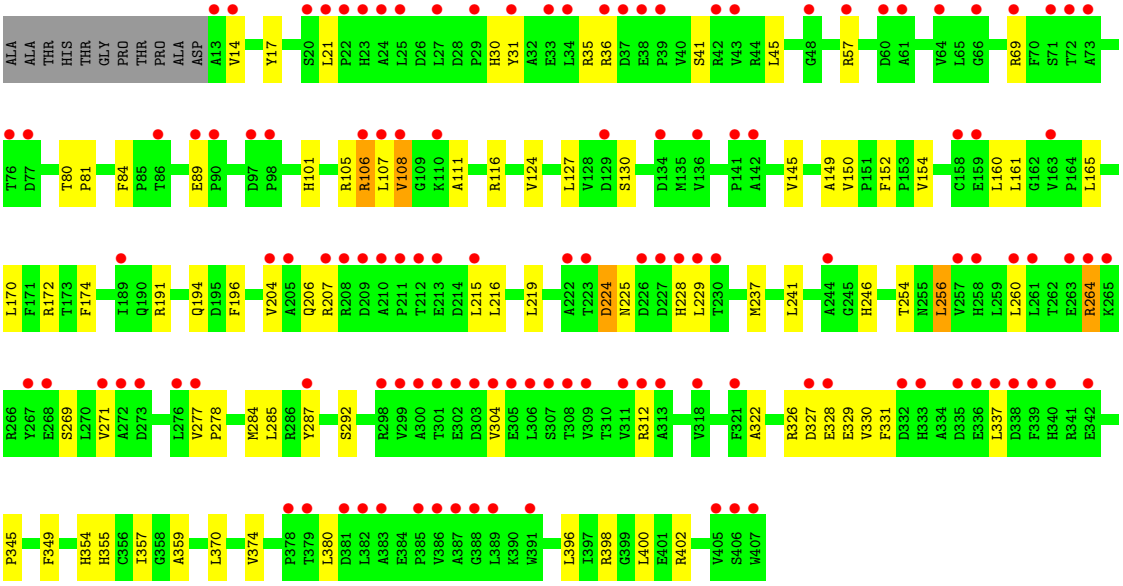
• Molecule 1: Cytochrome P-450

Chain D:



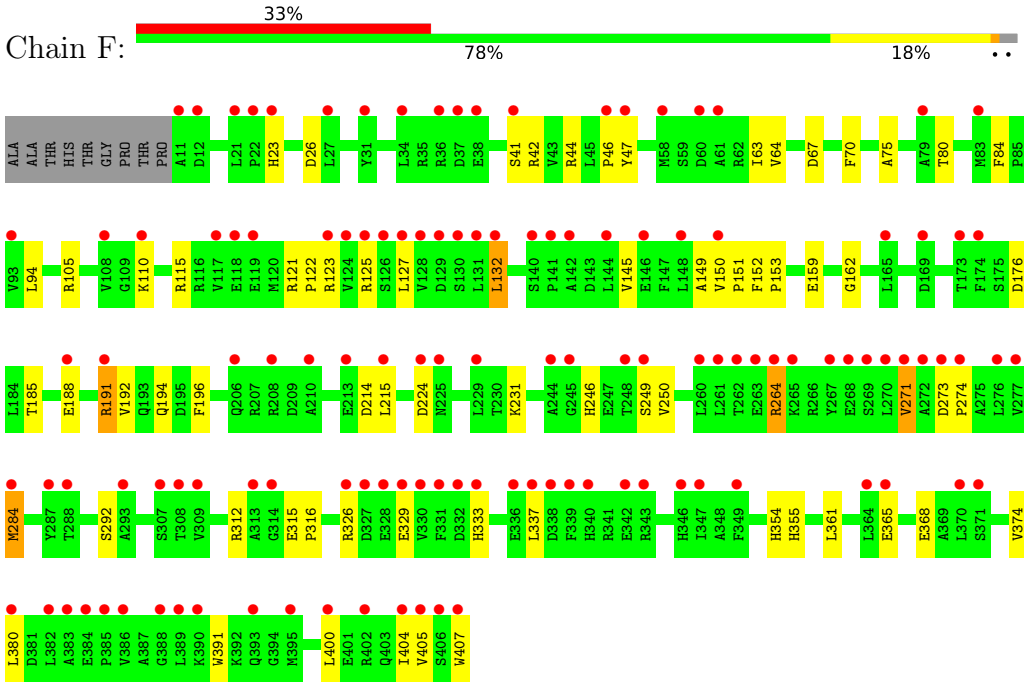
• Molecule 1: Cytochrome P-450

Chain E:



• Molecule 1: Cytochrome P-450

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.62Å 110.36Å 160.05Å 90.00° 129.63° 90.00°	Depositor
Resolution (Å)	51.34 – 2.70 51.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.34-2.70) 99.8 (51.29-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.268 0.206 , 0.268	Depositor DCC
R_{free} test set	5559 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	75.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20720	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8308e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: HEM, FMT, DEB

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	0.68	0/3543	0.84	0/4812
1	B	0.68	0/3531	0.85	0/4801
1	C	0.66	0/3395	0.82	0/4620
1	D	0.70	0/3617	0.83	0/4912
1	E	0.69	0/3446	0.84	0/4679
1	F	0.73	0/3622	0.84	1/4917 (0.0%)
All	All	0.69	0/21154	0.84	1/28741 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	274	PRO	N-CA-CB	5.33	109.70	103.30

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	3355	0	3408	58	0
1	B	3361	0	3417	49	0
1	C	3262	0	3270	47	0
1	D	3396	0	3492	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3282	0	3347	58	0
1	F	3402	0	3487	37	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	7	0
2	D	43	0	30	7	0
2	E	43	0	30	2	0
2	F	43	0	30	4	0
3	A	27	0	38	0	0
3	B	27	0	38	0	0
3	C	27	0	38	0	0
3	D	27	0	38	1	0
3	E	27	0	38	0	0
3	F	27	0	38	1	0
4	A	9	0	3	1	0
4	C	3	0	1	0	0
4	D	3	0	1	0	0
4	E	3	0	1	0	0
5	A	38	0	0	2	0
5	B	48	0	0	0	0
5	C	55	0	0	3	0
5	D	19	0	0	4	0
5	E	28	0	0	1	0
5	F	36	0	0	1	0
All	All	20720	0	20835	336	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 8.

All (336) 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:D:42[A]:ARG:NE	5:D:601[A]:HOH:O	1.80	1.15
1:E:106[A]:ARG:CG	1:E:106[A]:ARG:HH21	1.61	1.14
1:E:106[B]:ARG:HH11	1:E:106[B]:ARG:HG2	0.95	1.09
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:HG2	1.13	1.08
1:A:106[B]:ARG:HG2	1:A:106[B]:ARG:HH11	1.14	1.06
1:B:154[B]:VAL:HG11	1:B:168[B]:ARG:HD2	1.43	1.00
1:E:106[B]:ARG:HG2	1:E:106[B]:ARG:NH1	1.71	0.97
1:E:36[B]:ARG:NH1	1:E:328[B]:GLU:OE1	1.99	0.96
1:E:101[B]:HIS:CE1	1:E:354[B]:HIS:CD2	2.58	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42[A]:ARG:HG2	5:C:612[A]:HOH:O	1.71	0.91
1:A:106[B]:ARG:HH11	1:A:106[B]:ARG:CG	1.86	0.87
1:B:264:ARG:NH1	1:B:380:LEU:O	2.09	0.85
1:E:106[B]:ARG:HH11	1:E:106[B]:ARG:CG	1.85	0.83
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.58	0.82
1:D:100[B]:ASP:OD1	1:D:228[B]:HIS:HE1	1.63	0.81
1:A:150:VAL:O	1:A:154:VAL:HG23	1.79	0.81
1:C:105[A]:ARG:HG3	1:C:105[A]:ARG:HH11	1.47	0.80
1:D:297:VAL:HG22	1:D:318:VAL:CG2	2.12	0.79
1:E:224:ASP:OD2	5:E:601:HOH:O	2.03	0.77
1:E:107[A]:LEU:HD11	1:E:229:LEU:CD1	2.16	0.76
1:E:106[A]:ARG:HG2	1:E:106[A]:ARG:NH2	1.94	0.76
1:B:256:LEU:HD22	1:B:284:MET:HB3	1.67	0.75
1:A:106[B]:ARG:HG2	1:A:106[B]:ARG:NH1	1.95	0.74
1:E:106[A]:ARG:CG	1:E:106[A]:ARG:NH2	2.32	0.74
1:D:287:TYR:O	1:D:287:TYR:HD1	1.71	0.73
1:E:105:ARG:NH2	1:E:355:HIS:O	2.19	0.73
1:A:343[A]:ARG:NH2	5:A:601:HOH:O	2.21	0.72
1:D:42[A]:ARG:CD	5:D:601[A]:HOH:O	2.32	0.71
1:E:101[B]:HIS:HE1	1:E:354[B]:HIS:CD2	2.07	0.71
1:B:270:LEU:HB2	1:B:374[A]:VAL:HG21	1.72	0.71
1:E:216:LEU:HD23	1:E:219:LEU:HD12	1.73	0.71
1:F:145:VAL:HA	1:F:149:ALA:HB3	1.73	0.71
1:D:297:VAL:HG22	1:D:318:VAL:HG23	1.71	0.70
1:A:106[A]:ARG:NH2	5:A:602:HOH:O	2.24	0.70
1:D:102:THR:OG1	5:D:602:HOH:O	2.08	0.70
1:E:107[A]:LEU:HD21	1:E:229:LEU:HD12	1.73	0.70
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:HG3	1.54	0.70
1:A:101[B]:HIS:CE1	1:A:354[B]:HIS:CD2	2.80	0.70
1:B:123[B]:ARG:HH22	1:B:159[B]:GLU:HG2	1.55	0.69
1:F:105:ARG:NH2	1:F:355:HIS:O	2.25	0.69
1:D:287:TYR:O	1:D:287:TYR:CD1	2.45	0.69
1:B:270:LEU:CB	1:B:374[A]:VAL:HG21	2.24	0.67
1:C:101[B]:HIS:CE1	1:C:354[B]:HIS:CD2	2.82	0.67
1:C:91:ASP:OD1	5:C:601:HOH:O	2.15	0.65
1:D:152:PHE:HB3	1:D:153:PRO:HD3	1.78	0.65
1:E:101[B]:HIS:HE1	1:E:354[B]:HIS:HD2	1.43	0.65
1:B:392:LYS:HG3	1:B:399:GLY:O	1.96	0.65
1:C:145:VAL:HA	1:C:149:ALA:HB3	1.78	0.65
1:D:383:ALA:HB3	1:D:404:ILE:HG22	1.79	0.64
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106[A]:ARG:NH2	1:E:106[A]:ARG:HG3	2.09	0.64
1:B:188:GLU:O	1:B:191[B]:ARG:HG2	1.99	0.63
1:A:145:VAL:HA	1:A:149:ALA:HB3	1.80	0.63
1:F:42:ARG:NH2	5:F:602:HOH:O	2.31	0.63
1:C:9[B]:THR:HA	1:C:12[B]:ASP:OD1	1.99	0.63
1:E:17:TYR:HE1	1:E:31:TYR:HH	1.45	0.63
1:E:35:ARG:HG2	1:E:57[A]:ARG:HG2	1.81	0.62
1:B:123[B]:ARG:NH2	1:B:159[B]:GLU:HG2	2.15	0.62
1:D:232:GLY:O	1:D:236:ASN:HB2	2.00	0.62
1:D:101[B]:HIS:CE1	1:D:354[B]:HIS:CD2	2.89	0.61
1:E:107[A]:LEU:HD11	1:E:229:LEU:HD13	1.83	0.61
1:A:106[B]:ARG:CG	1:A:106[B]:ARG:NH1	2.51	0.61
1:D:49[C]:GLU:OE1	1:D:49[C]:GLU:HA	2.01	0.61
1:A:283:GLU:HG3	1:A:337:LEU:HD22	1.83	0.60
1:D:106[A]:ARG:NH2	1:D:110[A]:LYS:CE	2.65	0.60
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.83	0.60
1:F:177:ALA:HB3	1:F:192:VAL:HG11	1.84	0.60
1:C:105[A]:ARG:HH11	1:C:105[A]:ARG:CG	2.13	0.59
1:D:45:LEU:HB2	1:D:81:PRO:HB3	1.84	0.59
1:D:270:LEU:HB3	1:D:374:VAL:HG21	1.82	0.59
1:B:123[B]:ARG:HH12	1:B:159[B]:GLU:HG2	1.68	0.59
1:A:204:VAL:HG12	1:A:216:LEU:HD22	1.84	0.58
1:B:207:ARG:NH2	1:B:214:ASP:OD2	2.36	0.58
1:B:309:VAL:HG13	1:C:122:PRO:HA	1.84	0.58
1:D:100[B]:ASP:OD1	1:D:228[B]:HIS:CE1	2.52	0.58
1:D:106[A]:ARG:HH22	1:D:110[A]:LYS:HE2	1.69	0.58
1:E:69[A]:ARG:HE	1:E:304:VAL:HG22	1.69	0.58
1:C:105[A]:ARG:NH2	1:C:355:HIS:O	2.37	0.58
1:C:251:ASN:HD22	1:C:397:ILE:HD12	1.68	0.58
1:E:108:VAL:HG22	1:E:215[B]:LEU:HD11	1.85	0.58
1:C:9[B]:THR:N	1:C:10[B]:PRO:CD	2.67	0.57
1:E:292:SER:HA	1:E:398:ARG:HE	1.70	0.56
1:F:280:ALA:O	1:F:284[B]:MET:HG3	2.06	0.56
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.87	0.56
1:B:161:LEU:O	1:B:214:ASP:HB3	2.06	0.56
1:C:14:VAL:HG21	1:C:51[B]:THR:HG23	1.86	0.56
1:F:361:LEU:O	1:F:365[B]:GLU:HG2	2.05	0.56
1:A:256:LEU:HD22	1:A:284[B]:MET:HB3	1.88	0.56
1:D:64:VAL:HA	1:D:70:PHE:CD2	2.40	0.56
1:D:271:VAL:HA	1:D:374:VAL:HG13	1.88	0.56
1:F:121:ARG:N	1:F:122:PRO:HD2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107[A]:LEU:HD21	1:E:229:LEU:CD1	2.35	0.55
1:A:185:THR:OG1	1:A:188:GLU:HG3	2.07	0.55
1:C:208[B]:ARG:HH21	1:C:208[B]:ARG:HB2	1.72	0.55
1:B:256:LEU:HD22	1:B:284:MET:CB	2.37	0.54
1:A:290:LEU:HD22	2:A:501:HEM:HMB3	1.89	0.54
1:C:256:LEU:HD22	1:C:284:MET:HB3	1.90	0.54
1:C:230:THR:OG1	1:C:233:GLU:HG3	2.08	0.54
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.31	0.54
1:F:46:PRO:HB2	1:F:47:TYR:CD1	2.43	0.54
1:D:205:ALA:HA	1:D:208[B]:ARG:HG3	1.89	0.54
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.90	0.54
1:E:256:LEU:HD22	1:E:284:MET:HB3	1.89	0.53
1:D:391:TRP:O	1:D:393[A]:GLN:HG3	2.09	0.53
1:C:232:GLY:O	1:C:236:ASN:HB2	2.09	0.53
2:E:501:HEM:HHC	2:E:501:HEM:HBB2	1.90	0.53
1:B:64:VAL:HA	1:B:70:PHE:CD2	2.43	0.53
1:B:123[B]:ARG:NH1	1:B:159[B]:GLU:HG2	2.24	0.53
1:A:179:LEU:HD13	1:A:397[A]:ILE:CD1	2.39	0.52
1:C:252:GLN:O	1:C:256:LEU:HG	2.09	0.52
1:F:64:VAL:HA	1:F:70:PHE:CD2	2.43	0.52
1:B:133:ASP:O	1:B:136[A]:VAL:HG22	2.09	0.52
1:D:71:SER:OG	1:D:97:ASP:OD2	2.17	0.52
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.39	0.52
1:E:191[A]:ARG:NH2	1:E:194[A]:GLN:OE1	2.42	0.52
1:F:125[B]:ARG:HE	1:F:125[B]:ARG:HA	1.74	0.52
2:A:501:HEM:HBB2	2:A:501:HEM:HMB1	1.91	0.52
1:A:271:VAL:HA	1:A:374:VAL:HG13	1.92	0.52
1:D:322:ALA:O	1:D:326:ARG:HG2	2.10	0.52
1:C:132:LEU:O	1:C:136:VAL:HG13	2.10	0.51
1:D:106[A]:ARG:NH2	1:D:110[A]:LYS:NZ	2.58	0.51
1:A:174:PHE:HB3	1:A:196:PHE:CD2	2.45	0.51
1:F:23[A]:HIS:HD2	1:F:26[A]:ASP:OD2	1.93	0.51
1:B:252:GLN:OE1	1:B:252:GLN:HA	2.11	0.51
1:C:12[B]:ASP:OD1	1:C:12[B]:ASP:N	2.43	0.51
1:D:100[B]:ASP:HB2	5:D:606[B]:HOH:O	2.09	0.51
1:D:106[A]:ARG:HH22	1:D:110[A]:LYS:CE	2.23	0.51
1:B:105:ARG:NH2	1:B:355:HIS:O	2.44	0.51
1:B:256:LEU:CD2	1:B:284:MET:HB3	2.39	0.51
1:E:170:LEU:HD22	1:E:174:PHE:CZ	2.45	0.51
1:C:14:VAL:HG11	1:C:42[B]:ARG:HB3	1.92	0.51
1:A:105:ARG:HD2	1:A:357:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343[A]:ARG:HD3	1:A:345:PRO:HD3	1.92	0.51
1:A:366:LEU:HD11	2:A:501:HEM:HBB1	1.93	0.51
1:E:264:ARG:NH2	1:E:380:LEU:O	2.44	0.51
1:A:277:VAL:HB	1:A:278:PRO:HD3	1.92	0.51
1:E:349:PHE:CE1	1:E:359:ALA:HA	2.46	0.51
1:A:122:PRO:HB3	1:D:309:VAL:HG12	1.92	0.50
1:D:150:VAL:O	1:D:154:VAL:HG23	2.12	0.50
1:B:108:VAL:HG11	1:B:241:LEU:HD11	1.93	0.50
1:A:252:GLN:O	1:A:256:LEU:HG	2.12	0.50
1:B:101[B]:HIS:HE1	2:B:501:HEM:O2D	1.95	0.50
1:D:170:LEU:C	1:D:170:LEU:HD23	2.32	0.50
1:F:150:VAL:HB	1:F:151:PRO:HD3	1.94	0.50
1:F:379:THR:O	1:F:407:TRP:HA	2.11	0.50
1:D:45:LEU:HD12	1:D:81:PRO:HB2	1.95	0.49
1:B:105:ARG:HD2	1:B:357:ILE:HD12	1.94	0.49
2:D:501:HEM:HBA2	3:D:502:DEB:H253	1.94	0.49
1:C:99:PRO:HD2	5:C:625:HOH:O	2.12	0.49
1:E:105:ARG:HD3	1:E:357:ILE:HD12	1.93	0.49
1:A:384:GLU:OE1	1:A:389:LEU:HD23	2.12	0.49
1:B:383:ALA:HB3	1:B:404:ILE:HG22	1.93	0.49
1:F:94:LEU:HA	1:F:354[B]:HIS:HD2	1.77	0.49
1:A:144:LEU:HD21	1:A:257:VAL:HG21	1.95	0.49
1:C:55:VAL:HG13	1:C:60:ASP:HB2	1.95	0.49
1:C:9[B]:THR:CA	1:C:12[B]:ASP:OD1	2.60	0.49
1:D:256:LEU:CD2	1:D:284:MET:HB3	2.43	0.49
1:D:256:LEU:HD22	1:D:284:MET:HB3	1.95	0.49
1:D:266:ARG:CZ	1:D:337:LEU:HD12	2.42	0.49
1:A:108:VAL:HG22	1:A:215[A]:LEU:HD22	1.94	0.48
1:A:246:HIS:O	1:A:250:VAL:HG23	2.13	0.48
1:C:287:TYR:O	1:C:326:ARG:NH1	2.45	0.48
1:E:45:LEU:HD22	1:E:81:PRO:HB2	1.95	0.48
1:A:133:ASP:O	1:A:136:VAL:HG22	2.13	0.48
1:A:150:VAL:O	1:A:154:VAL:CG2	2.58	0.48
1:F:75:ALA:HA	1:F:80:THR:HG21	1.95	0.48
1:A:285:LEU:HD13	1:A:349:PHE:CE2	2.48	0.48
1:A:322:ALA:O	1:A:326:ARG:HG2	2.14	0.48
1:E:145:VAL:HA	1:E:149:ALA:HB3	1.95	0.48
1:E:322:ALA:O	1:E:326:ARG:HG2	2.14	0.48
1:F:283:GLU:HG3	1:F:337[B]:LEU:HD23	1.95	0.48
1:F:185:THR:HG23	1:F:188[A]:GLU:OE1	2.14	0.48
1:B:205:ALA:HA	1:B:208[B]:ARG:HE	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HG	1:B:284:MET:HE1	1.95	0.47
1:D:166[A]:GLU:HB2	1:E:228[A]:HIS:CE1	2.49	0.47
1:F:94:LEU:HD12	1:F:354[B]:HIS:HD2	1.80	0.47
1:B:67:ASP:CG	1:B:69:ARG:HE	2.17	0.47
1:D:149:ALA:O	1:D:250:VAL:HG22	2.14	0.47
1:D:260:LEU:HD22	1:D:267:TYR:HA	1.95	0.47
1:F:162:GLY:HA3	1:F:214:ASP:CG	2.35	0.47
1:A:64:VAL:HA	1:A:70:PHE:CD2	2.50	0.47
1:E:165:LEU:HD12	1:E:165:LEU:HA	1.80	0.47
1:D:101[A]:HIS:CD2	1:D:354[A]:HIS:CE1	3.02	0.47
1:C:105[A]:ARG:CG	1:C:105[A]:ARG:NH1	2.71	0.47
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.96	0.47
1:F:123[B]:ARG:NH2	1:F:127[B]:LEU:HD11	2.30	0.47
1:B:174:PHE:HB3	1:B:196:PHE:CD2	2.49	0.47
1:E:106[B]:ARG:NH1	1:E:106[B]:ARG:CG	2.54	0.47
1:D:42[B]:ARG:NH1	1:D:51[B]:THR:OG1	2.48	0.46
1:D:327:ASP:HB3	1:D:330:VAL:CG1	2.45	0.46
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.45	0.46
1:D:270:LEU:CB	1:D:374:VAL:HG21	2.46	0.46
1:D:283:GLU:HG3	1:D:337:LEU:CD2	2.45	0.46
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.97	0.46
1:C:349:PHE:CE1	1:C:359:ALA:HA	2.50	0.46
1:D:14:VAL:HG12	1:D:42[B]:ARG:HB3	1.98	0.46
1:A:130:SER:O	1:A:133:ASP:HB2	2.15	0.46
1:C:107:LEU:HD11	1:C:222:ALA:HB2	1.97	0.46
1:D:244:ALA:O	1:D:248:THR:OG1	2.25	0.46
1:D:277:VAL:HB	1:D:278:PRO:HD3	1.96	0.46
1:A:38[A]:GLU:CD	1:A:41:SER:HB3	2.36	0.46
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.98	0.46
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.98	0.46
1:B:186:ALA:O	1:B:190:GLN:HB2	2.17	0.45
1:A:116:ARG:O	1:A:119:GLU:HB2	2.17	0.45
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.97	0.45
1:D:150:VAL:N	1:D:151:PRO:HD2	2.32	0.45
1:A:276:LEU:HD11	1:A:340:HIS:NE2	2.31	0.45
1:A:297:VAL:HG22	1:A:318:VAL:HB	1.98	0.45
1:D:349:PHE:CE1	1:D:359:ALA:HA	2.52	0.45
1:F:271:VAL:HA	1:F:374:VAL:HG13	1.99	0.45
1:F:23[A]:HIS:CD2	1:F:26[A]:ASP:OD2	2.70	0.45
1:A:14:VAL:HG12	1:A:43:VAL:HA	1.99	0.44
1:A:256:LEU:HD22	1:A:284[A]:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:GLN:O	1:C:371:SER:HB2	2.17	0.44
1:E:150:VAL:O	1:E:154:VAL:HG13	2.17	0.44
1:C:321:PHE:CZ	2:C:501:HEM:HBA2	2.53	0.44
1:F:152:PHE:HB3	1:F:153:PRO:HD3	1.98	0.44
1:A:179:LEU:HD13	1:A:397[A]:ILE:HD11	2.00	0.44
1:B:150:VAL:O	1:B:154[A]:VAL:HG22	2.17	0.44
1:B:309:VAL:HG13	1:C:122:PRO:CA	2.48	0.44
1:E:154:VAL:HG12	1:E:246:HIS:HB2	1.98	0.44
1:A:343[A]:ARG:NH2	4:A:504:FMT:O2	2.51	0.44
1:E:69[B]:ARG:HD2	1:E:304:VAL:HG22	1.99	0.44
1:F:264:ARG:NH2	1:F:380:LEU:O	2.51	0.44
1:A:265[B]:LYS:HA	1:A:265[B]:LYS:HD3	1.85	0.44
1:C:101[B]:HIS:NE2	1:C:105[B]:ARG:HD3	2.33	0.44
1:A:359:ALA:O	1:A:363:ARG:HG3	2.18	0.44
1:B:150:VAL:N	1:B:151:PRO:HD2	2.33	0.44
1:C:75:ALA:HA	1:C:80:THR:HG21	1.99	0.44
1:D:106[A]:ARG:NH2	1:D:110[A]:LYS:HE2	2.29	0.44
1:A:20:SER:OG	1:A:28:ASP:OD2	2.21	0.44
1:D:174:PHE:HB3	1:D:196:PHE:CD2	2.53	0.44
1:F:191[B]:ARG:NH2	1:F:194[B]:GLN:OE1	2.51	0.44
1:B:315:GLU:HA	1:B:316:PRO:HD3	1.86	0.44
1:E:215[A]:LEU:HD23	1:E:215[A]:LEU:HA	1.90	0.44
1:A:293:ALA:HA	1:A:320:HIS:CE1	2.53	0.43
1:B:77:ASP:HB3	1:B:80:THR:OG1	2.18	0.43
1:A:35:ARG:HG2	1:A:57[B]:ARG:HG3	1.99	0.43
1:D:46:PRO:HB2	1:D:47:TYR:CD1	2.53	0.43
1:D:101[A]:HIS:CE1	1:D:105:ARG:HD3	2.53	0.43
1:D:256:LEU:HD22	1:D:284:MET:CB	2.48	0.43
1:E:111:ALA:CB	1:E:215[A]:LEU:HD21	2.48	0.43
1:F:63:ILE:O	1:F:67:ASP:HB2	2.17	0.43
1:C:101[B]:HIS:HE1	2:C:501:HEM:O2D	2.00	0.43
1:D:58:MET:HE2	1:D:62:ARG:HG3	2.00	0.43
1:E:260:LEU:HD11	1:E:370[B]:LEU:HD11	2.00	0.43
1:B:270:LEU:HB3	1:B:374[A]:VAL:HG21	1.99	0.43
1:A:179:LEU:HD13	1:A:397[A]:ILE:HD13	1.99	0.43
1:D:252:GLN:OE1	1:D:252:GLN:HA	2.19	0.43
1:D:166[A]:GLU:HB2	1:E:228[A]:HIS:HE1	1.84	0.43
1:E:57[B]:ARG:HG3	1:E:327:ASP:OD2	2.18	0.43
1:E:111:ALA:HB2	1:E:215[A]:LEU:HD21	2.01	0.43
1:B:46:PRO:HB2	1:B:47:TYR:CD1	2.53	0.43
1:A:343[A]:ARG:HH11	1:A:344:ASN:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLY:O	1:B:366:LEU:HG	2.18	0.43
1:C:55:VAL:HG21	1:C:64:VAL:HG21	2.01	0.43
1:C:332:ASP:C	1:C:333:HIS:ND1	2.72	0.43
1:C:357:ILE:HG22	2:C:501:HEM:C2D	2.54	0.43
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.49	0.43
1:D:219:LEU:O	1:D:222:ALA:HB3	2.19	0.43
1:E:124:VAL:HG13	1:E:152:PHE:HE1	1.83	0.43
1:A:200:MET:O	1:A:204:VAL:HG13	2.19	0.42
1:B:324:ALA:CB	1:B:347:ILE:HD11	2.49	0.42
1:D:287:TYR:CD2	1:D:337:LEU:HG	2.54	0.42
1:E:287:TYR:CG	1:E:337:LEU:HD13	2.54	0.42
1:D:207:ARG:HB2	1:D:220:ALA:CB	2.49	0.42
1:B:123[B]:ARG:HH12	1:B:159[B]:GLU:CG	2.32	0.42
1:C:14:VAL:HG11	1:C:42[A]:ARG:HB3	2.02	0.42
1:C:208[B]:ARG:CB	1:C:208[B]:ARG:NH2	2.82	0.42
1:D:152:PHE:CB	1:D:153:PRO:HD3	2.45	0.42
1:F:176[B]:ASP:OD1	1:F:183[B]:ARG:CZ	2.67	0.42
1:F:125[B]:ARG:NH1	1:F:368:GLU:O	2.52	0.42
1:F:391:TRP:CE2	1:F:400:LEU:HD21	2.55	0.42
1:D:166[B]:GLU:OE1	1:D:166[B]:GLU:HA	2.19	0.42
1:E:69[B]:ARG:CD	1:E:304:VAL:HG22	2.49	0.42
1:B:123[B]:ARG:CZ	1:B:159[B]:GLU:HG2	2.50	0.42
1:B:152:PHE:CB	1:B:153:PRO:HD3	2.50	0.42
1:B:354[B]:HIS:HD2	2:B:501:HEM:O1D	2.02	0.42
1:B:295:SER:HB3	1:B:319:VAL:O	2.20	0.42
1:C:70:PHE:CE2	1:C:304:VAL:HG11	2.55	0.42
1:C:256:LEU:HD22	1:C:284:MET:CB	2.49	0.42
1:D:292:SER:CB	1:D:398:ARG:HE	2.32	0.42
1:D:249:SER:O	1:D:253:ILE:HG13	2.20	0.41
1:E:35:ARG:O	1:E:57[A]:ARG:HD2	2.19	0.41
1:C:64:VAL:HA	1:C:70:PHE:CD2	2.55	0.41
1:C:207:ARG:HD3	1:C:212:THR:OG1	2.20	0.41
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	2.03	0.41
1:D:107[A]:LEU:HD23	1:D:219:LEU:CD2	2.50	0.41
1:E:285:LEU:HD13	1:E:349:PHE:CE2	2.55	0.41
1:F:132:LEU:HD12	1:F:132:LEU:HA	1.89	0.41
1:D:17:TYR:CD1	1:D:18:PRO:HA	2.56	0.41
1:D:44[A]:ARG:HG3	1:D:50:GLY:HA2	2.03	0.41
1:C:221:LEU:HD23	1:C:221:LEU:HA	1.93	0.41
1:C:357:ILE:CG2	2:C:501:HEM:HMD2	2.51	0.41
1:D:283:GLU:HG3	1:D:337:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:GLU:HA	1:F:316:PRO:HD3	1.84	0.41
1:C:64:VAL:HA	1:C:70:PHE:CE2	2.55	0.41
1:D:36[A]:ARG:HE	1:D:36[A]:ARG:HB2	1.70	0.41
1:E:237:MET:O	1:E:241:LEU:HG	2.21	0.41
1:F:84:PHE:CD2	3:F:502:DEB:H182	2.56	0.41
2:F:501:HEM:HBB2	2:F:501:HEM:CMB	2.49	0.41
2:F:501:HEM:HBC2	2:F:501:HEM:CMC	2.51	0.41
1:D:321:PHE:HZ	2:D:501:HEM:O2A	2.04	0.41
1:A:123[B]:ARG:NH1	1:A:159[B]:GLU:OE2	2.46	0.41
1:A:150:VAL:N	1:A:151:PRO:HD2	2.36	0.41
1:A:287:TYR:O	1:A:326:ARG:NH1	2.54	0.41
1:B:121:ARG:HB3	1:B:122:PRO:HD3	2.03	0.41
1:B:312:ARG:NH2	1:C:129:ASP:OD2	2.46	0.41
1:D:101[B]:HIS:HE1	2:D:501:HEM:O2D	2.04	0.41
1:D:207:ARG:HD2	1:D:212:THR:OG1	2.21	0.41
1:E:84:PHE:HB3	1:E:396:LEU:HD11	2.02	0.41
1:B:17:TYR:HA	1:B:18:PRO:C	2.41	0.41
1:E:254:THR:HB	1:E:400:LEU:HB2	2.02	0.40
1:E:277:VAL:HB	1:E:278:PRO:HD3	2.03	0.40
1:F:284[B]:MET:HG2	1:F:337[B]:LEU:HD21	2.02	0.40
1:A:150:VAL:N	1:A:151:PRO:CD	2.85	0.40
1:B:107:LEU:HD11	1:B:229:LEU:HD13	2.03	0.40
1:E:160:LEU:HG	1:E:215[A]:LEU:HD12	2.03	0.40
1:F:123[B]:ARG:CZ	1:F:127[B]:LEU:HD11	2.51	0.40
1:A:28:ASP:HA	1:A:29:PRO:HD3	1.96	0.40
1:D:362:GLY:O	1:D:366:LEU:HG	2.21	0.40
1:A:383:ALA:HB3	1:A:404:ILE:HG22	2.04	0.40
2:A:501:HEM:HMD1	2:A:501:HEM:HBD2	2.03	0.40
1:D:145:VAL:HA	1:D:149:ALA:HB3	2.02	0.40
1:E:271:VAL:HA	1:E:374:VAL:HG13	2.03	0.40
1:E:331:PHE:CE1	1:E:345:PRO:HD2	2.56	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	436/406 (107%)	410 (94%)	26 (6%)	0	100	100
1	B	437/406 (108%)	417 (95%)	20 (5%)	0	100	100
1	C	420/406 (103%)	403 (96%)	17 (4%)	0	100	100
1	D	443/406 (109%)	410 (93%)	33 (7%)	0	100	100
1	E	424/406 (104%)	398 (94%)	26 (6%)	0	100	100
1	F	445/406 (110%)	423 (95%)	21 (5%)	1 (0%)	47	73
All	All	2605/2436 (107%)	2461 (94%)	143 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	273	ASP

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	373/338 (110%)	356 (95%)	17 (5%)	27	54
1	B	371/338 (110%)	349 (94%)	22 (6%)	19	43
1	C	355/338 (105%)	332 (94%)	23 (6%)	17	38
1	D	380/338 (112%)	358 (94%)	22 (6%)	20	43
1	E	362/338 (107%)	334 (92%)	28 (8%)	13	30
1	F	380/338 (112%)	348 (92%)	32 (8%)	11	25
All	All	2221/2028 (110%)	2077 (94%)	144 (6%)	19	38

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	45	LEU
1	A	86	THR
1	A	105	ARG
1	A	108	VAL
1	A	125	ARG
1	A	135	MET
1	A	196	PHE
1	A	224[A]	ASP
1	A	224[B]	ASP
1	A	337	LEU
1	A	343[A]	ARG
1	A	343[B]	ARG
1	A	370	LEU
1	A	371	SER
1	A	402[A]	ARG
1	A	402[B]	ARG
1	B	4	THR
1	B	21	LEU
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	105	ARG
1	B	127	LEU
1	B	166	GLU
1	B	171	PHE
1	B	196	PHE
1	B	215	LEU
1	B	228[A]	HIS
1	B	228[B]	HIS
1	B	236	ASN
1	B	264	ARG
1	B	309	VAL
1	B	317	CYS
1	B	371	SER
1	B	374[A]	VAL
1	B	374[B]	VAL
1	B	395	MET
1	B	401	GLU
1	B	402	ARG
1	C	12[A]	ASP
1	C	12[B]	ASP
1	C	27	LEU
1	C	42[A]	ARG

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Mol	Chain	Res	Type
1	C	42[B]	ARG
1	C	86	THR
1	C	105[A]	ARG
1	C	105[B]	ARG
1	C	115	ARG
1	C	126	SER
1	C	136	VAL
1	C	184	LEU
1	C	190	GLN
1	C	196	PHE
1	C	208[A]	ARG
1	C	208[B]	ARG
1	C	236	ASN
1	C	269	SER
1	C	326	ARG
1	C	329	GLU
1	C	370	LEU
1	C	371	SER
1	C	402	ARG
1	D	56	THR
1	D	67	ASP
1	D	115[A]	ARG
1	D	115[B]	ARG
1	D	127	LEU
1	D	173	THR
1	D	196	PHE
1	D	204	VAL
1	D	207	ARG
1	D	213[A]	GLU
1	D	213[B]	GLU
1	D	224[A]	ASP
1	D	224[B]	ASP
1	D	230	THR
1	D	264	ARG
1	D	265[A]	LYS
1	D	265[B]	LYS
1	D	309	VAL
1	D	318	VAL
1	D	330	VAL
1	D	343[A]	ARG
1	D	343[B]	ARG
1	E	14	VAL

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Mol	Chain	Res	Type
1	E	21	LEU
1	E	30	HIS
1	E	41	SER
1	E	80	THR
1	E	89	GLU
1	E	106[A]	ARG
1	E	106[B]	ARG
1	E	108	VAL
1	E	116	ARG
1	E	127	LEU
1	E	130	SER
1	E	161	LEU
1	E	172	ARG
1	E	196	PHE
1	E	204	VAL
1	E	206	GLN
1	E	207	ARG
1	E	224	ASP
1	E	225	ASN
1	E	256	LEU
1	E	264	ARG
1	E	269	SER
1	E	312[A]	ARG
1	E	312[B]	ARG
1	E	329	GLU
1	E	330	VAL
1	E	402	ARG
1	F	41	SER
1	F	86	THR
1	F	89[A]	GLU
1	F	89[B]	GLU
1	F	110[A]	LYS
1	F	110[B]	LYS
1	F	115	ARG
1	F	132	LEU
1	F	159	GLU
1	F	181	SER
1	F	191[A]	ARG
1	F	191[B]	ARG
1	F	196	PHE
1	F	215	LEU
1	F	224[A]	ASP

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Mol	Chain	Res	Type
1	F	224[B]	ASP
1	F	231	LYS
1	F	246[A]	HIS
1	F	246[B]	HIS
1	F	249	SER
1	F	264	ARG
1	F	271	VAL
1	F	284[A]	MET
1	F	284[B]	MET
1	F	292	SER
1	F	312	ARG
1	F	326	ARG
1	F	333	HIS
1	F	375[A]	ARG
1	F	375[B]	ARG
1	F	404	ILE
1	F	405	VAL

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

Mol	Chain	Res	Type
1	C	193	GLN
1	E	96	GLN
1	E	206	GLN
1	E	320	HIS
1	F	193	GLN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
4	FMT	E	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	503	-	0,2,2	-	-	0,1,1	-	-
2	HEM	C	501	1	27,50,50	1.04	2 (7%)	17,82,82	1.81	4 (23%)
3	DEB	B	502	-	27,27,27	0.47	0	35,39,39	0.89	1 (2%)
2	HEM	D	501	1	27,50,50	1.19	2 (7%)	17,82,82	1.63	6 (35%)
2	HEM	E	501	1	27,50,50	1.04	2 (7%)	17,82,82	1.74	5 (29%)
3	DEB	D	502	-	27,27,27	0.56	1 (3%)	35,39,39	0.90	1 (2%)
3	DEB	E	502	-	27,27,27	0.37	0	35,39,39	0.73	1 (2%)
3	DEB	F	502	-	27,27,27	0.29	0	35,39,39	0.67	0
3	DEB	A	502	-	27,27,27	0.48	0	35,39,39	0.97	2 (5%)
4	FMT	C	503	-	0,2,2	-	-	0,1,1	-	-
3	DEB	C	502	-	27,27,27	0.39	0	35,39,39	0.90	1 (2%)
4	FMT	D	503	-	0,2,2	-	-	0,1,1	-	-
2	HEM	A	501	1	27,50,50	1.31	6 (22%)	17,82,82	2.39	8 (47%)
4	FMT	A	505	-	0,2,2	-	-	0,1,1	-	-
2	HEM	B	501	1	27,50,50	1.13	3 (11%)	17,82,82	1.87	7 (41%)
4	FMT	A	504	-	0,2,2	-	-	0,1,1	-	-
2	HEM	F	501	1	27,50,50	0.72	1 (3%)	17,82,82	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	2/6/54/54	-
3	DEB	B	502	-	-	8/50/50/50	0/1/1/1
2	HEM	D	501	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	E	501	1	-	0/6/54/54	-
3	DEB	D	502	-	-	10/50/50/50	0/1/1/1
3	DEB	E	502	-	-	12/50/50/50	0/1/1/1
3	DEB	F	502	-	-	10/50/50/50	0/1/1/1
3	DEB	A	502	-	-	10/50/50/50	0/1/1/1
3	DEB	C	502	-	-	8/50/50/50	0/1/1/1
2	HEM	A	501	1	-	0/6/54/54	-
2	HEM	B	501	1	-	2/6/54/54	-
2	HEM	F	501	1	-	0/6/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C4D	3.46	1.50	1.42
2	D	501	HEM	C3B-C2B	-3.44	1.35	1.40
2	E	501	HEM	C3B-C2B	-2.83	1.36	1.40
2	C	501	HEM	C3D-C4D	2.60	1.48	1.42
2	B	501	HEM	C4B-NB	-2.55	1.30	1.36
2	B	501	HEM	C3B-C2B	-2.54	1.36	1.40
2	A	501	HEM	C3D-C2D	-2.51	1.30	1.37
2	D	501	HEM	C4B-NB	-2.43	1.31	1.36
2	E	501	HEM	C3D-C4D	2.41	1.48	1.42
2	C	501	HEM	C3B-C2B	-2.36	1.37	1.40
2	A	501	HEM	CAA-C2A	2.28	1.55	1.52
2	A	501	HEM	C4B-NB	-2.18	1.31	1.36
2	A	501	HEM	C1A-CHA	-2.17	1.35	1.41
3	D	502	DEB	C2-C1	2.16	1.56	1.51
2	A	501	HEM	C1D-CHD	-2.12	1.35	1.41
2	B	501	HEM	C3D-C4D	2.05	1.47	1.42
2	F	501	HEM	C3D-C4D	2.05	1.47	1.42

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C4A-C3A-C2A	4.75	110.30	107.00
2	C	501	HEM	CBA-CAA-C2A	3.95	119.77	112.49
2	A	501	HEM	CBA-CAA-C2A	3.90	119.69	112.49
2	A	501	HEM	C3B-C4B-NB	-3.57	104.59	109.21
2	E	501	HEM	C1D-C2D-C3D	-3.51	104.55	107.00
2	A	501	HEM	CAA-CBA-CGA	3.50	118.53	112.67
2	E	501	HEM	C4A-C3A-C2A	3.39	109.35	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	CMC-C2C-C3C	3.35	130.95	124.68
2	B	501	HEM	C4A-C3A-C2A	3.32	109.31	107.00
2	C	501	HEM	CMA-C3A-C4A	-3.12	123.67	128.46
2	B	501	HEM	CBA-CAA-C2A	3.09	118.18	112.49
2	C	501	HEM	C4A-C3A-C2A	3.03	109.11	107.00
2	C	501	HEM	CMC-C2C-C3C	3.03	130.34	124.68
2	D	501	HEM	CBA-CAA-C2A	3.02	118.06	112.49
2	E	501	HEM	CBD-CAD-C3D	-3.02	106.91	112.48
2	B	501	HEM	CBD-CAD-C3D	-2.97	107.00	112.48
2	A	501	HEM	C2C-C3C-C4C	-2.67	105.03	106.90
3	E	502	DEB	O21-C5-C6	-2.62	104.91	109.83
2	E	501	HEM	C3B-C4B-NB	-2.57	105.88	109.21
2	A	501	HEM	C1D-C2D-C3D	-2.55	105.22	107.00
2	B	501	HEM	CMC-C2C-C3C	2.51	129.38	124.68
2	B	501	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
2	B	501	HEM	CMB-C2B-C3B	2.33	129.04	124.68
2	B	501	HEM	CAA-C2A-C3A	-2.33	120.56	127.25
3	D	502	DEB	O16-C13-C14	2.32	110.63	106.92
2	D	501	HEM	CAD-CBD-CGD	-2.22	108.94	112.67
3	A	502	DEB	C25-C10-C9	2.22	111.94	108.08
2	E	501	HEM	CBA-CAA-C2A	2.22	116.58	112.49
3	A	502	DEB	C6-C5-C4	-2.22	112.84	116.27
3	B	502	DEB	O16-C13-C14	2.21	110.46	106.92
2	A	501	HEM	CAD-CBD-CGD	2.19	116.35	112.67
2	A	501	HEM	CMB-C2B-C3B	2.15	128.70	124.68
2	D	501	HEM	C2C-C3C-C4C	2.15	108.40	106.90
3	C	502	DEB	O19-C3-C2	2.14	113.79	108.82
2	D	501	HEM	C3C-C4C-NC	-2.09	106.99	110.94
2	F	501	HEM	CMC-C2C-C3C	2.06	128.53	124.68
2	D	501	HEM	CMA-C3A-C4A	-2.05	125.31	128.46

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
3	A	502	DEB	C12-C13-C14-C15
3	A	502	DEB	O16-C13-C14-C15
3	B	502	DEB	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	B	502	DEB	O16-C13-C14-C15
3	C	502	DEB	C12-C13-C14-C15
3	C	502	DEB	O16-C13-C14-C15
3	D	502	DEB	C12-C13-C14-C15
3	D	502	DEB	O16-C13-C14-C15
3	E	502	DEB	C18-C2-C3-C4
3	E	502	DEB	O16-C13-C14-C15
3	A	502	DEB	C3-C4-C5-O21
3	B	502	DEB	C3-C4-C5-O21
3	C	502	DEB	C3-C4-C5-O21
3	D	502	DEB	C3-C4-C5-O21
3	F	502	DEB	C3-C4-C5-O21
3	D	502	DEB	C20-C4-C5-O21
3	E	502	DEB	C3-C4-C5-O21
3	A	502	DEB	C18-C2-C3-O19
3	C	502	DEB	C18-C2-C3-O19
3	E	502	DEB	C18-C2-C3-O19
3	F	502	DEB	C18-C2-C3-O19
3	A	502	DEB	C20-C4-C5-O21
3	F	502	DEB	C18-C2-C3-C4
3	B	502	DEB	C20-C4-C5-O21
3	C	502	DEB	C20-C4-C5-O21
3	E	502	DEB	C20-C4-C5-O21
3	F	502	DEB	C20-C4-C5-O21
3	D	502	DEB	C18-C2-C3-O19
3	D	502	DEB	C3-C4-C5-C6
3	A	502	DEB	C18-C2-C3-C4
3	B	502	DEB	C18-C2-C3-C4
3	C	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C20-C4-C5-C6
3	B	502	DEB	C18-C2-C3-O19
3	A	502	DEB	C20-C4-C5-C6
3	C	502	DEB	C20-C4-C5-C6
3	E	502	DEB	C20-C4-C5-C6
3	B	502	DEB	C20-C4-C5-C6
3	E	502	DEB	C3-C4-C5-C6
3	A	502	DEB	C3-C4-C5-C6
3	B	502	DEB	C3-C4-C5-C6
3	C	502	DEB	C3-C4-C5-C6
3	F	502	DEB	C3-C4-C5-C6
3	E	502	DEB	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	E	502	DEB	C1-C2-C3-C4
3	E	502	DEB	C1-C2-C3-O19
3	F	502	DEB	C1-C2-C3-C4
3	F	502	DEB	C1-C2-C3-O19
3	F	502	DEB	C20-C4-C5-C6
3	A	502	DEB	C23-C8-C9-O24
3	D	502	DEB	C23-C8-C9-O24
3	E	502	DEB	C23-C8-C9-O24
3	F	502	DEB	C4-C5-C6-C22
3	A	502	DEB	C7-C8-C9-O24
3	D	502	DEB	C7-C8-C9-O24
3	E	502	DEB	C7-C8-C9-O24
3	F	502	DEB	C7-C8-C9-O24

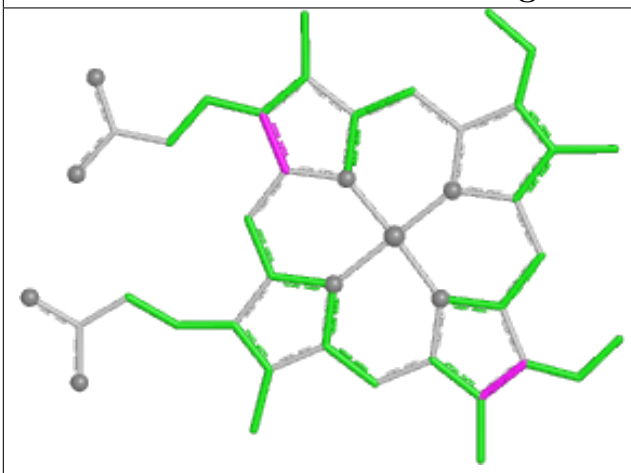
There are no ring outliers.

9 monomers are involved in 31 short contacts:

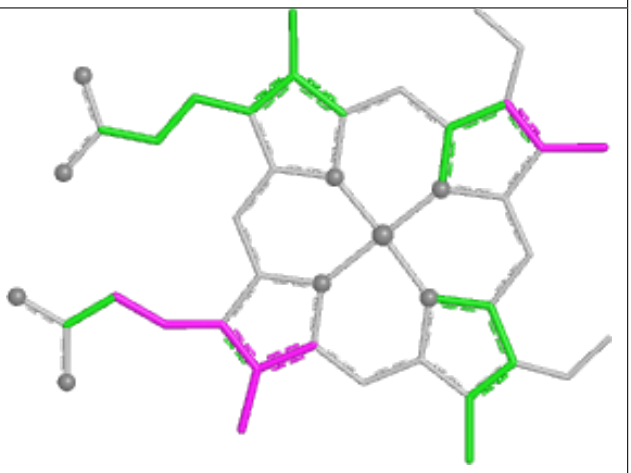
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	7	0
2	D	501	HEM	7	0
2	E	501	HEM	2	0
3	D	502	DEB	1	0
3	F	502	DEB	1	0
2	A	501	HEM	4	0
2	B	501	HEM	5	0
4	A	504	FMT	1	0
2	F	501	HEM	4	0

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.

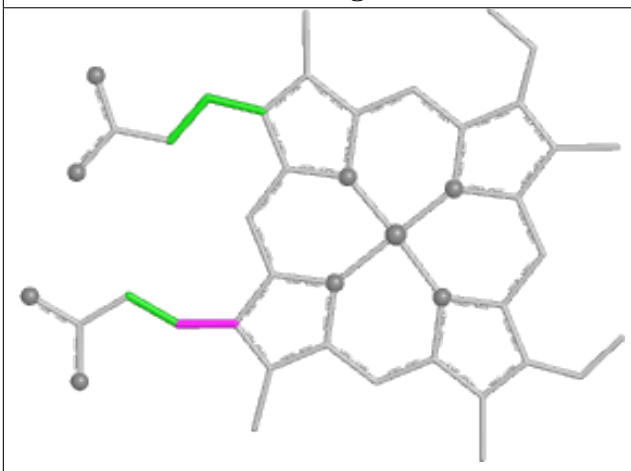
Ligand HEM C 501



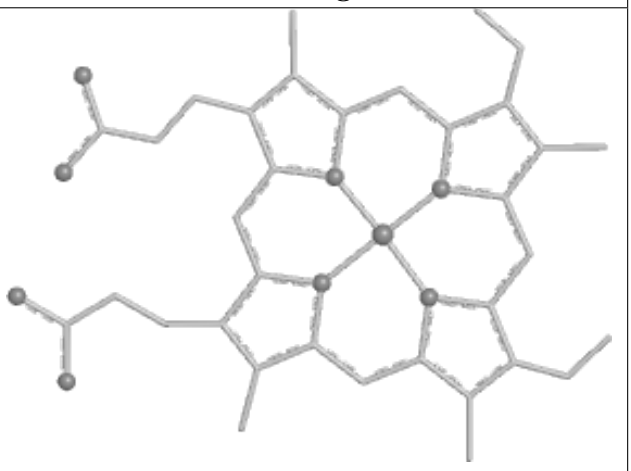
Bond lengths



Bond angles

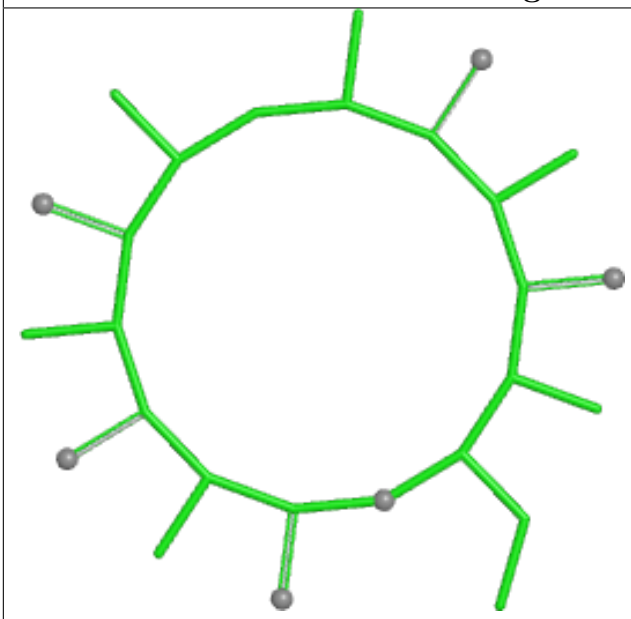


Torsions

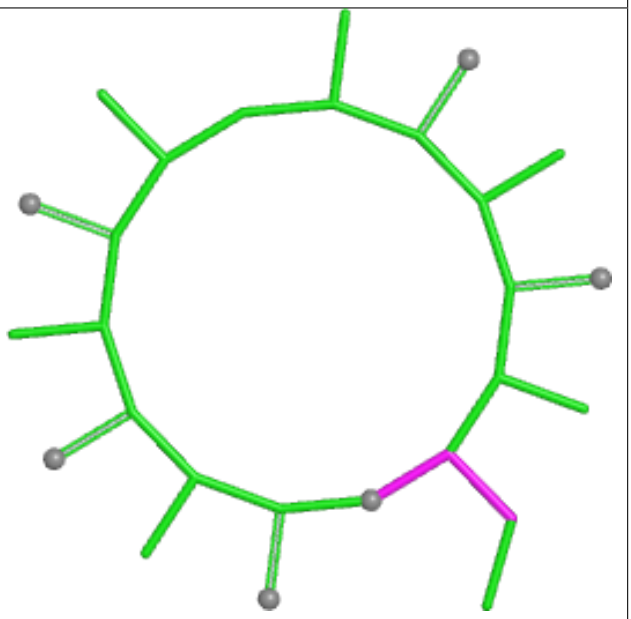


Rings

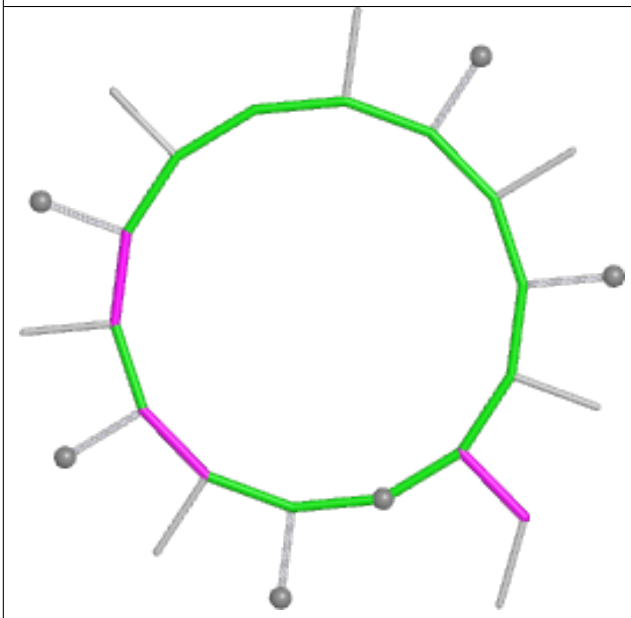
Ligand DEB B 502



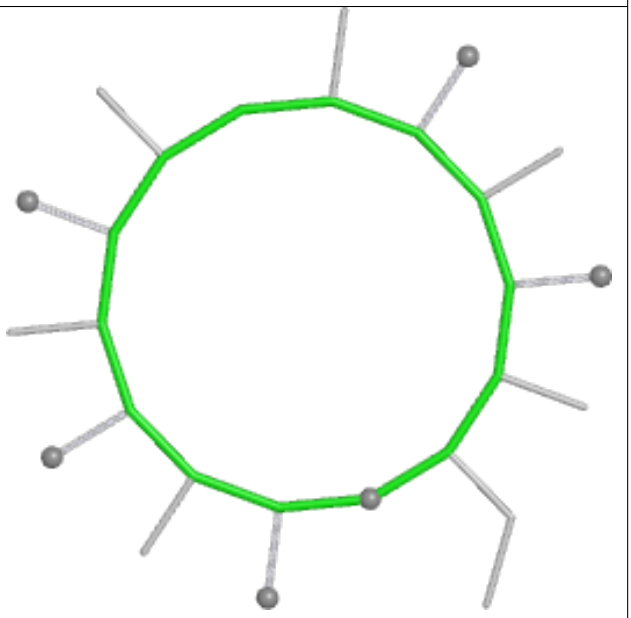
Bond lengths



Bond angles

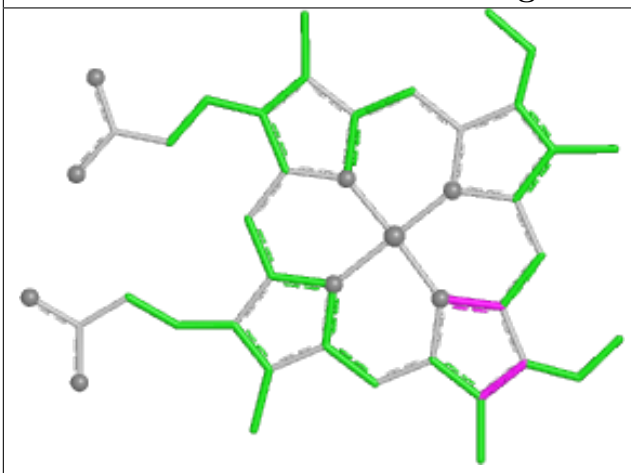


Torsions

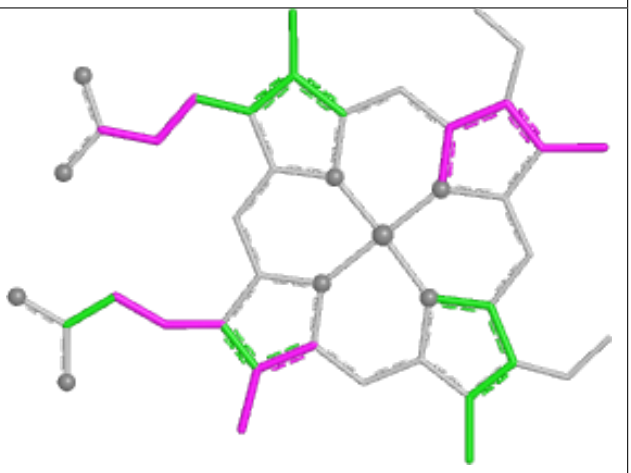


Rings

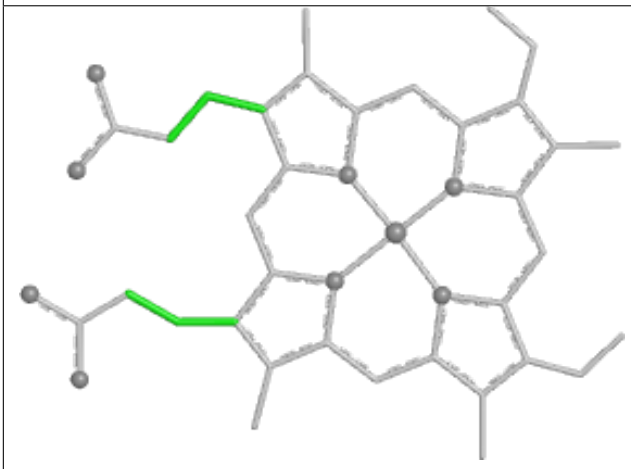
Ligand HEM D 501



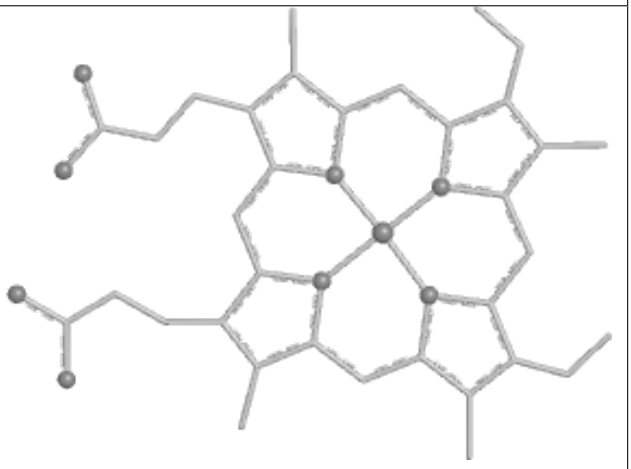
Bond lengths



Bond angles

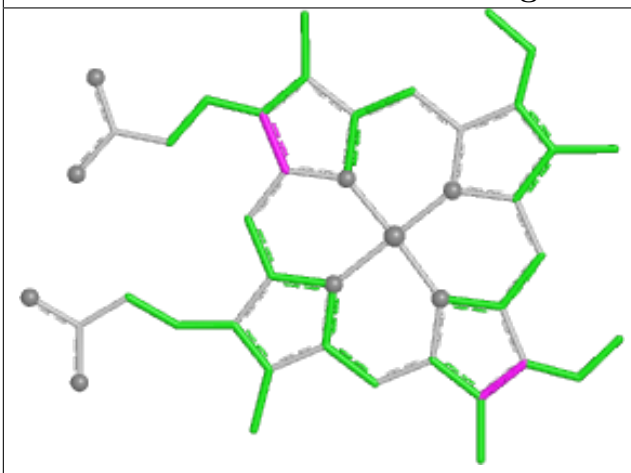


Torsions

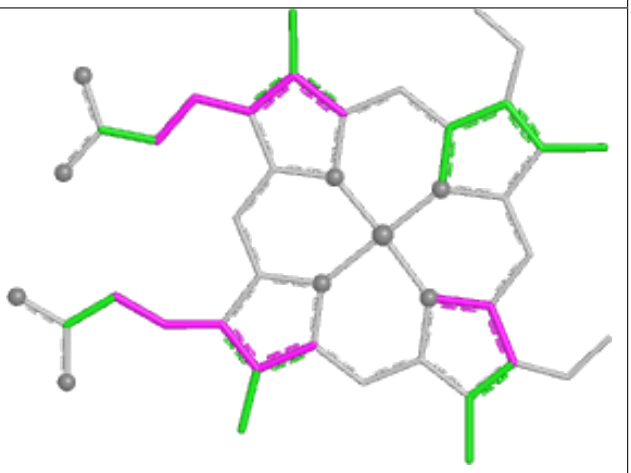


Rings

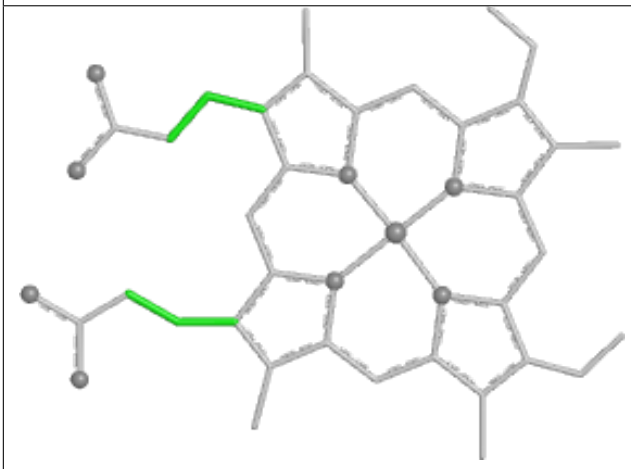
Ligand HEM E 501



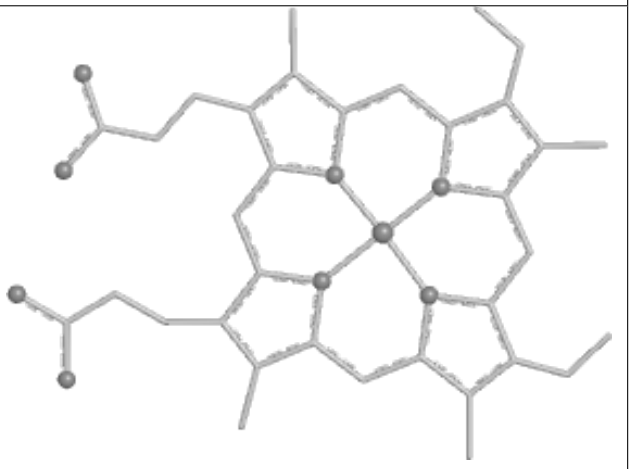
Bond lengths



Bond angles

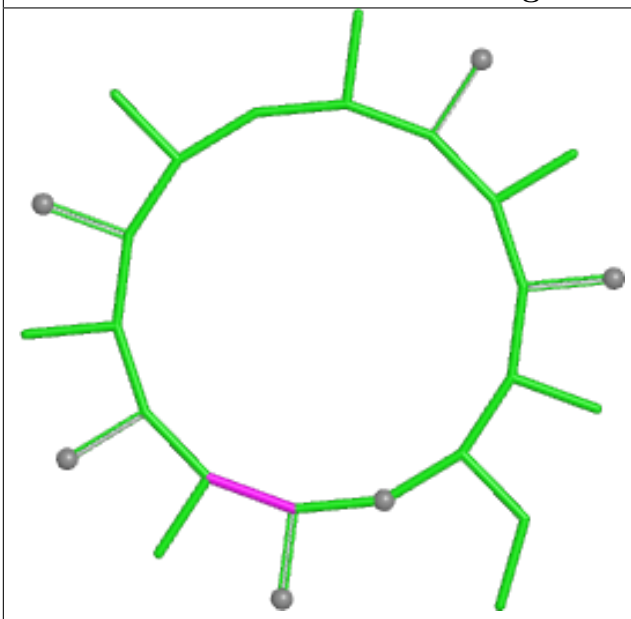


Torsions

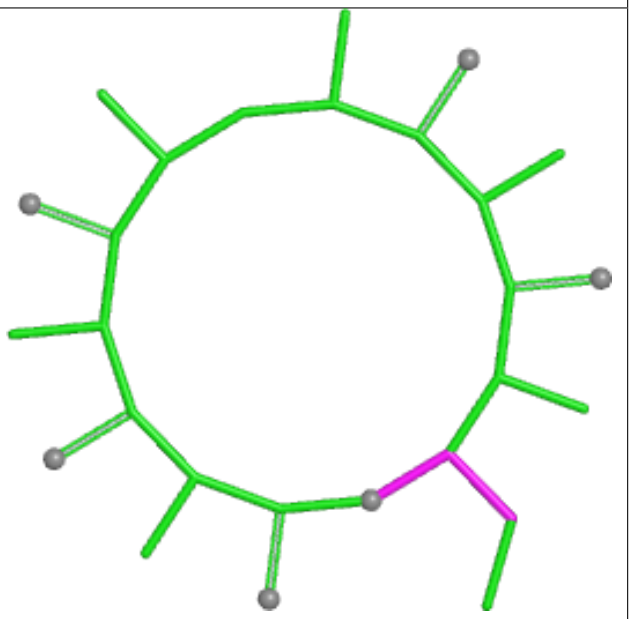


Rings

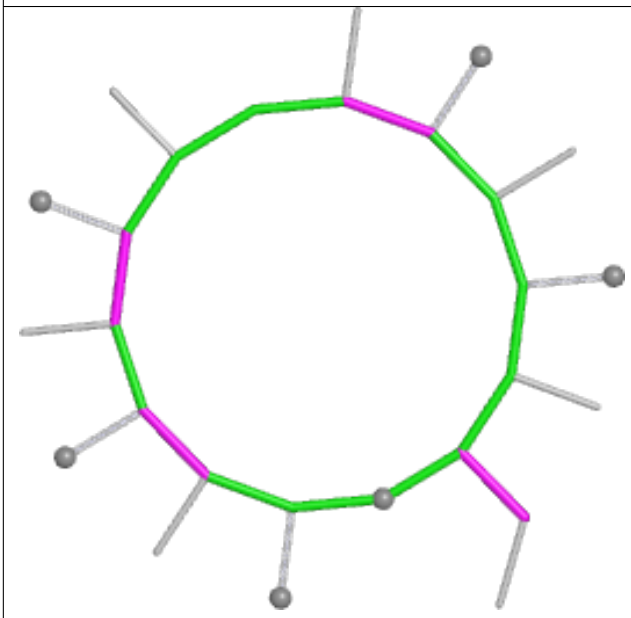
Ligand DEB D 502



Bond lengths



Bond angles



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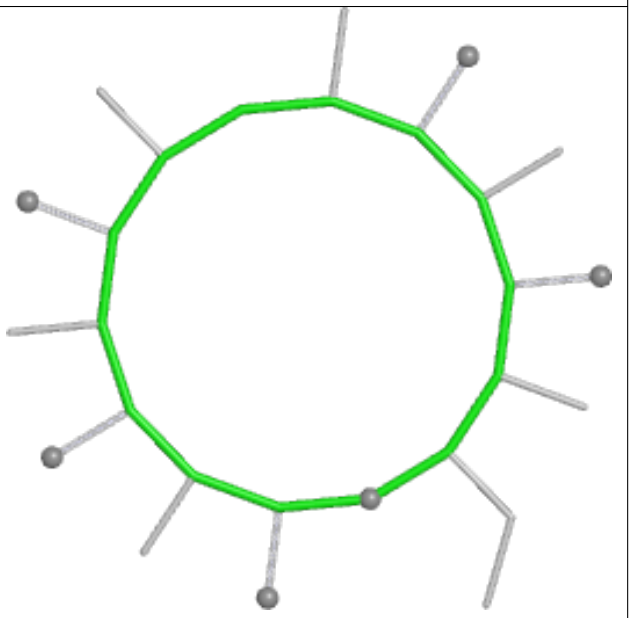
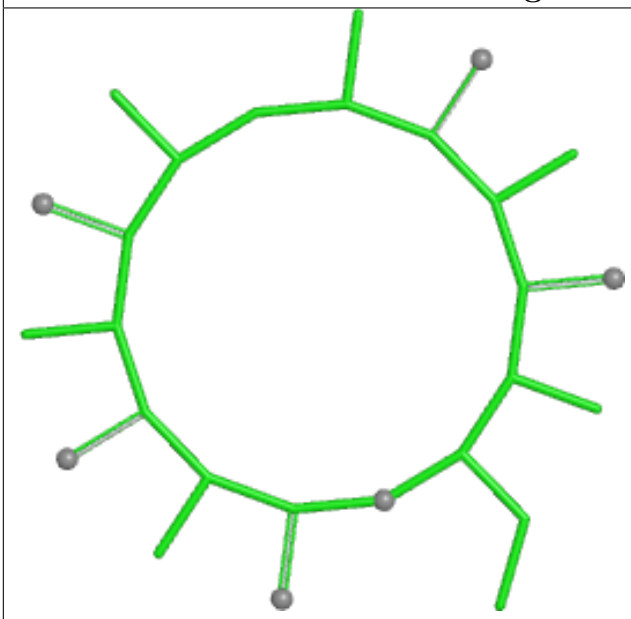
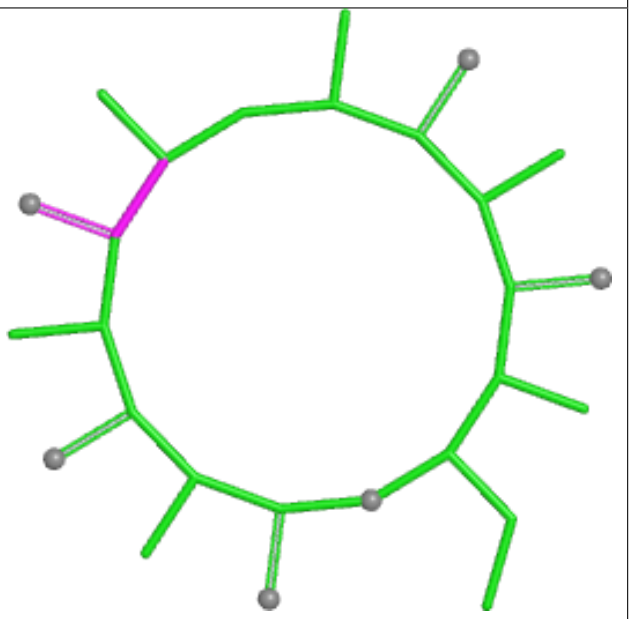


Rings

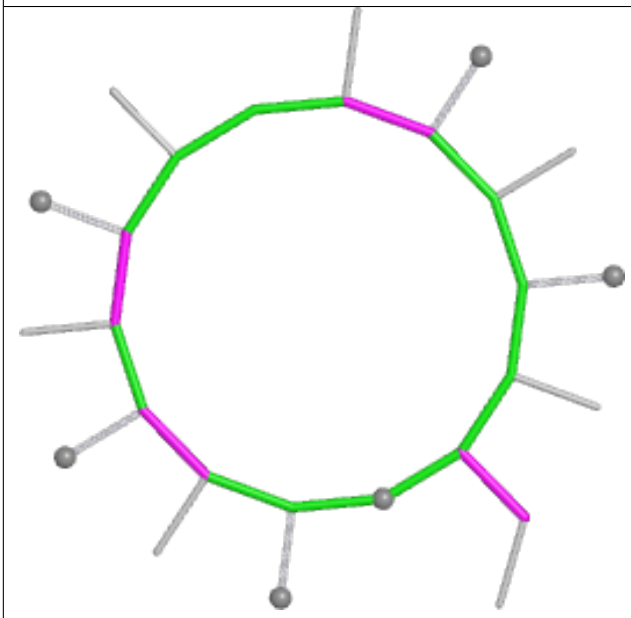
Ligand DEB E 502



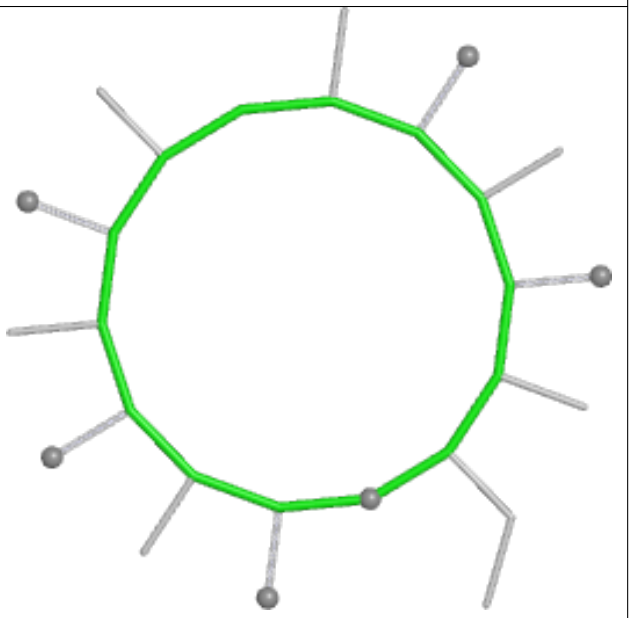
Bond lengths



Bond angles

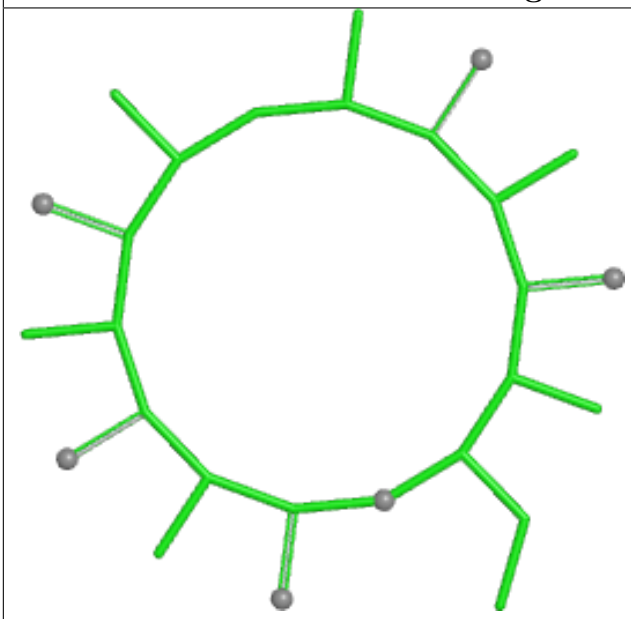


Torsions

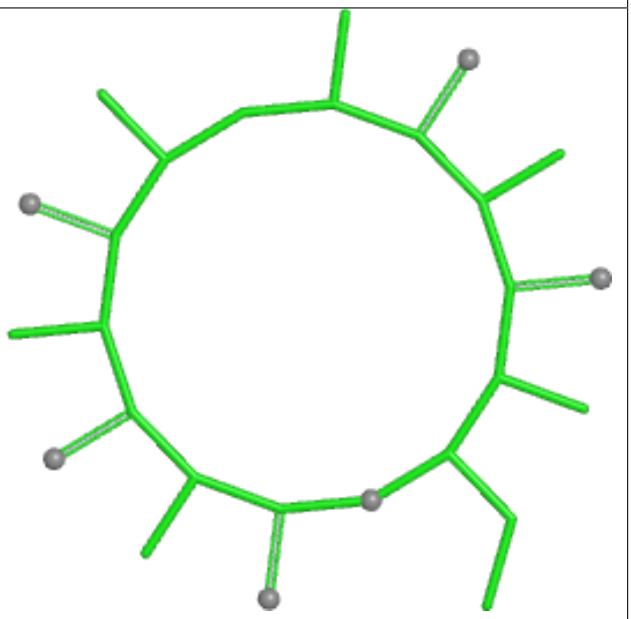


Rings

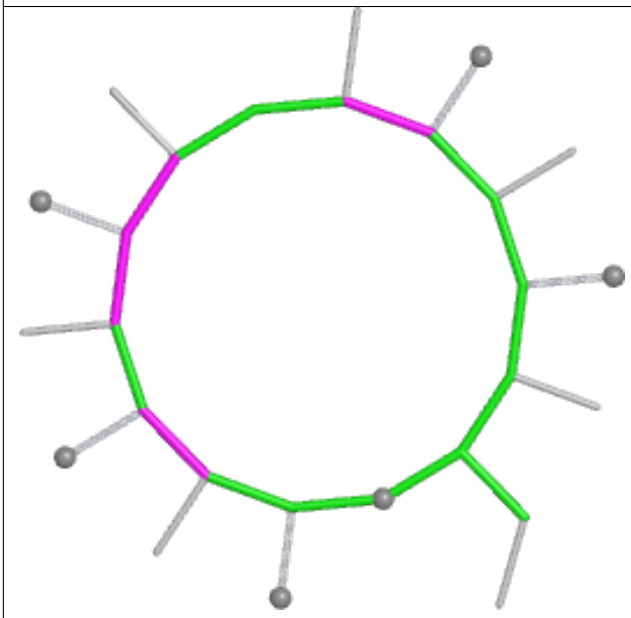
Ligand DEB F 502



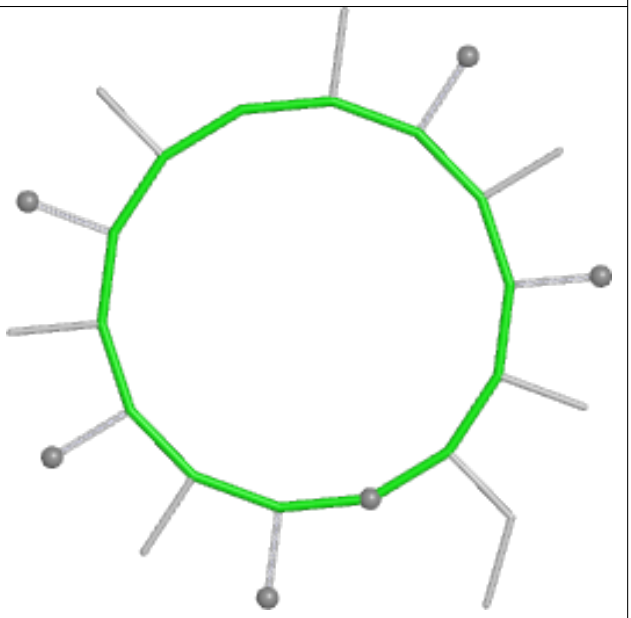
Bond lengths



Bond angles

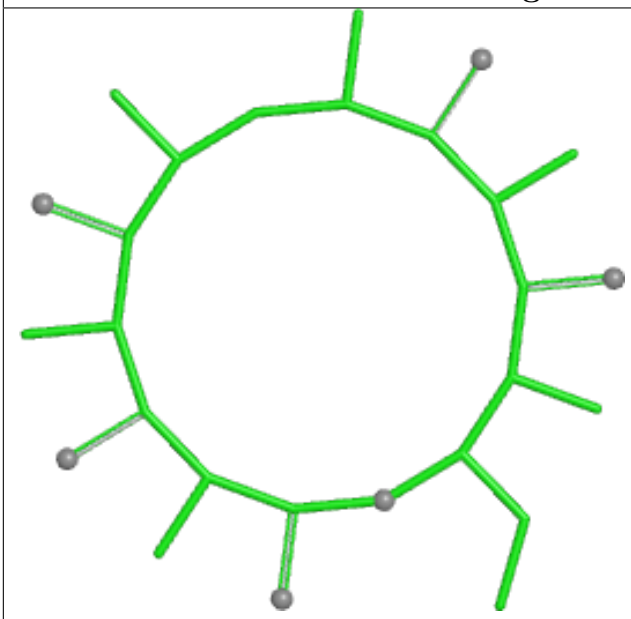


Torsions

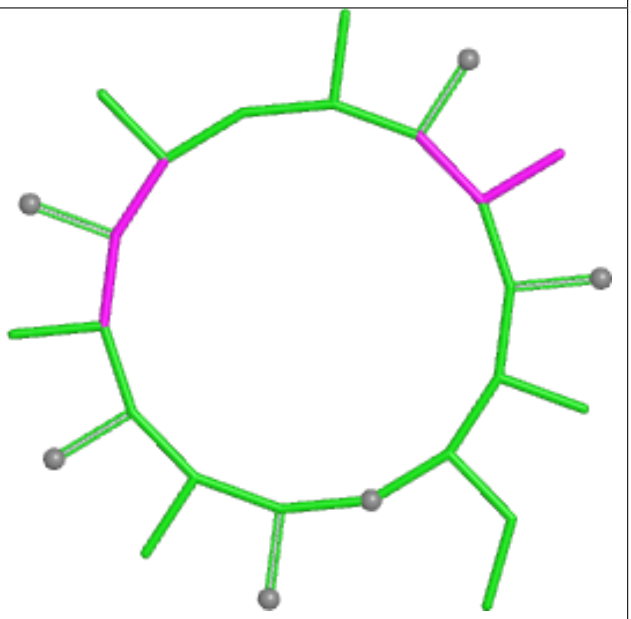


Rings

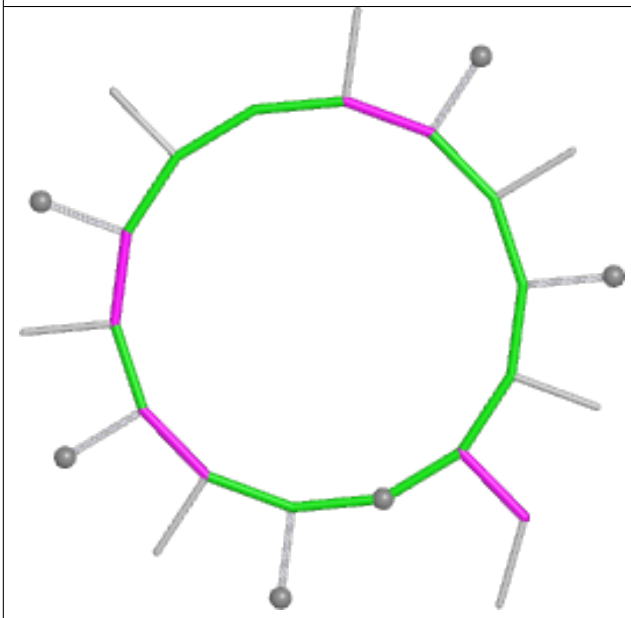
Ligand DEB A 502



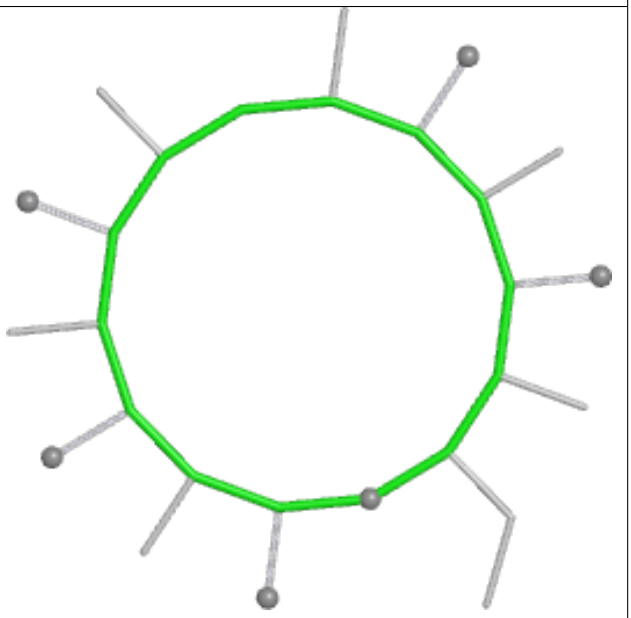
Bond lengths



Bond angles

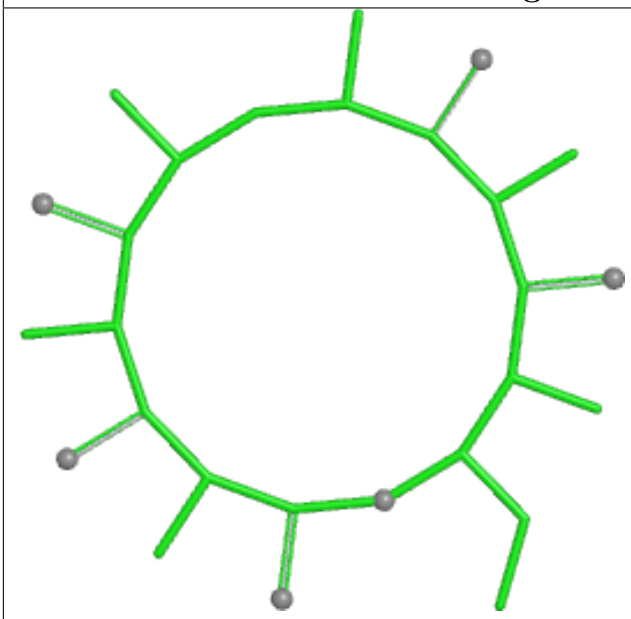


Torsions

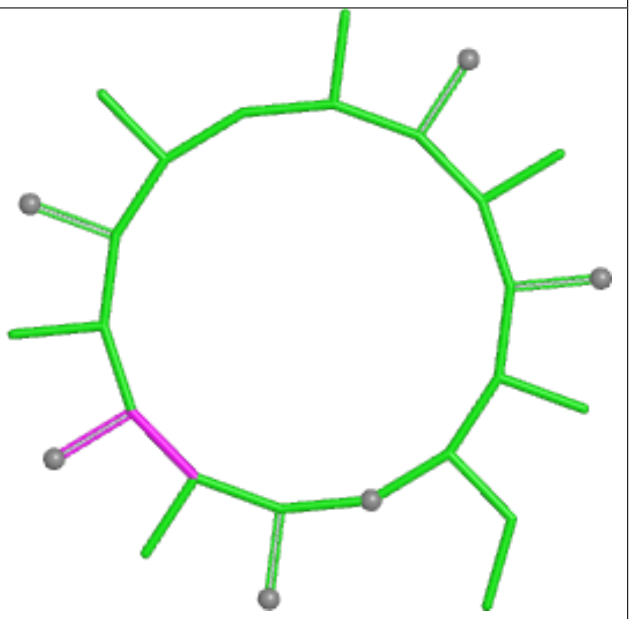


Rings

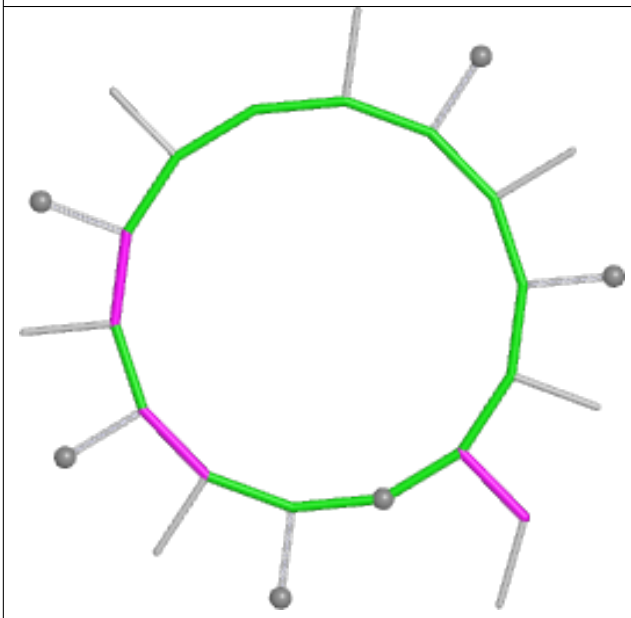
Ligand DEB C 502



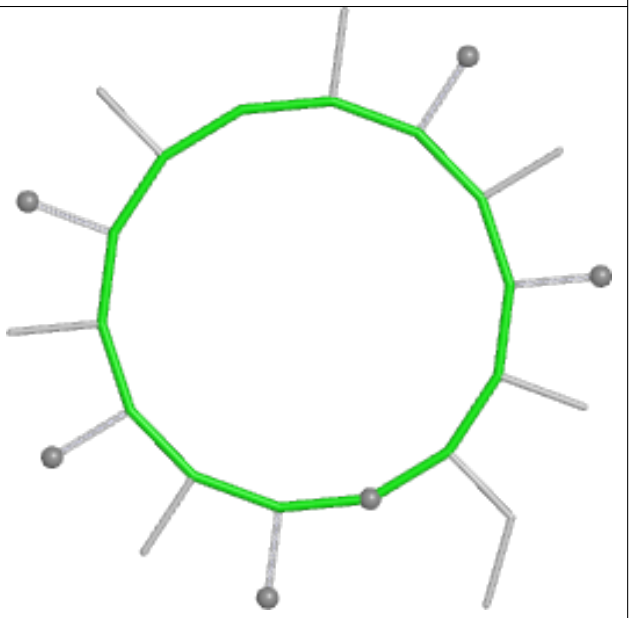
Bond lengths



Bond angles

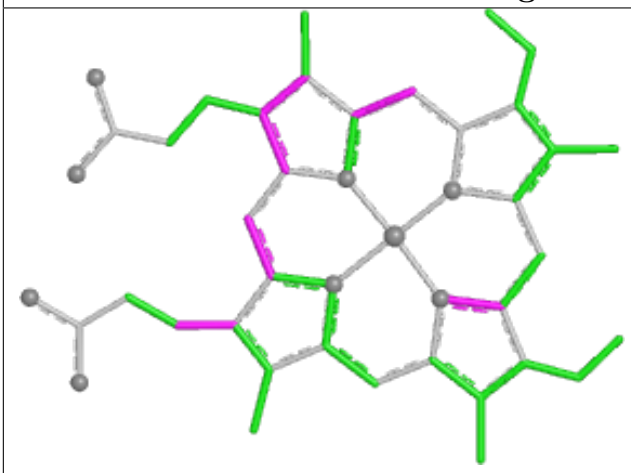


Torsions

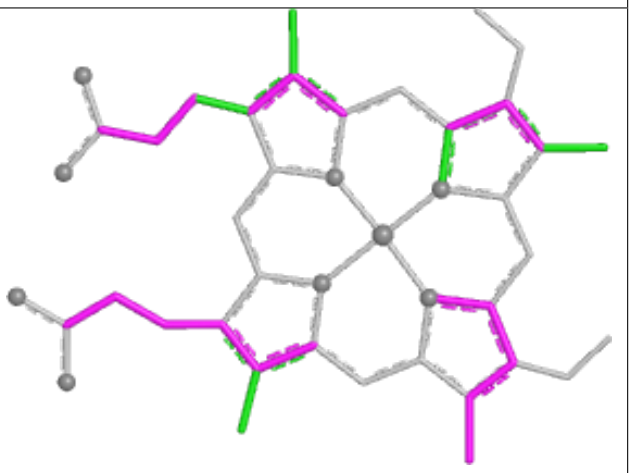


Rings

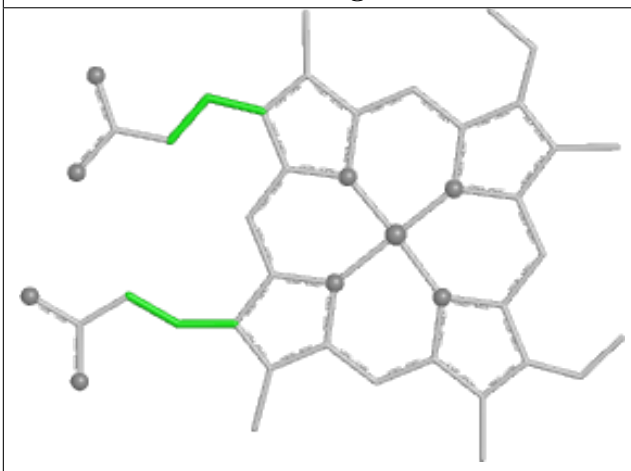
Ligand HEM A 501



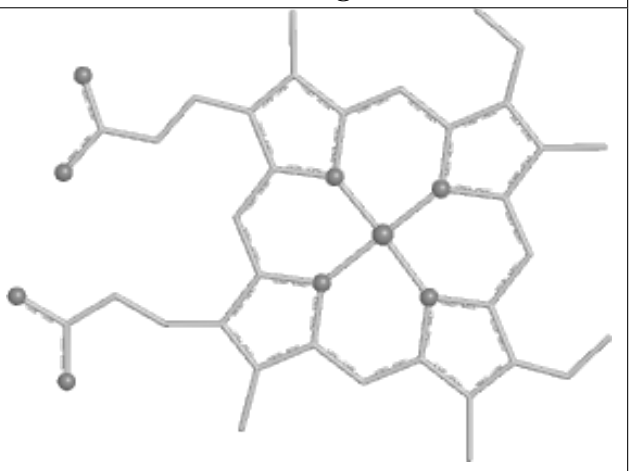
Bond lengths



Bond angles

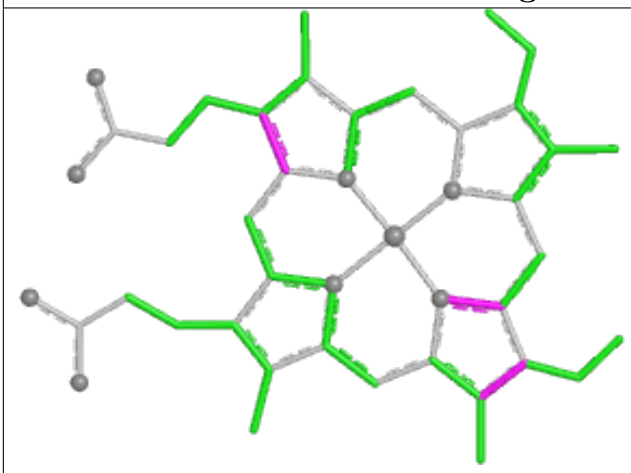


Torsions

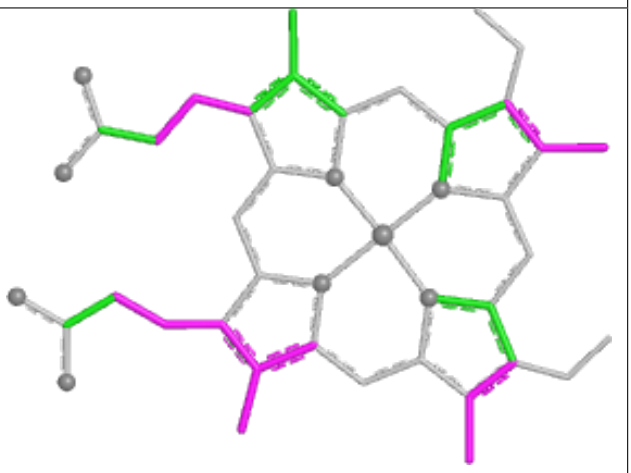


Rings

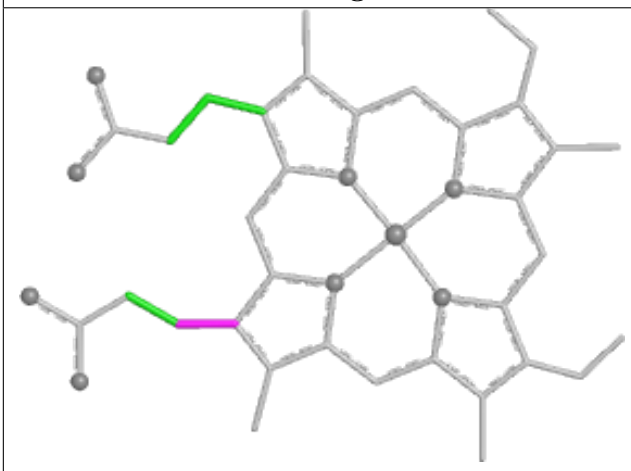
Ligand HEM B 501



Bond lengths



Bond angles



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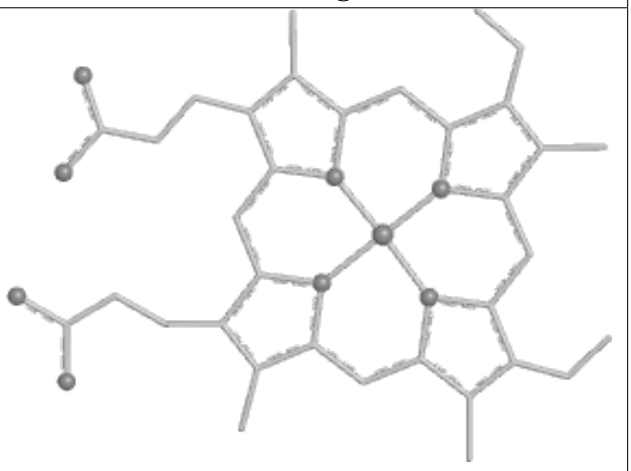
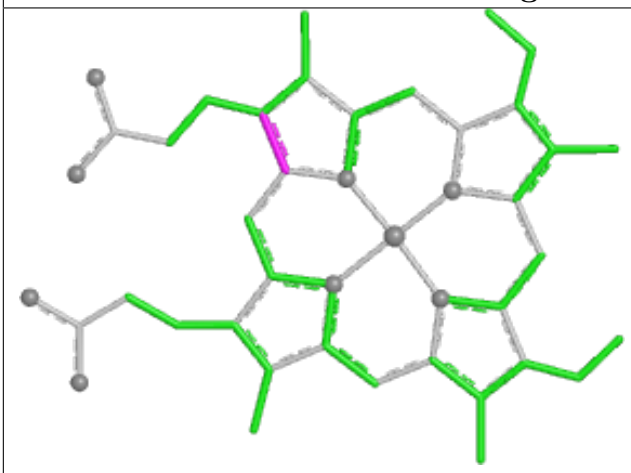
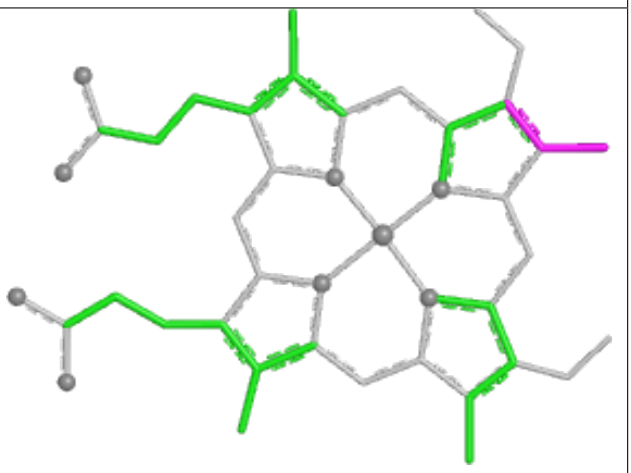


Rings

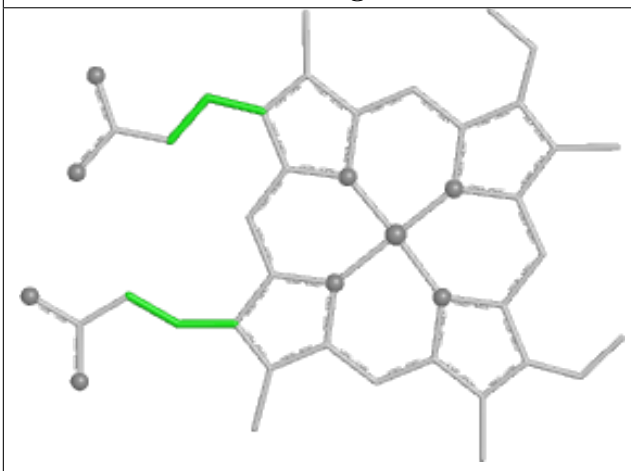
Ligand HEM F 501



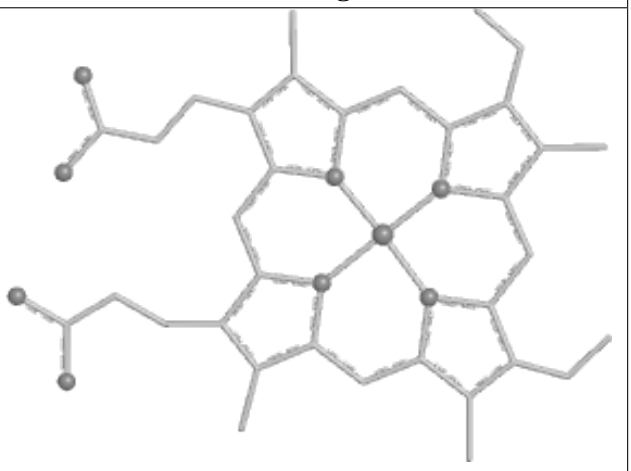
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	397/406 (97%)	0.84	38 (9%) 8 6	40, 60, 85, 129	0
1	B	406/406 (100%)	0.78	37 (9%) 9 7	35, 59, 89, 168	0
1	C	399/406 (98%)	0.77	20 (5%) 28 27	41, 55, 75, 98	0
1	D	396/406 (97%)	1.06	63 (15%) 1 1	46, 73, 100, 148	0
1	E	395/406 (97%)	1.54	124 (31%) 0 0	51, 74, 104, 150	0
1	F	397/406 (97%)	1.93	134 (33%) 0 0	54, 80, 115, 135	0
All	All	2390/2436 (98%)	1.15	416 (17%) 1 1	35, 66, 103, 168	0

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9[A]	THR	20.2
1	C	10[A]	PRO	12.7
1	F	129[A]	ASP	11.9
1	F	405	VAL	10.1
1	F	277	VAL	9.8
1	F	125[A]	ARG	9.5
1	F	364	LEU	9.4
1	F	127[A]	LEU	9.2
1	F	262	THR	9.0
1	F	124	VAL	8.5
1	F	224[A]	ASP	8.4
1	D	223	THR	8.3
1	B	209[A]	ASP	8.2
1	E	23	HIS	8.1
1	E	212	THR	7.7
1	F	385	PRO	7.6
1	F	126	SER	7.4
1	F	328[A]	GLU	7.3
1	B	3	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	E	209	ASP	6.9
1	F	132	LEU	6.8
1	F	11	ALA	6.7
1	E	335[A]	ASP	6.6
1	F	273	ASP	6.4
1	E	265[A]	LYS	6.2
1	E	313	ALA	6.0
1	E	226[A]	ASP	6.0
1	F	270[A]	LEU	6.0
1	F	377	PHE	5.9
1	F	269[A]	SER	5.9
1	E	306	LEU	5.8
1	F	271	VAL	5.8
1	F	267	TYR	5.8
1	F	130	SER	5.8
1	F	327	ASP	5.8
1	F	376	ARG	5.7
1	F	141	PRO	5.6
1	E	312[A]	ARG	5.6
1	D	333	HIS	5.6
1	F	23[A]	HIS	5.6
1	B	211	PRO	5.5
1	E	207	ARG	5.5
1	D	208[A]	ARG	5.4
1	A	224[A]	ASP	5.3
1	D	227[B]	ASP	5.3
1	E	332	ASP	5.2
1	E	98	PRO	5.2
1	C	11[A]	ALA	5.2
1	F	248	THR	5.2
1	A	11	ALA	5.1
1	F	382	LEU	5.1
1	F	12	ASP	5.0
1	E	71	SER	5.0
1	B	4	THR	5.0
1	F	263[A]	GLU	5.0
1	F	123[A]	ARG	5.0
1	E	90	PRO	5.0
1	E	24	ALA	4.9
1	F	406	SER	4.9
1	E	223	THR	4.9
1	A	209[A]	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	400	LEU	4.8
1	D	263[A]	GLU	4.8
1	F	393[A]	GLN	4.8
1	F	272	ALA	4.7
1	F	307	SER	4.7
1	F	343[A]	ARG	4.7
1	F	58	MET	4.7
1	D	210	ALA	4.6
1	B	265[A]	LYS	4.6
1	F	332	ASP	4.6
1	E	308	THR	4.6
1	E	39	PRO	4.5
1	E	229	LEU	4.5
1	F	337[A]	LEU	4.5
1	D	205	ALA	4.5
1	D	115[A]	ARG	4.4
1	D	138[A]	HIS	4.4
1	E	305[A]	GLU	4.4
1	D	191[A]	ARG	4.4
1	F	340	HIS	4.4
1	E	13	ALA	4.4
1	F	38	GLU	4.4
1	F	349	PHE	4.3
1	F	402[A]	ARG	4.3
1	E	60	ASP	4.3
1	D	225[A]	ASN	4.3
1	F	365[A]	GLU	4.3
1	F	384[A]	GLU	4.2
1	E	327	ASP	4.2
1	B	225[A]	ASN	4.2
1	F	386	VAL	4.2
1	B	115[A]	ARG	4.2
1	D	406	SER	4.2
1	D	27[A]	LEU	4.2
1	B	228[A]	HIS	4.1
1	F	347	ILE	4.1
1	E	211	PRO	4.1
1	E	208	ARG	4.1
1	F	225[A]	ASN	4.1
1	E	64	VAL	4.1
1	F	308	THR	4.1
1	E	336[A]	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	137	ALA	4.1
1	B	333	HIS	4.0
1	D	224[A]	ASP	4.0
1	E	107[A]	LEU	4.0
1	E	261	LEU	4.0
1	D	209[A]	ASP	4.0
1	E	311	VAL	4.0
1	A	38[A]	GLU	4.0
1	F	60	ASP	4.0
1	B	272	ALA	4.0
1	F	280	ALA	4.0
1	B	332	ASP	4.0
1	F	131	LEU	4.0
1	F	333	HIS	3.9
1	F	108	VAL	3.9
1	F	208[A]	ARG	3.9
1	D	222	ALA	3.9
1	E	76	THR	3.9
1	B	2	ALA	3.8
1	F	388	GLY	3.8
1	E	213[A]	GLU	3.8
1	F	213[A]	GLU	3.8
1	F	339	PHE	3.8
1	E	333	HIS	3.8
1	D	268	GLU	3.8
1	E	110[A]	LYS	3.8
1	F	284[A]	MET	3.7
1	F	380	LEU	3.7
1	E	228[A]	HIS	3.7
1	F	276	LEU	3.7
1	E	189	ILE	3.7
1	F	140	SER	3.7
1	B	342[A]	GLU	3.6
1	F	37	ASP	3.6
1	F	188[A]	GLU	3.6
1	E	382	LEU	3.6
1	B	214	ASP	3.6
1	F	117	VAL	3.6
1	E	302[A]	GLU	3.6
1	E	271	VAL	3.6
1	E	304	VAL	3.6
1	F	375[A]	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	37	ASP	3.5
1	E	385	PRO	3.5
1	F	379	THR	3.5
1	D	270	LEU	3.5
1	B	222	ALA	3.5
1	D	266	ARG	3.4
1	A	220	ALA	3.4
1	A	267	TYR	3.4
1	C	222	ALA	3.4
1	F	128	VAL	3.4
1	D	123[A]	ARG	3.4
1	F	371	SER	3.3
1	E	383	ALA	3.3
1	C	328[A]	GLU	3.3
1	D	271	VAL	3.3
1	F	244	ALA	3.3
1	A	210	ALA	3.3
1	A	211	PRO	3.3
1	E	338	ASP	3.3
1	D	393[A]	GLN	3.3
1	E	22	PRO	3.3
1	D	332	ASP	3.3
1	A	262	THR	3.3
1	E	309	VAL	3.3
1	D	342[A]	GLU	3.3
1	E	106[A]	ARG	3.3
1	D	220	ALA	3.3
1	B	10	PRO	3.3
1	F	330	VAL	3.2
1	A	328[A]	GLU	3.2
1	A	271	VAL	3.2
1	F	309	VAL	3.2
1	E	73	ALA	3.2
1	E	210	ALA	3.2
1	F	215	LEU	3.2
1	F	342[A]	GLU	3.2
1	F	183[A]	ARG	3.2
1	E	287	TYR	3.2
1	D	141	PRO	3.1
1	E	342[A]	GLU	3.1
1	E	77	ASP	3.1
1	E	136	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	188[A]	GLU	3.1
1	F	36[A]	ARG	3.1
1	D	407	TRP	3.1
1	F	191[A]	ARG	3.1
1	B	136[A]	VAL	3.1
1	B	5	HIS	3.1
1	F	268[A]	GLU	3.1
1	F	142	ALA	3.1
1	F	146[A]	GLU	3.1
1	A	228[A]	HIS	3.1
1	E	25	LEU	3.0
1	E	268	GLU	3.0
1	F	61	ALA	3.0
1	E	163	VAL	3.0
1	F	383	ALA	3.0
1	F	287	TYR	3.0
1	F	165	LEU	3.0
1	F	118	GLU	3.0
1	F	21[A]	LEU	3.0
1	F	329[A]	GLU	3.0
1	D	107[A]	LEU	3.0
1	A	342[A]	GLU	3.0
1	F	278	PRO	3.0
1	B	406	SER	3.0
1	F	245	GLY	3.0
1	E	337	LEU	2.9
1	C	307	SER	2.9
1	A	13	ALA	2.9
1	E	264	ARG	2.9
1	F	173	THR	2.9
1	B	210	ALA	2.9
1	E	227[A]	ASP	2.9
1	F	119[A]	GLU	2.9
1	A	141	PRO	2.9
1	E	307	SER	2.9
1	A	123[A]	ARG	2.9
1	E	159	GLU	2.9
1	F	27	LEU	2.8
1	C	271	VAL	2.8
1	F	389	LEU	2.8
1	E	129	ASP	2.8
1	F	331	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	109	GLY	2.8
1	B	235	VAL	2.8
1	E	42	ARG	2.8
1	E	299	VAL	2.8
1	F	395	MET	2.8
1	A	76	THR	2.8
1	C	223	THR	2.8
1	F	110[A]	LYS	2.8
1	A	206[A]	GLN	2.8
1	E	328[A]	GLU	2.8
1	B	327	ASP	2.8
1	A	221	LEU	2.8
1	D	219	LEU	2.8
1	D	108	VAL	2.7
1	F	336[A]	GLU	2.7
1	D	261	LEU	2.7
1	A	329	GLU	2.7
1	E	389	LEU	2.7
1	F	261	LEU	2.7
1	E	141	PRO	2.7
1	F	346	HIS	2.7
1	E	33[A]	GLU	2.7
1	A	407	TRP	2.7
1	E	303	ASP	2.7
1	F	174	PHE	2.7
1	B	221	LEU	2.7
1	A	335[A]	ASP	2.7
1	A	334	ALA	2.7
1	F	229	LEU	2.7
1	C	343[A]	ARG	2.7
1	E	391	TRP	2.7
1	C	308	THR	2.6
1	C	332	ASP	2.6
1	E	277	VAL	2.6
1	F	274	PRO	2.6
1	E	257	VAL	2.6
1	E	34	LEU	2.6
1	D	12	ASP	2.6
1	D	327	ASP	2.6
1	C	36	ARG	2.6
1	D	334	ALA	2.6
1	A	12	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	183[A]	ARG	2.6
1	E	272	ALA	2.5
1	F	407	TRP	2.5
1	A	386	VAL	2.5
1	E	388	GLY	2.5
1	D	49[A]	GLU	2.5
1	B	357	ILE	2.5
1	E	244	ALA	2.5
1	F	260	LEU	2.5
1	D	182	THR	2.5
1	E	258	HIS	2.5
1	B	224[A]	ASP	2.5
1	B	359	ALA	2.5
1	F	288	THR	2.5
1	E	43	VAL	2.5
1	E	20	SER	2.5
1	F	390[A]	LYS	2.4
1	B	268	GLU	2.4
1	F	83	MET	2.4
1	F	206[A]	GLN	2.4
1	D	226[A]	ASP	2.4
1	E	69[A]	ARG	2.4
1	E	222	ALA	2.4
1	E	318	VAL	2.4
1	A	377	PHE	2.4
1	E	339	PHE	2.4
1	D	267	TYR	2.4
1	E	379	THR	2.4
1	F	370	LEU	2.4
1	C	407	TRP	2.4
1	F	148	LEU	2.4
1	D	44[A]	ARG	2.4
1	D	142	ALA	2.4
1	E	27	LEU	2.4
1	E	48	GLY	2.4
1	D	36[A]	ARG	2.4
1	E	263	GLU	2.4
1	D	120	MET	2.3
1	A	182	THR	2.3
1	E	387	ALA	2.3
1	E	66	GLY	2.3
1	D	147	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	333	HIS	2.3
1	E	300	ALA	2.3
1	F	46	PRO	2.3
1	F	338	ASP	2.3
1	D	336[A]	GLU	2.3
1	E	276	LEU	2.3
1	F	264	ARG	2.3
1	D	381	ASP	2.3
1	D	217	GLY	2.3
1	E	61	ALA	2.3
1	E	205	ALA	2.3
1	E	321	PHE	2.3
1	F	326	ARG	2.3
1	F	265[A]	LYS	2.3
1	D	38[A]	GLU	2.3
1	B	335[A]	ASP	2.3
1	C	184	LEU	2.3
1	E	406	SER	2.3
1	F	41	SER	2.3
1	B	226[A]	ASP	2.3
1	F	314	GLY	2.3
1	D	184	LEU	2.3
1	D	228[A]	HIS	2.3
1	E	142	ALA	2.3
1	C	208[A]	ARG	2.3
1	D	394	GLY	2.2
1	F	22	PRO	2.2
1	E	89	GLU	2.2
1	D	47	TYR	2.2
1	A	189	ILE	2.2
1	E	381	ASP	2.2
1	F	92	GLY	2.2
1	E	38	GLU	2.2
1	E	29	PRO	2.2
1	A	341	ARG	2.2
1	C	272	ALA	2.2
1	F	313	ALA	2.2
1	A	37	ASP	2.2
1	F	93	VAL	2.2
1	E	260	LEU	2.2
1	F	144[A]	LEU	2.2
1	B	11	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	177	ALA	2.2
1	D	50	GLY	2.2
1	F	404	ILE	2.2
1	E	298	ARG	2.2
1	C	52	ALA	2.2
1	E	134	ASP	2.2
1	F	182	THR	2.2
1	B	147	PHE	2.2
1	E	21	LEU	2.2
1	D	329[A]	GLU	2.2
1	D	202	GLY	2.2
1	F	210	ALA	2.2
1	B	208[A]	ARG	2.2
1	E	267	TYR	2.2
1	D	163	VAL	2.2
1	F	249	SER	2.2
1	E	158	CYS	2.2
1	F	79	ALA	2.2
1	E	57[A]	ARG	2.2
1	D	277	VAL	2.1
1	E	72	THR	2.1
1	D	189	ILE	2.1
1	E	31	TYR	2.1
1	E	405	VAL	2.1
1	F	31	TYR	2.1
1	E	301	THR	2.1
1	A	332	ASP	2.1
1	A	337	LEU	2.1
1	D	231[A]	LYS	2.1
1	E	378	PRO	2.1
1	E	230	THR	2.1
1	A	183	ARG	2.1
1	C	381	ASP	2.1
1	E	97	ASP	2.1
1	A	107	LEU	2.1
1	A	42[A]	ARG	2.1
1	E	273	ASP	2.1
1	F	169[A]	ASP	2.1
1	F	150	VAL	2.1
1	F	293	ALA	2.1
1	A	115[A]	ARG	2.1
1	A	83	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	227[A]	ASP	2.1
1	B	116[A]	ARG	2.0
1	E	36[A]	ARG	2.0
1	D	262	THR	2.0
1	F	34	LEU	2.0
1	F	47	TYR	2.0
1	B	230	THR	2.0
1	E	86	THR	2.0
1	E	407	TRP	2.0
1	D	216	LEU	2.0
1	E	215[A]	LEU	2.0
1	D	192	VAL	2.0
1	E	108	VAL	2.0
1	B	213[B]	GLU	2.0
1	E	340	HIS	2.0
1	A	192	VAL	2.0
1	E	14	VAL	2.0
1	E	204	VAL	2.0
1	E	386	VAL	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)

There are no monosaccharides in this entry.

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
4	FMT	E	503	3/3	0.51	0.50	81,81,93,93	0
4	FMT	C	503	3/3	0.58	0.31	96,96,97,100	0
4	FMT	A	504	3/3	0.61	0.42	91,91,94,98	0
4	FMT	D	503	3/3	0.65	0.35	98,98,101,102	0

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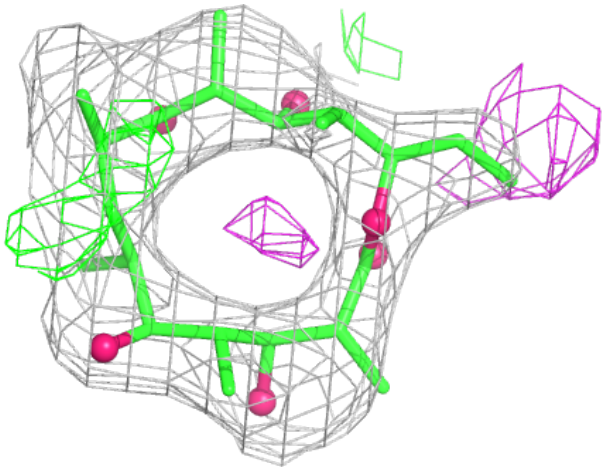
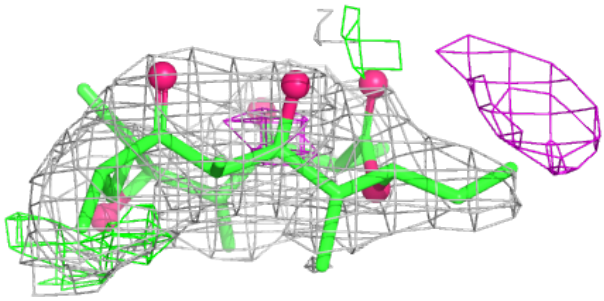
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DEB	F	502	27/27	0.73	0.32	66,74,81,87	0
4	FMT	A	503	3/3	0.76	0.17	87,87,92,93	0
2	HEM	E	501	43/43	0.79	0.24	44,51,57,58	0
2	HEM	F	501	43/43	0.83	0.29	55,62,69,75	0
3	DEB	E	502	27/27	0.83	0.28	58,63,67,68	0
3	DEB	C	502	27/27	0.85	0.28	46,52,56,57	0
4	FMT	A	505	3/3	0.86	0.26	59,59,62,66	0
3	DEB	D	502	27/27	0.87	0.32	58,64,68,78	0
3	DEB	A	502	27/27	0.88	0.28	45,49,52,54	0
3	DEB	B	502	27/27	0.92	0.28	47,50,55,57	0
2	HEM	A	501	43/43	0.93	0.21	38,42,47,48	0
2	HEM	D	501	43/43	0.93	0.24	40,43,55,61	0
2	HEM	B	501	43/43	0.94	0.23	36,40,49,52	0
2	HEM	C	501	43/43	0.95	0.23	39,43,48,54	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 DEB F 502:

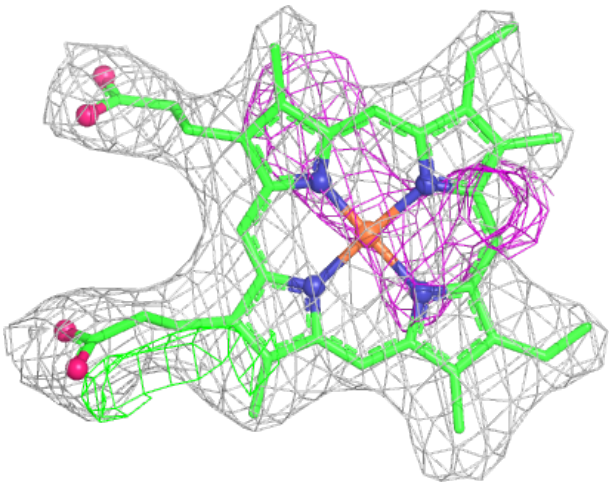
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

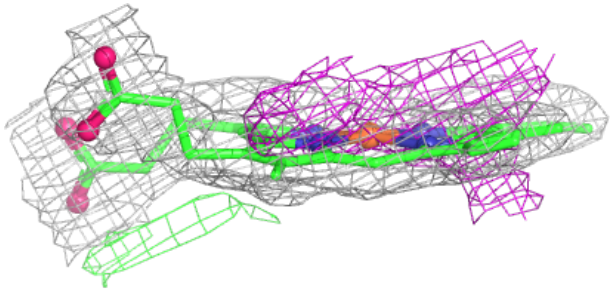


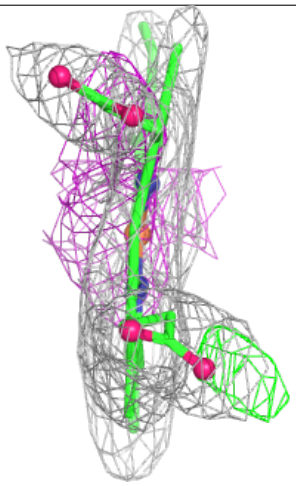


Electron density around HEM E 501:

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

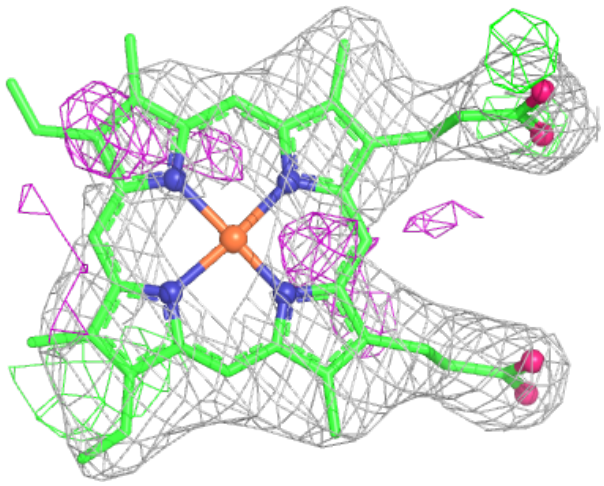


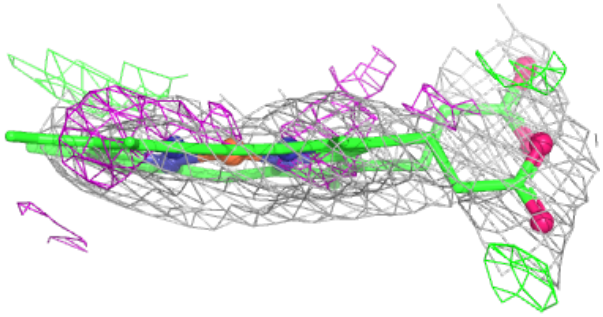




Electron density around HEM F 501:

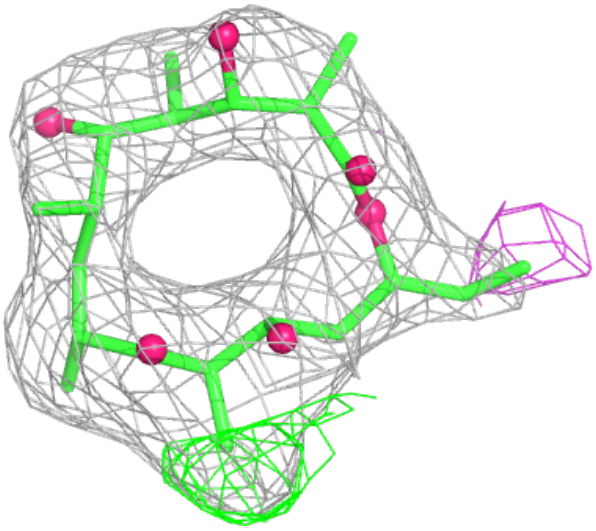
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

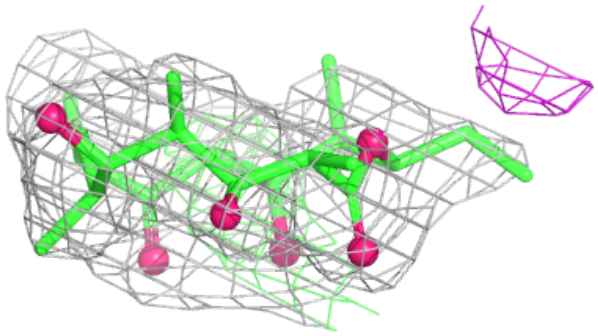


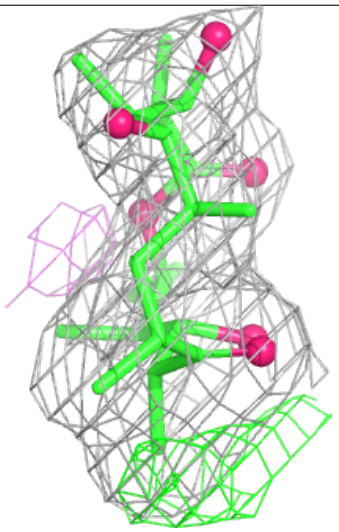


Electron density around DEB E 502:

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

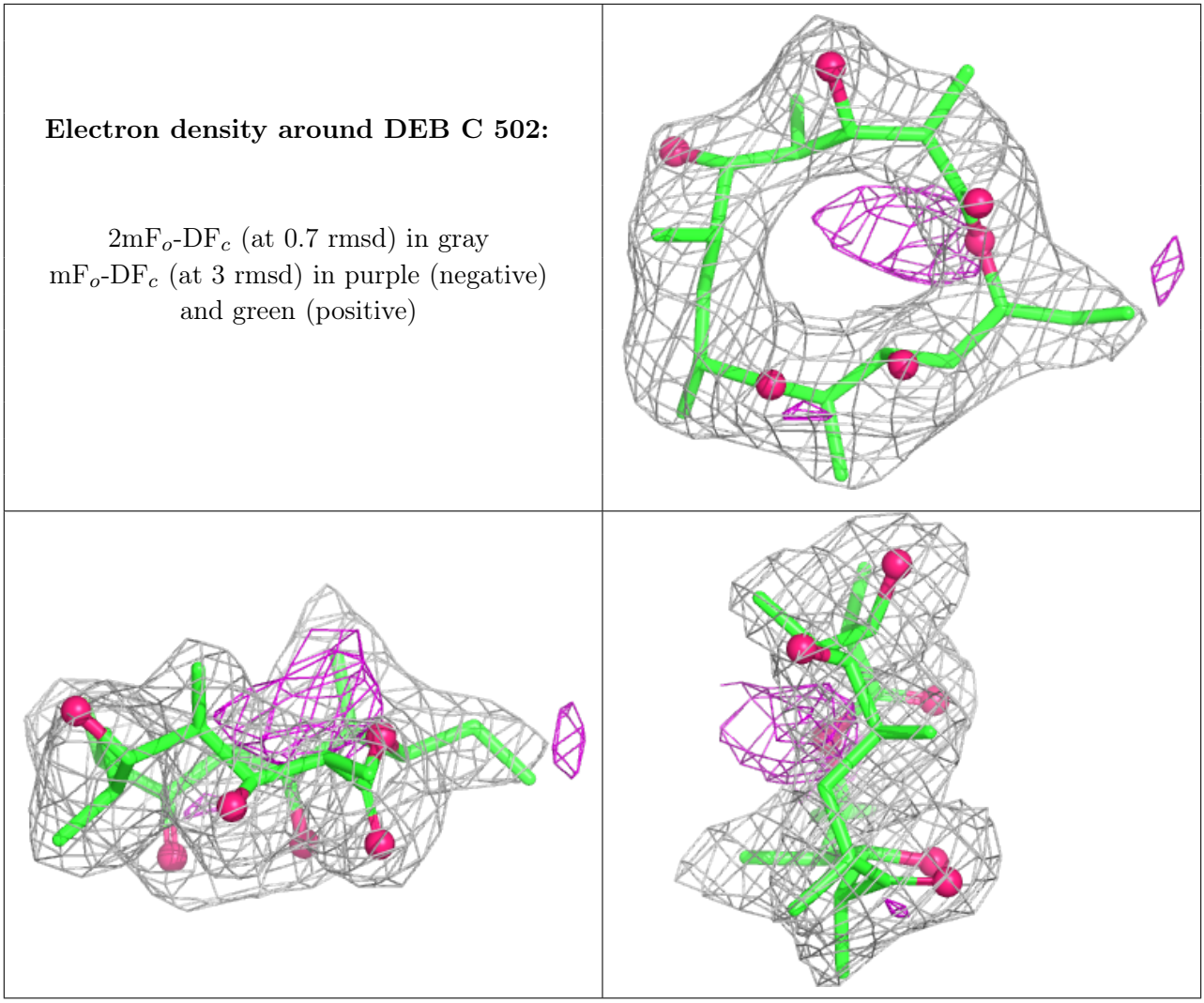






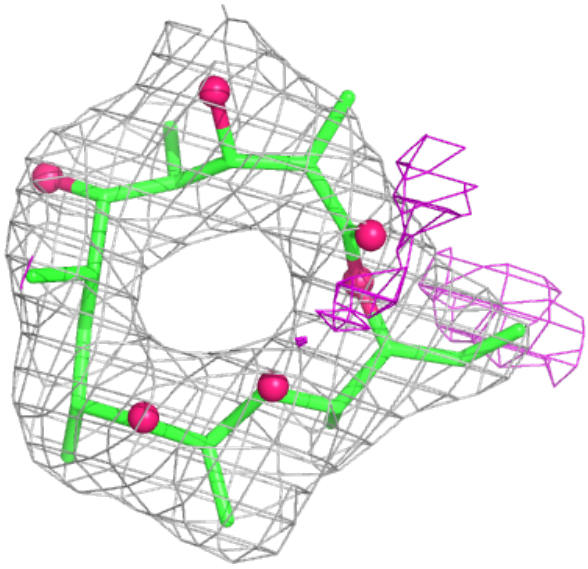
Electron density around DEB C 502:

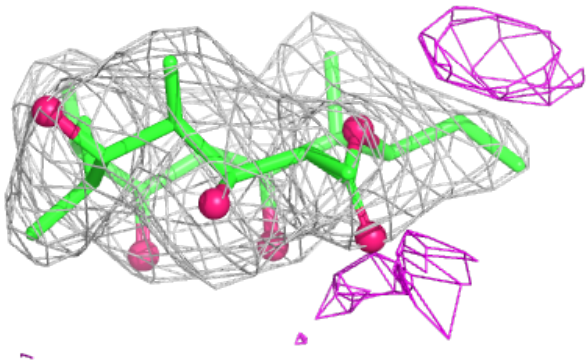
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

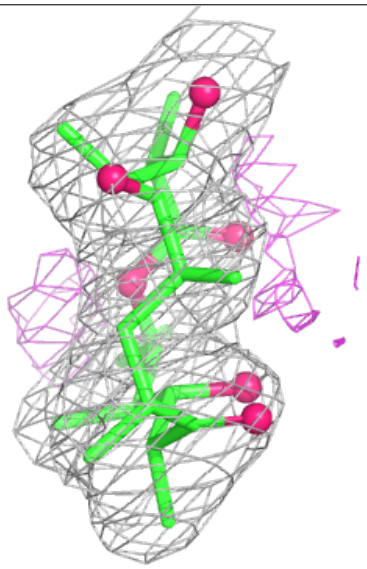


Electron density around DEB D 502:

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

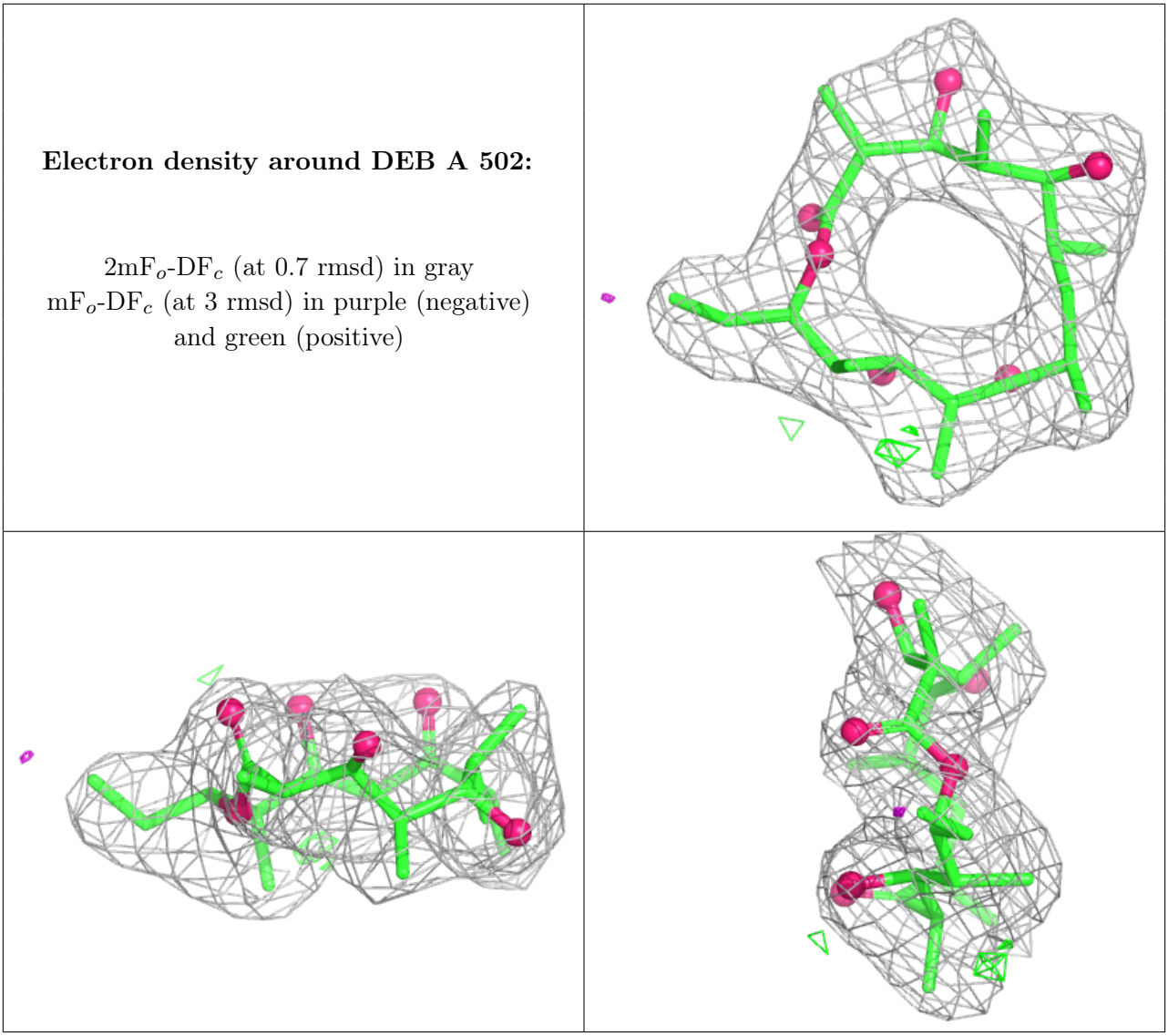






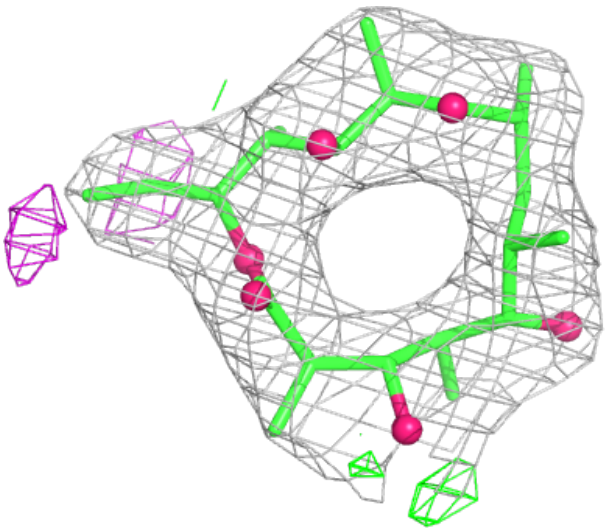
Electron density around DEB A 502:

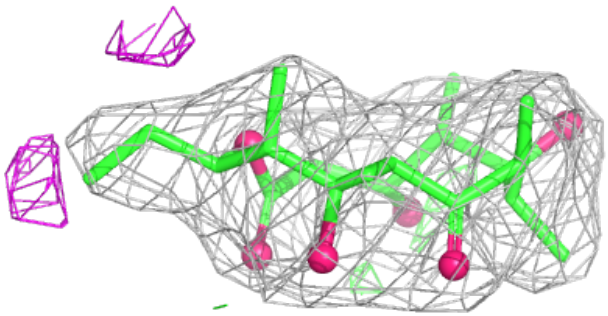
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

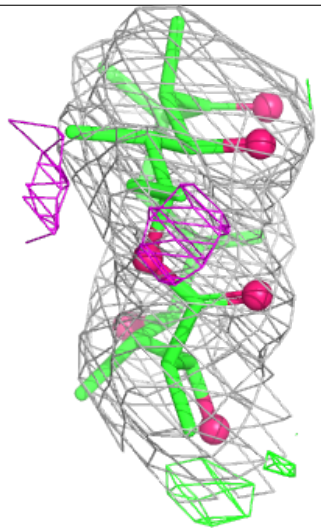


Electron density around DEB B 502:

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

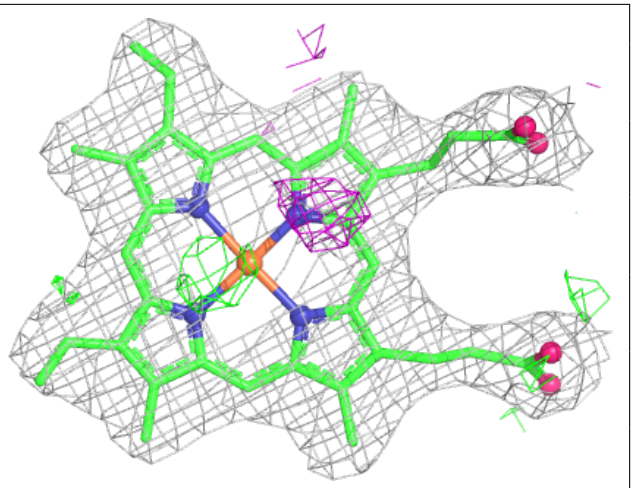


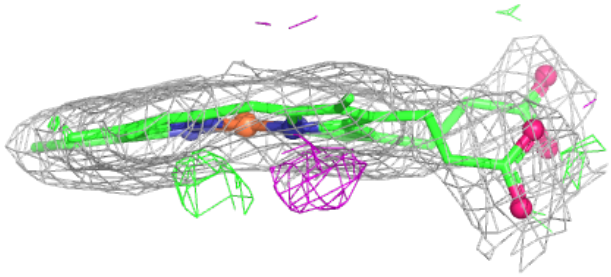


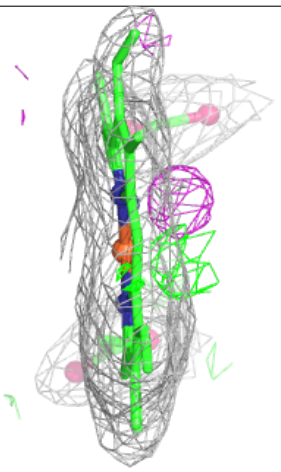


Electron density around HEM A 501:

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

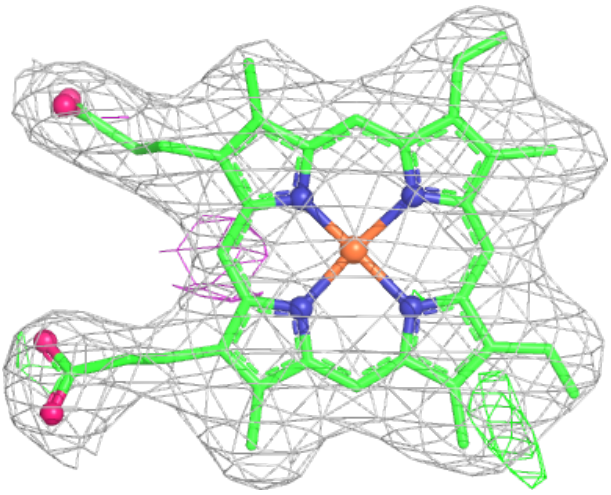


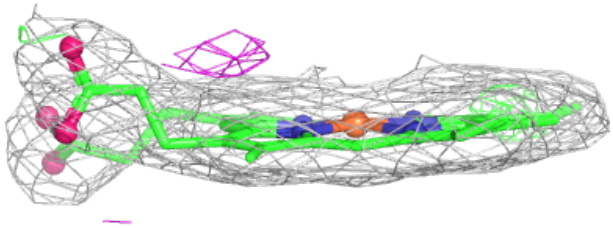


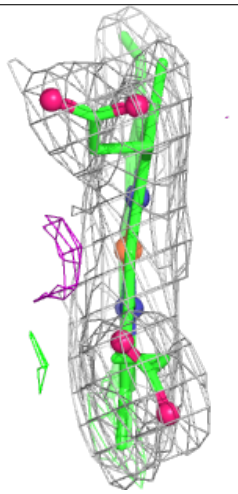


Electron density around HEM D 501:

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

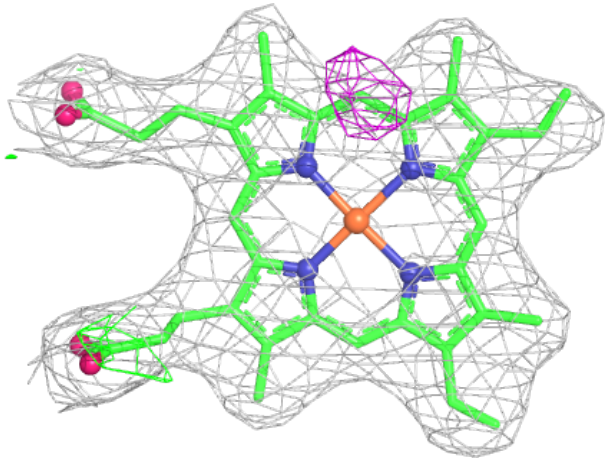


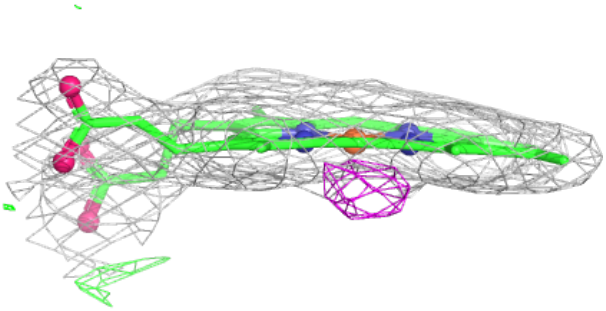


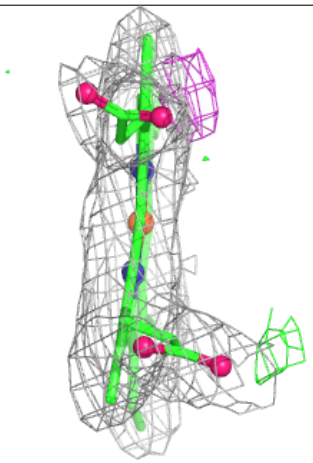


Electron density around HEM B 501:

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

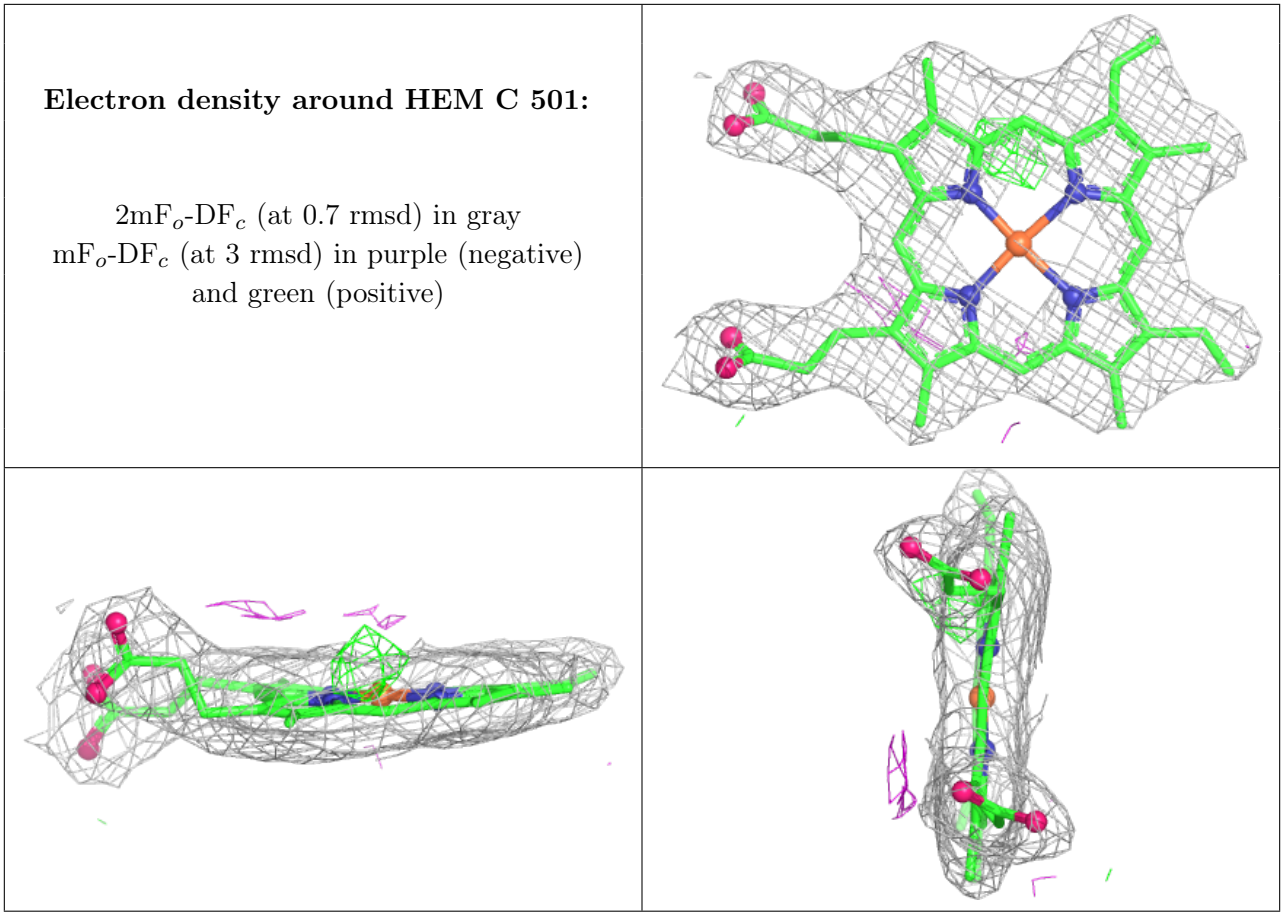






Electron density around HEM C 501:

$2mF_o$-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.