Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 04:13 pm BST

PDB ID	:	7AO7
Title	:	Structure of CYP153A from Polaromonas sp. in complex with octan-1-ol
Authors	:	Zukic, E.; Rowlinson, B.; Sharma, M.; Hoffmann, S.; Hauer, B.; Grogan, G.
Deposited on	:	2020-10-13
Resolution	:	2.55 Å(reported)

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

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

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

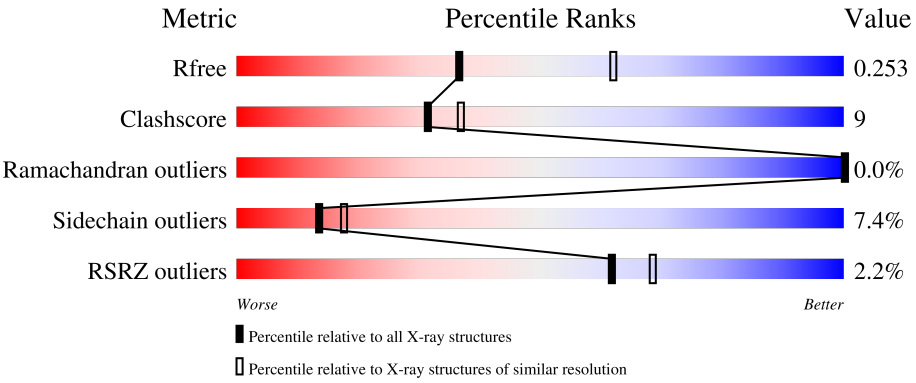
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	418	3% 81% 13%
1	B	418	2% 77% 16% 5%
1	C	418	2% 74% 17% 5%
1	D	418	% 78% 15% 5%
1	E	418	78% 16%

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Mol	Chain	Length	Quality of chain
1	F	418	

2 Entry composition

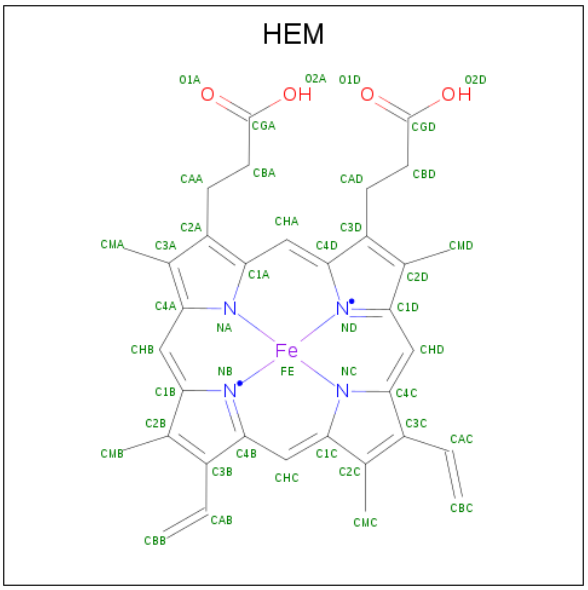
There are 4 unique types of molecules in this entry. The entry contains 19048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P450.

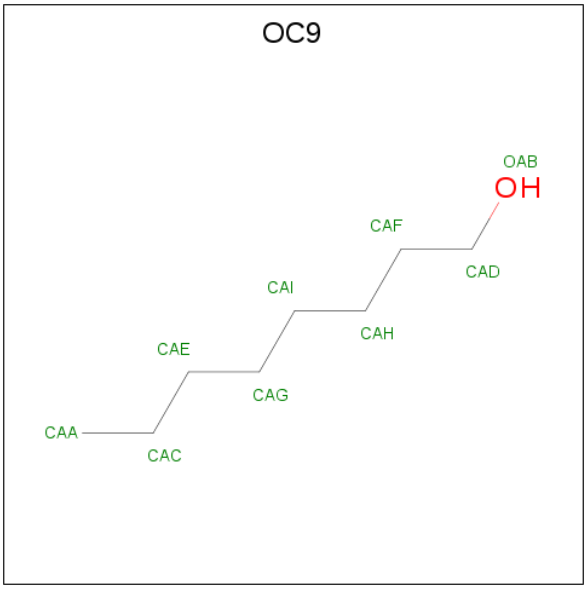
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3037	1934	524	558	21			
1	B	397	Total	C	N	O	S	0	0	0
			3061	1952	538	552	19			
1	C	401	Total	C	N	O	S	0	0	0
			3085	1965	529	571	20			
1	D	397	Total	C	N	O	S	0	0	0
			3107	1977	544	565	21			
1	E	402	Total	C	N	O	S	0	0	0
			3146	2007	544	574	21			
1	F	390	Total	C	N	O	S	0	0	0
			2947	1883	512	533	19			

- 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 OCTAN-1-OL (three-letter code: OC9) (formula: $C_8H_{18}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			9	8	1			
3	B	1	Total	C	O		0	0
			9	8	1			
3	C	1	Total	C	O		0	0
			9	8	1			
3	D	1	Total	C	O		0	0
			9	8	1			
3	E	1	Total	C	O		0	0
			9	8	1			

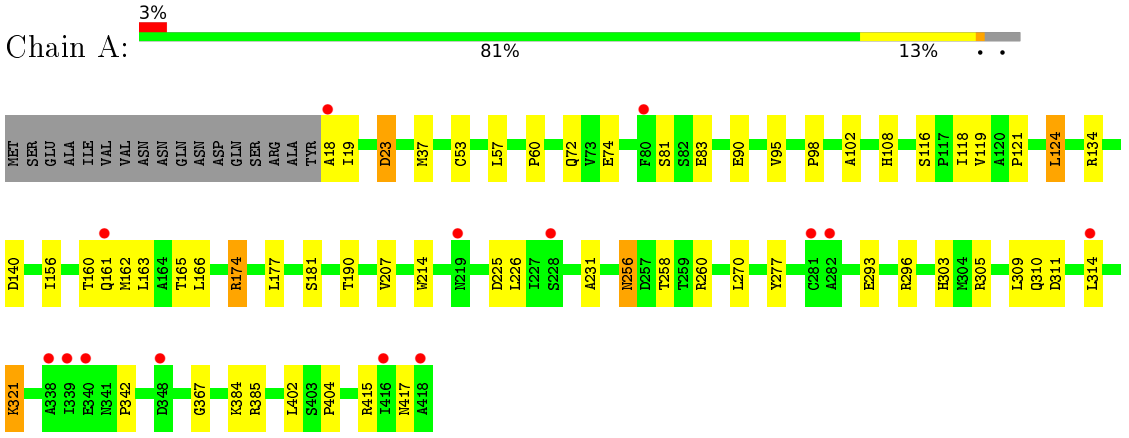
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	51	Total O 51 51	0	0
4	C	55	Total O 55 55	0	0
4	D	80	Total O 80 80	0	0
4	E	105	Total O 105 105	0	0
4	F	28	Total O 28 28	0	0

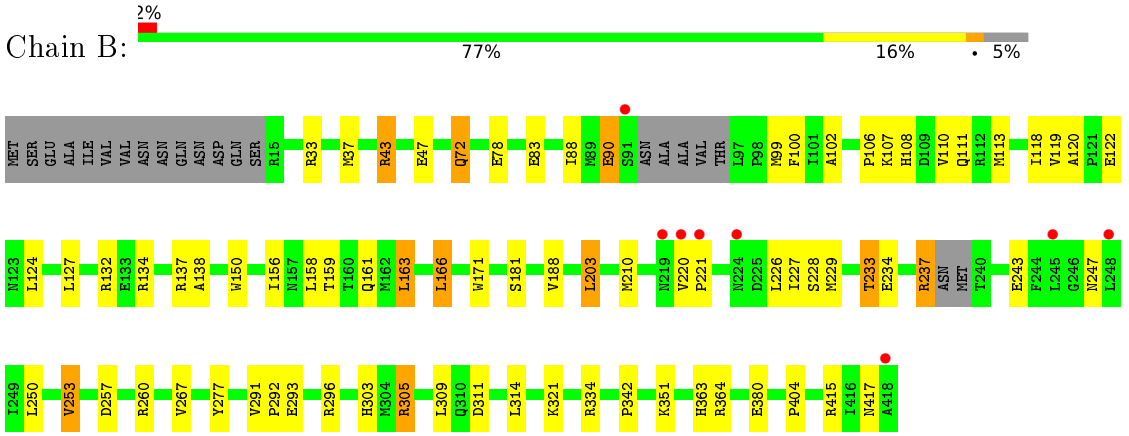
3 Residue-property plots (i)

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.

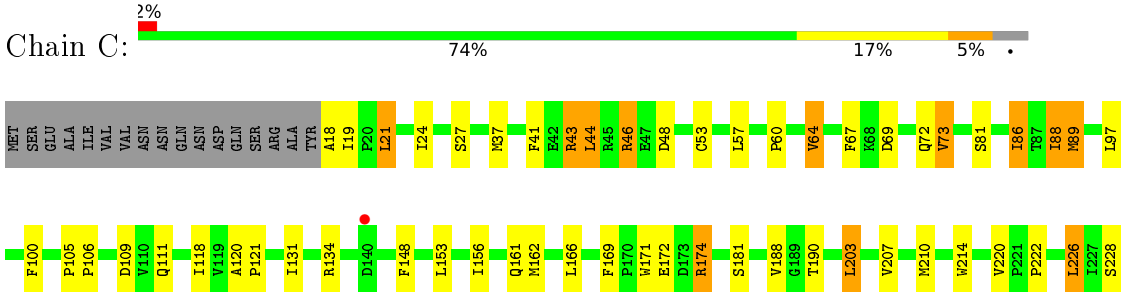
- Molecule 1: Cytochrome P450

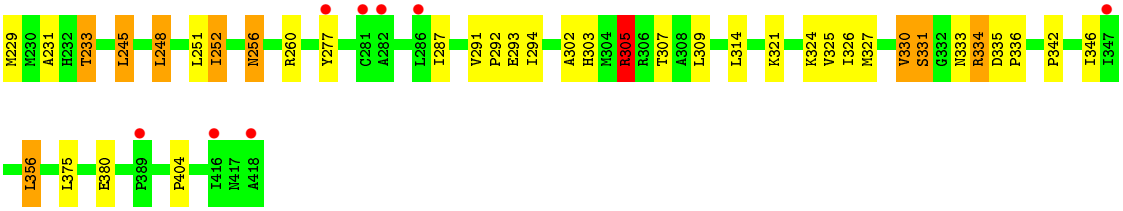


- Molecule 1: Cytochrome P450



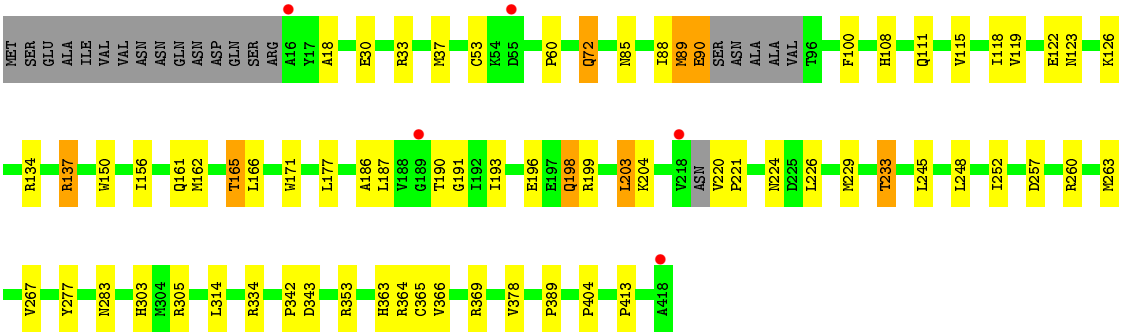
- Molecule 1: Cytochrome P450





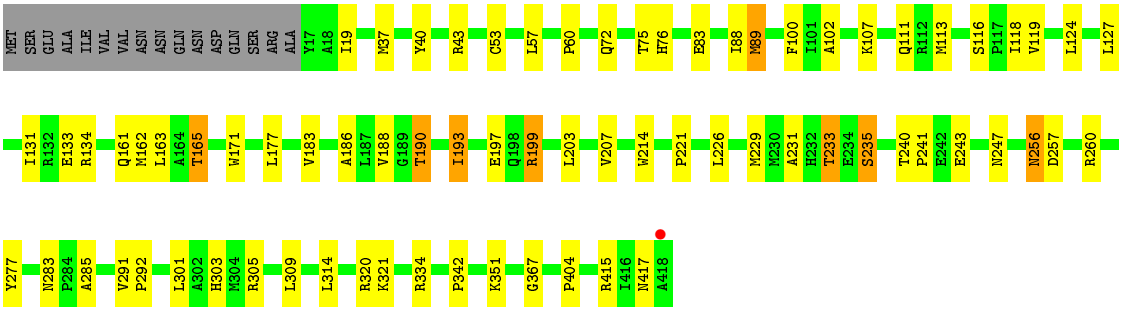
• Molecule 1: Cytochrome P450

Chain D:



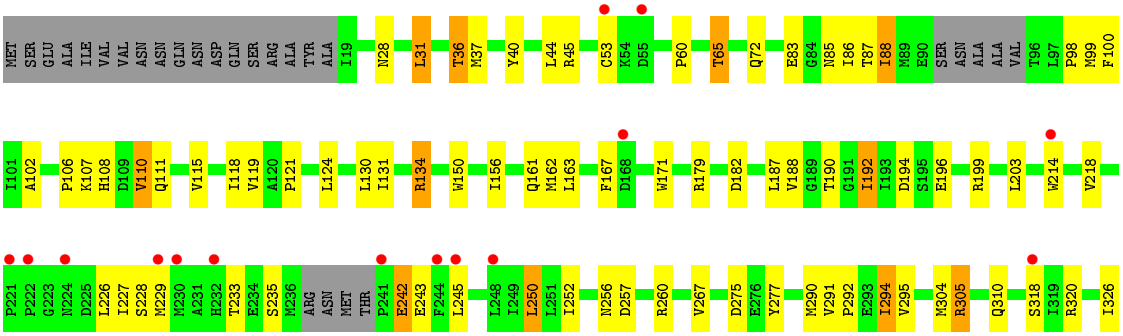
• Molecule 1: Cytochrome P450

Chain E:



• Molecule 1: Cytochrome P450

Chain F:




R334
P342
I346
R349
H363
R369
Q374
L375
K384
E393
R415
I416
N417
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.50Å 116.19Å 288.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 2.55 45.13 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.17-2.55) 99.9 (45.13-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.205 , 0.254 0.208 , 0.253	Depositor DCC
R_{free} test set	4029 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19048	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.29% 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: OC9, 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	0.71	0/3111	0.82	0/4254
1	B	0.70	0/3135	0.83	2/4273 (0.0%)
1	C	0.74	1/3160 (0.0%)	0.86	2/4317 (0.0%)
1	D	0.71	0/3181	0.86	0/4330
1	E	0.73	0/3222	0.85	2/4388 (0.0%)
1	F	0.70	0/3020	0.86	2/4123 (0.0%)
All	All	0.72	1/18829 (0.0%)	0.85	8/25685 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	PRO	C-N	7.72	1.49	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	305	ARG	CG-CD-NE	5.79	123.95	111.80
1	C	305	ARG	CG-CD-NE	-5.73	99.76	111.80
1	B	305	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	174	ARG	CB-CA-C	-5.34	99.72	110.40
1	B	90	GLU	CB-CA-C	5.27	120.94	110.40
1	E	199	ARG	CG-CD-NE	-5.15	100.99	111.80
1	F	199	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	E	43	ARG	CG-CD-NE	-5.05	101.20	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3037	0	2885	44	0
1	B	3061	0	2947	50	0
1	C	3085	0	2970	84	0
1	D	3107	0	3032	45	0
1	E	3146	0	3085	51	0
1	F	2947	0	2783	56	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0
2	D	43	0	30	1	0
2	E	43	0	30	3	0
2	F	43	0	30	3	0
3	A	9	0	18	1	0
3	B	9	0	17	0	0
3	C	9	0	18	0	0
3	D	9	0	17	0	0
3	E	9	0	18	1	0
4	A	43	0	0	3	0
4	B	51	0	0	4	0
4	C	55	0	0	3	0
4	D	80	0	0	3	0
4	E	105	0	0	4	0
4	F	28	0	0	4	0
All	All	19048	0	17970	329	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 9.

All (329) 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:111:GLN:NE2	1:B:247:ASN:HD21	1.55	1.04
1:B:132:ARG:NH2	1:B:380:GLU:OE1	1.97	0.98
1:F:100:PHE:HB3	1:F:111:GLN:HE21	1.27	0.97
1:D:343:ASP:CB	4:D:672:HOH:O	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:HG2	1:C:46:ARG:HH11	1.32	0.93
1:A:310:GLN:HA	1:A:321:LYS:HG2	1.49	0.92
1:E:186:ALA:O	1:E:199:ARG:NH2	2.02	0.92
1:F:100:PHE:HB3	1:F:111:GLN:NE2	1.85	0.89
1:B:110:VAL:HG12	1:C:19:ILE:HG13	1.53	0.88
1:E:118:ILE:HG23	1:E:119:VAL:HG23	1.58	0.86
1:C:169:PHE:HE1	1:C:210:MET:CE	1.89	0.85
1:C:169:PHE:HE1	1:C:210:MET:HE1	1.41	0.85
1:D:186:ALA:O	1:D:199:ARG:NH2	2.09	0.84
1:A:311:ASP:CB	4:A:635:HOH:O	2.26	0.83
1:A:310:GLN:HA	1:A:321:LYS:CG	2.07	0.83
1:B:321:LYS:CB	4:B:648:HOH:O	2.26	0.83
1:E:131:ILE:HG12	1:E:162:MET:HE3	1.61	0.81
1:C:287:ILE:CD1	1:C:380:GLU:HG3	2.11	0.80
1:C:333:ASN:HD21	1:C:356:LEU:H	1.25	0.80
1:F:384:LYS:CD	4:F:627:HOH:O	2.33	0.76
1:A:310:GLN:CA	1:A:321:LYS:HG2	2.14	0.76
1:F:203:LEU:CB	4:F:619:HOH:O	2.33	0.76
1:A:118:ILE:HG23	1:A:119:VAL:HG23	1.69	0.74
1:F:100:PHE:CB	1:F:111:GLN:HE21	2.00	0.73
1:B:181:SER:HA	1:B:253:VAL:CG2	2.19	0.73
1:C:88:ILE:CD1	1:C:324:LYS:HE3	2.19	0.73
1:E:162:MET:HE2	4:E:623:HOH:O	1.89	0.73
1:B:111:GLN:HE21	1:B:247:ASN:HD21	1.34	0.73
1:F:393:GLU:CB	4:F:624:HOH:O	2.38	0.72
1:E:131:ILE:HG12	1:E:162:MET:CE	2.20	0.71
1:E:134:ARG:HH12	1:E:165:THR:CG2	2.04	0.71
1:F:40:TYR:O	1:F:44:LEU:CD1	2.40	0.70
1:B:78:GLU:O	1:E:221:PRO:HG2	1.93	0.69
1:A:119:VAL:HG11	1:A:367:GLY:HA2	1.75	0.68
1:C:248:LEU:O	1:C:252:ILE:HG23	1.93	0.68
1:F:118:ILE:HG22	1:F:226:LEU:HD22	1.74	0.68
2:E:501:HEM:HBC2	2:E:501:HEM:HHD	1.75	0.68
1:C:100:PHE:HB3	1:C:111:GLN:HE21	1.59	0.68
1:E:162:MET:CE	4:E:623:HOH:O	2.41	0.67
1:F:167:PHE:O	1:F:227:ILE:HD12	1.94	0.67
1:E:134:ARG:HH12	1:E:165:THR:HG21	1.59	0.67
1:A:309:LEU:O	1:A:321:LYS:HD2	1.94	0.67
1:F:243:GLU:HA	1:F:243:GLU:OE1	1.93	0.66
1:D:89:MET:O	1:D:90:GLU:HB2	1.96	0.66
1:A:83:GLU:O	1:A:102:ALA:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ALA:HB1	1:C:57:LEU:HD21	1.78	0.65
1:A:108:HIS:HE1	2:A:501:HEM:O1D	1.79	0.65
1:B:363:HIS:HD2	2:B:501:HEM:O2D	1.79	0.65
1:D:126:LYS:CB	1:D:224:ASN:HD21	2.08	0.65
1:F:242:GLU:HG2	1:F:242:GLU:O	1.94	0.65
1:E:111:GLN:HE22	1:E:247:ASN:HD21	1.41	0.65
1:E:83:GLU:O	1:E:102:ALA:O	2.15	0.64
1:C:181:SER:N	1:C:252:ILE:HD11	2.13	0.64
1:A:81:SER:HB2	1:A:309:LEU:HD11	1.79	0.64
1:A:90:GLU:HA	1:A:90:GLU:OE1	1.98	0.64
1:C:287:ILE:HD11	1:C:380:GLU:HG3	1.79	0.63
1:F:45:ARG:HG2	1:F:65:THR:HG23	1.81	0.63
1:F:83:GLU:O	1:F:102:ALA:O	2.17	0.63
1:E:415:ARG:HE	1:E:417:ASN:HD21	1.47	0.63
1:C:64:VAL:HG13	1:C:326:ILE:O	2.00	0.62
1:C:46:ARG:HG2	1:C:46:ARG:NH1	2.08	0.62
1:F:40:TYR:O	1:F:44:LEU:HD12	1.99	0.62
1:B:415:ARG:HE	1:B:417:ASN:HD21	1.47	0.62
1:A:270:LEU:CB	4:A:640:HOH:O	2.46	0.62
1:D:100:PHE:CZ	1:D:115:VAL:HG21	2.35	0.62
1:E:119:VAL:HG11	1:E:367:GLY:HA2	1.81	0.62
1:F:156:ILE:HG12	1:F:260:ARG:HD2	1.80	0.61
1:F:162:MET:SD	1:F:374:GLN:OE1	2.58	0.61
1:F:415:ARG:HE	1:F:417:ASN:HD21	1.47	0.61
1:F:88:ILE:HD13	1:F:326:ILE:HD11	1.81	0.61
1:A:162:MET:HE3	1:A:165:THR:HB	1.82	0.60
1:C:287:ILE:HD11	1:C:380:GLU:CG	2.31	0.60
1:A:415:ARG:HE	1:A:417:ASN:HD21	1.47	0.60
1:C:131:ILE:CG1	1:C:162:MET:HE1	2.31	0.60
1:C:169:PHE:CE1	1:C:210:MET:CE	2.80	0.60
1:B:83:GLU:O	1:B:102:ALA:O	2.19	0.60
1:D:193:ILE:HA	1:D:198:GLN:HE21	1.66	0.60
1:F:40:TYR:O	1:F:44:LEU:HD13	2.02	0.60
1:B:33:ARG:CD	4:B:640:HOH:O	2.50	0.60
1:C:169:PHE:CE1	1:C:210:MET:HE1	2.32	0.60
1:E:161:GLN:HE21	1:E:171:TRP:HZ2	1.50	0.59
1:B:243:GLU:CB	4:B:643:HOH:O	2.50	0.59
1:F:161:GLN:HG2	1:F:171:TRP:CZ2	2.38	0.59
1:C:210:MET:HG3	1:C:248:LEU:HG	1.85	0.58
1:E:161:GLN:O	1:E:165:THR:HG22	2.02	0.58
1:A:225:ASP:O	1:A:226:LEU:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:PHE:CE2	1:C:356:LEU:HD22	2.38	0.58
1:D:156:ILE:HG12	1:D:260:ARG:HD2	1.83	0.58
1:C:161:GLN:HE21	1:C:171:TRP:HZ2	1.50	0.58
1:B:120:ALA:CB	1:C:57:LEU:HD21	2.33	0.58
1:C:19:ILE:HD12	1:C:19:ILE:H	1.68	0.58
1:E:118:ILE:CG2	1:E:119:VAL:HG23	2.33	0.58
1:B:159:THR:O	1:B:163:LEU:HG	2.04	0.57
1:C:21:LEU:HD11	1:C:48:ASP:HB2	1.86	0.57
1:B:111:GLN:NE2	1:B:247:ASN:ND2	2.40	0.57
1:A:119:VAL:HG12	1:A:119:VAL:O	2.03	0.57
1:C:118:ILE:HG21	1:C:226:LEU:HD13	1.86	0.57
1:D:161:GLN:HG2	1:D:171:TRP:CZ2	2.40	0.57
1:F:179:ARG:NH1	1:F:192:ILE:HD12	2.20	0.57
1:D:85:ASN:ND2	1:D:90:GLU:HA	2.19	0.57
1:D:89:MET:HE1	1:D:404:PRO:HG2	1.87	0.57
1:E:119:VAL:HG12	1:E:119:VAL:O	2.05	0.57
1:B:364:ARG:HD2	4:B:620:HOH:O	2.03	0.57
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.85	0.56
1:C:302:ALA:O	1:C:330:VAL:HG22	2.05	0.56
1:F:182:ASP:HB3	1:F:192:ILE:HD13	1.87	0.56
1:C:88:ILE:HD13	1:C:326:ILE:HD11	1.88	0.56
1:B:106:PRO:HB2	1:C:18:ALA:HB1	1.88	0.55
1:B:90:GLU:OE2	1:B:90:GLU:HA	2.06	0.55
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.88	0.55
1:A:95:VAL:HG12	3:A:502:OC9:CAA	2.37	0.55
1:B:156:ILE:HG12	1:B:260:ARG:HD2	1.88	0.55
1:A:118:ILE:CG2	1:A:119:VAL:HG23	2.37	0.55
1:D:122:GLU:CD	1:D:369:ARG:HH12	2.10	0.55
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.89	0.55
1:B:296:ARG:NH2	1:B:342:PRO:O	2.40	0.55
1:C:106:PRO:HD2	4:C:638:HOH:O	2.07	0.54
1:C:131:ILE:HG12	1:C:162:MET:CE	2.37	0.54
1:D:353:ARG:HD2	4:D:662:HOH:O	2.07	0.54
1:E:240:THR:HG23	1:E:243:GLU:H	1.71	0.54
1:B:118:ILE:HG22	1:B:226:LEU:HD22	1.88	0.54
1:D:85:ASN:HD21	1:D:90:GLU:H	1.55	0.54
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.89	0.54
1:A:296:ARG:NH2	1:A:342:PRO:O	2.41	0.54
2:C:501:HEM:HBC2	2:C:501:HEM:HHD	1.90	0.54
1:D:118:ILE:HG22	1:D:226:LEU:HD22	1.90	0.54
1:C:287:ILE:CD1	1:C:380:GLU:CG	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLN:HG2	1:C:171:TRP:CZ2	2.44	0.53
1:B:161:GLN:HG2	1:B:171:TRP:CZ2	2.43	0.53
1:C:134:ARG:HG2	1:C:161:GLN:NE2	2.24	0.53
1:C:169:PHE:CE1	1:C:210:MET:HE3	2.43	0.53
1:B:108:HIS:HE1	2:B:501:HEM:O1D	1.92	0.53
1:C:156:ILE:HG12	1:C:260:ARG:HD2	1.91	0.53
1:F:98:PRO:HG2	1:F:243:GLU:HG3	1.91	0.53
1:A:98:PRO:HG3	1:D:137:ARG:HD2	1.89	0.52
1:B:181:SER:HA	1:B:253:VAL:HG23	1.92	0.52
1:E:118:ILE:HG21	1:E:226:LEU:HD21	1.91	0.52
1:D:126:LYS:CB	1:D:224:ASN:ND2	2.73	0.52
1:D:161:GLN:O	1:D:165:THR:HG22	2.09	0.52
1:E:351:LYS:NZ	4:E:602:HOH:O	2.38	0.52
1:E:134:ARG:NH1	1:E:165:THR:HG21	2.24	0.52
1:E:303:HIS:HD2	1:E:404:PRO:O	1.93	0.52
1:E:161:GLN:HG2	1:E:171:TRP:CZ2	2.45	0.52
1:C:305:ARG:NH1	1:C:307:THR:OG1	2.43	0.51
1:C:88:ILE:CD1	1:C:324:LYS:CE	2.89	0.51
1:A:118:ILE:HG21	1:A:226:LEU:HD21	1.92	0.51
1:A:134:ARG:HG2	1:A:161:GLN:NE2	2.26	0.51
1:A:181:SER:CB	1:A:256:ASN:HD21	2.23	0.51
1:E:134:ARG:HG2	1:E:161:GLN:NE2	2.26	0.51
1:F:156:ILE:CG1	1:F:260:ARG:HD2	2.40	0.51
1:B:122:GLU:HB2	1:C:57:LEU:CD2	2.41	0.50
2:E:501:HEM:HBB2	2:E:501:HEM:HMB2	1.94	0.50
1:B:156:ILE:CG1	1:B:260:ARG:HD2	2.41	0.50
1:C:291:VAL:HA	1:C:294:ILE:HG12	1.93	0.50
1:F:346:ILE:HG12	1:F:349:ARG:HG3	1.93	0.50
1:C:131:ILE:HG13	1:C:162:MET:HE1	1.94	0.50
1:E:72:GLN:HG2	1:E:314:LEU:CD1	2.41	0.50
1:C:88:ILE:HD11	1:C:324:LYS:HE3	1.94	0.50
1:C:162:MET:HE2	4:C:640:HOH:O	2.12	0.49
1:A:303:HIS:HD2	1:A:404:PRO:O	1.95	0.49
1:C:334:ARG:HA	1:C:342:PRO:HB2	1.94	0.49
1:F:229:MET:O	1:F:233:THR:HG23	2.12	0.49
1:F:245:LEU:HD23	1:F:245:LEU:N	2.27	0.49
1:B:303:HIS:HD2	1:B:404:PRO:O	1.95	0.49
1:D:303:HIS:HD2	1:D:404:PRO:O	1.95	0.49
1:E:229:MET:O	1:E:233:THR:HG22	2.11	0.49
1:C:346:ILE:HG13	1:C:346:ILE:O	2.12	0.49
1:C:291:VAL:HB	1:C:292:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:HIS:HD2	1:C:404:PRO:O	1.95	0.49
1:E:111:GLN:NE2	1:E:247:ASN:HD21	2.09	0.49
1:A:23:ASP:HB3	1:F:235:SER:HB3	1.93	0.49
1:A:156:ILE:HG12	1:A:260:ARG:HD2	1.93	0.49
1:C:294:ILE:HD11	1:C:375:LEU:HD13	1.94	0.49
2:E:501:HEM:HBB2	2:E:501:HEM:CMB	2.42	0.49
1:E:190:THR:HG22	4:E:634:HOH:O	2.12	0.49
1:C:203:LEU:HB3	1:C:245:LEU:HD11	1.95	0.49
1:C:229:MET:O	1:C:233:THR:HG22	2.13	0.49
1:B:181:SER:HA	1:B:253:VAL:HG22	1.94	0.49
1:F:86:ILE:HB	1:F:304:MET:HE3	1.94	0.49
1:E:19:ILE:HD12	1:E:19:ILE:H	1.78	0.48
1:F:318:SER:HB3	1:F:320:ARG:HH12	1.78	0.48
1:E:214:TRP:CH2	1:E:231:ALA:HA	2.49	0.48
2:F:501:HEM:HBC2	2:F:501:HEM:CMC	2.44	0.48
1:C:118:ILE:CG2	1:C:226:LEU:HD13	2.44	0.48
1:C:156:ILE:CG1	1:C:260:ARG:HD2	2.43	0.48
1:C:335:ASP:OD1	1:C:336:PRO:HD2	2.13	0.48
1:E:256:ASN:HD21	1:E:260:ARG:NH1	2.11	0.48
1:A:156:ILE:CG1	1:A:260:ARG:HD2	2.44	0.48
1:A:293:GLU:HA	1:A:293:GLU:OE1	2.14	0.48
1:C:162:MET:CE	4:C:640:HOH:O	2.61	0.48
1:E:256:ASN:ND2	1:E:260:ARG:HH11	2.11	0.48
1:C:131:ILE:HG12	1:C:162:MET:HE1	1.96	0.48
1:C:222:PRO:HA	1:C:228:SER:OG	2.14	0.48
1:C:88:ILE:HD12	1:C:324:LYS:HZ2	1.79	0.47
1:D:191:GLY:HA2	1:E:75:THR:HG21	1.94	0.47
1:F:111:GLN:O	1:F:115:VAL:HG23	2.15	0.47
1:D:156:ILE:CG1	1:D:260:ARG:HD2	2.43	0.47
1:E:100:PHE:HB3	1:E:111:GLN:HE21	1.78	0.47
1:C:73:VAL:HG22	1:C:327:MET:SD	2.53	0.47
1:C:226:LEU:HG	1:C:251:LEU:HD13	1.97	0.47
1:F:163:LEU:HD11	1:F:256:ASN:HA	1.97	0.47
1:F:214:TRP:CD1	1:F:218:VAL:HG13	2.49	0.47
1:C:333:ASN:HD21	1:C:356:LEU:N	2.03	0.47
1:F:28:ASN:HB3	1:F:31:LEU:HD22	1.96	0.47
1:D:187:LEU:HB2	1:D:190:THR:HG21	1.96	0.47
1:F:107:LYS:O	1:F:110:VAL:HG13	2.15	0.47
1:D:30:GLU:OE1	1:D:33:ARG:NH2	2.48	0.47
1:B:363:HIS:CD2	2:B:501:HEM:O2D	2.65	0.47
1:A:214:TRP:CH2	1:A:231:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:PHE:HB3	1:C:331:SER:HB2	1.95	0.46
1:C:214:TRP:CH2	1:C:231:ALA:HA	2.50	0.46
1:D:196:GLU:HA	1:D:196:GLU:OE2	2.16	0.46
1:F:290:MET:O	1:F:294:ILE:HG23	2.15	0.46
1:D:203:LEU:C	1:D:203:LEU:HD23	2.36	0.46
1:B:293:GLU:OE1	1:B:293:GLU:HA	2.15	0.46
1:E:134:ARG:HH12	1:E:165:THR:HG22	1.77	0.46
1:B:43:ARG:NH1	1:B:47:GLU:OE1	2.49	0.46
1:D:229:MET:O	1:D:233:THR:HG22	2.16	0.46
1:A:163:LEU:HD23	1:A:177:LEU:HB3	1.98	0.46
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.98	0.46
1:A:140:ASP:OD1	1:A:385:ARG:NH1	2.49	0.45
1:C:293:GLU:OE1	1:C:293:GLU:HA	2.16	0.45
1:D:413:PRO:HG3	1:E:113:MET:HG3	1.97	0.45
1:E:88:ILE:H	1:E:303:HIS:HE1	1.64	0.45
1:C:46:ARG:NH1	1:C:46:ARG:CG	2.73	0.45
1:C:291:VAL:O	1:C:294:ILE:HG12	2.16	0.45
1:C:69:ASP:O	1:C:73:VAL:HG12	2.17	0.45
1:D:72:GLN:HG2	1:D:314:LEU:CD1	2.47	0.45
1:D:177:LEU:HD22	1:D:252:ILE:HG23	1.98	0.45
1:D:85:ASN:HD22	1:D:90:GLU:HA	1.82	0.45
1:F:85:ASN:OD1	1:F:87:THR:HG22	2.17	0.45
1:C:88:ILE:H	1:C:303:HIS:HE1	1.63	0.45
1:C:53:CYS:O	1:C:60:PRO:HA	2.17	0.45
1:C:131:ILE:HG12	1:C:162:MET:HE3	1.99	0.45
1:C:256:ASN:HD21	1:C:260:ARG:NH1	2.15	0.45
1:C:148:PHE:CD2	1:C:153:LEU:HD12	2.52	0.44
1:D:220:VAL:HG13	1:D:221:PRO:HD2	1.99	0.44
1:F:108:HIS:CD2	1:F:363:HIS:CE1	3.05	0.44
1:B:88:ILE:H	1:B:303:HIS:HE1	1.66	0.44
1:A:321:LYS:HE2	1:A:321:LYS:HB3	1.37	0.44
1:D:108:HIS:CD2	1:D:363:HIS:CE1	3.05	0.44
1:D:364:ARG:NH2	1:D:365:CYS:O	2.51	0.44
1:E:89:MET:CE	1:E:404:PRO:HG2	2.48	0.44
1:B:122:GLU:HB2	1:C:57:LEU:HD22	2.00	0.44
1:F:194:ASP:C	1:F:194:ASP:OD1	2.56	0.44
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.48	0.44
1:C:81:SER:HB2	1:C:309:LEU:HD11	1.99	0.44
1:D:122:GLU:OE1	1:D:369:ARG:NH1	2.48	0.44
1:B:72:GLN:HG2	1:B:314:LEU:CD1	2.48	0.44
1:B:100:PHE:HB3	1:B:111:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HD12	1:B:229:MET:HB3	1.99	0.44
1:C:88:ILE:HD12	1:C:324:LYS:CE	2.48	0.44
1:F:310:GLN:CB	4:F:622:HOH:O	2.65	0.44
1:B:234:GLU:HA	1:B:237:ARG:HD3	2.00	0.44
1:E:291:VAL:HB	1:E:292:PRO:HD3	1.98	0.44
1:F:291:VAL:HB	1:F:292:PRO:HD3	2.00	0.44
1:D:263:MET:HE2	1:D:378:VAL:HG21	2.00	0.43
2:C:501:HEM:HBB2	2:C:501:HEM:CMB	2.47	0.43
1:D:18:ALA:HB1	1:E:285:ALA:HB1	1.99	0.43
1:F:36:THR:HG23	1:F:40:TYR:HE1	1.82	0.43
1:D:100:PHE:HB3	1:D:111:GLN:HE21	1.84	0.43
1:F:294:ILE:HD11	1:F:375:LEU:HD13	1.99	0.43
1:B:220:VAL:HB	1:B:221:PRO:HD2	2.01	0.43
1:B:203:LEU:O	1:B:203:LEU:HD12	2.19	0.43
1:B:138:ALA:HB3	1:B:158:LEU:HD21	2.01	0.43
1:A:19:ILE:HG13	1:F:110:VAL:HB	2.01	0.43
1:D:72:GLN:CD	4:D:634:HOH:O	2.57	0.43
1:B:107:LYS:O	1:B:110:VAL:HG22	2.18	0.42
1:B:150:TRP:CE2	1:B:267:VAL:HG21	2.54	0.42
1:A:18:ALA:HB1	1:F:106:PRO:HB2	2.01	0.42
1:C:120:ALA:N	1:C:121:PRO:CD	2.82	0.42
1:D:88:ILE:H	1:D:303:HIS:HE1	1.67	0.42
1:C:88:ILE:HD12	1:C:324:LYS:NZ	2.33	0.42
1:F:334:ARG:HA	1:F:342:PRO:HB2	2.01	0.42
1:A:258:THR:HB	2:A:501:HEM:C3B	2.54	0.42
2:A:501:HEM:HBC2	2:A:501:HEM:HHD	2.00	0.42
1:C:291:VAL:O	1:C:294:ILE:CG1	2.68	0.42
1:E:72:GLN:HE21	1:E:76:HIS:CD2	2.38	0.42
1:F:121:PRO:HD2	1:F:369:ARG:NH1	2.35	0.42
1:A:367:GLY:HA3	2:A:501:HEM:C3C	2.54	0.42
1:B:291:VAL:HB	1:B:292:PRO:HD3	2.02	0.42
1:F:86:ILE:HB	1:F:304:MET:CE	2.49	0.42
1:A:121:PRO:HA	1:A:124:LEU:HB2	2.01	0.42
1:F:187:LEU:HB2	1:F:190:THR:HG21	2.02	0.42
1:D:334:ARG:HA	1:D:342:PRO:HB2	2.02	0.42
1:E:131:ILE:CG1	1:E:162:MET:CE	2.95	0.42
1:E:162:MET:O	1:E:165:THR:HG23	2.20	0.42
1:B:113:MET:HE1	1:C:24:ILE:HA	2.02	0.42
1:E:53:CYS:O	1:E:60:PRO:HA	2.20	0.41
1:F:150:TRP:CE2	1:F:267:VAL:HG21	2.55	0.41
1:F:294:ILE:HG12	1:F:295:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:MET:HE1	1:B:227:ILE:HD11	2.03	0.41
1:C:86:ILE:HA	1:C:86:ILE:HD12	1.77	0.41
1:F:107:LYS:HA	1:F:110:VAL:CG1	2.50	0.41
1:A:160:THR:HG22	1:A:174:ARG:HG2	2.03	0.41
1:C:89:MET:CE	1:C:404:PRO:HG2	2.50	0.41
1:D:123:ASN:HD22	1:D:123:ASN:HA	1.58	0.41
1:D:150:TRP:CE2	1:D:267:VAL:HG21	2.55	0.41
1:A:53:CYS:O	1:A:60:PRO:HA	2.20	0.41
1:C:44:LEU:HD12	1:C:44:LEU:HA	1.81	0.41
1:C:89:MET:HE1	1:C:404:PRO:HG2	2.03	0.41
1:D:203:LEU:HD23	1:D:204:LYS:N	2.36	0.41
1:E:19:ILE:HD13	1:E:40:TYR:HE2	1.85	0.41
1:E:301:LEU:HD11	3:E:502:OC9:HAF1	2.03	0.41
1:E:309:LEU:O	1:E:321:LYS:HG3	2.21	0.41
1:E:334:ARG:HA	1:E:342:PRO:HB2	2.01	0.41
1:F:100:PHE:CB	1:F:111:GLN:NE2	2.68	0.41
1:A:162:MET:HE2	1:A:166:LEU:HG	2.03	0.41
1:A:384:LYS:CB	4:A:641:HOH:O	2.69	0.41
1:C:333:ASN:HD22	1:C:333:ASN:HA	1.69	0.41
1:D:162:MET:O	1:D:165:THR:HG23	2.21	0.41
1:F:53:CYS:O	1:F:60:PRO:HA	2.21	0.41
1:F:130:LEU:O	1:F:134:ARG:HD3	2.21	0.41
1:B:229:MET:O	1:B:233:THR:HG23	2.21	0.40
1:E:183:VAL:HG22	1:E:193:ILE:HD13	2.02	0.40
1:A:181:SER:HB2	1:A:256:ASN:HD21	1.86	0.40
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.95	0.40
1:E:163:LEU:HD23	1:E:177:LEU:HB3	2.03	0.40
1:A:190:THR:CG2	1:A:402:LEU:HD23	2.51	0.40
1:A:309:LEU:C	1:A:321:LYS:HD2	2.41	0.40
1:B:334:ARG:HA	1:B:342:PRO:HB2	2.03	0.40
1:C:19:ILE:O	1:C:43:ARG:NH2	2.54	0.40
1:D:53:CYS:O	1:D:60:PRO:HA	2.21	0.40
1:C:88:ILE:HD12	1:C:88:ILE:O	2.21	0.40
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.81	0.40
2:D:501:HEM:HMC2	2:D:501:HEM:HAC	1.82	0.40
1:E:240:THR:OG1	1:E:241:PRO:HD2	2.21	0.40
1:F:250:LEU:HD23	1:F:250:LEU:O	2.21	0.40
1:B:166:LEU:HD12	1:B:166:LEU:HA	1.98	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	399/418 (96%)	387 (97%)	12 (3%)	0	100 100
1	B	391/418 (94%)	382 (98%)	9 (2%)	0	100 100
1	C	399/418 (96%)	390 (98%)	9 (2%)	0	100 100
1	D	391/418 (94%)	383 (98%)	8 (2%)	0	100 100
1	E	400/418 (96%)	389 (97%)	10 (2%)	1 (0%)	41 51
1	F	384/418 (92%)	368 (96%)	16 (4%)	0	100 100
All	All	2364/2508 (94%)	2299 (97%)	64 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	235	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	311/366 (85%)	297 (96%)	14 (4%)	27 37
1	B	314/366 (86%)	291 (93%)	23 (7%)	14 18
1	C	324/366 (88%)	287 (89%)	37 (11%)	5 5
1	D	329/366 (90%)	310 (94%)	19 (6%)	20 26
1	E	334/366 (91%)	311 (93%)	23 (7%)	15 20
1	F	295/366 (81%)	270 (92%)	25 (8%)	10 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1907/2196 (87%)	1766 (93%)	141 (7%)	13 18

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	37	MET
1	A	57	LEU
1	A	72	GLN
1	A	74	GLU
1	A	116	SER
1	A	124	LEU
1	A	174	ARG
1	A	207	VAL
1	A	256	ASN
1	A	277	TYR
1	A	305	ARG
1	A	314	LEU
1	A	321	LYS
1	B	37	MET
1	B	43	ARG
1	B	72	GLN
1	B	99	MET
1	B	119	VAL
1	B	124	LEU
1	B	127	LEU
1	B	134	ARG
1	B	137	ARG
1	B	163	LEU
1	B	166	LEU
1	B	188	VAL
1	B	203	LEU
1	B	228	SER
1	B	233	THR
1	B	237	ARG
1	B	250	LEU
1	B	253	VAL
1	B	257	ASP
1	B	277	TYR
1	B	305	ARG
1	B	311	ASP
1	B	351	LYS

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Mol	Chain	Res	Type
1	C	21	LEU
1	C	27	SER
1	C	37	MET
1	C	43	ARG
1	C	44	LEU
1	C	46	ARG
1	C	64	VAL
1	C	72	GLN
1	C	73	VAL
1	C	86	ILE
1	C	88	ILE
1	C	89	MET
1	C	97	LEU
1	C	109	ASP
1	C	166	LEU
1	C	172	GLU
1	C	174	ARG
1	C	188	VAL
1	C	190	THR
1	C	203	LEU
1	C	207	VAL
1	C	220	VAL
1	C	226	LEU
1	C	233	THR
1	C	245	LEU
1	C	248	LEU
1	C	252	ILE
1	C	256	ASN
1	C	277	TYR
1	C	305	ARG
1	C	314	LEU
1	C	321	LYS
1	C	325	VAL
1	C	330	VAL
1	C	331	SER
1	C	334	ARG
1	C	356	LEU
1	D	37	MET
1	D	72	GLN
1	D	89	MET
1	D	90	GLU
1	D	119	VAL

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Mol	Chain	Res	Type
1	D	134	ARG
1	D	137	ARG
1	D	165	THR
1	D	166	LEU
1	D	198	GLN
1	D	203	LEU
1	D	233	THR
1	D	245	LEU
1	D	257	ASP
1	D	277	TYR
1	D	283	ASN
1	D	305	ARG
1	D	366	VAL
1	D	389	PRO
1	E	37	MET
1	E	57	LEU
1	E	89	MET
1	E	107	LYS
1	E	116	SER
1	E	124	LEU
1	E	127	LEU
1	E	133	GLU
1	E	165	THR
1	E	188	VAL
1	E	190	THR
1	E	193	ILE
1	E	197	GLU
1	E	203	LEU
1	E	207	VAL
1	E	233	THR
1	E	235	SER
1	E	256	ASN
1	E	257	ASP
1	E	277	TYR
1	E	283	ASN
1	E	305	ARG
1	E	320	ARG
1	F	31	LEU
1	F	36	THR
1	F	37	MET
1	F	65	THR
1	F	72	GLN

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Mol	Chain	Res	Type
1	F	88	ILE
1	F	99	MET
1	F	110	VAL
1	F	119	VAL
1	F	124	LEU
1	F	131	ILE
1	F	134	ARG
1	F	188	VAL
1	F	192	ILE
1	F	196	GLU
1	F	228	SER
1	F	242	GLU
1	F	250	LEU
1	F	252	ILE
1	F	257	ASP
1	F	275	ASP
1	F	277	TYR
1	F	294	ILE
1	F	305	ARG
1	F	346	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	161	GLN
1	A	224	ASN
1	A	232	HIS
1	A	273	ASN
1	A	303	HIS
1	A	417	ASN
1	B	108	HIS
1	B	111	GLN
1	B	215	ASN
1	B	303	HIS
1	B	363	HIS
1	B	417	ASN
1	C	111	GLN
1	C	161	GLN
1	C	198	GLN
1	C	215	ASN
1	C	261	ASN

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Mol	Chain	Res	Type
1	C	273	ASN
1	C	303	HIS
1	C	333	ASN
1	D	111	GLN
1	D	123	ASN
1	D	198	GLN
1	D	215	ASN
1	D	224	ASN
1	D	232	HIS
1	D	247	ASN
1	D	283	ASN
1	D	303	HIS
1	E	76	HIS
1	E	111	GLN
1	E	161	GLN
1	E	215	ASN
1	E	219	ASN
1	E	232	HIS
1	E	238	ASN
1	E	256	ASN
1	E	261	ASN
1	E	283	ASN
1	E	303	HIS
1	E	417	ASN
1	F	76	HIS
1	F	111	GLN
1	F	215	ASN
1	F	298	GLN
1	F	374	GLN
1	F	417	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
3	OC9	D	502	2	8,8,8	0.23	0	7,7,7	0.59	0
3	OC9	A	502	2	8,8,8	0.35	0	7,7,7	0.59	0
2	HEM	A	501	1,3	27,50,50	1.53	6 (22%)	17,82,82	1.76	6 (35%)
3	OC9	E	502	2	8,8,8	0.30	0	7,7,7	1.10	1 (14%)
2	HEM	E	501	1,3	27,50,50	1.21	3 (11%)	17,82,82	1.28	3 (17%)
2	HEM	C	501	1,3	27,50,50	1.15	2 (7%)	17,82,82	1.42	5 (29%)
2	HEM	F	501	1	27,50,50	1.25	2 (7%)	17,82,82	1.19	2 (11%)
3	OC9	B	502	2	8,8,8	0.29	0	7,7,7	0.49	0
2	HEM	B	501	1,3	27,50,50	1.23	4 (14%)	17,82,82	1.88	4 (23%)
3	OC9	C	502	2	8,8,8	0.26	0	7,7,7	0.75	0
2	HEM	D	501	1,3	27,50,50	1.23	2 (7%)	17,82,82	1.65	4 (23%)

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
3	OC9	D	502	2	-	4/6/6/6	-
3	OC9	A	502	2	-	0/6/6/6	-
2	HEM	A	501	1,3	-	0/6/54/54	-
3	OC9	E	502	2	-	2/6/6/6	-
2	HEM	E	501	1,3	-	0/6/54/54	-
2	HEM	C	501	1,3	-	0/6/54/54	-
2	HEM	F	501	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OC9	B	502	2	-	4/6/6/6	-
2	HEM	B	501	1,3	-	0/6/54/54	-
3	OC9	C	502	2	-	3/6/6/6	-
2	HEM	D	501	1,3	-	2/6/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-C2C	-3.63	1.35	1.40
2	A	501	HEM	C4D-C3D	3.52	1.50	1.42
2	B	501	HEM	C3B-C2B	-3.24	1.35	1.40
2	A	501	HEM	C3C-C2C	-2.87	1.36	1.40
2	D	501	HEM	C3B-C2B	-2.85	1.36	1.40
2	E	501	HEM	C3C-C2C	-2.83	1.36	1.40
2	D	501	HEM	C1D-ND	-2.68	1.30	1.36
2	A	501	HEM	C4A-CHB	-2.64	1.33	1.41
2	E	501	HEM	C4B-NB	-2.64	1.30	1.36
2	A	501	HEM	C4B-NB	-2.53	1.31	1.36
2	A	501	HEM	C4A-NA	-2.43	1.31	1.36
2	F	501	HEM	C3B-C2B	-2.38	1.37	1.40
2	B	501	HEM	C4B-NB	-2.25	1.31	1.36
2	F	501	HEM	C4D-C3D	2.25	1.47	1.42
2	C	501	HEM	C4D-C3D	2.21	1.47	1.42
2	A	501	HEM	C3B-C2B	-2.17	1.37	1.40
2	B	501	HEM	C3D-C2D	-2.15	1.31	1.37
2	E	501	HEM	C4D-C3D	2.15	1.47	1.42
2	B	501	HEM	C1A-CHA	-2.06	1.35	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CAA-CBA-CGA	5.31	121.58	112.67
2	D	501	HEM	C4C-C3C-C2C	-4.03	104.08	106.90
2	A	501	HEM	CAD-CBD-CGD	3.35	118.29	112.67
2	A	501	HEM	C4C-C3C-C2C	-3.13	104.71	106.90
2	D	501	HEM	C1D-C2D-C3D	2.87	109.00	107.00
2	C	501	HEM	C1D-C2D-C3D	2.51	108.74	107.00
2	C	501	HEM	C3C-C4C-NC	-2.49	106.23	110.94
2	A	501	HEM	CAA-CBA-CGA	2.49	116.85	112.67
2	E	501	HEM	CMB-C2B-C3B	2.39	129.14	124.68
3	E	502	OC9	CAH-CAI-CAG	-2.32	102.66	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	CBD-CAD-C3D	-2.31	108.22	112.48
2	B	501	HEM	C4C-C3C-C2C	-2.27	105.31	106.90
2	F	501	HEM	C3B-C4B-NB	-2.23	106.33	109.21
2	C	501	HEM	CBD-CAD-C3D	-2.17	108.48	112.48
2	B	501	HEM	CMB-C2B-C3B	2.16	128.71	124.68
2	F	501	HEM	CMC-C2C-C3C	2.15	128.69	124.68
2	B	501	HEM	CBD-CAD-C3D	-2.14	108.54	112.48
2	A	501	HEM	CMA-C3A-C2A	-2.11	120.97	124.94
2	E	501	HEM	CBA-CAA-C2A	-2.09	108.64	112.49
2	C	501	HEM	CAD-CBD-CGD	2.07	116.14	112.67
2	C	501	HEM	CMA-C3A-C4A	-2.04	125.32	128.46
2	D	501	HEM	CMA-C3A-C4A	-2.04	125.32	128.46
2	E	501	HEM	CAD-CBD-CGD	2.01	116.05	112.67
2	A	501	HEM	CBA-CAA-C2A	-2.01	108.78	112.49
2	D	501	HEM	CAD-CBD-CGD	2.01	116.04	112.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
3	C	502	OC9	CAE-CAG-CAI-CAH
3	B	502	OC9	CAD-CAF-CAH-CAI
3	D	502	OC9	OAB-CAD-CAF-CAH
3	E	502	OC9	CAE-CAG-CAI-CAH
3	C	502	OC9	CAF-CAH-CAI-CAG
3	B	502	OC9	CAA-CAC-CAE-CAG
3	D	502	OC9	CAD-CAF-CAH-CAI
3	D	502	OC9	CAF-CAH-CAI-CAG
3	B	502	OC9	CAF-CAH-CAI-CAG
3	B	502	OC9	CAC-CAE-CAG-CAI
3	C	502	OC9	OAB-CAD-CAF-CAH
3	D	502	OC9	CAE-CAG-CAI-CAH
3	E	502	OC9	CAA-CAC-CAE-CAG

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	OC9	1	0

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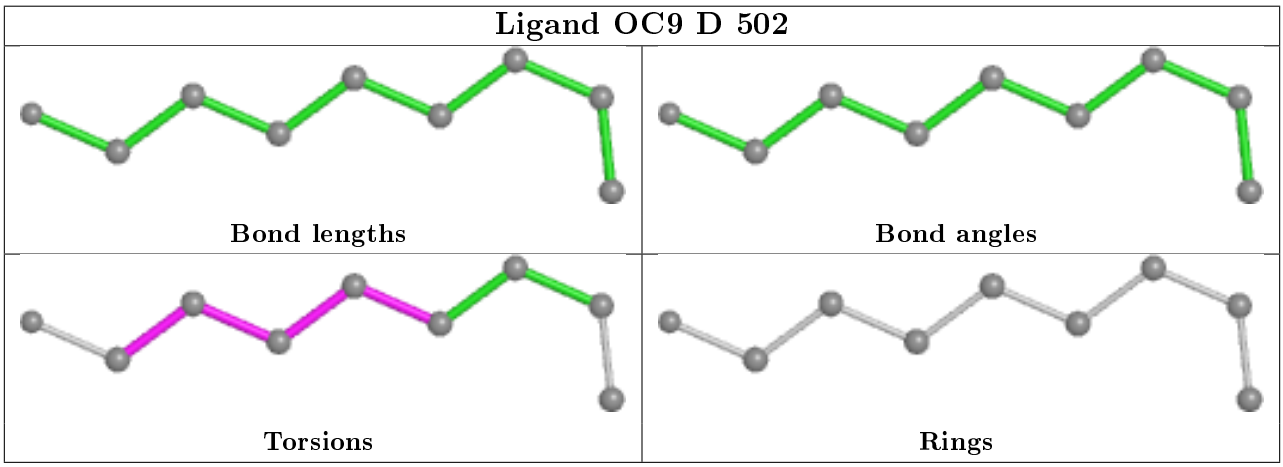
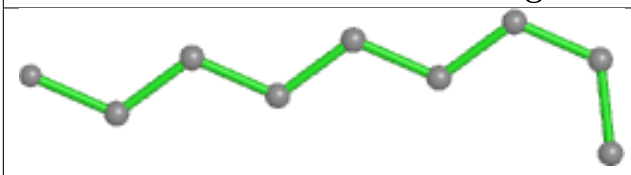
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
3	E	502	OC9	1	0
2	E	501	HEM	3	0
2	C	501	HEM	3	0
2	F	501	HEM	3	0
2	B	501	HEM	5	0
2	D	501	HEM	1	0

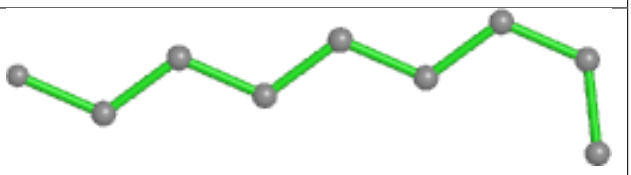
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



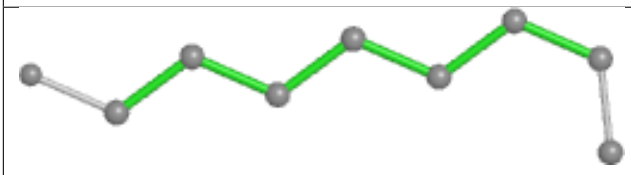
Ligand OC9 A 502



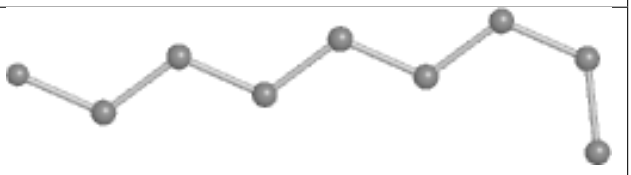
Bond lengths



Bond angles

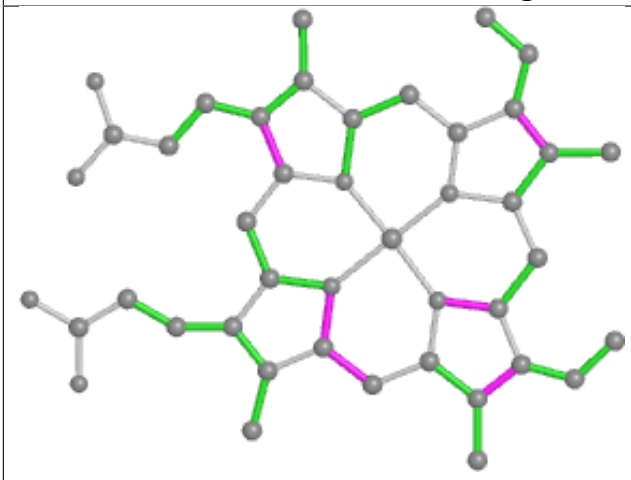


Torsions

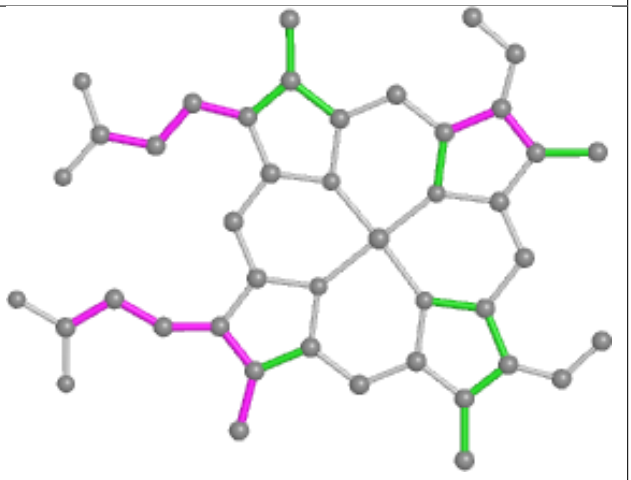


Rings

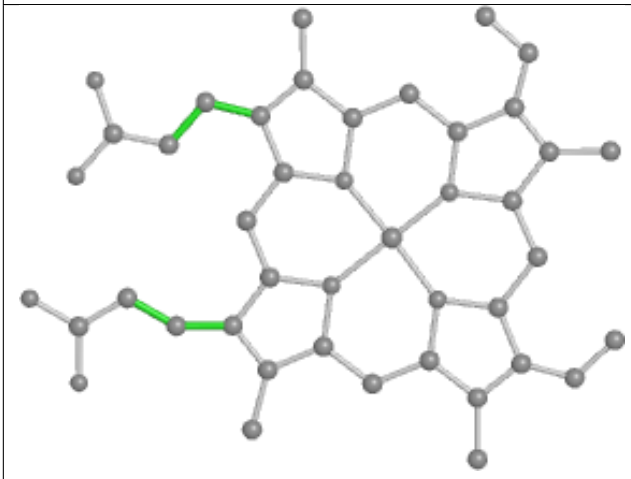
Ligand HEM A 501



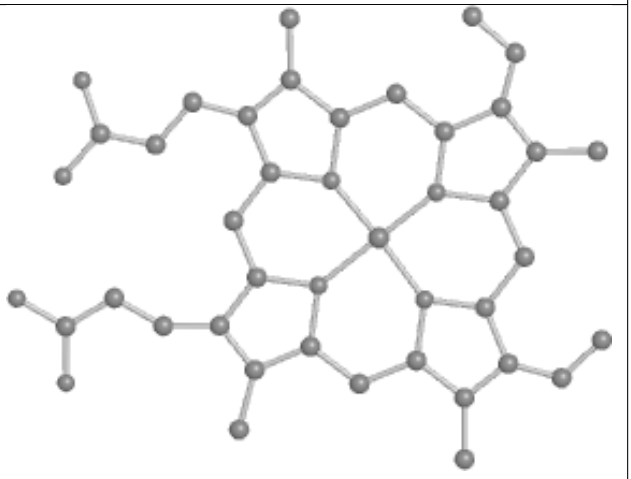
Bond lengths



Bond angles

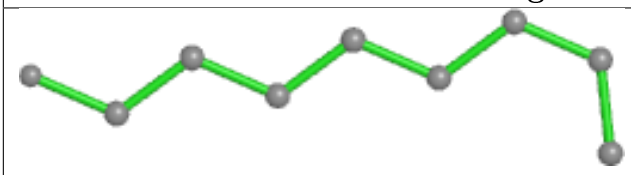


Torsions

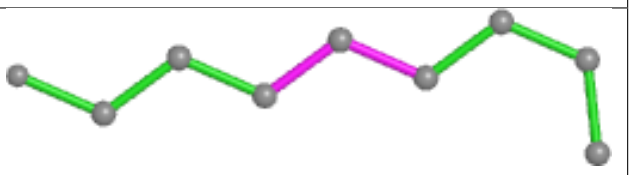


Rings

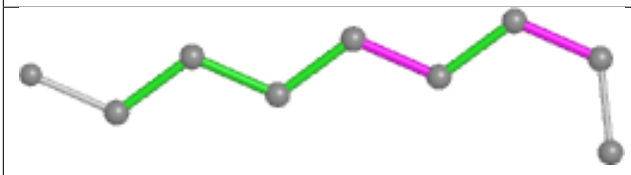
Ligand OC9 E 502



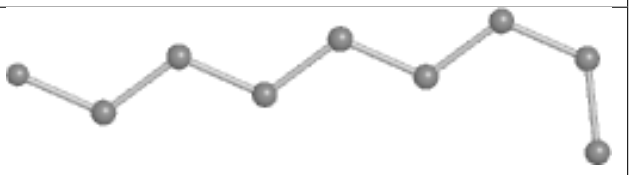
Bond lengths



Bond angles

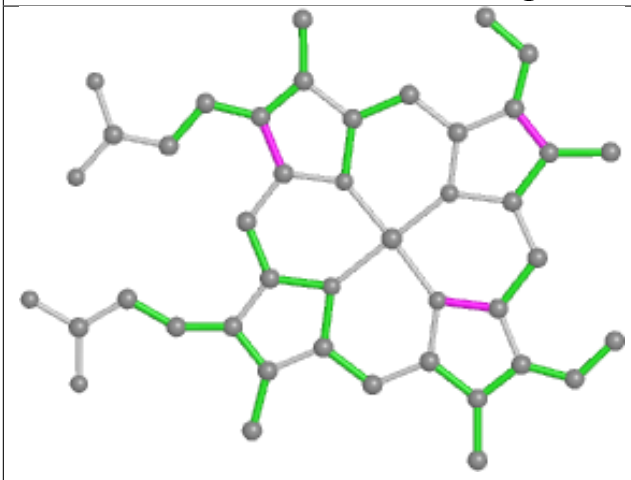


Torsions

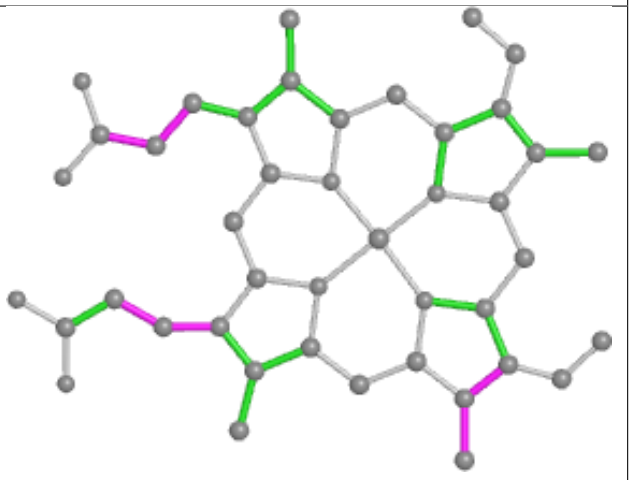


Rings

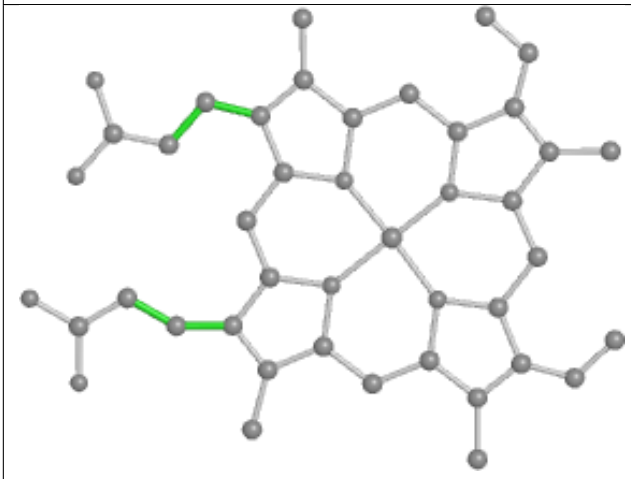
Ligand HEM E 501



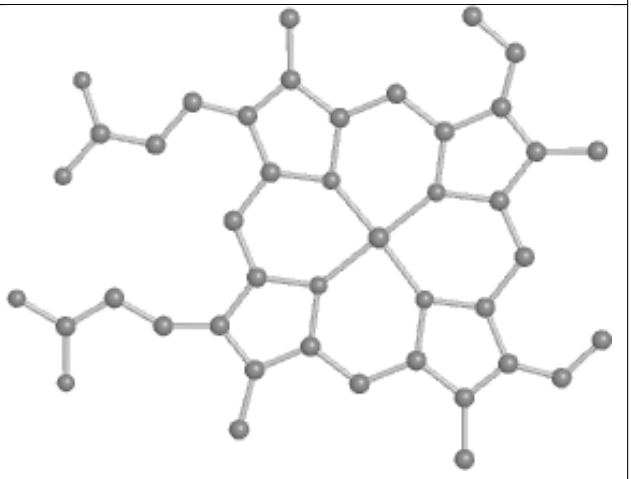
Bond lengths



Bond angles

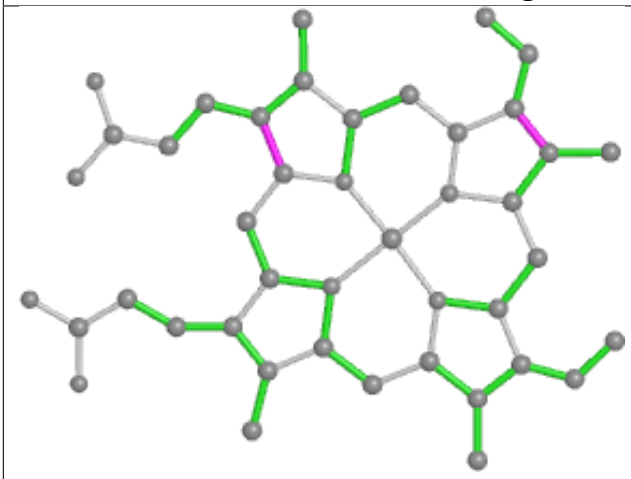


Torsions

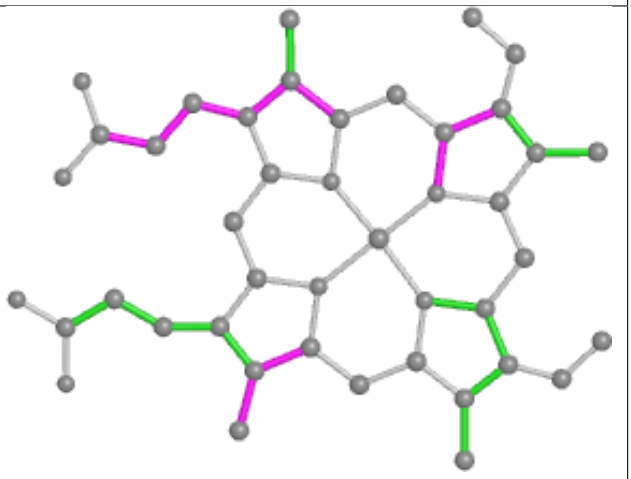


Rings

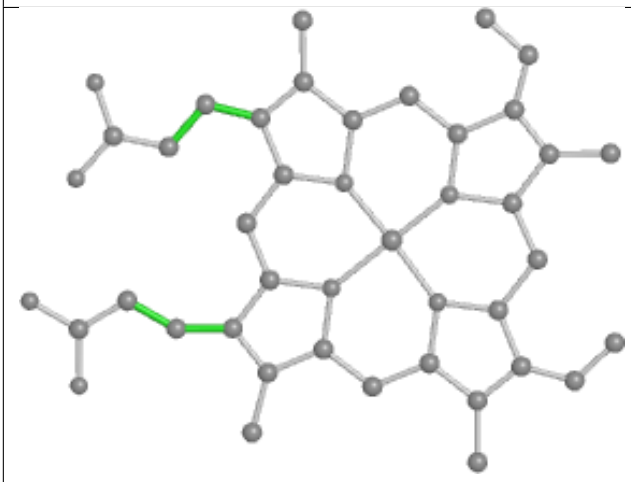
Ligand HEM C 501



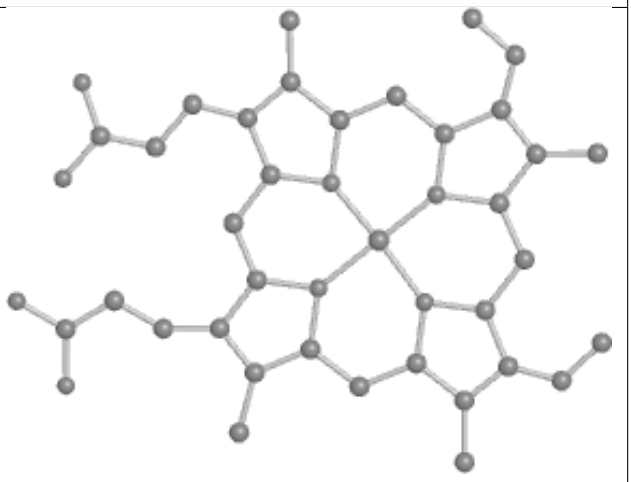
Bond lengths



Bond angles

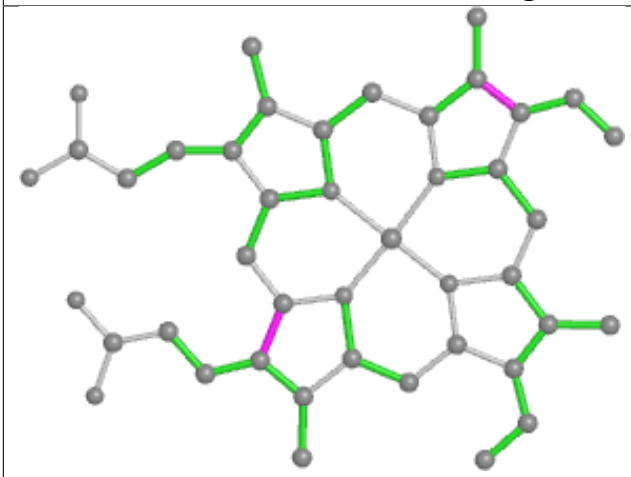


Torsions

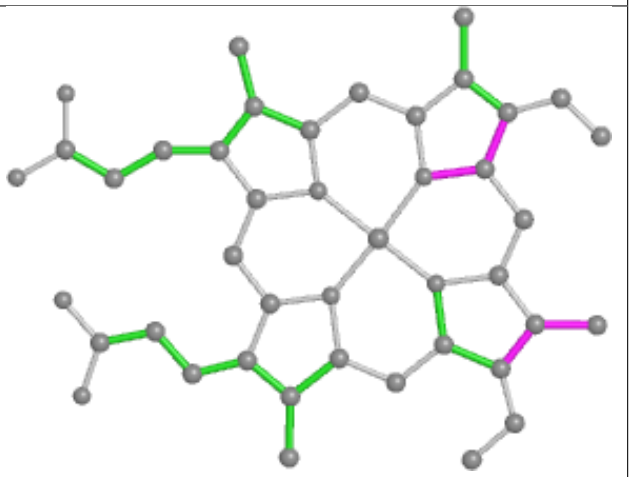


Rings

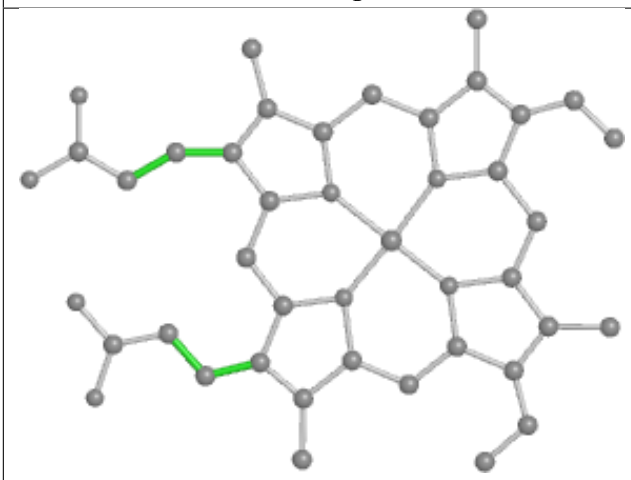
Ligand HEM F 501



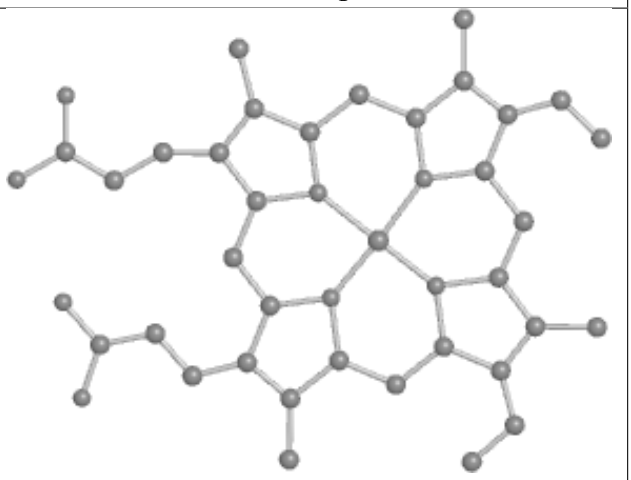
Bond lengths



Bond angles

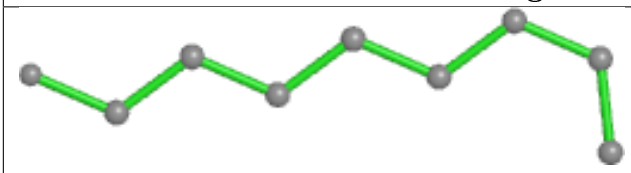


Torsions

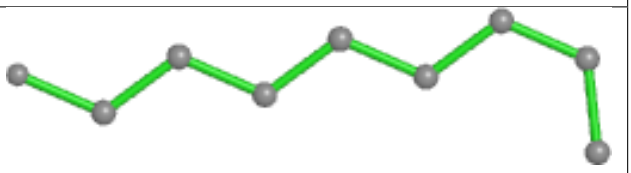


Rings

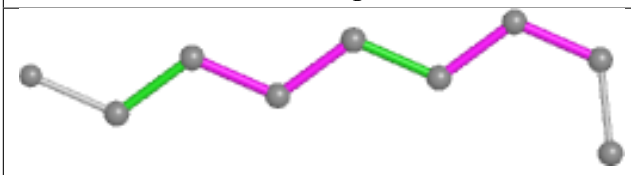
Ligand OC9 B 502



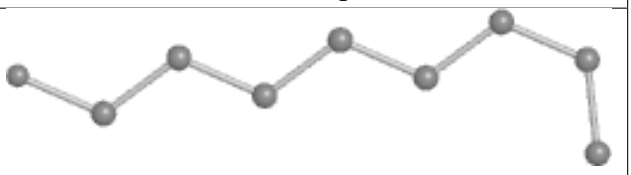
Bond lengths



Bond angles

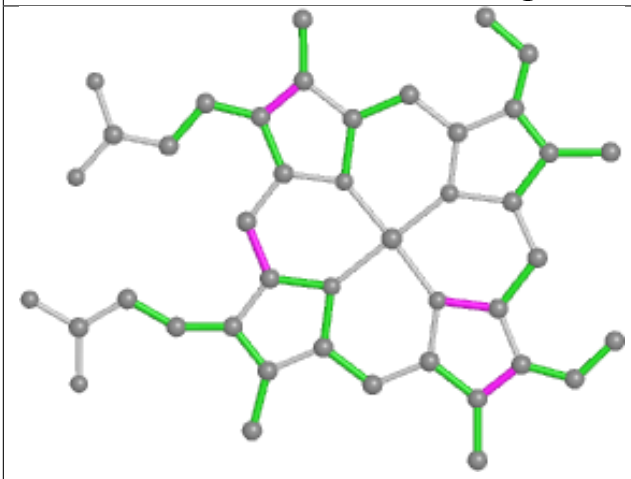


Torsions

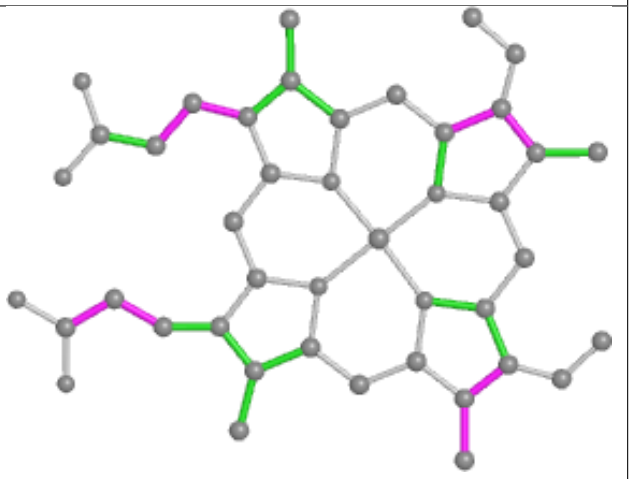


Rings

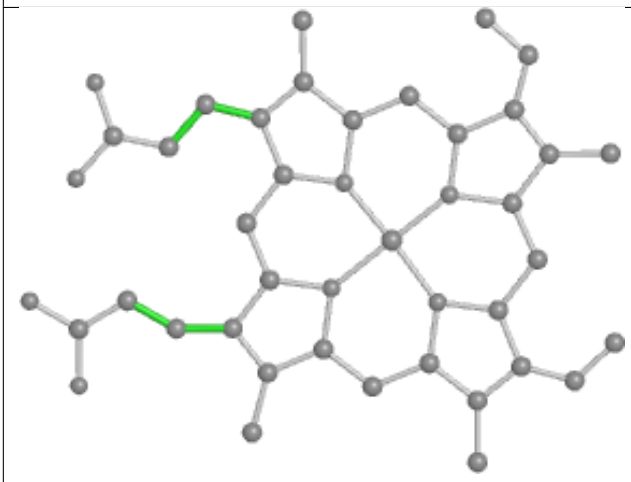
Ligand HEM B 501



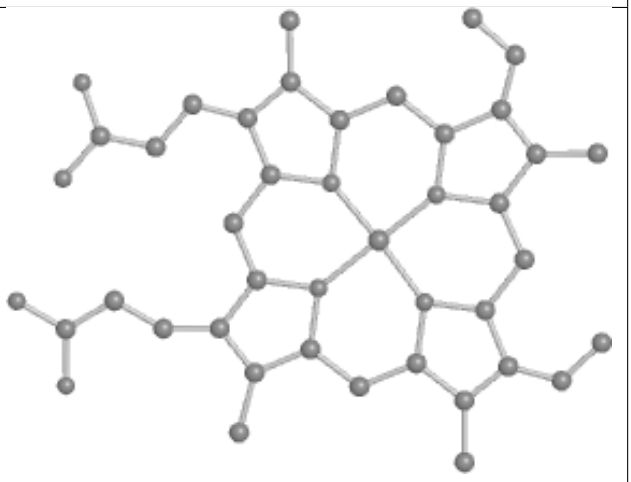
Bond lengths



Bond angles

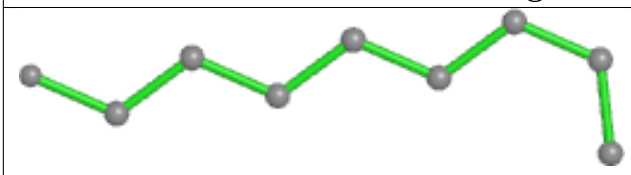


Torsions

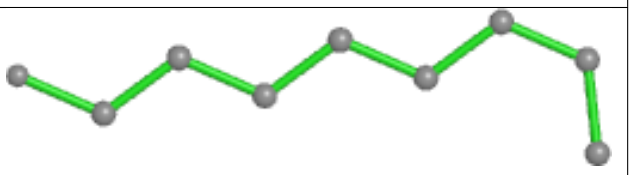


Rings

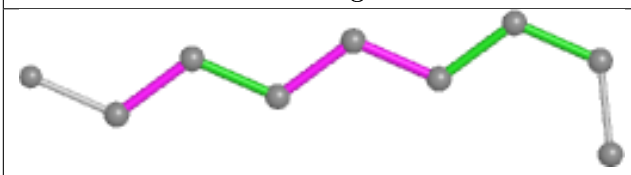
Ligand OC9 C 502



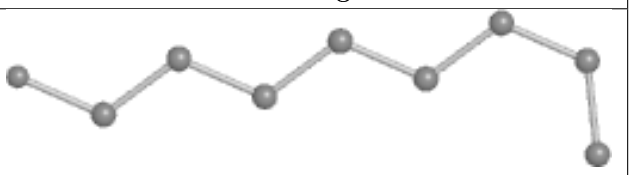
Bond lengths



Bond angles

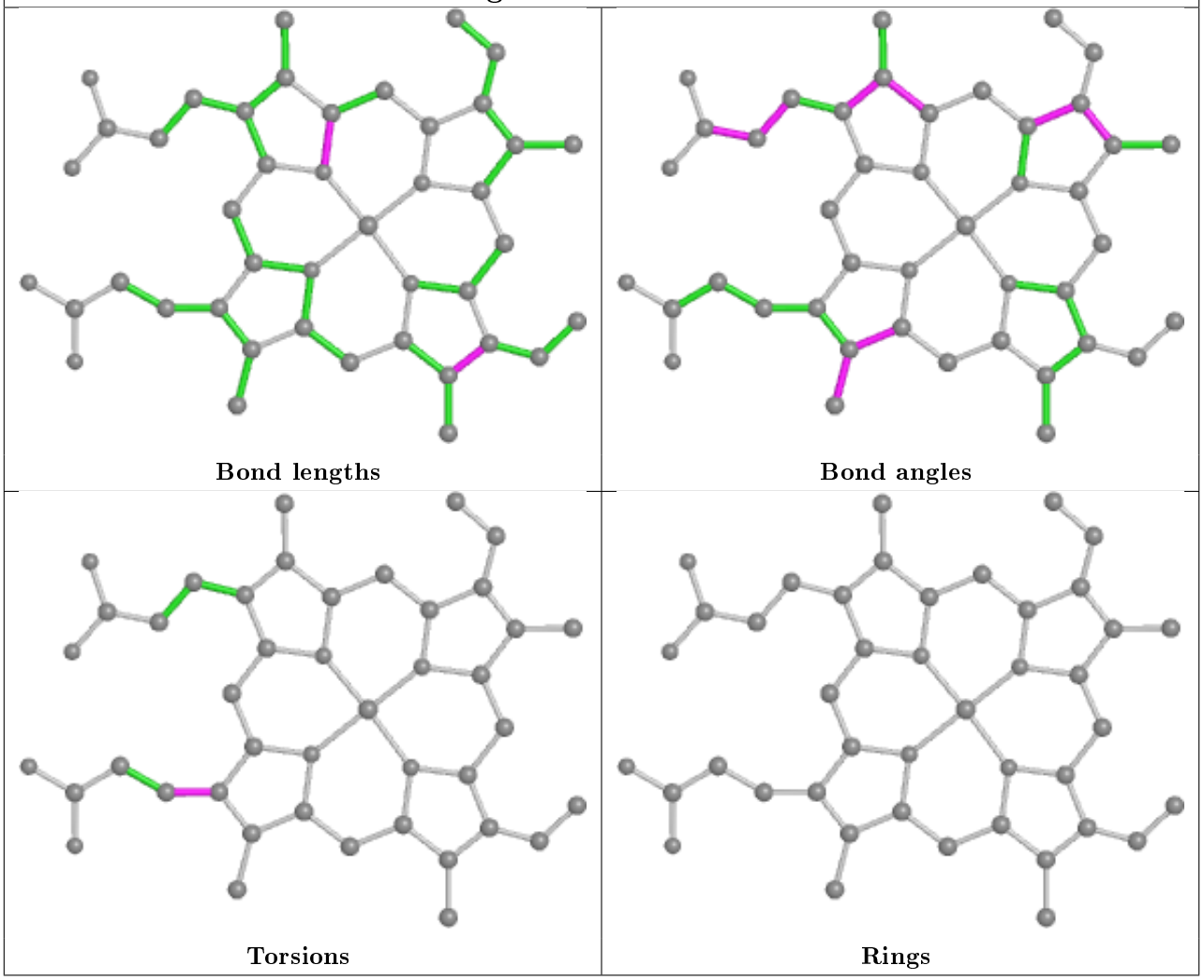


Torsions



Rings

Ligand HEM D 501



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	401/418 (95%)	0.35	14 (3%)	44	51	31, 58, 82, 101	0
1	B	397/418 (94%)	0.03	8 (2%)	65	72	30, 49, 80, 107	0
1	C	401/418 (95%)	-0.06	9 (2%)	62	68	26, 46, 72, 88	0
1	D	397/418 (94%)	-0.12	5 (1%)	77	82	24, 39, 75, 115	0
1	E	402/418 (96%)	-0.24	1 (0%)	95	97	20, 37, 56, 85	0
1	F	390/418 (93%)	0.27	15 (3%)	40	47	29, 57, 92, 114	0
All	All	2388/2508 (95%)	0.04	52 (2%)	62	68	20, 48, 80, 115	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ALA	4.2
1	A	418	ALA	4.0
1	E	418	ALA	3.7
1	F	224	ASN	3.6
1	F	248	LEU	3.5
1	C	418	ALA	3.5
1	C	416	ILE	3.2
1	C	282	ALA	3.1
1	F	244	PHE	3.1
1	F	232	HIS	3.0
1	F	53	CYS	3.0
1	F	222	PRO	3.0
1	A	228	SER	3.0
1	C	140	ASP	3.0
1	D	218	VAL	2.9
1	C	389	PRO	2.9
1	B	248	LEU	2.7
1	D	418	ALA	2.6
1	D	189	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	55	ASP	2.5
1	B	245	LEU	2.5
1	B	224	ASN	2.5
1	A	314	LEU	2.5
1	A	416	ILE	2.5
1	F	214	TRP	2.5
1	A	281	CYS	2.4
1	F	229	MET	2.4
1	B	219	ASN	2.4
1	B	91	SER	2.4
1	F	318	SER	2.4
1	A	340	GLU	2.4
1	F	241	PRO	2.4
1	C	281	CYS	2.4
1	D	55	ASP	2.3
1	A	80	PHE	2.3
1	F	230	MET	2.3
1	F	245	LEU	2.3
1	C	347	ILE	2.2
1	A	219	ASN	2.2
1	A	348	ASP	2.2
1	A	282	ALA	2.2
1	F	221	PRO	2.2
1	A	161	GLN	2.2
1	A	338	ALA	2.2
1	B	220	VAL	2.2
1	A	339	ILE	2.2
1	C	277	TYR	2.1
1	A	18	ALA	2.1
1	F	168	ASP	2.1
1	C	286	LEU	2.1
1	B	418	ALA	2.0
1	B	221	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)

There are no monosaccharides in this entry.

6.4 Ligands

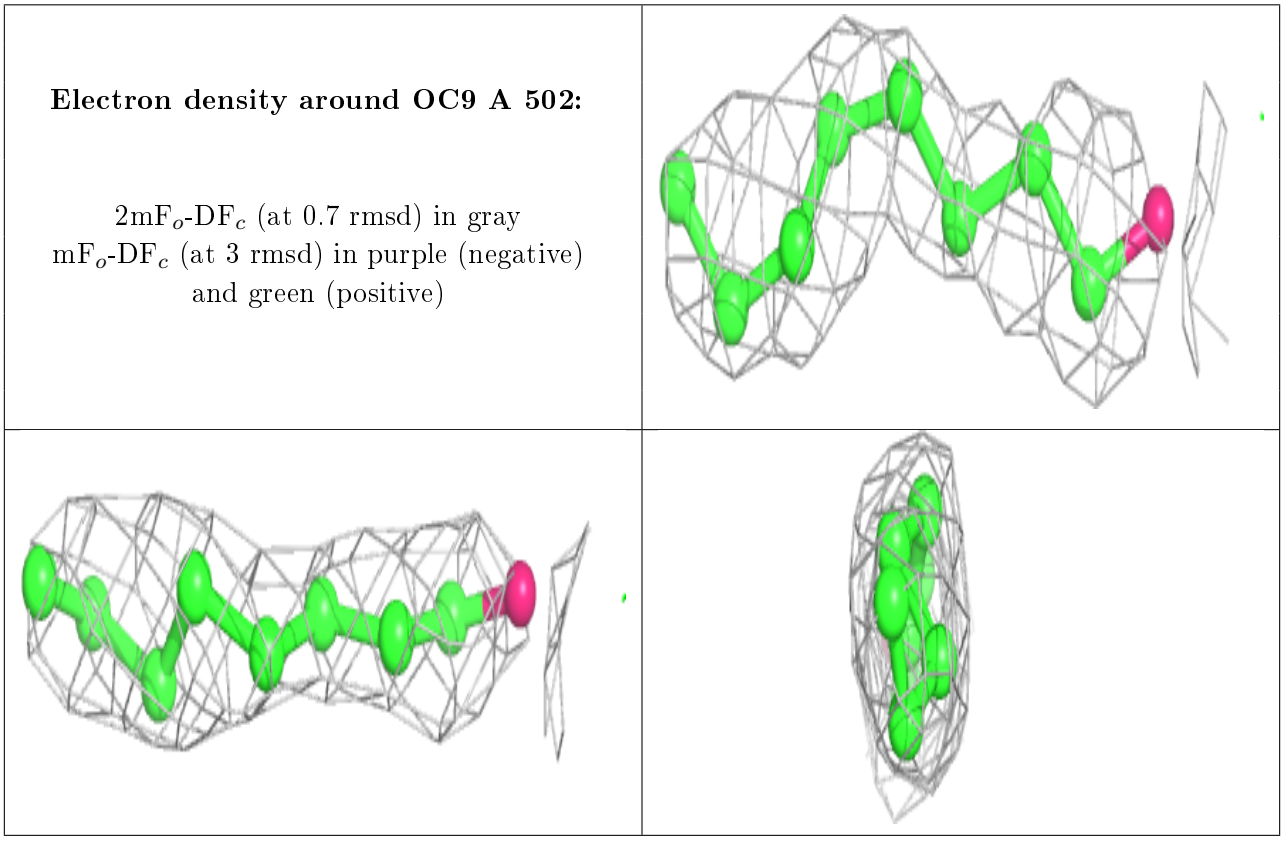
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	OC9	A	502	9/9	0.91	0.23	47,52,59,59	0
2	HEM	A	501	43/43	0.97	0.16	27,34,42,47	0
3	OC9	B	502	9/9	0.97	0.21	46,47,63,64	0
3	OC9	C	502	9/9	0.97	0.24	35,37,47,50	0
3	OC9	D	502	9/9	0.97	0.24	42,47,75,82	0
2	HEM	D	501	43/43	0.98	0.14	20,23,30,34	0
2	HEM	F	501	43/43	0.98	0.14	22,28,47,55	0
2	HEM	C	501	43/43	0.98	0.12	22,28,32,36	0
3	OC9	E	502	9/9	0.98	0.20	26,29,33,35	0
2	HEM	B	501	43/43	0.99	0.12	22,27,31,34	0
2	HEM	E	501	43/43	0.99	0.14	21,24,26,29	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.

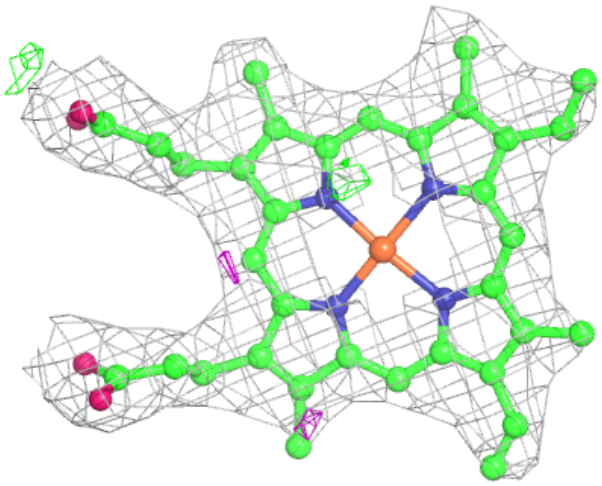
Electron density around OC9 A 502:

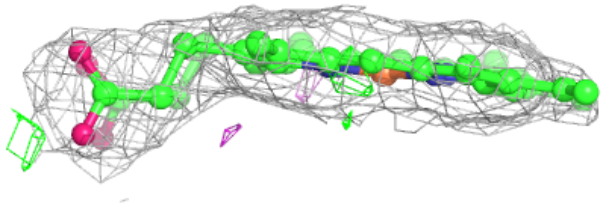
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

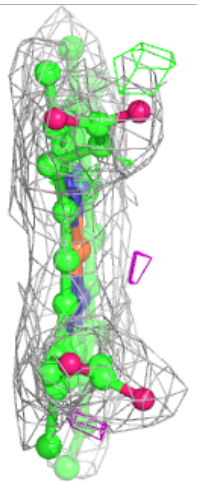


Electron density around HEM A 501:

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

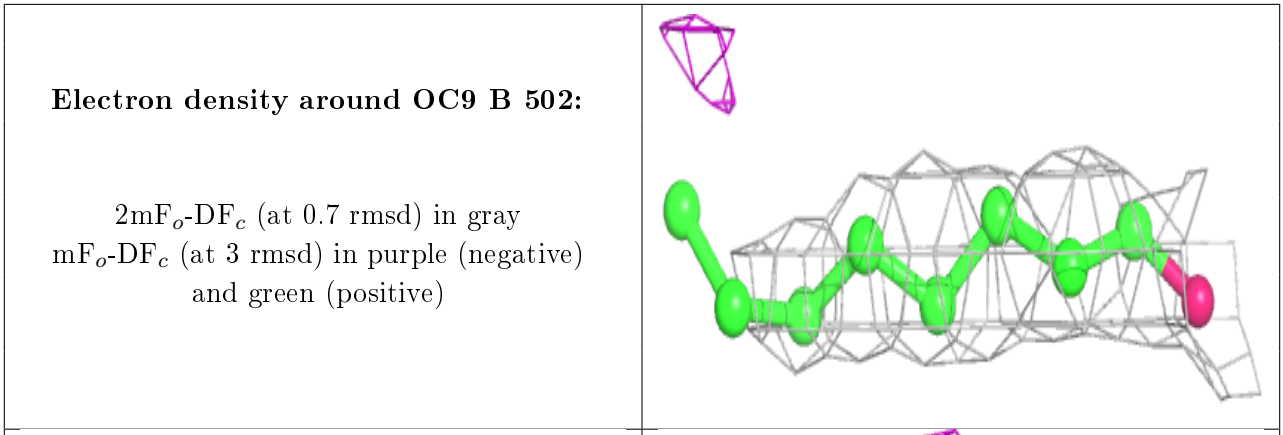


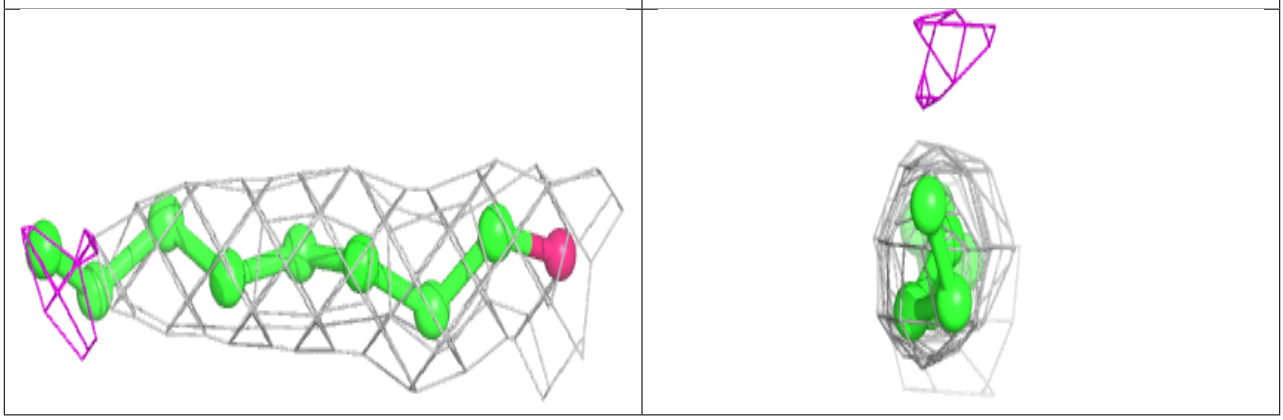




Electron density around OC9 B 502:

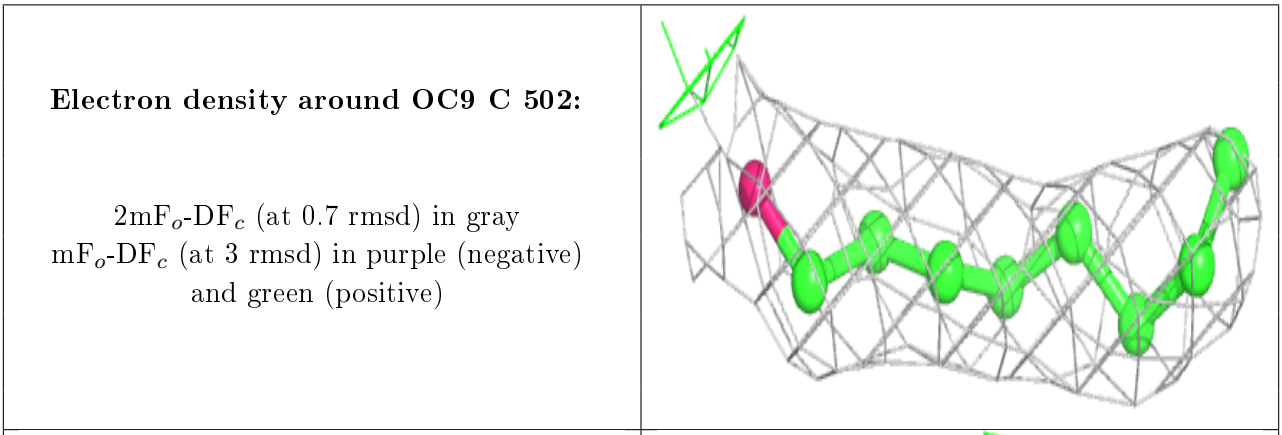
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

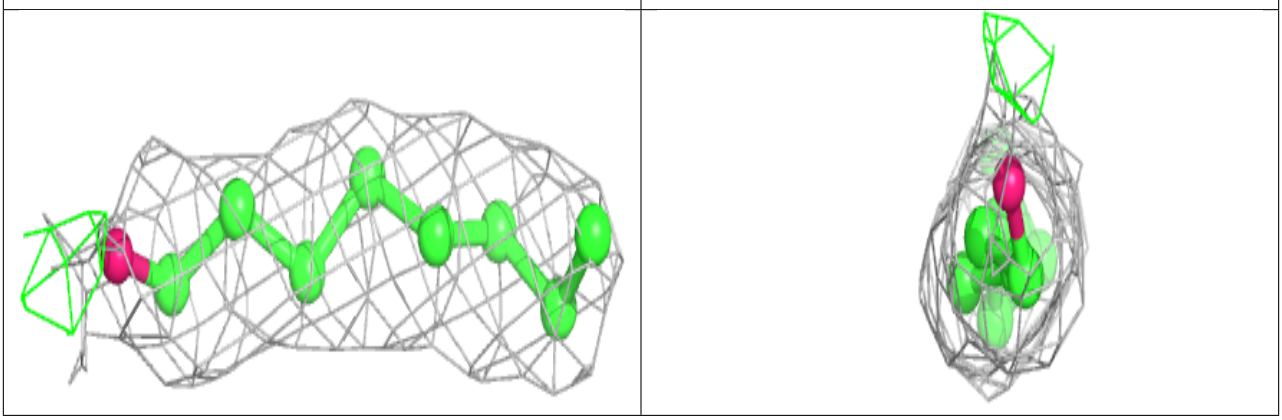




Electron density around OC9 C 502:

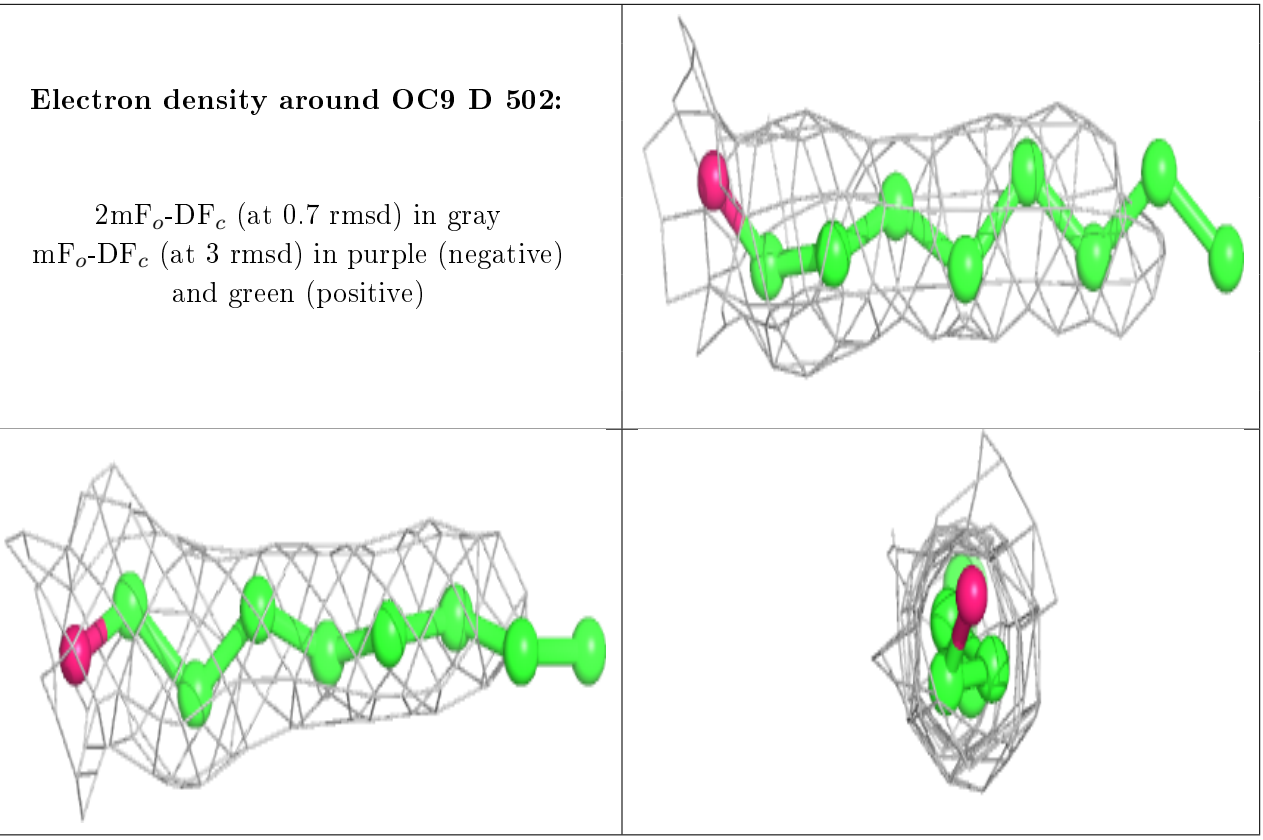
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





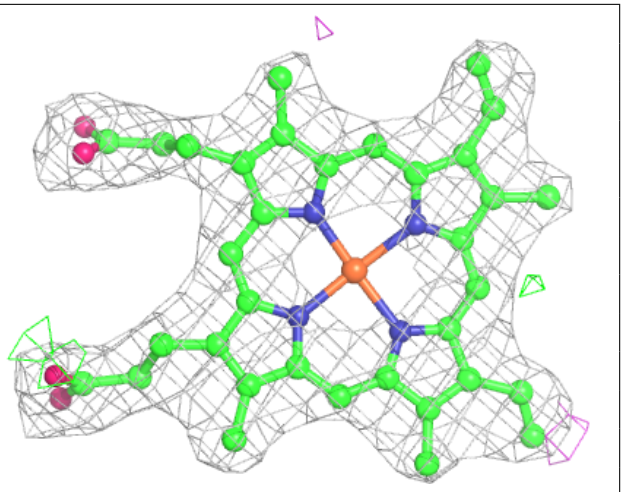
Electron density around OC9 D 502:

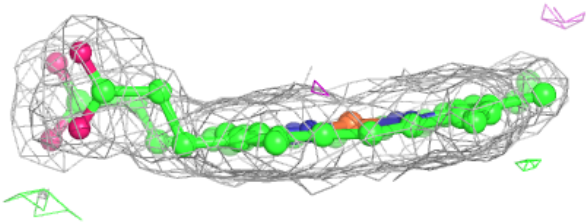
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

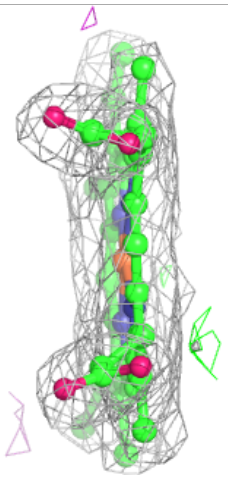


Electron density around HEM D 501:

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

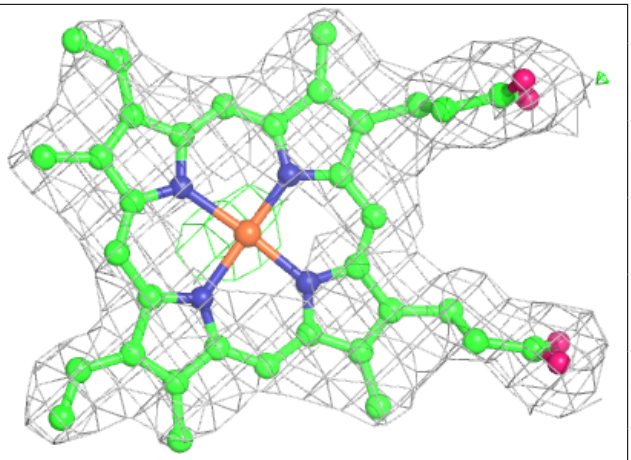


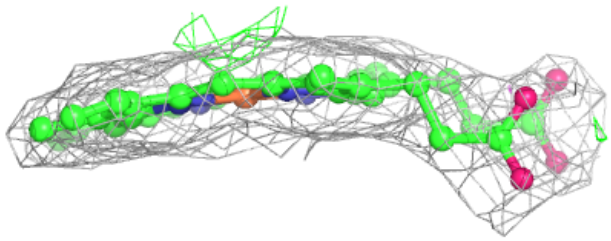


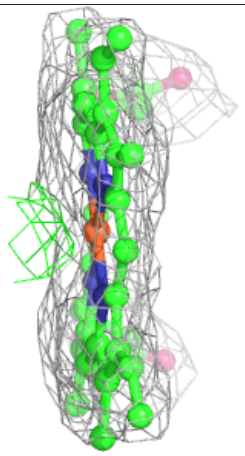


Electron density around HEM F 501:

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

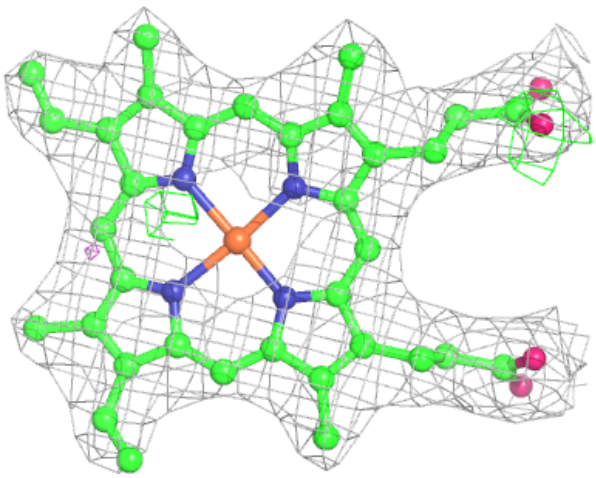


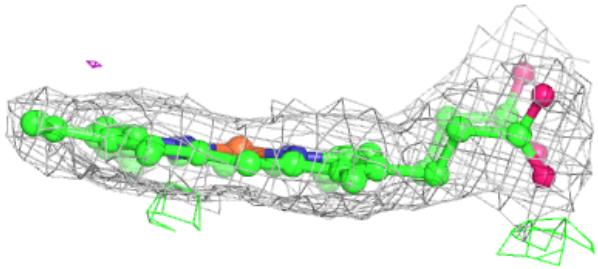


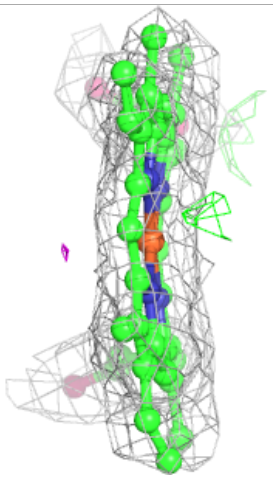


Electron density around HEM C 501:

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

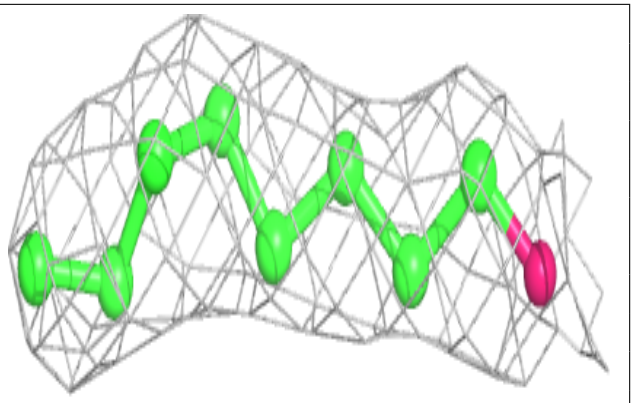


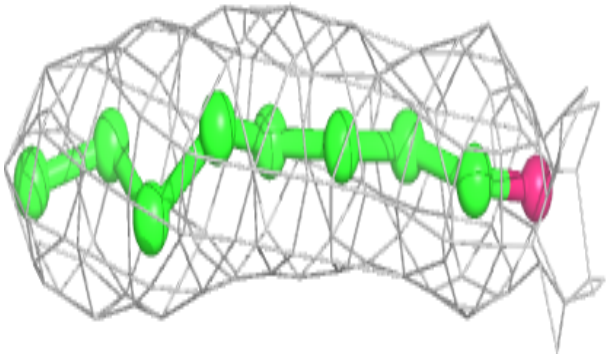


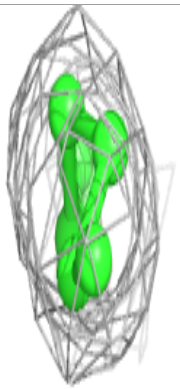


Electron density around OC9 E 502:

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

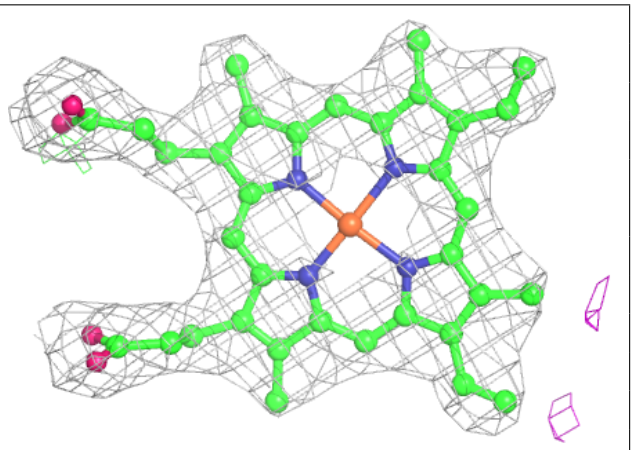


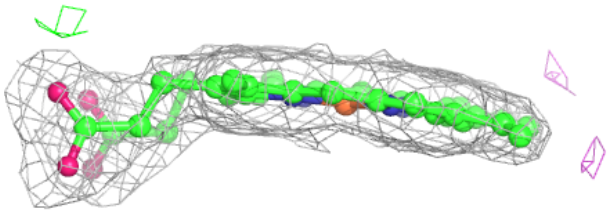


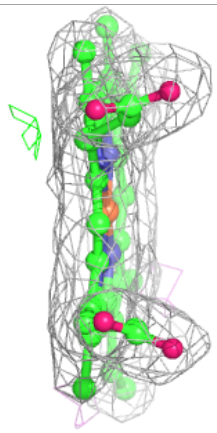


Electron density around HEM B 501:

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

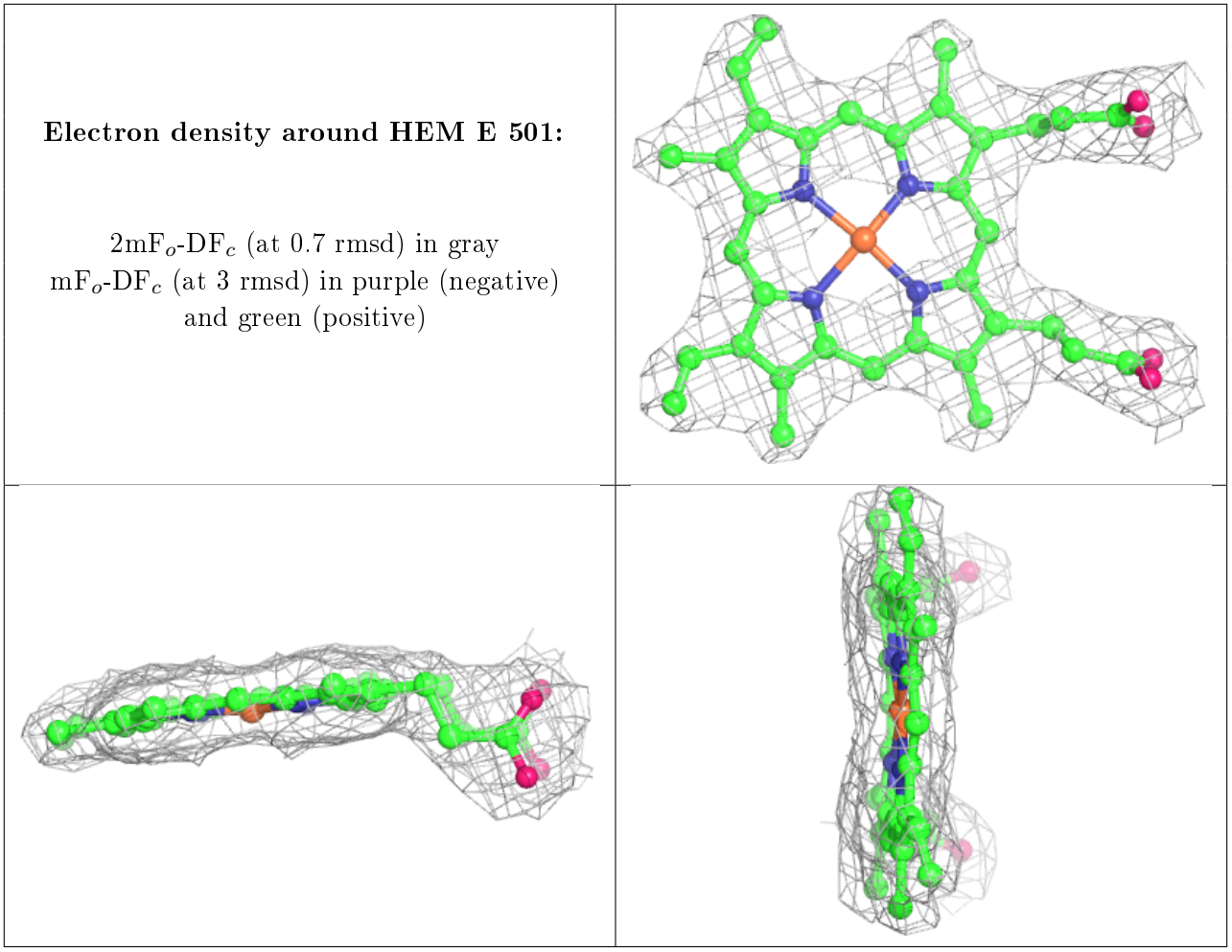






Electron density around HEM E 501:

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



6.5 Other polymers

There are no such residues in this entry.