Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 08:01 am BST

PDB ID	:	6YRC / pdb_00006yrc
Title	:	Spectroscopically-validated structure of DtpB from Streptomyces lividans in the ferric state
Authors	:	Lucic, M.; Dworkowski, F.S.N.; Worrall, J.A.R.; Hough, M.A.
Deposited on	:	2020-04-20
Resolution	:	1.99 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

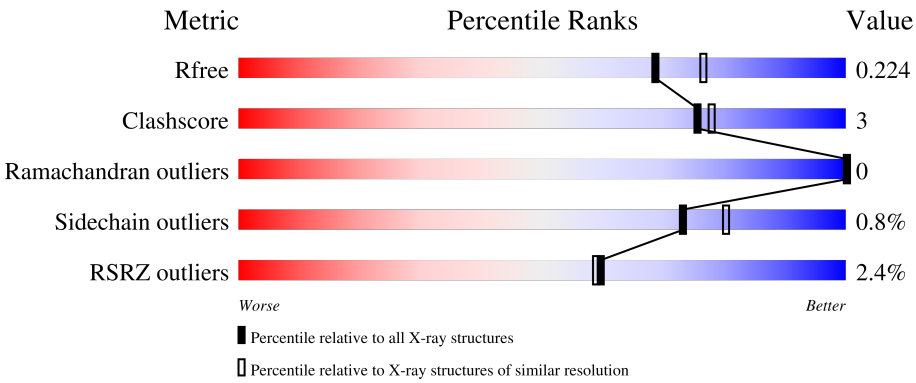
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	.% 88% 9% •
1	B	316	3% 92% • •
1	C	316	2% 92% 5% •
1	D	316	3% 91% 6% •
1	E	316	3% 94% • •

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Mol	Chain	Length	Quality of chain
1	F	316	3% 90% 7%

2 Entry composition (i)

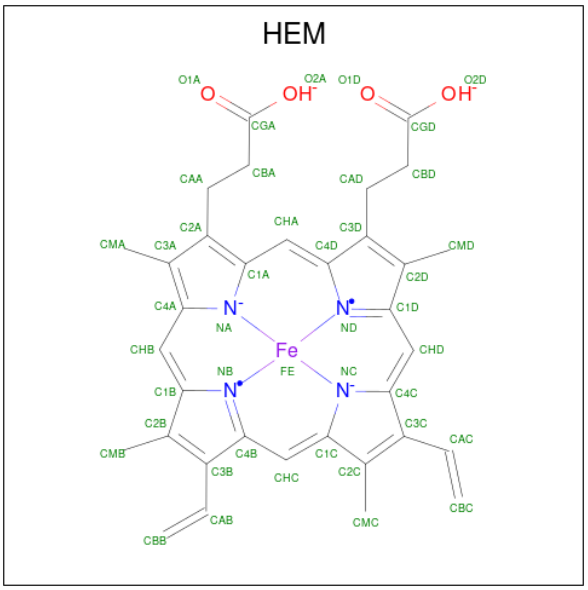
There are 6 unique types of molecules in this entry. The entry contains 15579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative iron-dependent peroxidase.

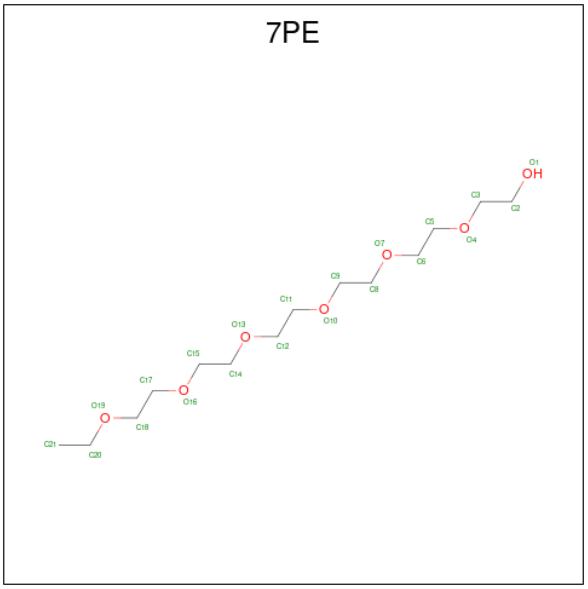
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2372	1488	414	461	9	0	5	0
1	B	306	2328	1466	404	449	9	0	1	0
1	C	306	2330	1468	398	454	10	0	1	0
1	D	306	2348	1474	407	458	9	0	2	0
1	E	306	2335	1471	401	454	9	0	2	0
1	F	308	2349	1476	401	463	9	0	5	0

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



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

- Molecule 3 is 2-(2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (CCD ID: 7PE) (formula: $C_{14}H_{30}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	4	2	0	0
3	A	1	4	2	2	0	0
3	B	1	5	4	1	0	0
3	B	1	5	3	2	0	0
3	D	1	6	4	2	0	0

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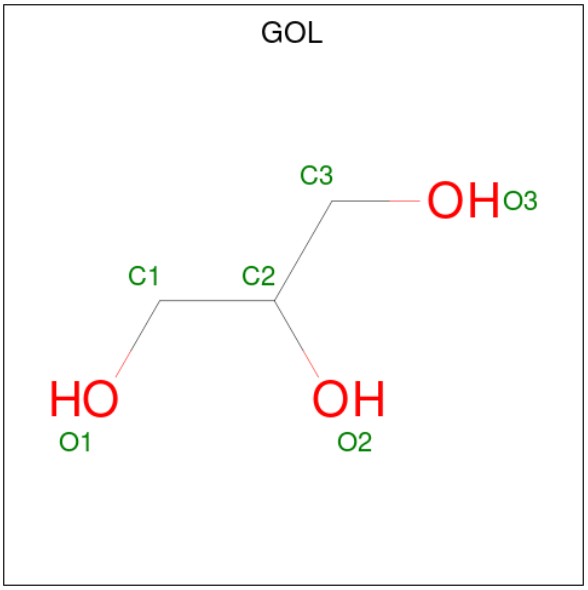
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 9 6 3	0	0
3	F	1	Total C O 6 4 2	0	1
3	F	1	Total C O 5 3 2	0	0
3	F	1	Total C O 7 5 2	0	0
3	F	1	Total C O 5 3 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	6	3	3	0	0
5	C	1	6	3	3	0	0
5	C	1	6	3	3	0	0
5	C	1	6	3	3	0	0
5	F	1	6	3	3	0	0
5	F	1	6	3	3	0	0
5	F	1	6	3	3	0	0
5	F	1	6	3	3	0	0

- Molecule 6 is water.

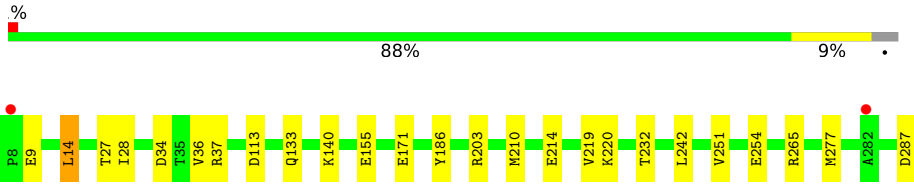
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	216	216	216	0	0
6	B	147	147	147	0	0
6	C	205	205	205	0	0
6	D	198	198	198	0	0
6	E	189	189	189	0	0
6	F	187	187	187	0	0

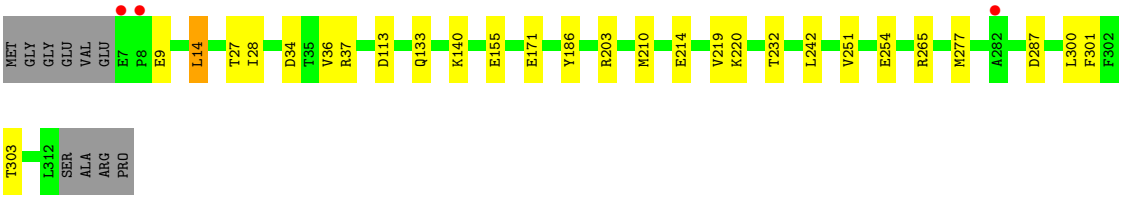
3 Residue-property plots (i)

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: Putative iron-dependent peroxidase

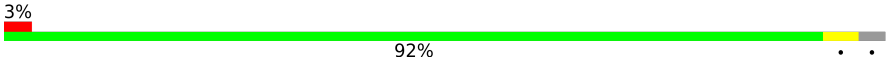
Chain A:

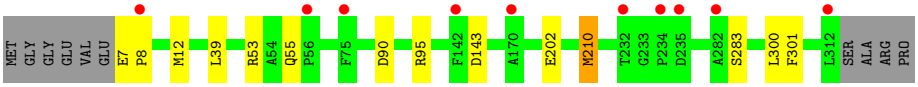




• Molecule 1: Putative iron-dependent peroxidase

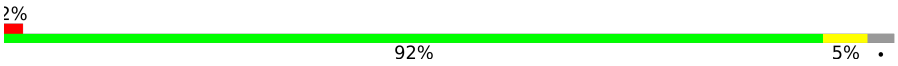
Chain B:

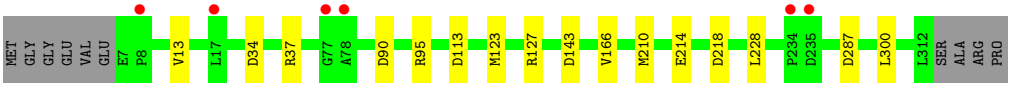




• Molecule 1: Putative iron-dependent peroxidase

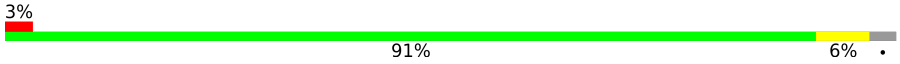
Chain C:

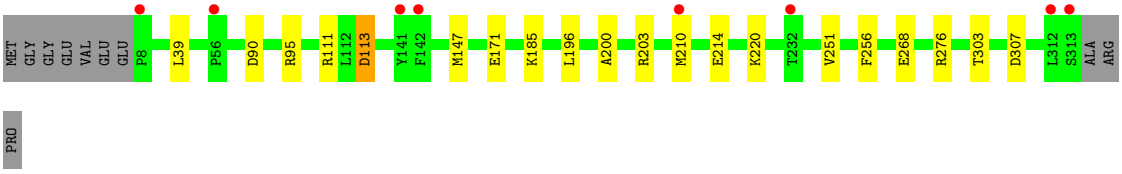




• Molecule 1: Putative iron-dependent peroxidase

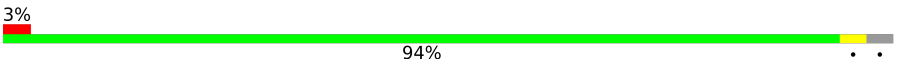
Chain D:





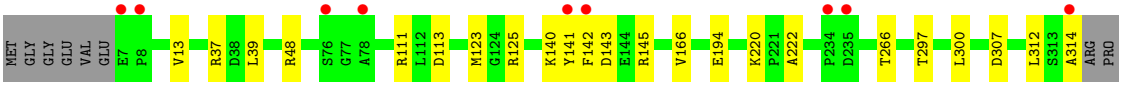
• Molecule 1: Putative iron-dependent peroxidase

Chain E:



• Molecule 1: Putative iron-dependent peroxidase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.79Å 120.27Å 196.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 1.99 49.05 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.05-1.99) 99.0 (49.05-1.99)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.176 , 0.218 0.185 , 0.224	Depositor DCC
R_{free} test set	6824 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15579	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 7PE, GOL, MG, 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	1.09	0/2422	1.28	3/3289 (0.1%)
1	B	1.06	0/2378	1.33	0/3231
1	C	1.05	0/2380	1.29	0/3233
1	D	1.07	0/2398	1.34	2/3256 (0.1%)
1	E	1.08	1/2385 (0.0%)	1.32	0/3241
1	F	1.09	0/2398	1.31	0/3259
All	All	1.07	1/14361 (0.0%)	1.31	5/19509 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	137	HIS	CE1-NE2	6.39	1.39	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	9	GLU	CB-CA-C	6.37	117.14	109.31
1	A	303	THR	CB-CA-C	5.67	115.55	110.44
1	D	113	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	303	THR	CB-CA-C	5.28	115.20	110.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	312	LEU	Peptide

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	2372	0	2288	18	0
1	B	2328	0	2251	10	0
1	C	2330	0	2251	14	0
1	D	2348	0	2272	16	0
1	E	2335	0	2249	9	0
1	F	2349	0	2233	21	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
2	E	43	0	30	0	0
2	F	43	0	30	0	0
3	A	10	0	10	6	0
3	B	10	0	8	1	0
3	D	6	0	6	1	0
3	F	32	0	28	5	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	B	12	0	16	0	0
5	C	18	0	24	2	0
5	F	24	0	32	1	0
6	A	216	0	0	4	0
6	B	147	0	0	0	0
6	C	205	0	0	4	0
6	D	198	0	0	5	0
6	E	189	0	0	1	0
6	F	187	0	0	3	0
All	All	15579	0	13848	84	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 3.

All (84) 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:A:210:MET:HB2	1:D:210:MET:HE1	1.59	0.83
1:C:214:GLU:OE1	6:C:501:HOH:O	2.05	0.74
1:E:48:ARG:CZ	3:F:410:7PE:H61	2.19	0.73
1:D:214:GLU:OE1	6:D:501:HOH:O	2.13	0.66
1:D:111[B]:ARG:NH1	1:F:142:PHE:HB3	2.10	0.65
1:F:37:ARG:HD2	1:F:314:ALA:HA	1.78	0.65
1:E:143:ASP:N	1:E:143:ASP:OD1	2.30	0.64
1:C:210[B]:MET:SD	1:E:210:MET:HE3	2.39	0.63
1:F:297:THR:HG22	3:F:405[A]:7PE:H62	1.80	0.62
1:D:214:GLU:OE2	1:D:220:LYS:NZ	2.21	0.61
1:D:90:ASP:OD1	1:D:95:ARG:NH1	2.33	0.61
1:F:111[B]:ARG:HD2	1:F:113:ASP:OD1	2.01	0.61
1:B:210:MET:HE1	1:F:145:ARG:CZ	2.31	0.60
2:B:401:HEM:HBC2	2:B:401:HEM:HMC2	1.83	0.59
1:A:214:GLU:OE2	1:A:220:LYS:NZ	2.20	0.59
1:A:232:THR:HG23	6:A:691:HOH:O	2.03	0.59
1:C:37:ARG:HD3	6:C:681:HOH:O	2.03	0.58
1:A:34:ASP:OD1	1:A:37:ARG:NH2	2.35	0.58
1:D:111[B]:ARG:NH1	1:F:142:PHE:CB	2.66	0.58
1:C:218:ASP:OD1	6:C:502:HOH:O	2.17	0.58
1:F:194:GLU:OE1	6:F:501:HOH:O	2.16	0.58
2:A:401:HEM:HMC2	2:A:401:HEM:HBC2	1.87	0.55
1:B:53:ARG:HD2	1:C:143:ASP:OD2	2.07	0.54
1:F:140:LYS:HG3	1:F:141:TYR:O	2.07	0.53
1:D:171:GLU:OE2	3:D:402:7PE:C8	2.57	0.52
1:C:210[A]:MET:SD	5:C:405:GOL:H31	2.51	0.51
3:A:402:7PE:H91	1:F:48:ARG:CD	2.41	0.51
1:A:155:GLU:OE1	3:A:402:7PE:O13	2.29	0.50
1:D:147:MET:HE3	1:D:256:PHE:HA	1.94	0.50
1:F:140:LYS:CG	1:F:141:TYR:O	2.60	0.49
3:A:402:7PE:H91	1:F:48:ARG:HD3	1.93	0.49
3:A:402:7PE:H111	1:F:48:ARG:CZ	2.42	0.49
1:B:300:LEU:C	1:B:300:LEU:HD23	2.38	0.49
1:F:13:VAL:HG11	1:F:166:VAL:CG1	2.42	0.48
2:A:401:HEM:HBC2	2:A:401:HEM:CMC	2.44	0.48
1:F:300:LEU:C	1:F:300:LEU:HD23	2.39	0.48
1:A:203[B]:ARG:NH1	6:A:501:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:VAL:HG11	1:C:166:VAL:CG1	2.45	0.47
1:F:13:VAL:HG11	1:F:166:VAL:HG11	1.96	0.47
1:A:171:GLU:HG2	3:A:403:7PE:H171	1.96	0.47
1:D:113:ASP:HB3	6:F:611:HOH:O	2.13	0.47
1:D:196:LEU:HB3	1:D:200:ALA:HB3	1.97	0.46
1:C:210[B]:MET:HE1	1:E:210:MET:HB2	1.97	0.46
2:B:401:HEM:HBC2	2:B:401:HEM:CMC	2.46	0.46
1:C:228:LEU:HD12	1:C:287:ASP:HA	1.99	0.45
1:E:48:ARG:NE	3:F:410:7PE:H61	2.31	0.45
1:A:14:LEU:HD23	1:A:242:LEU:HD22	1.99	0.44
1:C:34:ASP:OD1	1:C:37:ARG:NH1	2.50	0.44
1:C:300:LEU:C	1:C:300:LEU:HD23	2.42	0.44
5:C:403:GOL:H11	6:C:649:HOH:O	2.16	0.44
1:F:220:LYS:O	3:F:402:7PE:H61	2.16	0.44
1:A:254:GLU:OE1	6:A:502:HOH:O	2.21	0.44
1:D:185:LYS:NZ	6:D:504:HOH:O	2.41	0.44
3:A:403:7PE:C18	6:A:521:HOH:O	2.66	0.44
1:E:300:LEU:HD23	1:E:301:PHE:N	2.32	0.43
1:D:39:LEU:C	1:D:39:LEU:HD13	2.43	0.43
1:D:276:ARG:CZ	6:D:562:HOH:O	2.66	0.43
1:B:55:GLN:HA	1:B:55:GLN:OE1	2.17	0.43
1:B:90:ASP:OD1	1:B:95:ARG:NE	2.51	0.43
1:E:34:ASP:OD1	1:E:37[A]:ARG:NH2	2.40	0.43
1:E:300:LEU:HD23	1:E:300:LEU:C	2.44	0.43
1:B:7:GLU:N	1:B:8:PRO:CD	2.82	0.43
1:D:251:VAL:HG12	1:F:123:MET:HG3	2.01	0.43
1:C:90:ASP:OD1	1:C:95:ARG:NH1	2.52	0.42
1:E:88:GLU:CD	6:E:605:HOH:O	2.61	0.42
1:A:27:THR:HG23	1:A:133[A]:GLN:HG3	2.01	0.42
1:B:39:LEU:C	1:B:39:LEU:HD13	2.44	0.42
1:A:186:TYR:CG	2:A:401:HEM:HBB1	2.55	0.42
1:A:251:VAL:HG12	1:C:123:MET:HG3	2.01	0.42
1:A:300:LEU:HD23	1:A:301:PHE:N	2.34	0.42
1:B:300:LEU:HD23	1:B:301:PHE:N	2.35	0.42
1:B:202:GLU:OE1	3:B:402:7PE:H141	2.20	0.41
1:A:300:LEU:HD23	1:A:300:LEU:C	2.45	0.41
1:F:222:ALA:O	3:F:402:7PE:C11	2.68	0.41
1:D:276:ARG:HD2	6:D:562:HOH:O	2.20	0.41
1:D:203:ARG:NE	6:D:502:HOH:O	2.26	0.41
1:F:125:ARG:HD3	6:F:538:HOH:O	2.21	0.41
1:A:140:LYS:O	1:C:113:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143[A]:ASP:OD1	5:F:407:GOL:H11	2.20	0.41
1:F:39:LEU:C	1:F:39:LEU:HD13	2.46	0.40
1:A:277:MET:HA	1:A:287:ASP:HB2	2.03	0.40
1:B:12:MET:O	1:B:12:MET:HG3	2.21	0.40
1:A:27:THR:HG23	1:A:133[A]:GLN:CG	2.52	0.40
1:A:28:ILE:HG12	1:A:36:VAL:HG21	2.03	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	309/316 (98%)	300 (97%)	9 (3%)	0	100	100
1	B	305/316 (96%)	299 (98%)	6 (2%)	0	100	100
1	C	305/316 (96%)	298 (98%)	7 (2%)	0	100	100
1	D	306/316 (97%)	300 (98%)	6 (2%)	0	100	100
1	E	306/316 (97%)	299 (98%)	7 (2%)	0	100	100
1	F	311/316 (98%)	307 (99%)	4 (1%)	0	100	100
All	All	1842/1896 (97%)	1803 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/252 (98%)	244 (98%)	4 (2%)	55	62
1	B	241/252 (96%)	238 (99%)	3 (1%)	63	70
1	C	243/252 (96%)	242 (100%)	1 (0%)	84	89
1	D	247/252 (98%)	244 (99%)	3 (1%)	63	70
1	E	242/252 (96%)	241 (100%)	1 (0%)	84	89
1	F	241/252 (96%)	239 (99%)	2 (1%)	73	80
All	All	1462/1512 (97%)	1448 (99%)	14 (1%)	73	75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	219	VAL
1	A	265[A]	ARG
1	A	265[B]	ARG
1	B	143	ASP
1	B	210	MET
1	B	283	SER
1	C	127	ARG
1	D	268	GLU
1	D	307[A]	ASP
1	D	307[B]	ASP
1	E	143	ASP
1	F	266	THR
1	F	307	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 5 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	7PE	B	404	-	4,4,20	0.33	0	3,3,19	0.19	0
3	7PE	A	403	-	3,3,20	0.38	0	2,2,19	0.06	0
3	7PE	B	402	-	4,4,20	0.34	0	3,3,19	0.22	0
2	HEM	C	401	1	50,50,50	1.35	6 (12%)	66,82,82	1.51	12 (18%)
2	HEM	B	401	1	50,50,50	1.34	4 (8%)	66,82,82	1.63	12 (18%)
3	7PE	A	402	-	5,5,20	0.36	0	4,4,19	0.23	0
3	7PE	F	409	-	6,6,20	0.41	0	5,5,19	0.17	0
5	GOL	C	402	-	5,5,5	0.13	0	5,5,5	0.21	0
5	GOL	F	406	-	5,5,5	0.10	0	5,5,5	0.25	0
5	GOL	B	405	-	5,5,5	0.14	0	5,5,5	0.34	0
3	7PE	D	402	-	5,5,20	0.30	0	4,4,19	0.30	0
2	HEM	D	401	1	50,50,50	1.40	8 (16%)	66,82,82	1.57	13 (19%)
5	GOL	C	403	-	5,5,5	0.12	0	5,5,5	0.13	0
5	GOL	F	407	-	5,5,5	0.15	0	5,5,5	0.37	0
2	HEM	F	401	1	50,50,50	1.44	6 (12%)	66,82,82	1.60	13 (19%)
2	HEM	A	401	1	50,50,50	1.39	7 (14%)	66,82,82	1.63	17 (25%)
5	GOL	F	403	-	5,5,5	0.15	0	5,5,5	0.38	0
5	GOL	B	403	-	5,5,5	0.11	0	5,5,5	0.27	0
5	GOL	F	404	-	5,5,5	0.09	0	5,5,5	0.38	0
3	7PE	F	402	-	8,8,20	0.35	0	7,7,19	0.15	0
2	HEM	E	401	1	50,50,50	1.48	8 (16%)	66,82,82	1.66	12 (18%)
5	GOL	C	405	-	5,5,5	0.16	0	5,5,5	0.39	0
3	7PE	F	410	-	4,4,20	0.26	0	3,3,19	0.17	0
3	7PE	F	408	-	4,4,20	0.35	0	3,3,19	0.24	0
3	7PE	F	405[A]	-	5,5,20	0.10	0	4,4,19	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7PE	B	404	-	-	2/2/2/18	-
3	7PE	A	403	-	-	0/1/1/18	-
3	7PE	B	402	-	-	1/2/2/18	-
2	HEM	C	401	1	-	5/14/54/54	-
2	HEM	B	401	1	-	4/14/54/54	-
3	7PE	A	402	-	-	1/3/3/18	-
3	7PE	F	409	-	-	1/4/4/18	-
5	GOL	C	402	-	-	2/4/4/4	-
5	GOL	F	406	-	-	1/4/4/4	-
5	GOL	B	405	-	-	3/4/4/4	-
3	7PE	D	402	-	-	3/3/3/18	-
2	HEM	D	401	1	-	4/14/54/54	-
5	GOL	C	403	-	-	2/4/4/4	-
5	GOL	F	407	-	-	0/4/4/4	-
2	HEM	F	401	1	-	4/14/54/54	-
2	HEM	A	401	1	-	4/14/54/54	-
5	GOL	F	403	-	-	0/4/4/4	-
5	GOL	B	403	-	-	2/4/4/4	-
5	GOL	F	404	-	-	2/4/4/4	-
3	7PE	F	402	-	-	3/6/6/18	-
2	HEM	E	401	1	-	4/14/54/54	-
5	GOL	C	405	-	-	2/4/4/4	-
3	7PE	F	410	-	-	0/2/2/18	-
3	7PE	F	408	-	-	2/2/2/18	-
3	7PE	F	405[A]	-	-	1/3/3/18	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	FE-NB	4.52	2.08	1.94
2	F	401	HEM	FE-NC	4.27	2.09	1.95
2	C	401	HEM	FE-NB	4.18	2.07	1.94
2	A	401	HEM	FE-NB	4.05	2.07	1.94
2	E	401	HEM	FE-NB	4.01	2.07	1.94
2	C	401	HEM	FE-NC	3.98	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C1B-NB	-3.95	1.33	1.40
2	E	401	HEM	FE-NC	3.94	2.08	1.95
2	D	401	HEM	FE-NC	3.85	2.08	1.95
2	F	401	HEM	FE-NB	3.85	2.06	1.94
2	D	401	HEM	FE-NB	3.78	2.06	1.94
2	A	401	HEM	FE-NC	3.72	2.07	1.95
2	F	401	HEM	C1B-NB	-3.70	1.33	1.40
2	B	401	HEM	FE-NC	3.30	2.06	1.95
2	E	401	HEM	C4D-ND	-3.23	1.34	1.40
2	E	401	HEM	C4B-NB	-3.18	1.32	1.38
2	D	401	HEM	C4B-NB	-2.96	1.32	1.38
2	A	401	HEM	C4D-ND	-2.94	1.35	1.40
2	A	401	HEM	C4D-C3D	2.93	1.50	1.45
2	A	401	HEM	C1B-NB	-2.93	1.35	1.40
2	C	401	HEM	C1B-NB	-2.82	1.35	1.40
2	F	401	HEM	C3C-C2C	2.58	1.42	1.37
2	A	401	HEM	C3B-C4B	2.55	1.50	1.44
2	E	401	HEM	C1C-NC	-2.34	1.35	1.39
2	E	401	HEM	O1A-CGA	2.33	1.29	1.22
2	D	401	HEM	C4D-ND	-2.32	1.36	1.40
2	D	401	HEM	C3D-C2D	-2.30	1.31	1.36
2	D	401	HEM	C3B-C4B	2.29	1.49	1.44
2	B	401	HEM	C4D-ND	-2.25	1.36	1.40
2	D	401	HEM	C1B-NB	-2.23	1.36	1.40
2	E	401	HEM	C1B-NB	-2.21	1.36	1.40
2	A	401	HEM	C4B-NB	-2.17	1.34	1.38
2	D	401	HEM	O2A-CGA	-2.09	1.23	1.30
2	C	401	HEM	O2A-CGA	-2.07	1.23	1.30
2	C	401	HEM	C4B-NB	-2.05	1.34	1.38
2	C	401	HEM	C3B-C4B	2.04	1.48	1.44
2	F	401	HEM	C4D-C3D	2.03	1.48	1.45
2	F	401	HEM	C1D-ND	-2.03	1.34	1.38
2	E	401	HEM	FE-NA	2.01	2.01	1.95

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HEM	C1B-NB-C4B	5.61	110.86	105.07
2	E	401	HEM	C1B-NB-C4B	5.38	110.63	105.07
2	F	401	HEM	CHC-C4B-NB	5.17	130.04	124.42
2	B	401	HEM	C1B-NB-C4B	4.97	110.20	105.07
2	B	401	HEM	CHC-C4B-NB	4.82	129.66	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	HEM	CHC-C4B-NB	4.57	129.39	124.42
2	C	401	HEM	CHC-C4B-NB	4.50	129.30	124.42
2	D	401	HEM	CHC-C4B-NB	4.31	129.10	124.42
2	F	401	HEM	C1B-NB-C4B	4.10	109.31	105.07
2	D	401	HEM	C1B-NB-C4B	3.93	109.13	105.07
2	B	401	HEM	CHD-C1D-ND	3.82	128.57	124.42
2	C	401	HEM	C1B-NB-C4B	3.47	108.65	105.07
2	F	401	HEM	CHD-C1D-ND	3.46	128.17	124.42
2	D	401	HEM	CHD-C1D-ND	3.41	128.12	124.42
2	A	401	HEM	CHD-C1D-C2D	-3.40	119.67	124.98
2	E	401	HEM	CMD-C2D-C1D	3.35	130.13	125.04
2	A	401	HEM	CHD-C1D-ND	3.30	128.00	124.42
2	E	401	HEM	CHA-C4D-ND	3.28	128.42	124.37
2	C	401	HEM	CHD-C1D-ND	3.17	127.86	124.42
2	A	401	HEM	CHC-C4B-NB	3.11	127.80	124.42
2	F	401	HEM	CHD-C1D-C2D	-3.11	120.12	124.98
2	B	401	HEM	CHD-C1D-C2D	-3.10	120.14	124.98
2	F	401	HEM	C4C-NC-C1C	3.10	108.38	105.35
2	E	401	HEM	CHB-C1B-NB	2.96	128.02	124.37
2	D	401	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
2	D	401	HEM	CHA-C4D-C3D	-2.90	119.89	125.33
2	E	401	HEM	CHD-C1D-C2D	-2.86	120.51	124.98
2	D	401	HEM	CHA-C4D-ND	2.79	127.81	124.37
2	C	401	HEM	CHD-C1D-C2D	-2.75	120.69	124.98
2	A	401	HEM	C4C-NC-C1C	2.74	108.03	105.35
2	B	401	HEM	CAD-C3D-C4D	2.70	129.38	124.66
2	B	401	HEM	CHA-C4D-ND	2.62	127.61	124.37
2	C	401	HEM	CHD-C4C-NC	2.62	127.27	124.44
2	A	401	HEM	CMB-C2B-C1B	2.61	129.02	125.04
2	C	401	HEM	CHA-C4D-ND	2.57	127.55	124.37
2	F	401	HEM	CHA-C4D-C3D	-2.57	120.50	125.33
2	F	401	HEM	O2D-CGD-CBD	2.54	122.18	114.03
2	A	401	HEM	CHB-C1B-NB	2.50	127.46	124.37
2	D	401	HEM	C4C-CHD-C1D	-2.50	120.67	126.06
2	E	401	HEM	CHA-C4D-C3D	-2.50	120.64	125.33
2	D	401	HEM	C4A-NA-C1A	2.47	107.76	105.35
2	C	401	HEM	C4C-NC-C1C	2.46	107.75	105.35
2	B	401	HEM	CHD-C4C-NC	2.45	127.08	124.44
2	D	401	HEM	CAD-C3D-C4D	2.43	128.91	124.66
2	A	401	HEM	O2D-CGD-CBD	2.43	121.84	114.03
2	A	401	HEM	CAD-C3D-C4D	2.41	128.88	124.66
2	E	401	HEM	CHD-C1D-ND	2.40	127.02	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	HEM	CHB-C1B-NB	2.38	127.31	124.37
2	D	401	HEM	CMD-C2D-C1D	2.37	128.65	125.04
2	A	401	HEM	CHA-C4D-ND	2.33	127.25	124.37
2	C	401	HEM	CHA-C4D-C3D	-2.33	120.95	125.33
2	A	401	HEM	C1A-CHA-C4D	-2.31	120.85	126.34
2	E	401	HEM	O2D-CGD-CBD	2.30	121.42	114.03
2	A	401	HEM	CHA-C4D-C3D	-2.29	121.02	125.33
2	B	401	HEM	C4C-CHD-C1D	-2.29	121.12	126.06
2	D	401	HEM	CHD-C4C-NC	2.29	126.91	124.44
2	B	401	HEM	CHA-C4D-C3D	-2.28	121.05	125.33
2	C	401	HEM	CMD-C2D-C1D	2.25	128.46	125.04
2	F	401	HEM	CAD-C3D-C4D	2.25	128.59	124.66
2	F	401	HEM	CHA-C4D-ND	2.23	127.12	124.37
2	A	401	HEM	CAB-C3B-C2B	-2.22	121.30	128.60
2	E	401	HEM	CAD-C3D-C4D	2.20	128.51	124.66
2	F	401	HEM	O1D-CGD-CBD	-2.18	116.09	123.08
2	B	401	HEM	CHB-C1B-NB	2.16	127.04	124.37
2	E	401	HEM	C2D-C1D-ND	2.16	112.46	109.88
2	D	401	HEM	C1A-CHA-C4D	-2.13	121.29	126.34
2	D	401	HEM	CHA-C1A-NA	2.13	127.76	123.85
2	A	401	HEM	CMD-C2D-C1D	2.13	128.28	125.04
2	B	401	HEM	C4C-NC-C1C	2.11	107.42	105.35
2	B	401	HEM	CMD-C2D-C1D	2.11	128.25	125.04
2	F	401	HEM	C4C-CHD-C1D	-2.11	121.51	126.06
2	C	401	HEM	C4C-CHD-C1D	-2.10	121.52	126.06
2	C	401	HEM	CAD-C3D-C4D	2.07	128.28	124.66
2	A	401	HEM	CHD-C4C-NC	2.05	126.66	124.44
2	A	401	HEM	C2D-C1D-ND	2.04	112.33	109.88
2	E	401	HEM	C4C-NC-C1C	2.02	107.33	105.35
2	A	401	HEM	O2D-CGD-O1D	-2.02	118.26	123.30
2	C	401	HEM	C1A-CHA-C4D	-2.01	121.56	126.34
2	F	401	HEM	O2A-CGA-CBA	2.01	120.49	114.03

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	402	GOL	O1-C1-C2-O2
5	C	402	GOL	O1-C1-C2-C3
5	C	403	GOL	C1-C2-C3-O3
5	C	403	GOL	O2-C2-C3-O3
5	C	405	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	F	402	7PE	O7-C8-C9-O10
5	B	405	GOL	O1-C1-C2-O2
3	F	409	7PE	O13-C14-C15-O16
3	F	402	7PE	O4-C5-C6-O7
3	F	405[A]	7PE	O4-C5-C6-O7
5	B	403	GOL	C1-C2-C3-O3
5	B	405	GOL	O1-C1-C2-C3
5	F	404	GOL	C1-C2-C3-O3
5	F	404	GOL	O2-C2-C3-O3
3	B	404	7PE	O10-C11-C12-O13
3	F	408	7PE	O13-C14-C15-O16
3	B	402	7PE	C15-C14-O13-C12
3	A	402	7PE	C8-C9-O10-C11
5	B	403	GOL	O2-C2-C3-O3
5	B	405	GOL	O2-C2-C3-O3
3	B	404	7PE	C12-C11-O10-C9
3	F	402	7PE	C8-C9-O10-C11
3	D	402	7PE	O10-C11-C12-O13
2	F	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O2D
3	F	408	7PE	C14-C15-O16-C17
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	F	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O1A
5	F	406	GOL	C1-C2-C3-O3
3	D	402	7PE	C12-C11-O10-C9
2	B	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	E	401	HEM	CAA-CBA-CGA-O2A
5	C	405	GOL	O1-C1-C2-O2
2	D	401	HEM	CAA-CBA-CGA-O2A
2	E	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAD-CBD-CGD-O2D
3	D	402	7PE	C8-C9-O10-C11

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Mol	Chain	Res	Type	Atoms
2	B	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	C4B-C3B-CAB-CBB
2	B	401	HEM	CAA-CBA-CGA-O1A

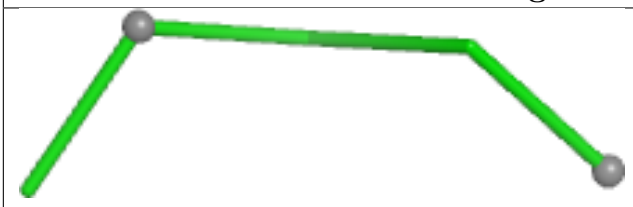
There are no ring outliers.

12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	7PE	2	0
3	B	402	7PE	1	0
2	B	401	HEM	2	0
3	A	402	7PE	4	0
3	D	402	7PE	1	0
5	C	403	GOL	1	0
5	F	407	GOL	1	0
2	A	401	HEM	3	0
3	F	402	7PE	2	0
5	C	405	GOL	1	0
3	F	410	7PE	2	0
3	F	405[A]	7PE	1	0

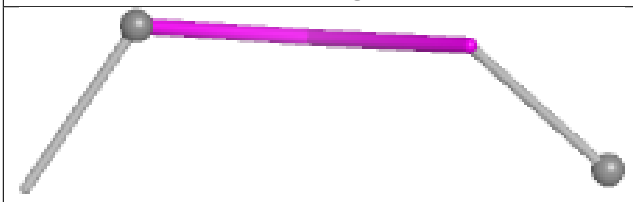
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 7PE B 404

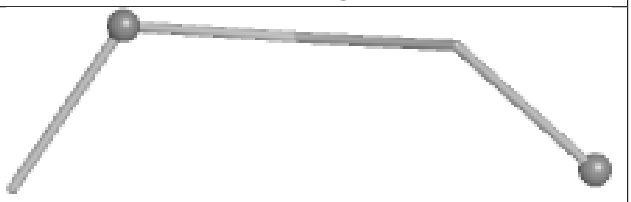


Bond lengths

Bond angles

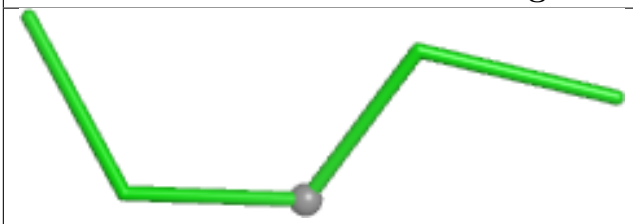


Torsions

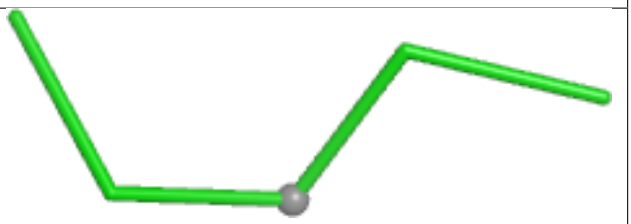


Rings

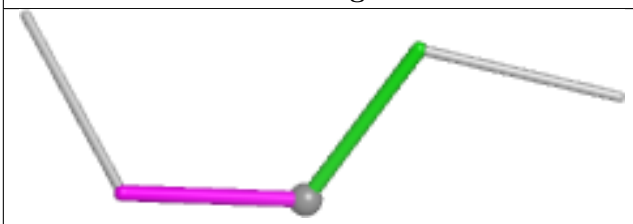
Ligand 7PE B 402



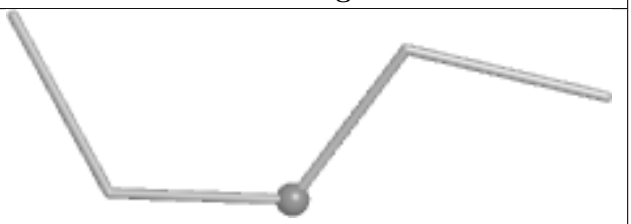
Bond lengths



Bond angles

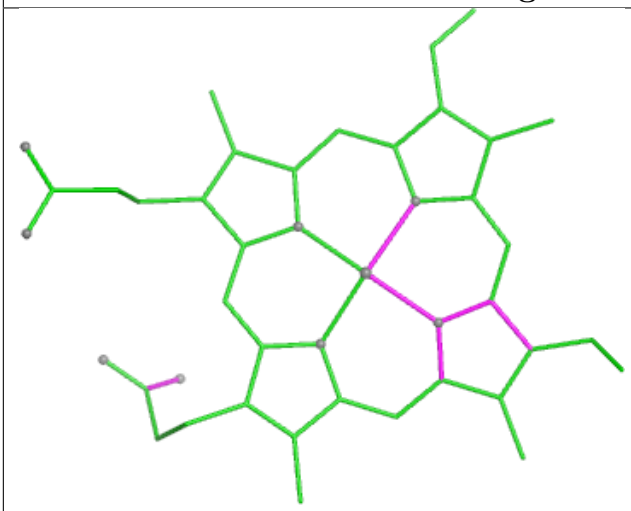


Torsions

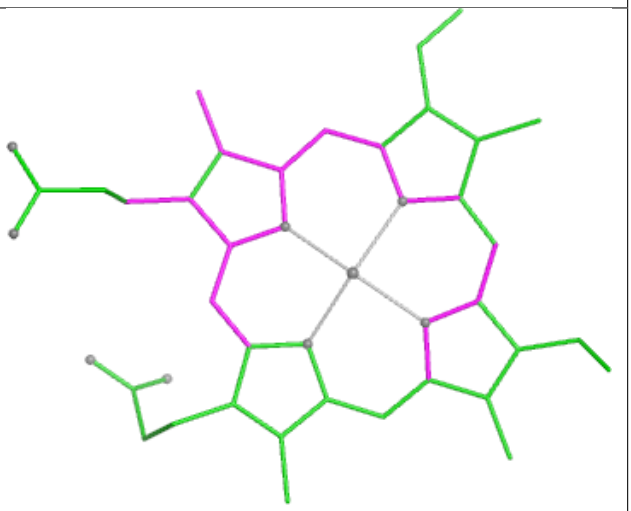


Rings

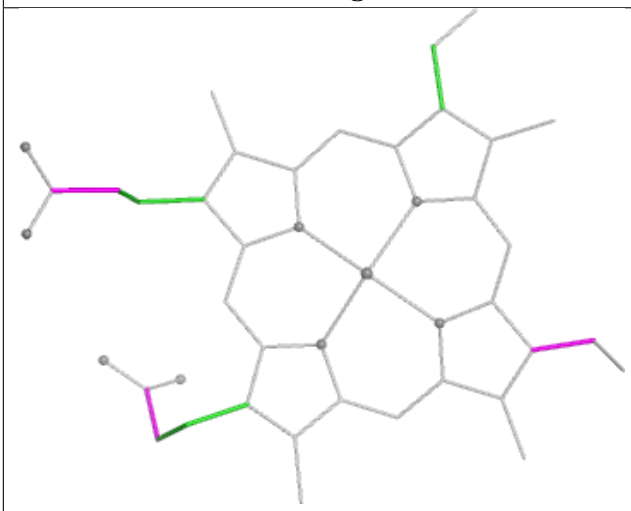
Ligand HEM C 401



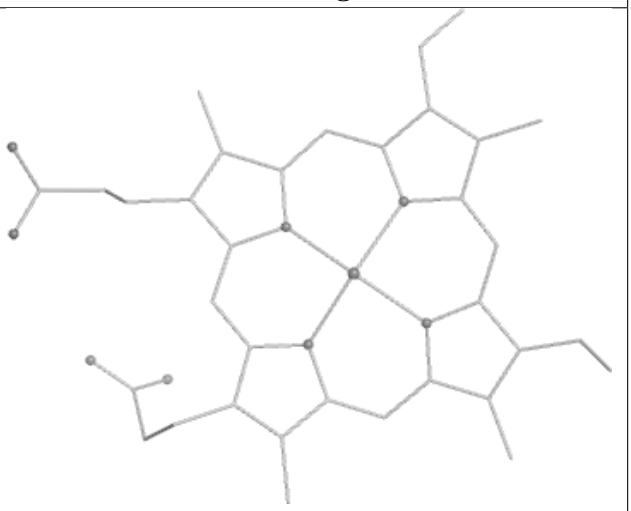
Bond lengths



Bond angles

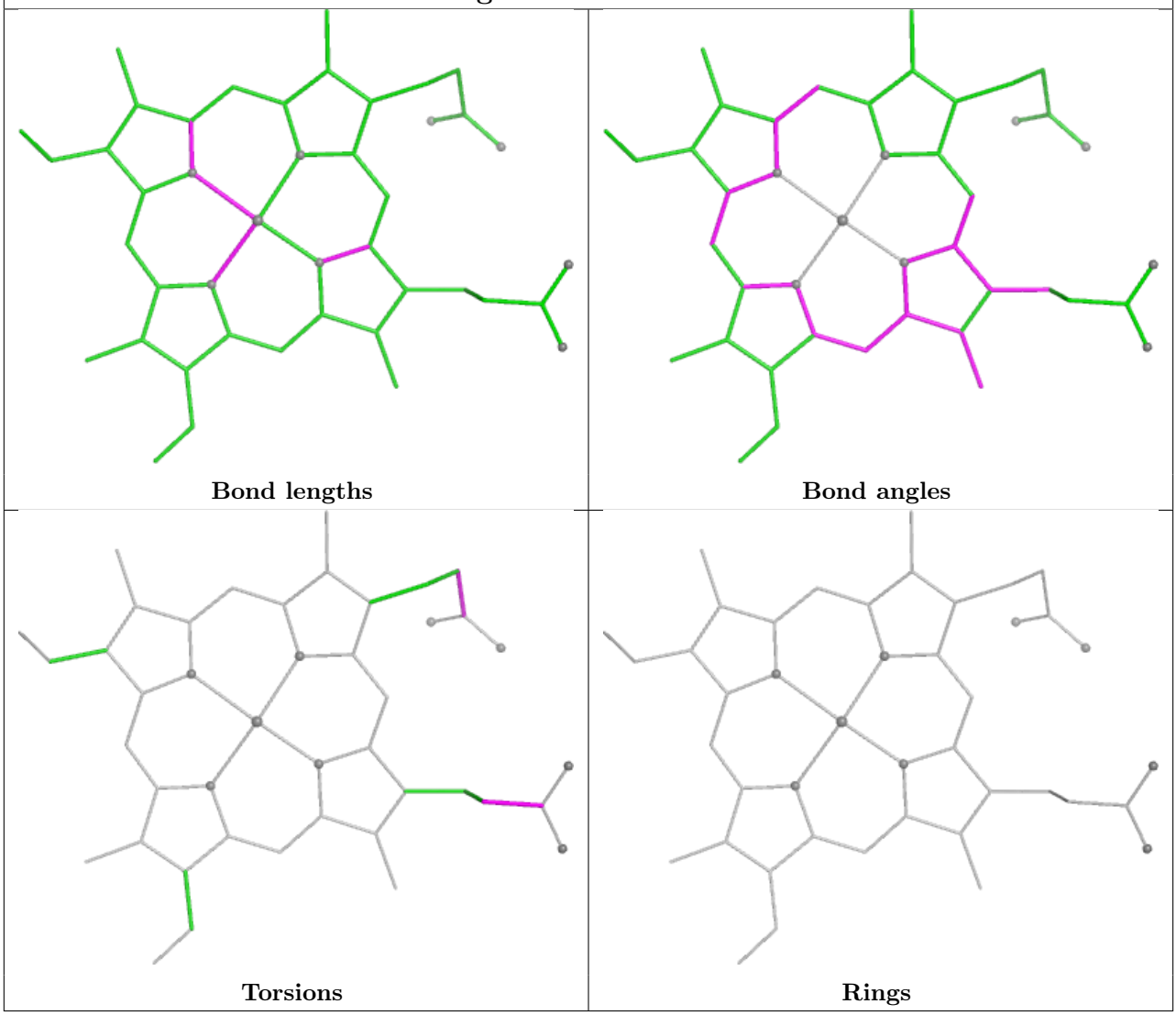


Torsions

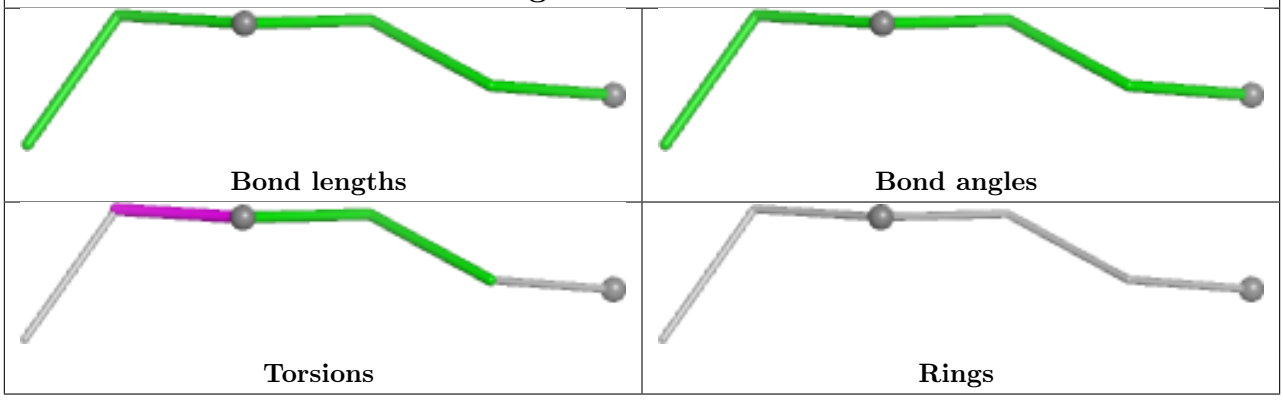


Rings

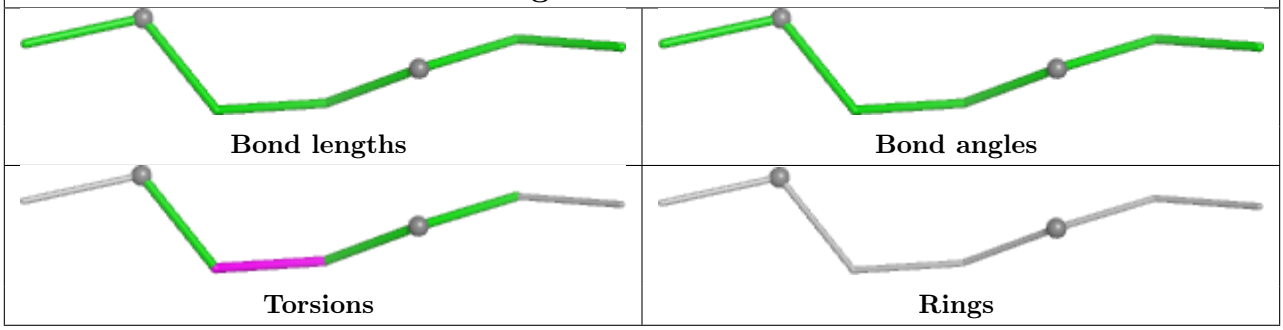
Ligand HEM B 401



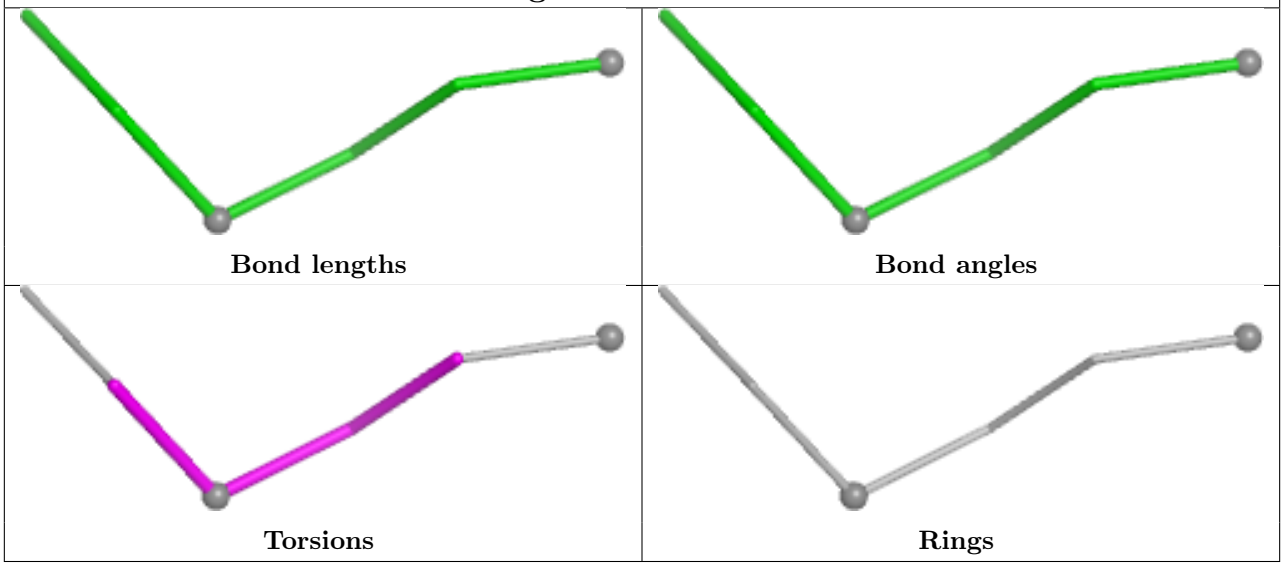
Ligand 7PE A 402



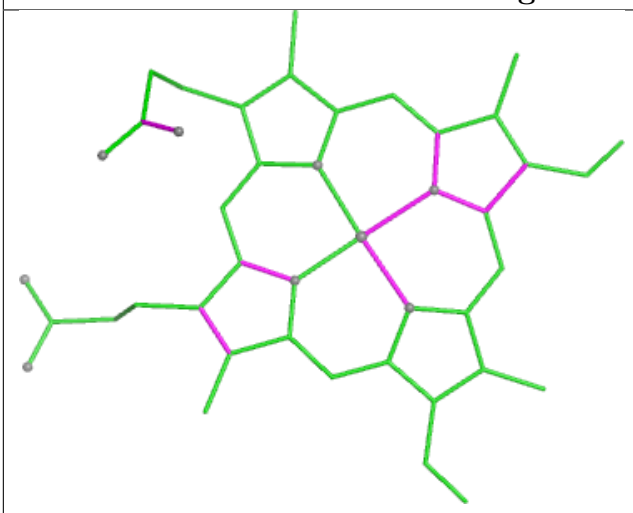
Ligand 7PE F 409



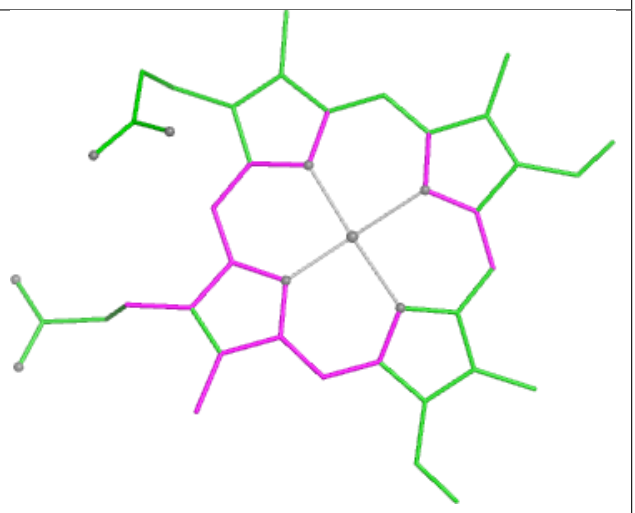
Ligand 7PE D 402



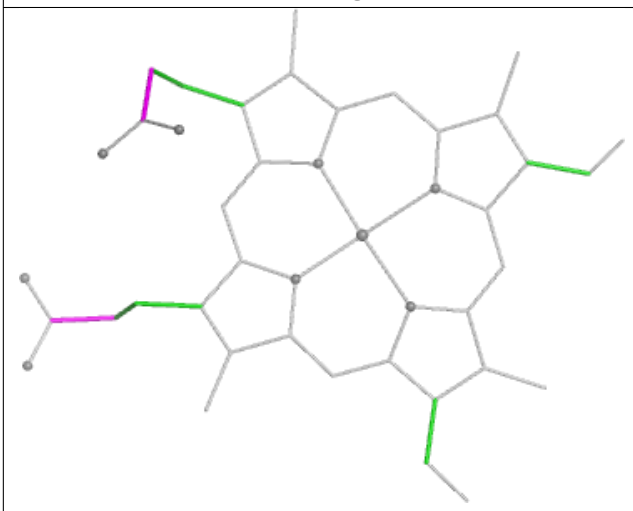
Ligand HEM D 401



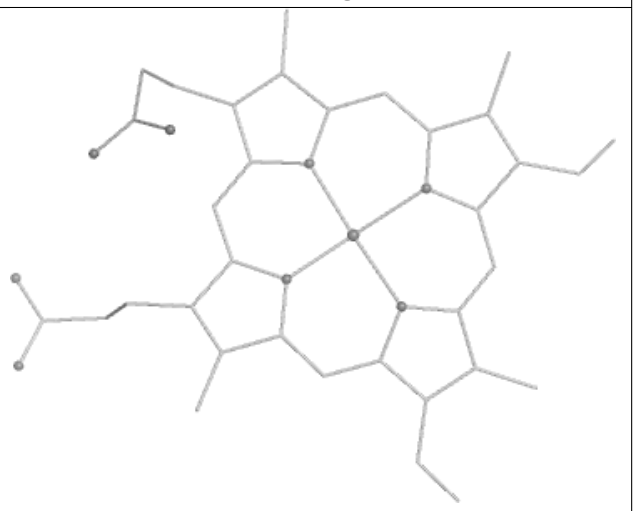
Bond lengths



Bond angles

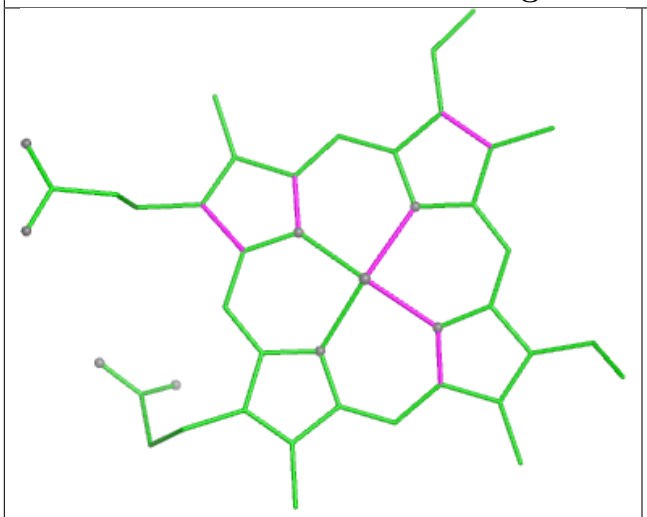


Torsions

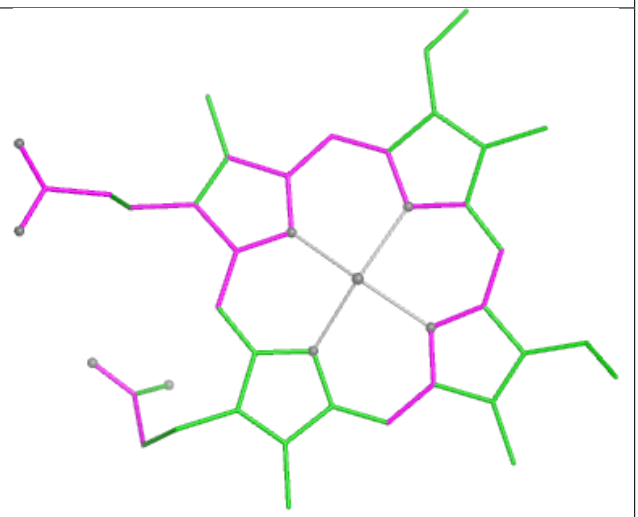


Rings

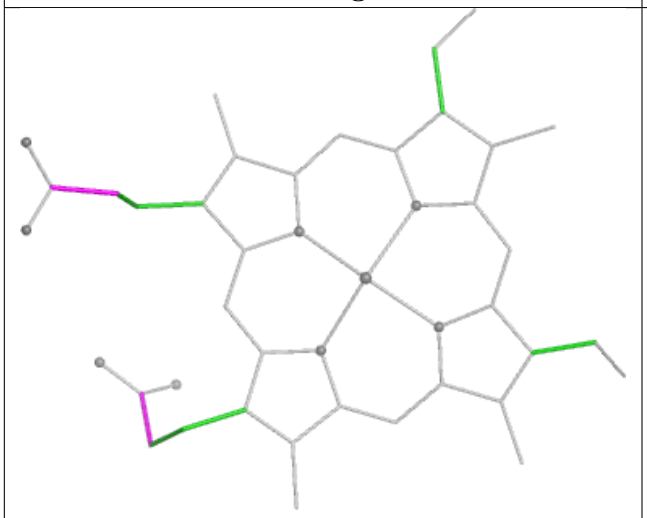
Ligand HEM F 401



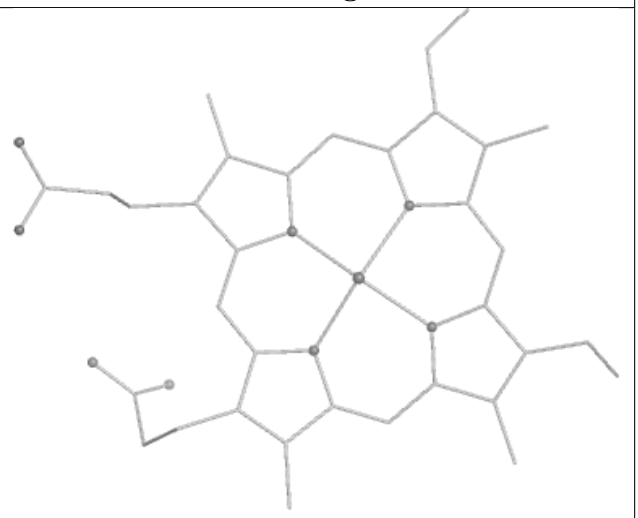
Bond lengths



Bond angles

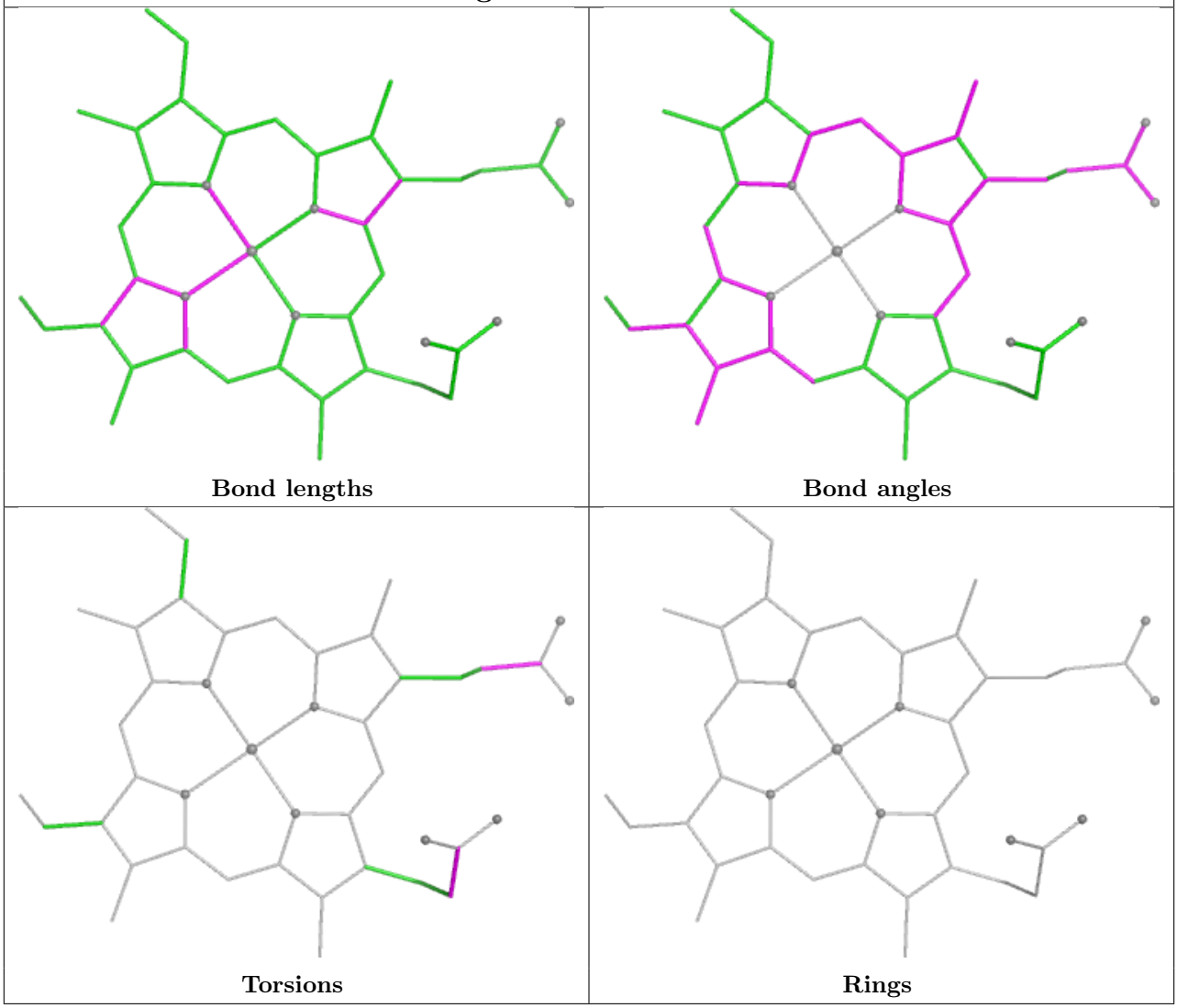


Torsions

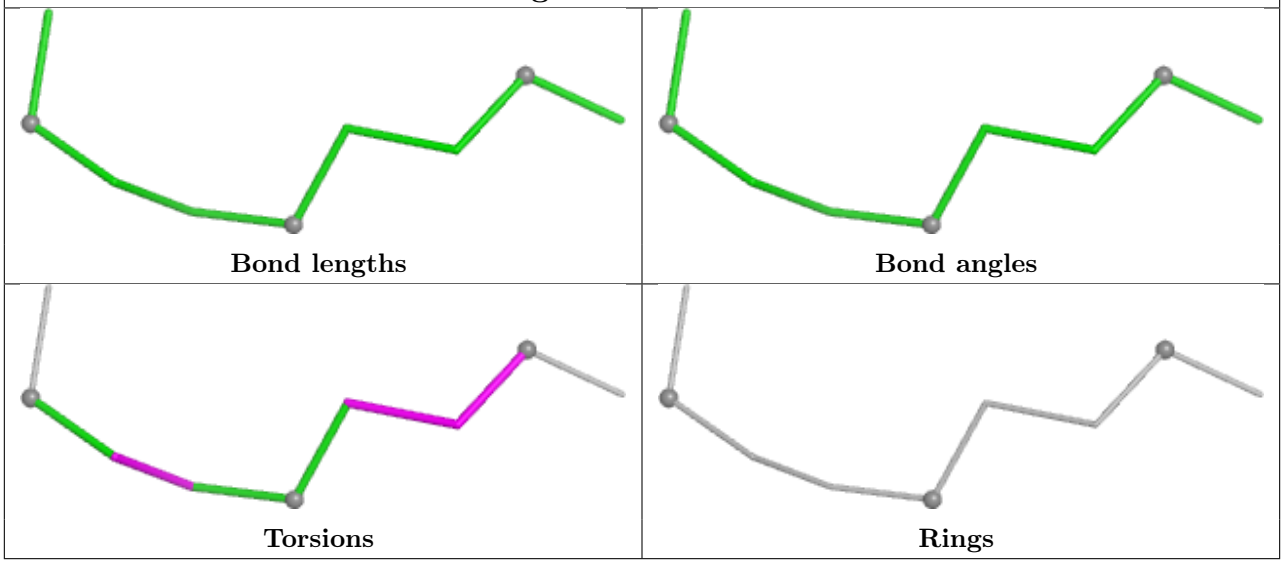


Rings

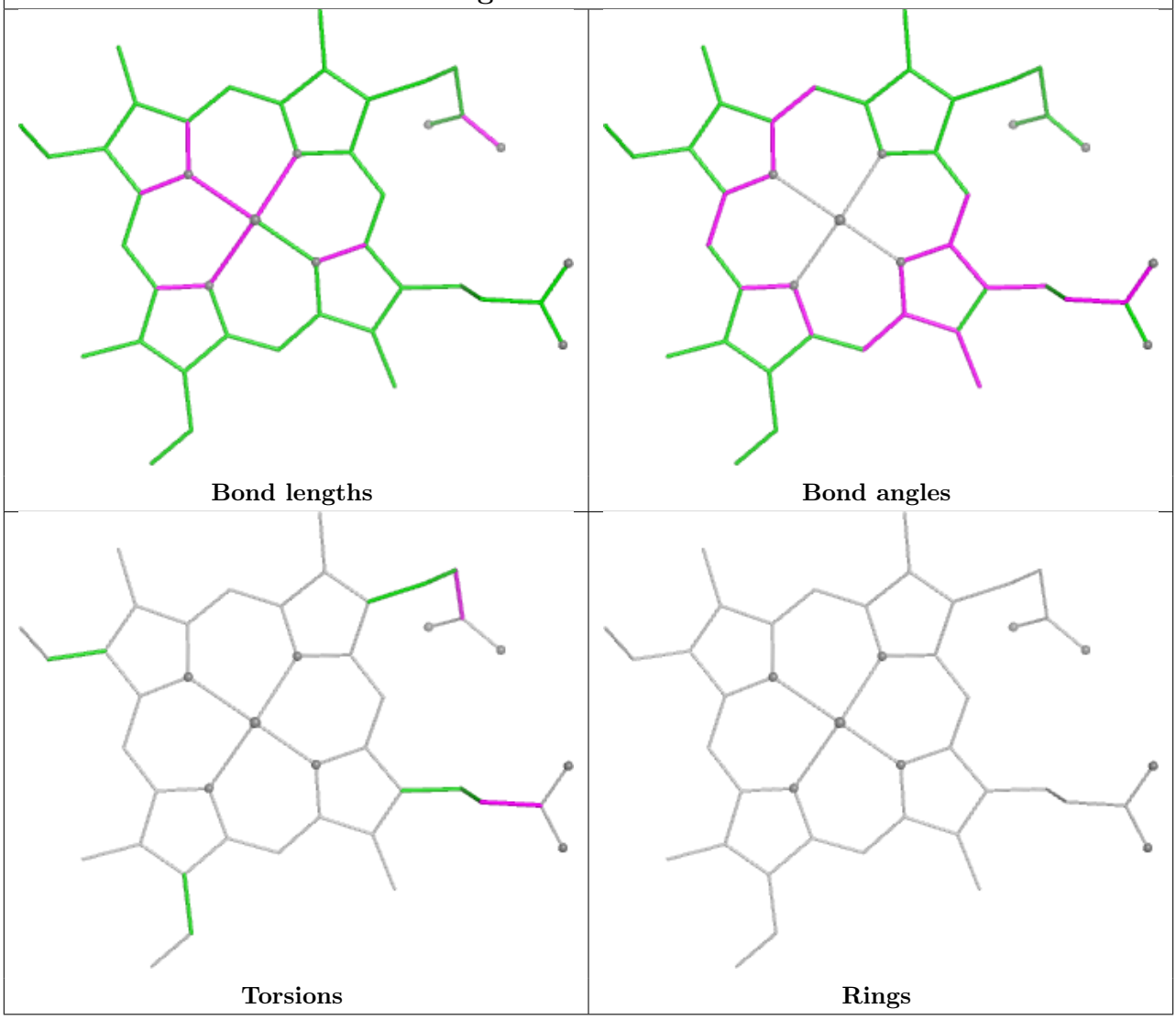
Ligand HEM A 401



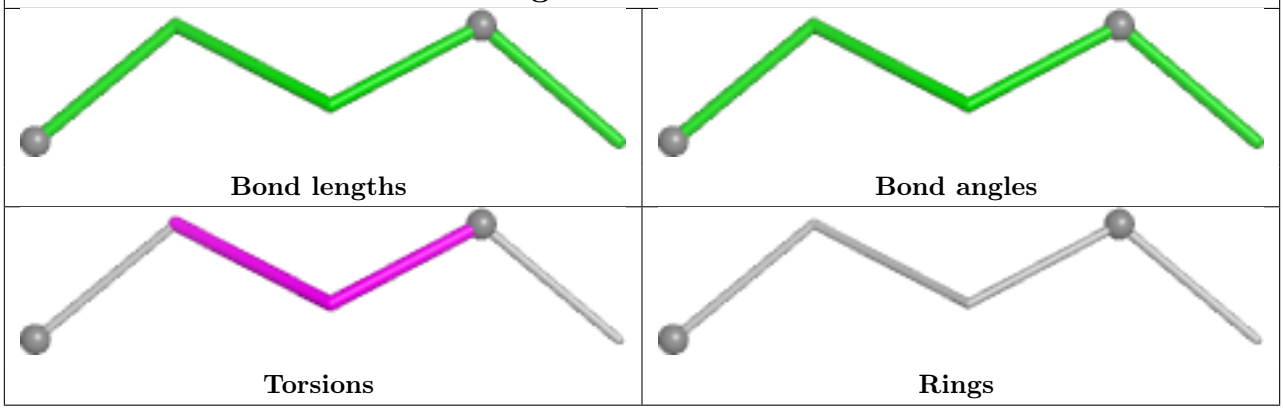
Ligand 7PE F 402

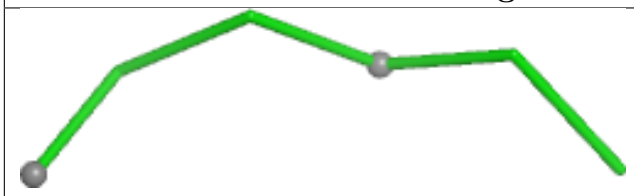
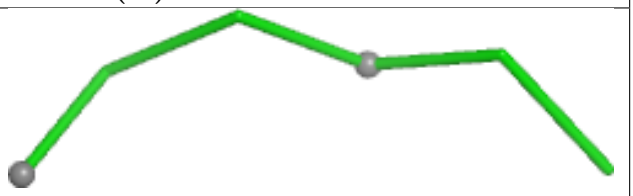
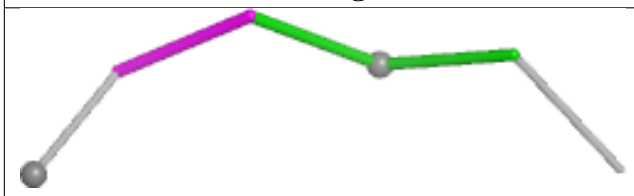
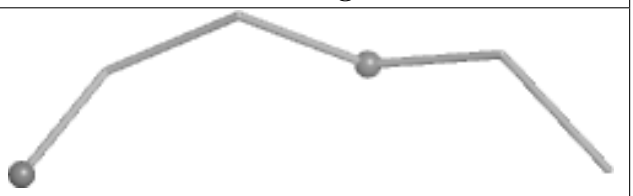


Ligand HEM E 401



Ligand 7PE F 408



Ligand 7PE F 405 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	306/316 (96%)	-0.06	3 (0%)	79	79	13, 28, 45, 69	5 (1%)
1	B	306/316 (96%)	0.21	10 (3%)	49	48	18, 33, 53, 80	1 (0%)
1	C	306/316 (96%)	0.01	6 (1%)	65	64	16, 29, 46, 70	1 (0%)
1	D	306/316 (96%)	0.06	8 (2%)	57	56	17, 29, 48, 67	2 (0%)
1	E	306/316 (96%)	0.10	8 (2%)	57	56	13, 30, 49, 91	2 (0%)
1	F	308/316 (97%)	0.08	9 (2%)	53	52	13, 29, 48, 73	5 (1%)
All	All	1838/1896 (96%)	0.07	44 (2%)	59	59	13, 30, 49, 91	16 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	142	PHE	5.5
1	F	314	ALA	4.7
1	F	142	PHE	4.6
1	D	141	TYR	4.5
1	B	142	PHE	4.3
1	F	141	TYR	4.2
1	E	235	ASP	4.2
1	D	142	PHE	4.0
1	F	76[A]	SER	3.9
1	D	313	SER	3.6
1	B	56	PRO	3.6
1	B	235	ASP	3.6
1	D	312	LEU	3.5
1	E	7	GLU	3.3
1	A	7	GLU	3.2
1	C	78	ALA	3.1
1	C	235	ASP	3.1
1	E	237	SER	3.1
1	C	17	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	8	PRO	3.0
1	B	312	LEU	2.8
1	E	234	PRO	2.8
1	C	77	GLY	2.7
1	A	8	PRO	2.7
1	F	8	PRO	2.7
1	B	234	PRO	2.6
1	F	7	GLU	2.6
1	F	78	ALA	2.5
1	D	8	PRO	2.5
1	F	234	PRO	2.5
1	E	56	PRO	2.4
1	C	8	PRO	2.3
1	D	232	THR	2.3
1	B	232	THR	2.2
1	C	234	PRO	2.2
1	A	282	ALA	2.2
1	B	282	ALA	2.2
1	B	75	PHE	2.2
1	D	210	MET	2.1
1	E	143	ASP	2.1
1	D	56	PRO	2.1
1	B	170	ALA	2.1
1	E	161	ALA	2.0
1	F	235	ASP	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 oligosaccharides in this entry.

6.4 Ligands (i)

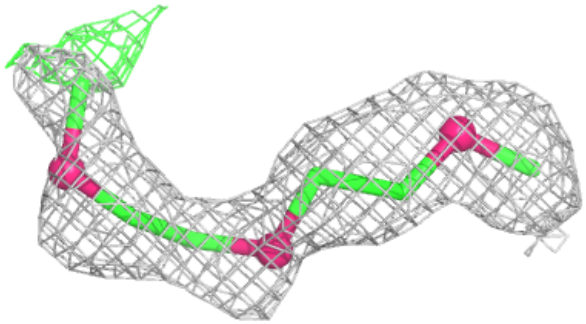
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

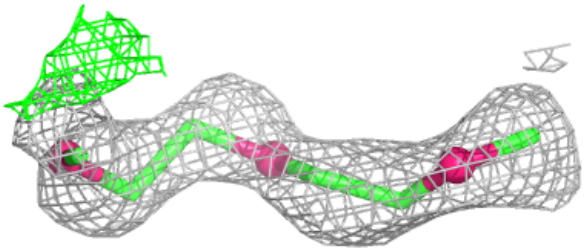
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	C	403	6/6	0.65	0.17	47,61,62,68	0
5	GOL	B	405	6/6	0.71	0.15	54,58,59,60	0
3	7PE	F	402	9/21	0.71	0.20	39,57,65,72	0
3	7PE	A	402	6/21	0.72	0.20	48,52,55,57	0
3	7PE	F	409	7/21	0.74	0.22	62,69,74,77	0
5	GOL	B	403	6/6	0.75	0.19	49,59,64,67	0
5	GOL	C	402	6/6	0.77	0.15	44,52,54,63	0
3	7PE	B	402	5/21	0.77	0.22	50,53,56,58	0
5	GOL	F	403	6/6	0.77	0.17	58,66,68,69	0
5	GOL	F	407	6/6	0.77	0.20	59,63,67,69	0
4	MG	A	406	1/1	0.78	0.11	56,56,56,56	0
5	GOL	F	406	6/6	0.80	0.15	38,60,65,67	0
3	7PE	B	404	5/21	0.81	0.17	49,56,59,60	0
5	GOL	C	405	6/6	0.82	0.14	48,58,60,62	0
5	GOL	F	404	6/6	0.85	0.12	59,62,64,65	0
3	7PE	F	410	5/21	0.85	0.18	38,46,49,50	0
3	7PE	F	408	5/21	0.85	0.16	51,54,56,57	0
3	7PE	F	405[A]	6/21	0.87	0.20	14,21,25,25	6
3	7PE	D	402	6/21	0.88	0.14	49,56,56,59	0
4	MG	E	402	1/1	0.89	0.08	54,54,54,54	0
3	7PE	A	403	4/21	0.94	0.16	42,42,43,45	0
4	MG	A	404	1/1	0.97	0.03	27,27,27,27	0
4	MG	C	404	1/1	0.97	0.03	30,30,30,30	0
2	HEM	F	401	43/43	0.98	0.06	21,24,26,27	0
2	HEM	A	401	43/43	0.98	0.06	21,24,26,32	0
2	HEM	B	401	43/43	0.98	0.06	23,25,28,30	0
2	HEM	C	401	43/43	0.98	0.06	21,25,28,29	0
2	HEM	D	401	43/43	0.98	0.06	21,23,26,27	0
2	HEM	E	401	43/43	0.98	0.06	22,25,28,29	0
4	MG	A	405	1/1	0.99	0.04	41,41,41,41	0

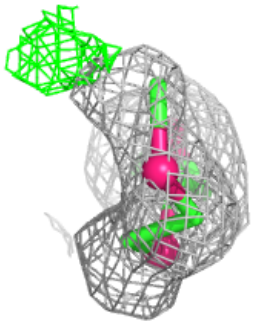
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 7PE F 402:

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

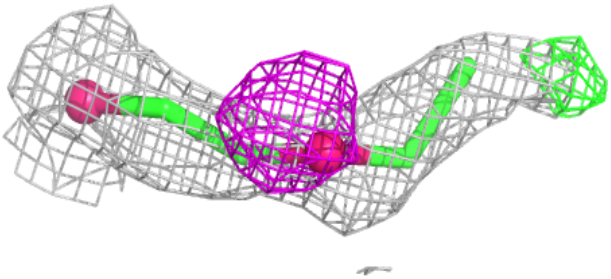


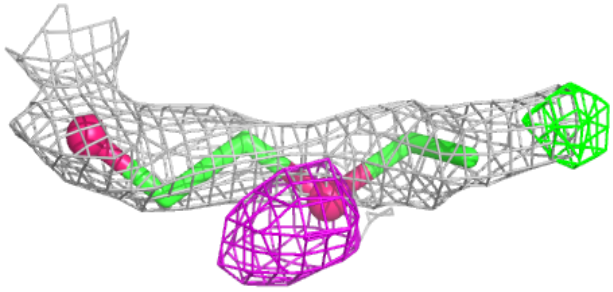


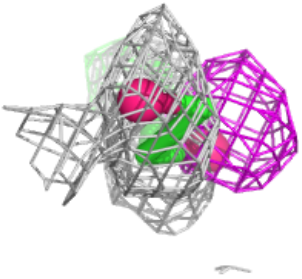


Electron density around 7PE A 402:

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

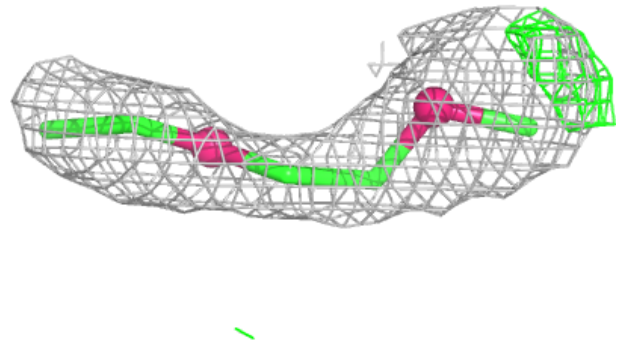


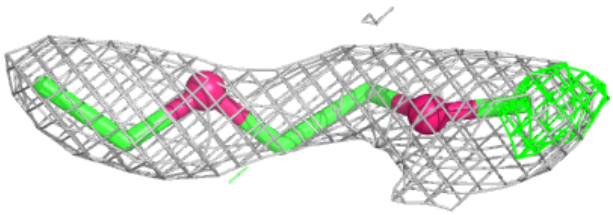


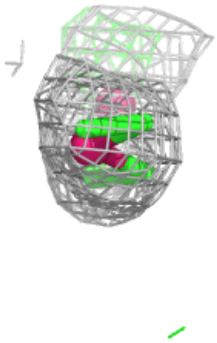


Electron density around 7PE F 409:

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

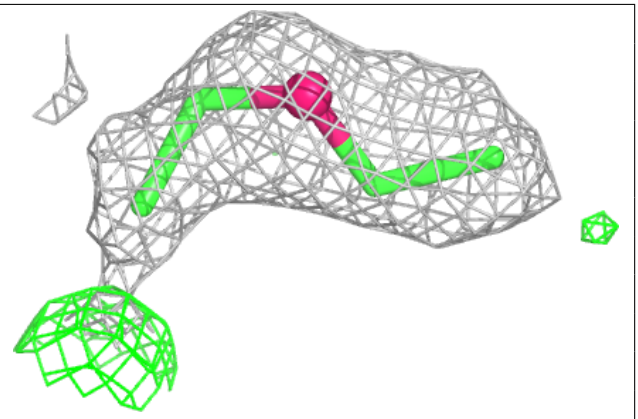


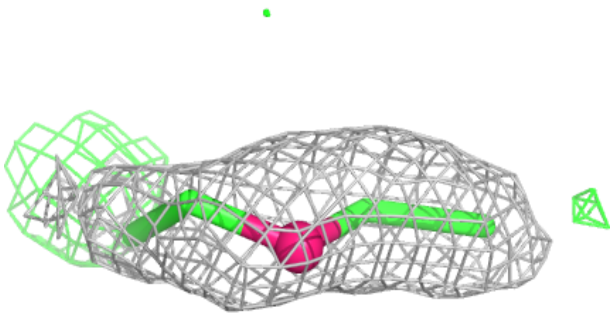


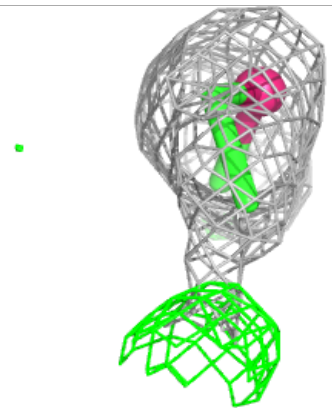


Electron density around 7PE B 402:

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

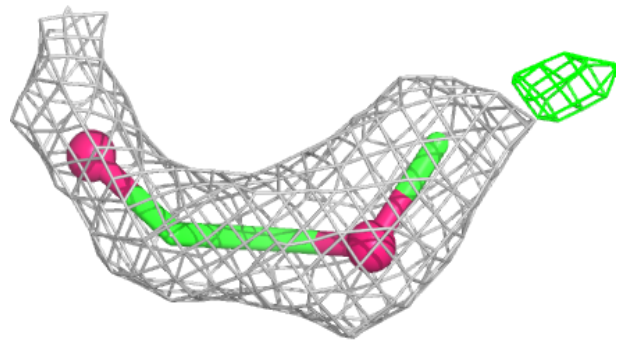


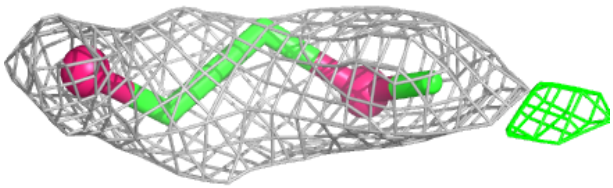


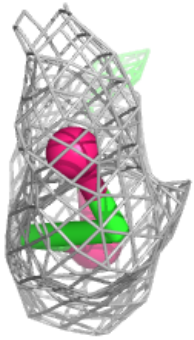


Electron density around 7PE B 404:

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

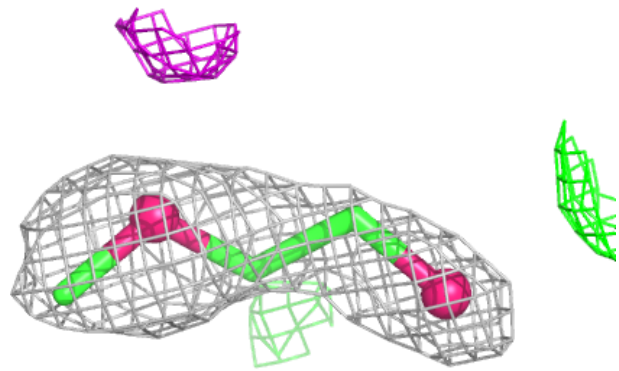


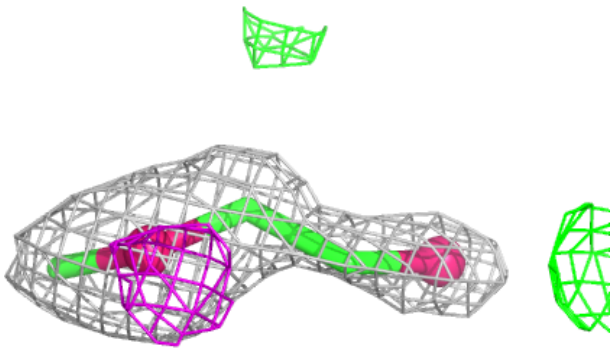


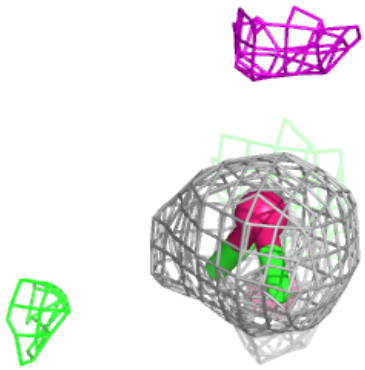


Electron density around 7PE F 408:

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

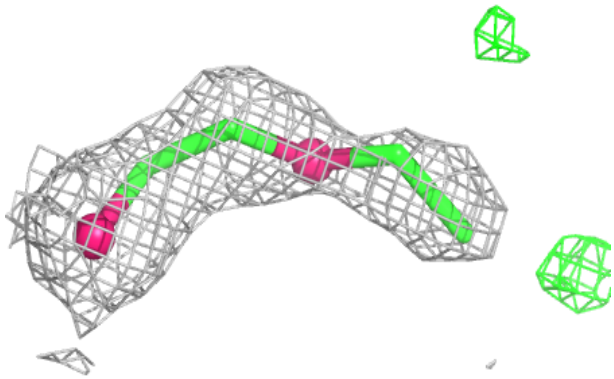


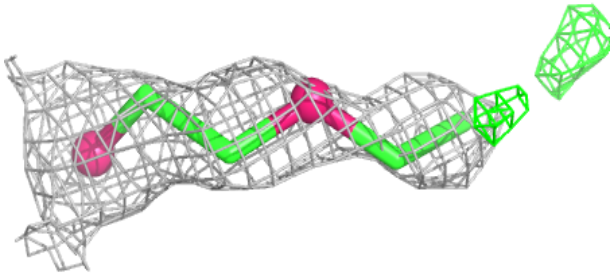


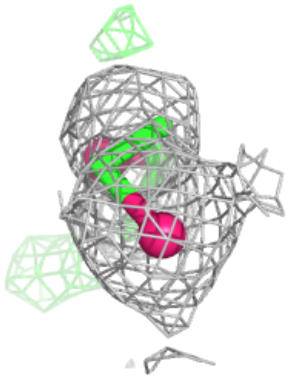


Electron density around 7PE F 405 (A):

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

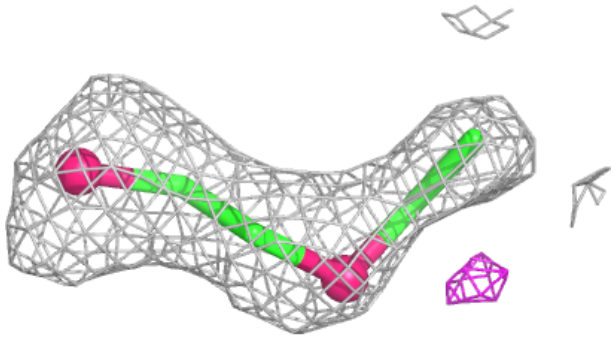


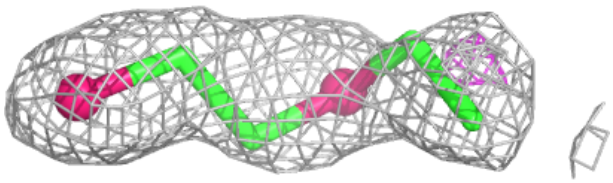


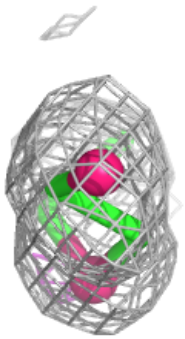


Electron density around 7PE D 402:

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

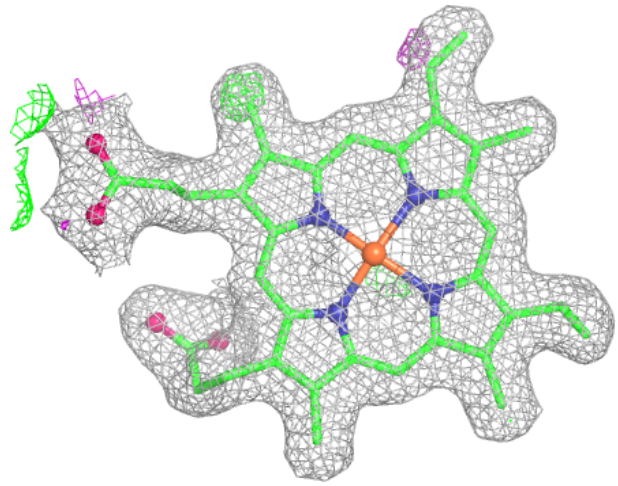


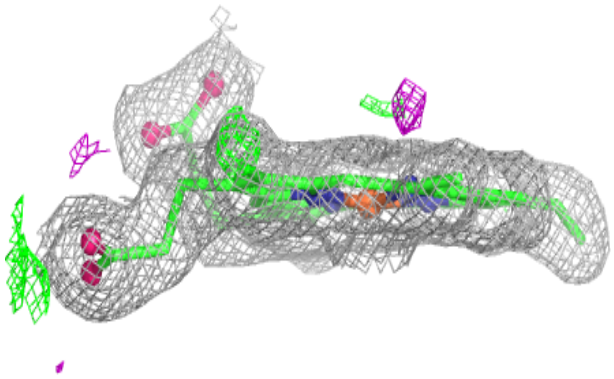


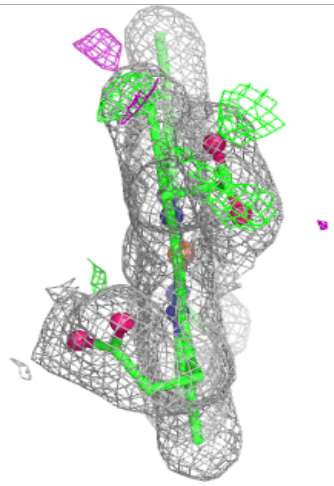


Electron density around HEM F 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

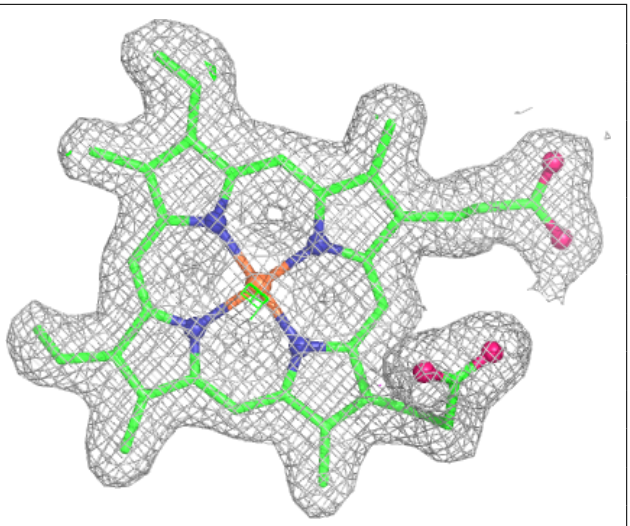


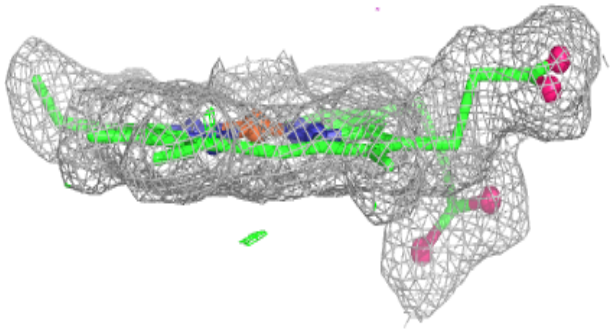


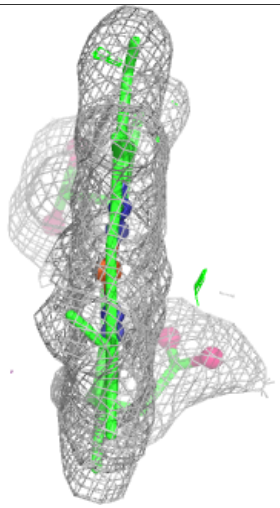


Electron density around HEM A 401:

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

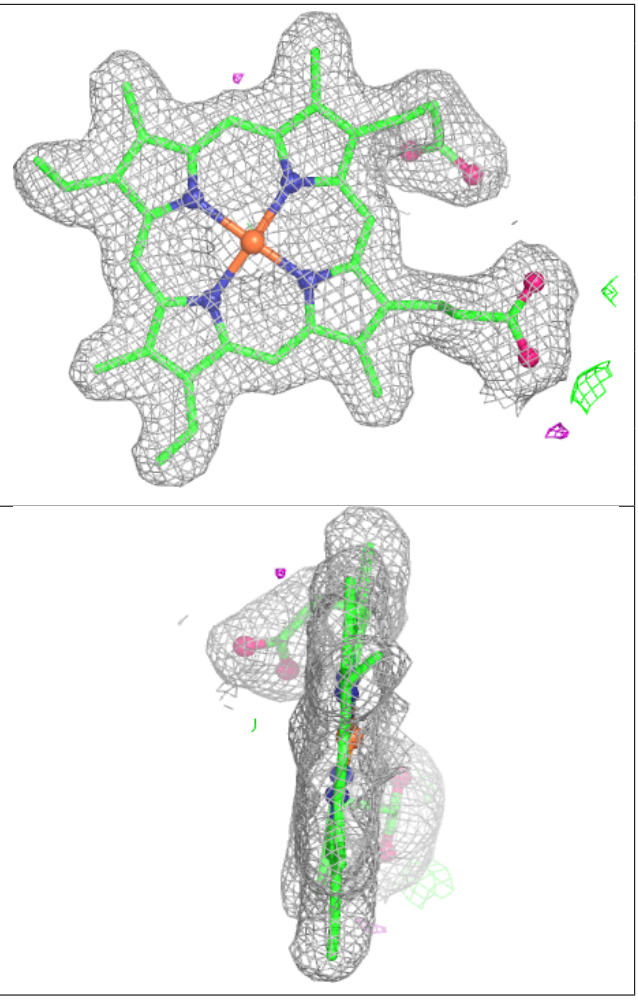






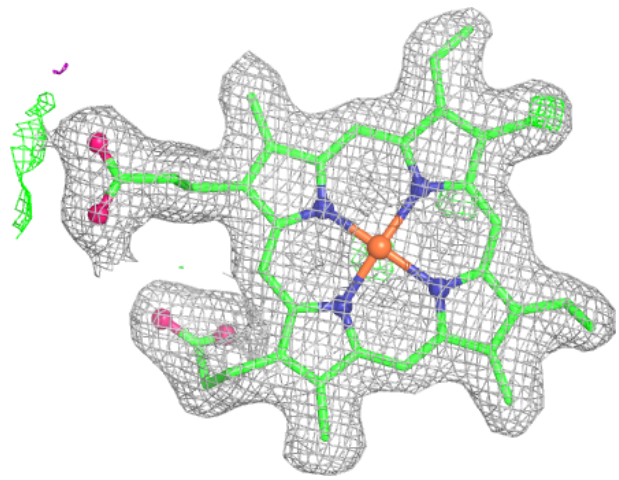
Electron density around HEM B 401:

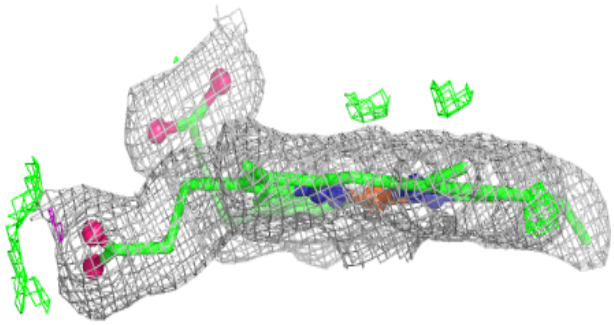
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

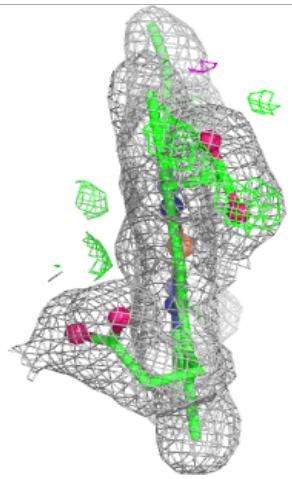


Electron density around HEM C 401:

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

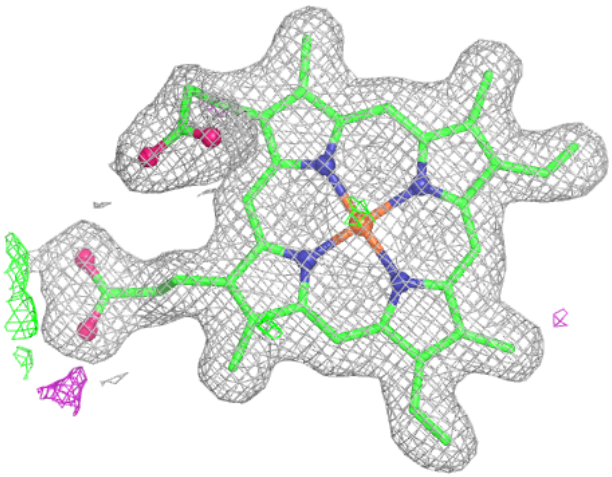


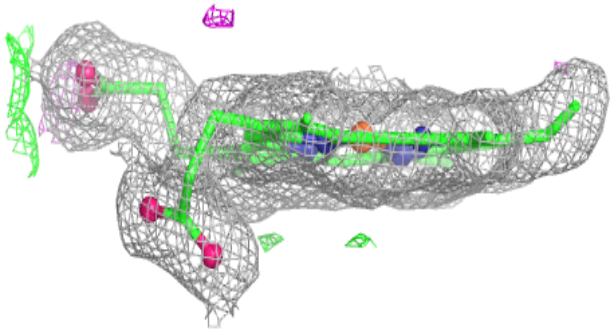


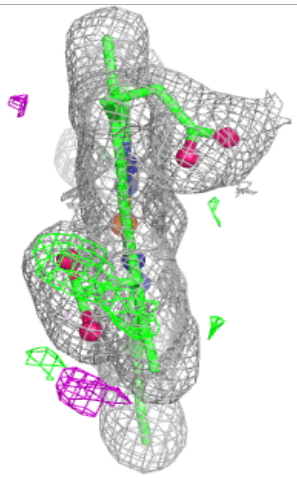


Electron density around HEM D 401:

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

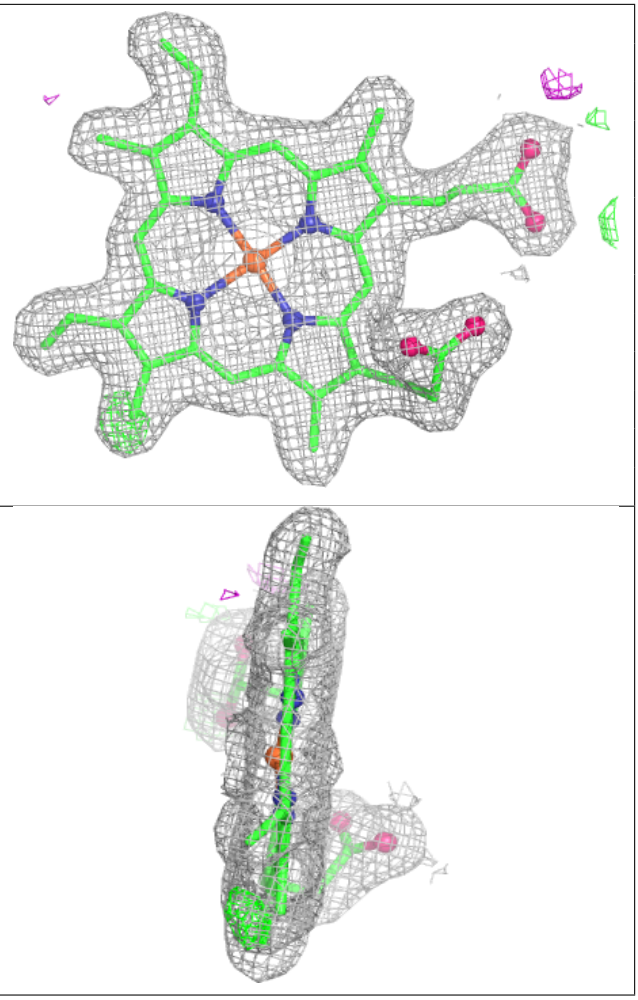






Electron density around HEM E 401:

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 (i)

There are no such residues in this entry.