



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:40 PM UTC

PDB ID : 5MMS / pdb_00005mms
Title : Human cystathionine beta-synthase (CBS) p.P49L delta409-551 variant
Authors : Vicente, J.B.; Colaco, H.G.; Malagrino, F.; Santo, P.E.; Gutierrez, A.; Bandediras, T.M.; Leandro, P.; Brito, J.A.; Giuffre, A.
Deposited on : 2016-12-12
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

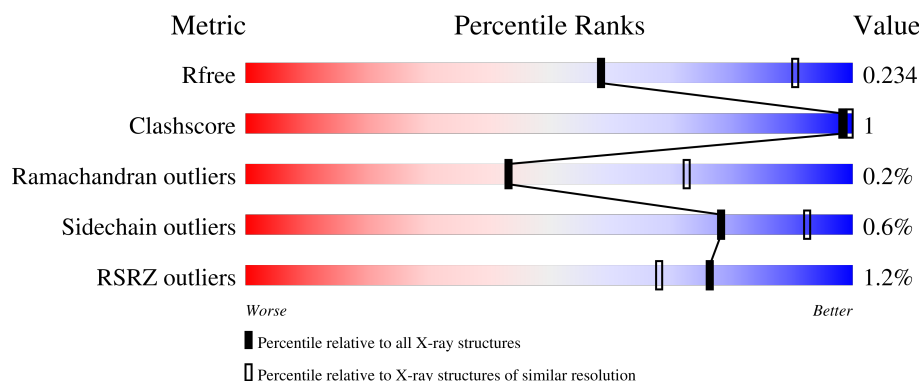
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	408	% 82% 17%
1	B	408	82% 15%
1	C	408	% 82% 16%
1	D	408	% 85% 13%
1	E	408	% 83% 14%

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Mol	Chain	Length	Quality of chain
1	F	408	% 81% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16452 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2604	1639	458	490	17			
1	B	348	Total	C	N	O	S	0	0	0
			2666	1673	468	508	17			
1	C	343	Total	C	N	O	S	0	0	0
			2625	1646	462	501	16			
1	D	356	Total	C	N	O	S	0	0	0
			2735	1715	481	522	17			
1	E	349	Total	C	N	O	S	0	0	0
			2675	1682	471	505	17			
1	F	341	Total	C	N	O	S	0	0	0
			2611	1641	460	494	16			

There are 6 discrepancies between the modelled and reference sequences:

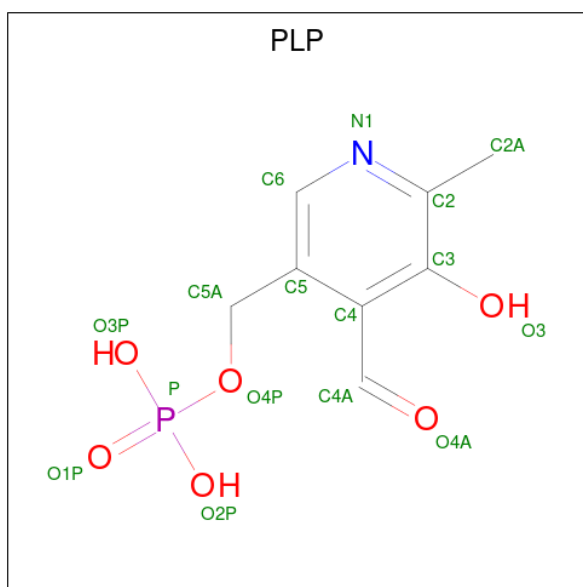
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	LEU	PRO	engineered mutation	UNP P35520
B	49	LEU	PRO	engineered mutation	UNP P35520
C	49	LEU	PRO	engineered mutation	UNP P35520
D	49	LEU	PRO	engineered mutation	UNP P35520
E	49	LEU	PRO	engineered mutation	UNP P35520
F	49	LEU	PRO	engineered mutation	UNP P35520

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



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total	Na	0	0
			2	2		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

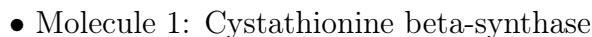
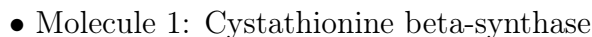
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		

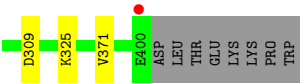
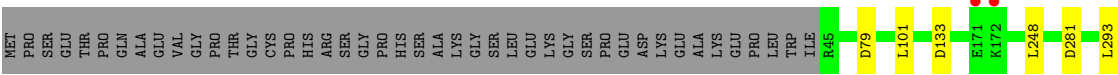
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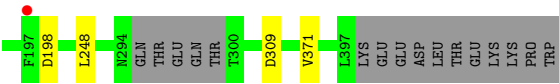
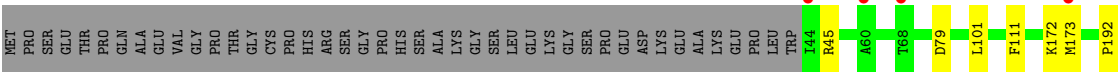
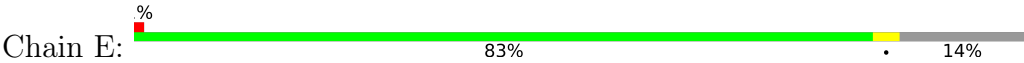
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	30	Total 30	O 30	0	0
5	C	22	Total 22	O 22	0	0
5	D	32	Total 32	O 32	0	0
5	E	38	Total 38	O 38	0	0
5	F	37	Total 37	O 37	0	0

- Molecule 1: Cystathionine beta-synthase

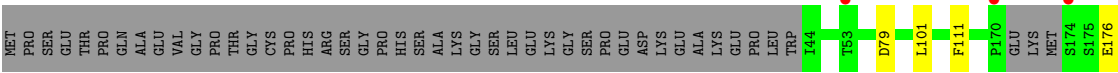
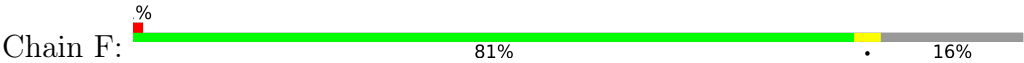




● Molecule 1: Cystathionine beta-synthase



● Molecule 1: Cystathionine beta-synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.17Å 86.78Å 97.79Å 102.67° 103.07° 111.19°	Depositor
Resolution (Å)	76.35 – 2.80 76.35 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (76.35-2.80) 98.5 (76.35-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.82Å)	Xtriage
Refinement program	PHENIX, BUSTER 2.10.3	Depositor
R, R_{free}	0.182 , 0.221 0.195 , 0.234	Depositor DCC
R_{free} test set	2836 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16452	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.83	0/2649	1.12	3/3577 (0.1%)
1	B	0.84	0/2712	1.12	2/3666 (0.1%)
1	C	0.82	0/2669	1.12	2/3609 (0.1%)
1	D	0.84	0/2783	1.14	3/3762 (0.1%)
1	E	0.84	1/2722 (0.0%)	1.15	6/3679 (0.2%)
1	F	0.83	0/2654	1.13	4/3586 (0.1%)
All	All	0.83	1/16189 (0.0%)	1.13	20/21879 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	MET	SD-CE	5.12	1.92	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	173	MET	CA-C-N	9.09	133.71	120.90
1	E	173	MET	C-N-CA	9.09	133.71	120.90
1	E	198	ASP	CA-CB-CG	6.52	119.12	112.60
1	C	79	ASP	CA-CB-CG	6.23	118.83	112.60
1	D	79	ASP	CA-CB-CG	6.01	118.61	112.60
1	F	79	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	79	ASP	CA-CB-CG	5.91	118.51	112.60
1	E	79	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	79	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	133	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	111	PHE	CA-CB-CG	5.42	119.22	113.80
1	F	303	VAL	N-CA-CB	5.31	116.84	110.31
1	D	309	ASP	CA-CB-CG	5.29	117.89	112.60
1	F	111	PHE	CA-CB-CG	5.29	119.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	PHE	CA-CB-CG	5.26	119.06	113.80
1	B	309	ASP	CA-CB-CG	5.22	117.82	112.60
1	E	309	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	45	ARG	N-CA-C	5.07	121.02	109.81
1	E	111	PHE	CA-CB-CG	5.04	118.84	113.80
1	F	309	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	0	2642	2	0
1	B	2666	0	2694	4	0
1	C	2625	0	2653	4	0
1	D	2735	0	2760	2	0
1	E	2675	0	2709	1	0
1	F	2611	0	2647	3	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	2	0
2	E	43	0	30	0	0
2	F	43	0	30	0	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
3	C	15	0	6	0	0
3	D	15	0	6	0	0
3	E	15	0	6	0	0
3	F	15	0	6	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
5	A	26	0	0	0	0
5	B	30	0	0	0	0
5	C	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	32	0	0	0	0
5	E	38	0	0	0	0
5	F	37	0	0	0	0
All	All	16452	0	16321	18	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 1.

All (18) 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)
2:D:1001:HEM:HMB2	2:D:1001:HEM:HBB2	1.93	0.51
1:B:191:THR:HG21	1:B:203:HIS:HA	1.94	0.50
1:F:281:ASP:O	1:F:325:LYS:HA	2.15	0.47
2:D:1001:HEM:HBC2	2:D:1001:HEM:HMC2	1.97	0.47
1:C:204:VAL:O	1:C:208:TRP:HD1	1.98	0.46
1:C:248:LEU:CD1	1:C:371:VAL:HG23	2.45	0.46
1:E:248:LEU:HD13	1:E:371:VAL:HG23	1.99	0.45
1:B:248:LEU:HD13	1:B:371:VAL:HG23	2.00	0.44
1:A:248:LEU:HD13	1:A:371:VAL:HG23	1.99	0.44
1:F:248:LEU:HD13	1:F:371:VAL:HG23	2.00	0.44
1:D:248:LEU:HD13	1:D:371:VAL:HG23	2.00	0.44
1:B:106:LEU:HD11	1:B:369:ARG:HD3	2.00	0.44
1:B:281:ASP:O	1:B:325:LYS:HA	2.18	0.43
1:A:45:ARG:HD3	1:A:47:ASP:OD2	2.19	0.42
1:C:248:LEU:HD13	1:C:371:VAL:HG23	2.02	0.42
1:C:276:ARG:HD3	5:C:1119:HOH:O	2.19	0.42
1:F:328:ASP:O	1:F:332:PHE:CD2	2.74	0.41
1:D:281:ASP:O	1:D:325:LYS:HA	2.21	0.41

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	334/408 (82%)	324 (97%)	9 (3%)	1 (0%)	36	66
1	B	344/408 (84%)	334 (97%)	10 (3%)	0	100	100
1	C	337/408 (83%)	326 (97%)	11 (3%)	0	100	100
1	D	354/408 (87%)	345 (98%)	9 (2%)	0	100	100
1	E	345/408 (85%)	328 (95%)	14 (4%)	3 (1%)	14	41
1	F	335/408 (82%)	323 (96%)	12 (4%)	0	100	100
All	All	2049/2448 (84%)	1980 (97%)	65 (3%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	172	LYS
1	E	45	ARG
1	A	45	ARG
1	E	192	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/341 (83%)	280 (99%)	2 (1%)	76	91
1	B	290/341 (85%)	288 (99%)	2 (1%)	76	91
1	C	286/341 (84%)	284 (99%)	2 (1%)	76	91
1	D	297/341 (87%)	295 (99%)	2 (1%)	76	91
1	E	290/341 (85%)	289 (100%)	1 (0%)	86	95
1	F	283/341 (83%)	281 (99%)	2 (1%)	76	91
All	All	1728/2046 (84%)	1717 (99%)	11 (1%)	78	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	101	LEU
1	B	45	ARG
1	B	101	LEU
1	C	101	LEU
1	C	135	THR
1	D	101	LEU
1	D	293	LEU
1	E	101	LEU
1	F	101	LEU
1	F	176	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	242	GLN
1	C	298	GLN
1	E	66	HIS
1	E	341	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 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	PLP	A	1002	1	15,15,16	0.99	1 (6%)	21,22,23	0.74	0
3	PLP	B	1002	1	15,15,16	0.88	1 (6%)	21,22,23	0.84	0
2	HEM	D	1001	1	50,50,50	1.98	15 (30%)	67,82,82	2.02	17 (25%)
2	HEM	C	1001	1	50,50,50	1.69	13 (26%)	67,82,82	1.37	10 (14%)
2	HEM	F	502	1	50,50,50	1.51	11 (22%)	67,82,82	1.43	9 (13%)
3	PLP	D	1002	1	15,15,16	0.92	1 (6%)	21,22,23	0.82	0
3	PLP	E	503	1	15,15,16	0.93	2 (13%)	21,22,23	0.84	0
2	HEM	B	1001	1	50,50,50	1.48	9 (18%)	67,82,82	1.46	11 (16%)
2	HEM	E	502	1	50,50,50	1.50	9 (18%)	67,82,82	1.47	9 (13%)
2	HEM	A	1001	1	50,50,50	1.57	11 (22%)	67,82,82	1.37	10 (14%)
3	PLP	C	1002	1	15,15,16	0.95	1 (6%)	21,22,23	0.82	0
3	PLP	F	503	1	15,15,16	1.05	2 (13%)	21,22,23	0.75	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	PLP	A	1002	1	-	0/6/6/8	0/1/1/1
3	PLP	B	1002	1	-	0/6/6/8	0/1/1/1
2	HEM	D	1001	1	-	4/14/54/54	-
2	HEM	C	1001	1	-	2/14/54/54	-
2	HEM	F	502	1	-	3/14/54/54	-
3	PLP	D	1002	1	-	0/6/6/8	0/1/1/1
3	PLP	E	503	1	-	0/6/6/8	0/1/1/1
2	HEM	B	1001	1	-	2/14/54/54	-
2	HEM	E	502	1	-	2/14/54/54	-
2	HEM	A	1001	1	-	2/14/54/54	-
3	PLP	C	1002	1	-	0/6/6/8	0/1/1/1
3	PLP	F	503	1	-	0/6/6/8	0/1/1/1

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	HEM	C4B-NB	-5.61	1.27	1.38
2	D	1001	HEM	C1D-ND	-4.08	1.30	1.38
2	C	1001	HEM	C4D-ND	-3.96	1.33	1.40
2	D	1001	HEM	C1B-NB	-3.91	1.33	1.40
2	C	1001	HEM	C1D-ND	-3.81	1.31	1.38
2	E	502	HEM	C3B-C4B	3.75	1.52	1.44
2	A	1001	HEM	C3B-C4B	3.58	1.51	1.44
2	F	502	HEM	C1A-C2A	-3.41	1.37	1.44
2	D	1001	HEM	C4D-ND	-3.34	1.34	1.40
2	A	1001	HEM	C4D-ND	-3.34	1.34	1.40
2	D	1001	HEM	CAD-C3D	3.33	1.59	1.51
2	F	502	HEM	C4B-NB	-3.32	1.32	1.38
2	F	502	HEM	C3B-C4B	3.30	1.51	1.44
2	A	1001	HEM	C3C-C2C	3.28	1.43	1.37
2	A	1001	HEM	C1D-ND	-3.28	1.32	1.38
2	D	1001	HEM	C2A-C3A	-3.15	1.30	1.38
2	B	1001	HEM	C4D-ND	-3.13	1.34	1.40
2	B	1001	HEM	C3B-C4B	3.04	1.50	1.44
2	C	1001	HEM	C1A-C2A	-2.99	1.38	1.44
2	C	1001	HEM	C1B-NB	-2.98	1.35	1.40
2	D	1001	HEM	C1C-C2C	-2.94	1.39	1.45
2	C	1001	HEM	C3B-C4B	2.90	1.50	1.44
2	F	502	HEM	C1B-NB	-2.81	1.35	1.40
2	B	1001	HEM	C1D-ND	-2.80	1.33	1.38
2	E	502	HEM	C1D-ND	-2.78	1.33	1.38
2	A	1001	HEM	O2A-CGA	2.76	1.40	1.30
2	E	502	HEM	C1A-C2A	-2.74	1.39	1.44
2	B	1001	HEM	CMC-C2C	2.72	1.56	1.50
2	B	1001	HEM	C3C-C2C	2.70	1.42	1.37
2	D	1001	HEM	CAB-C3B	2.68	1.54	1.47
2	E	502	HEM	C4D-ND	-2.67	1.35	1.40
2	C	1001	HEM	C4B-NB	-2.66	1.33	1.38
2	B	1001	HEM	C1A-C2A	-2.60	1.39	1.44
2	A	1001	HEM	C1A-C2A	-2.60	1.39	1.44
2	B	1001	HEM	C4B-NB	-2.57	1.33	1.38
2	B	1001	HEM	C1B-NB	-2.56	1.35	1.40
2	C	1001	HEM	CMA-C3A	2.55	1.56	1.50
3	B	1002	PLP	C4A-C4	-2.54	1.46	1.51
2	D	1001	HEM	CMC-C2C	2.53	1.56	1.50
2	E	502	HEM	CHD-C4C	2.50	1.43	1.38
2	C	1001	HEM	C3C-C2C	2.50	1.42	1.37
3	A	1002	PLP	C4A-C4	-2.50	1.46	1.51
2	D	1001	HEM	C3C-C2C	2.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	PLP	C4A-C4	-2.47	1.46	1.51
2	F	502	HEM	C1D-ND	-2.47	1.34	1.38
2	C	1001	HEM	O2D-CGD	2.46	1.38	1.30
3	D	1002	PLP	C4A-C4	-2.45	1.46	1.51
2	A	1001	HEM	C4B-NB	-2.44	1.34	1.38
2	A	1001	HEM	O2D-CGD	2.44	1.38	1.30
2	E	502	HEM	C1C-C2C	-2.44	1.40	1.45
3	C	1002	PLP	C4A-C4	-2.41	1.46	1.51
2	A	1001	HEM	C2A-C3A	-2.39	1.32	1.38
2	D	1001	HEM	C3B-C4B	2.35	1.49	1.44
2	F	502	HEM	CMC-C2C	2.33	1.55	1.50
2	E	502	HEM	CMA-C3A	2.33	1.55	1.50
2	C	1001	HEM	C2A-C3A	-2.33	1.32	1.38
2	F	502	HEM	C3C-C2C	2.30	1.41	1.37
2	F	502	HEM	C2A-C3A	-2.28	1.33	1.38
2	C	1001	HEM	CMC-C2C	2.27	1.55	1.50
2	D	1001	HEM	CHA-C4D	-2.25	1.34	1.38
2	B	1001	HEM	C2A-C3A	-2.24	1.33	1.38
2	D	1001	HEM	CMD-C2D	-2.23	1.46	1.50
2	C	1001	HEM	C4A-NA	-2.22	1.35	1.39
2	E	502	HEM	FE-NB	2.20	2.01	1.94
2	D	1001	HEM	CHB-C4A	-2.19	1.34	1.39
3	E	503	PLP	P-O4P	2.12	1.67	1.60
2	C	1001	HEM	C3D-C2D	-2.10	1.32	1.36
2	F	502	HEM	C4D-ND	-2.09	1.36	1.40
3	F	503	PLP	C4A-C4	-2.07	1.47	1.51
2	E	502	HEM	O2D-CGD	2.07	1.37	1.30
2	A	1001	HEM	CMC-C2C	2.07	1.55	1.50
2	F	502	HEM	CMA-C3A	2.05	1.55	1.50
2	A	1001	HEM	C1B-NB	-2.04	1.36	1.40
3	F	503	PLP	P-O1P	2.03	1.56	1.50
2	D	1001	HEM	C3C-C4C	-2.01	1.42	1.46
2	F	502	HEM	O2D-CGD	2.01	1.37	1.30

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	HEM	C3B-C4B-NB	7.06	114.54	109.47
2	D	1001	HEM	C4B-C3B-C2B	-5.48	102.25	107.28
2	E	502	HEM	C2B-C1B-NB	4.34	114.83	109.84
2	B	1001	HEM	C2B-C1B-NB	4.31	114.80	109.84
2	C	1001	HEM	C2B-C1B-NB	4.22	114.69	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	HEM	C2B-C1B-NB	4.19	114.65	109.84
2	D	1001	HEM	CMD-C2D-C1D	4.16	131.54	125.03
2	F	502	HEM	C2B-C1B-NB	4.06	114.51	109.84
2	F	502	HEM	C4B-C3B-C2B	-4.02	103.58	107.28
2	F	502	HEM	C3B-C4B-NB	3.97	112.32	109.47
2	D	1001	HEM	CAA-CBA-CGA	-3.82	103.54	113.67
2	B	1001	HEM	C3B-C4B-NB	3.62	112.07	109.47
2	D	1001	HEM	CBA-CAA-C2A	3.62	122.53	112.53
2	D	1001	HEM	C3D-C4D-ND	3.56	114.07	110.17
2	C	1001	HEM	CAA-CBA-CGA	-3.56	104.23	113.67
2	E	502	HEM	C4B-C3B-C2B	-3.52	104.05	107.28
2	D	1001	HEM	CAA-C2A-C1A	-3.49	118.13	124.94
2	B	1001	HEM	C4B-C3B-C2B	-3.34	104.21	107.28
2	D	1001	HEM	C2B-C1B-NB	3.32	113.65	109.84
2	E	502	HEM	CAA-CBA-CGA	-3.30	104.92	113.67
2	D	1001	HEM	CHA-C4D-C3D	-3.21	119.30	125.23
2	A	1001	HEM	C4B-C3B-C2B	-3.04	104.48	107.28
2	C	1001	HEM	C4B-C3B-C2B	-2.99	104.53	107.28
2	B	1001	HEM	C4A-NA-C1A	-2.89	101.11	105.82
2	D	1001	HEM	CMA-C3A-C4A	2.87	129.79	125.42
2	C	1001	HEM	C3B-C4B-NB	2.85	111.52	109.47
2	D	1001	HEM	CAA-C2A-C3A	2.78	133.30	127.07
2	D	1001	HEM	C4D-C3D-C2D	-2.73	102.92	106.89
2	F	502	HEM	CMD-C2D-C1D	2.68	129.23	125.03
2	D	1001	HEM	CMB-C2B-C1B	2.67	129.20	125.03
2	A	1001	HEM	C3B-C4B-NB	2.62	111.35	109.47
2	A	1001	HEM	CMD-C2D-C1D	2.59	129.08	125.03
2	E	502	HEM	O2D-CGD-CBD	2.56	122.09	114.00
2	A	1001	HEM	CMB-C2B-C1B	2.55	129.02	125.03
2	F	502	HEM	C4A-NA-C1A	-2.54	101.67	105.82
2	B	1001	HEM	CMD-C2D-C1D	2.52	128.97	125.03
2	D	1001	HEM	C2D-C1D-ND	2.51	112.81	109.90
2	E	502	HEM	C4A-C3A-C2A	-2.51	103.94	106.82
2	C	1001	HEM	C4A-NA-C1A	-2.51	101.73	105.82
2	C	1001	HEM	C3D-C4D-ND	2.48	112.89	110.17
2	A	1001	HEM	C4A-NA-C1A	-2.48	101.78	105.82
2	F	502	HEM	CHB-C1B-C2B	-2.39	120.17	126.95
2	B	1001	HEM	CMB-C2B-C1B	2.38	128.75	125.03
2	D	1001	HEM	O2D-CGD-O1D	-2.36	117.25	123.33
2	B	1001	HEM	C3A-C4A-NA	2.35	113.90	110.14
2	F	502	HEM	CMB-C2B-C1B	2.30	128.63	125.03
2	D	1001	HEM	O2D-CGD-CBD	2.30	121.26	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	HEM	CMB-C2B-C1B	2.27	128.59	125.03
2	B	1001	HEM	C3D-C4D-ND	2.25	112.64	110.17
2	A	1001	HEM	C4C-C3C-C2C	-2.25	104.87	106.81
2	F	502	HEM	CAA-CBA-CGA	-2.24	107.73	113.67
2	D	1001	HEM	C4A-NA-C1A	-2.22	102.21	105.82
2	C	1001	HEM	C3A-C4A-NA	2.21	113.69	110.14
2	A	1001	HEM	CAA-CBA-CGA	-2.19	107.85	113.67
2	B	1001	HEM	CHB-C1B-C2B	-2.19	120.73	126.95
2	E	502	HEM	C4A-NA-C1A	-2.18	102.26	105.82
2	C	1001	HEM	CMD-C2D-C1D	2.18	128.44	125.03
2	A	1001	HEM	CHB-C1B-C2B	-2.18	120.75	126.95
2	E	502	HEM	O2D-CGD-O1D	-2.18	117.73	123.33
2	C	1001	HEM	CHB-C1B-C2B	-2.16	120.81	126.95
2	B	1001	HEM	C4C-C3C-C2C	-2.15	104.95	106.81
2	A	1001	HEM	C4A-C3A-C2A	-2.14	104.36	106.82
2	E	502	HEM	CMB-C2B-C1B	2.10	128.32	125.03
2	E	502	HEM	CHB-C1B-C2B	-2.10	120.99	126.95
2	F	502	HEM	C3D-C4D-ND	2.06	112.43	110.17
2	B	1001	HEM	C4A-C3A-C2A	-2.02	104.51	106.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

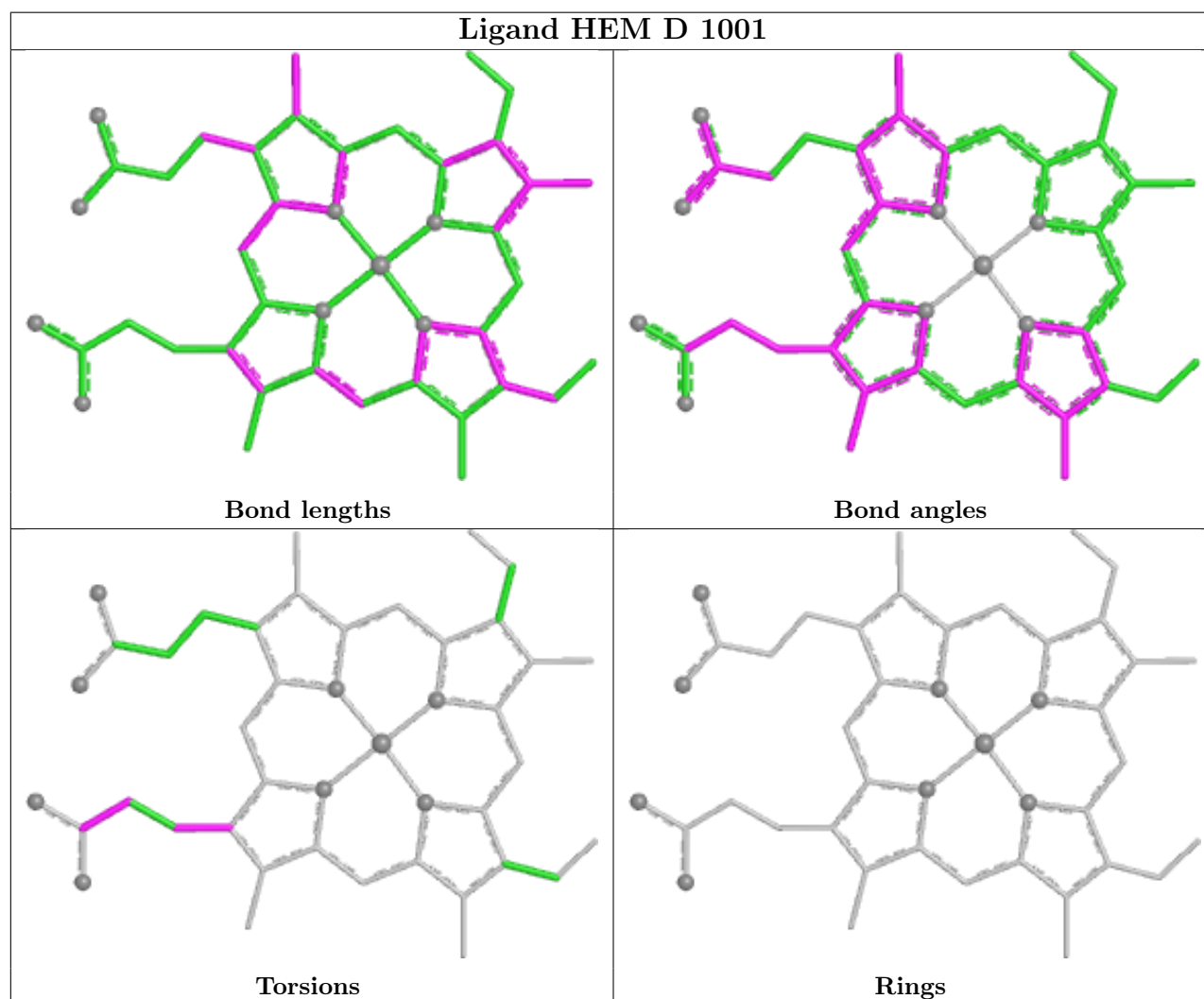
Mol	Chain	Res	Type	Atoms
2	D	1001	HEM	C3A-C2A-CAA-CBA
2	D	1001	HEM	C1A-C2A-CAA-CBA
2	A	1001	HEM	CAA-CBA-CGA-O2A
2	B	1001	HEM	CAA-CBA-CGA-O2A
2	A	1001	HEM	CAA-CBA-CGA-O1A
2	B	1001	HEM	CAA-CBA-CGA-O1A
2	F	502	HEM	CAA-CBA-CGA-O1A
2	F	502	HEM	CAA-CBA-CGA-O2A
2	C	1001	HEM	CAA-CBA-CGA-O2A
2	C	1001	HEM	CAA-CBA-CGA-O1A
2	E	502	HEM	CAA-CBA-CGA-O1A
2	D	1001	HEM	CAA-CBA-CGA-O2A
2	E	502	HEM	CAA-CBA-CGA-O2A
2	D	1001	HEM	CAA-CBA-CGA-O1A
2	F	502	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

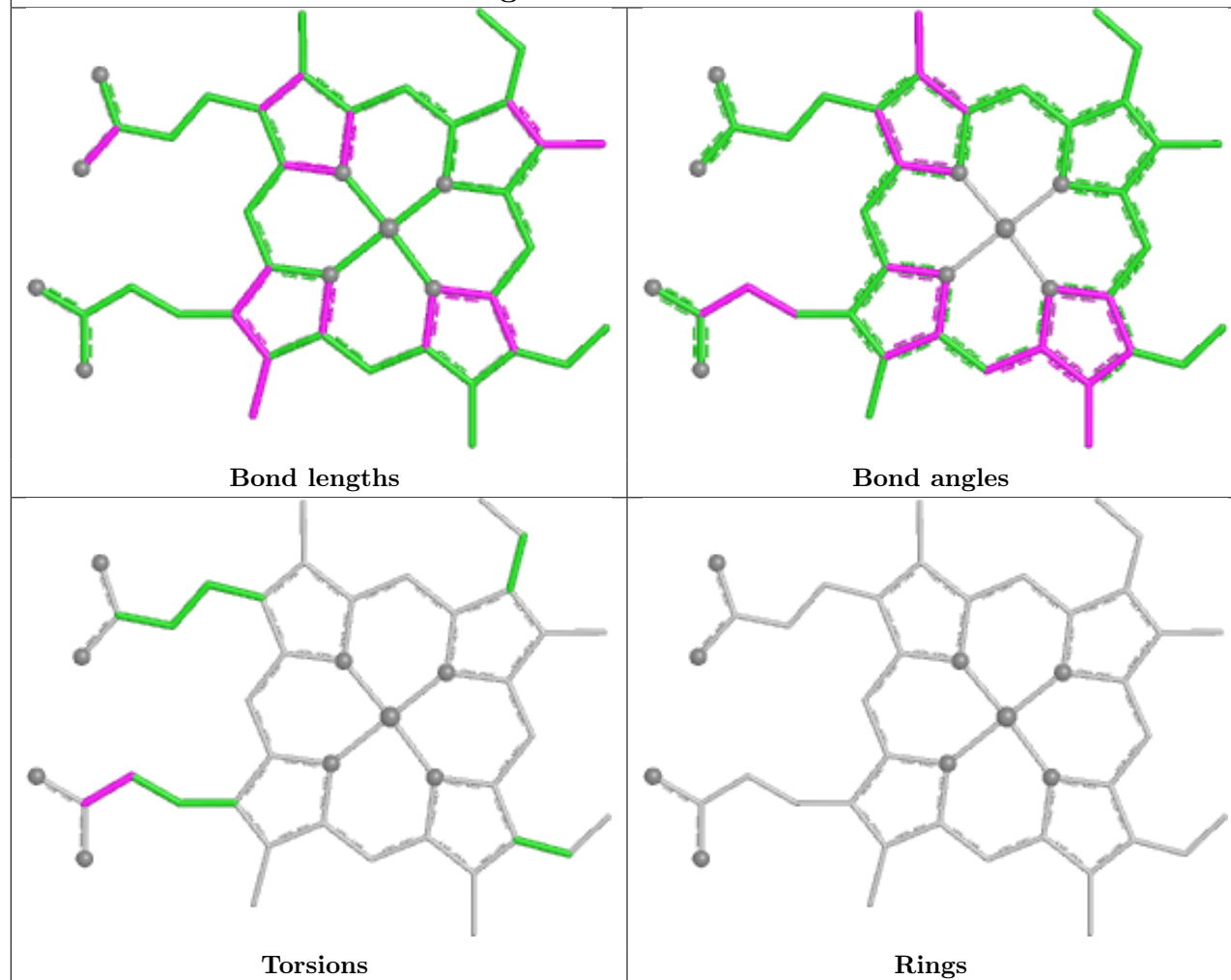
1 monomer is involved in 2 short contacts:

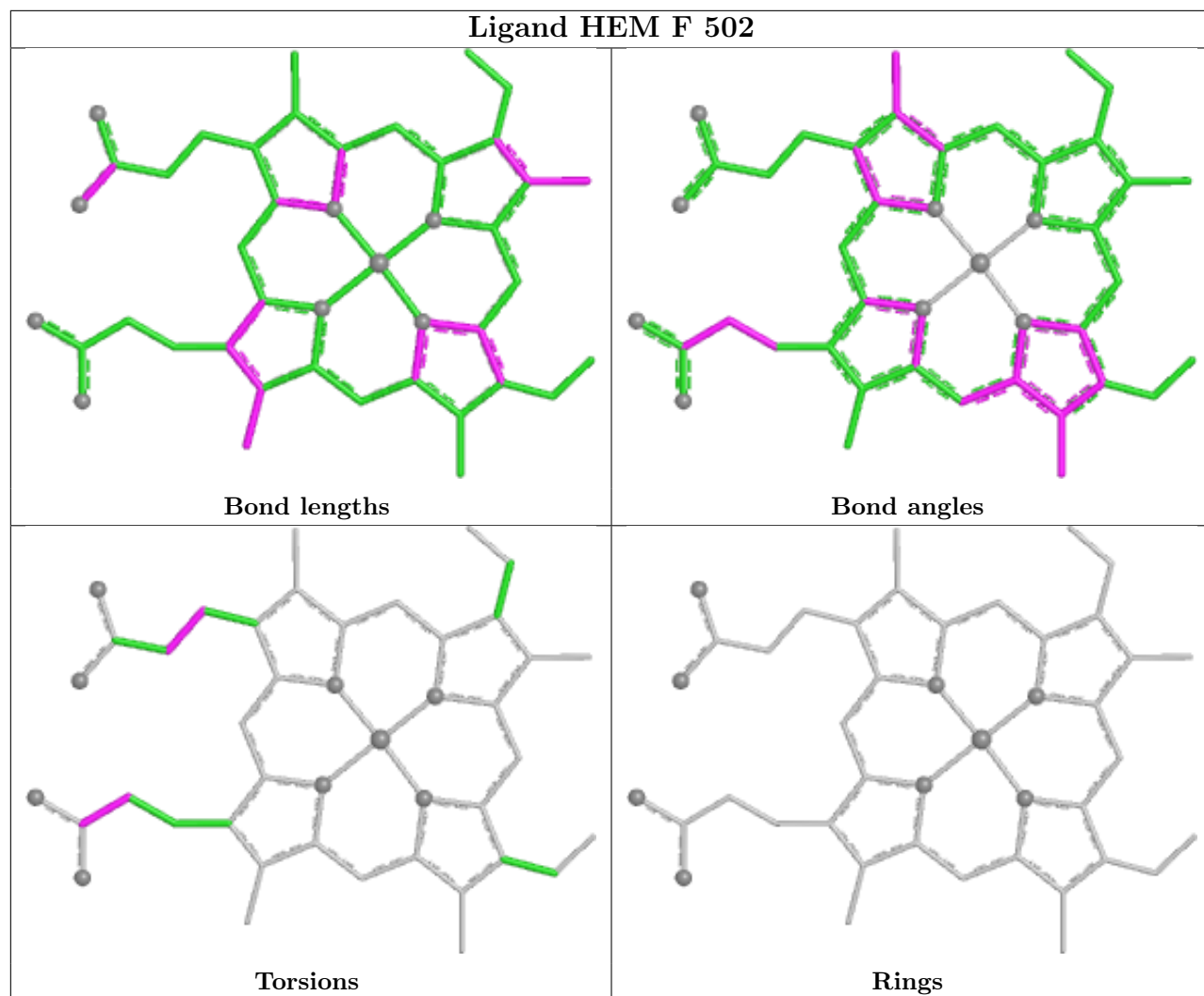
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	HEM	2	0

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

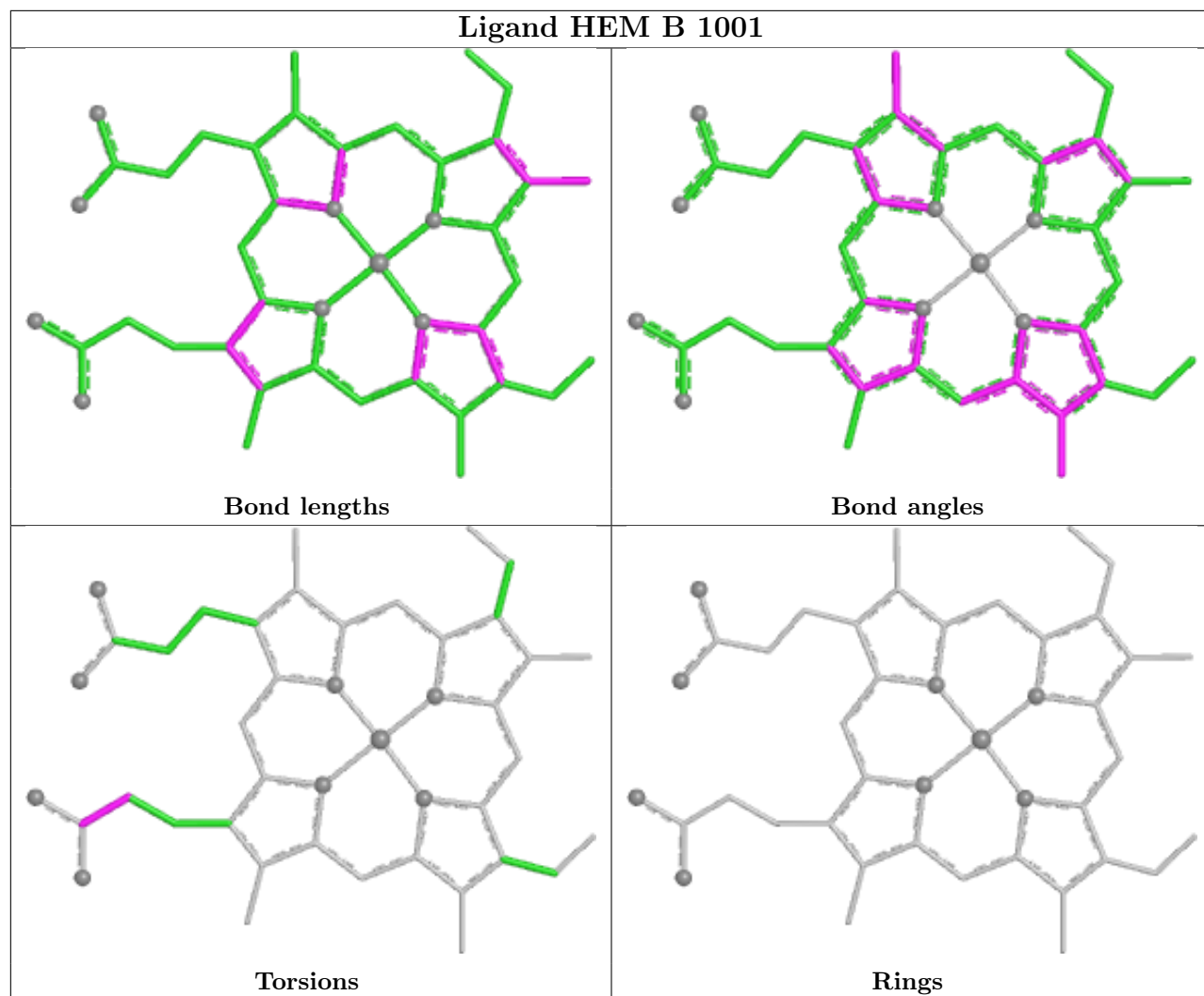


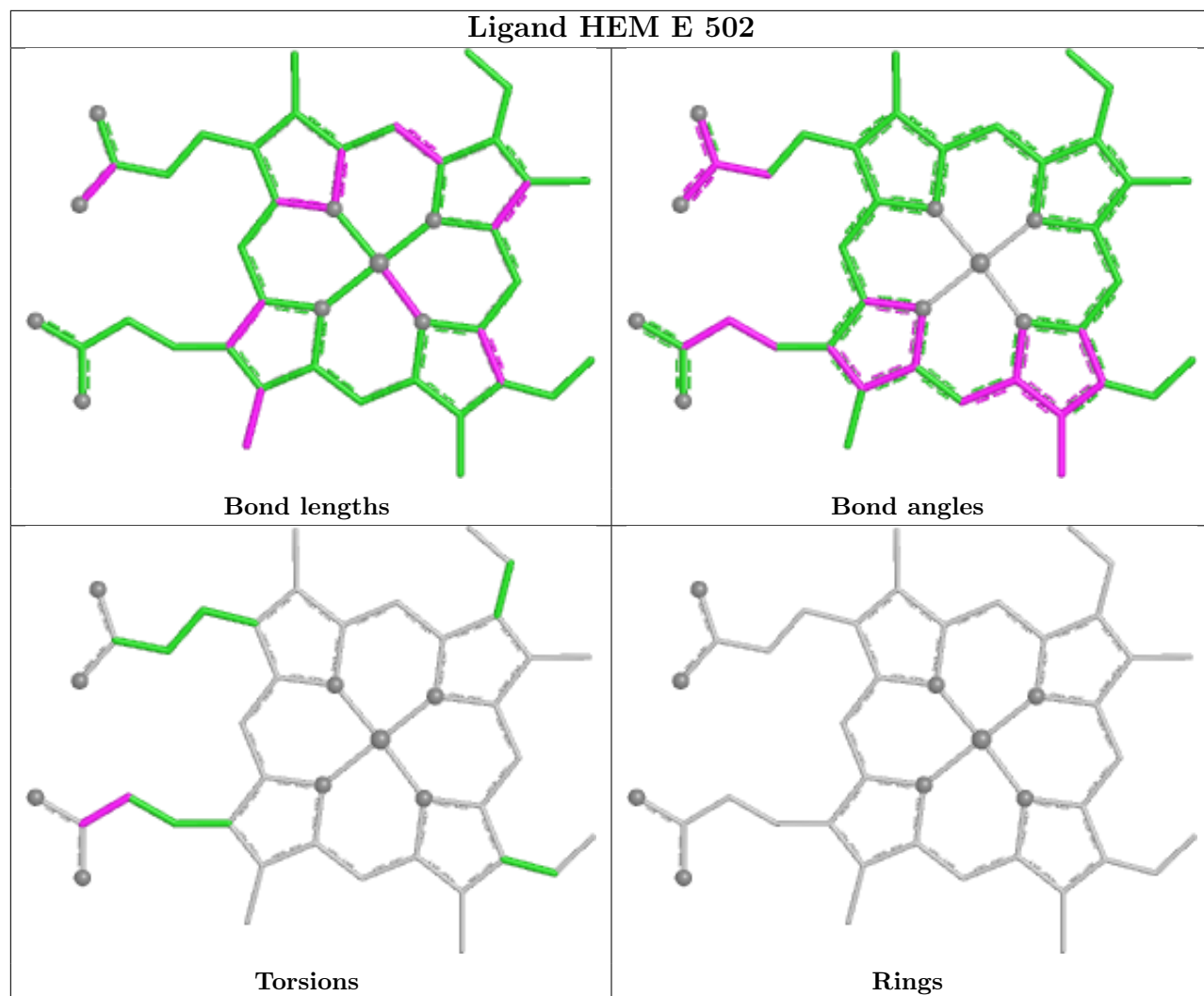
Ligand HEM C 1001

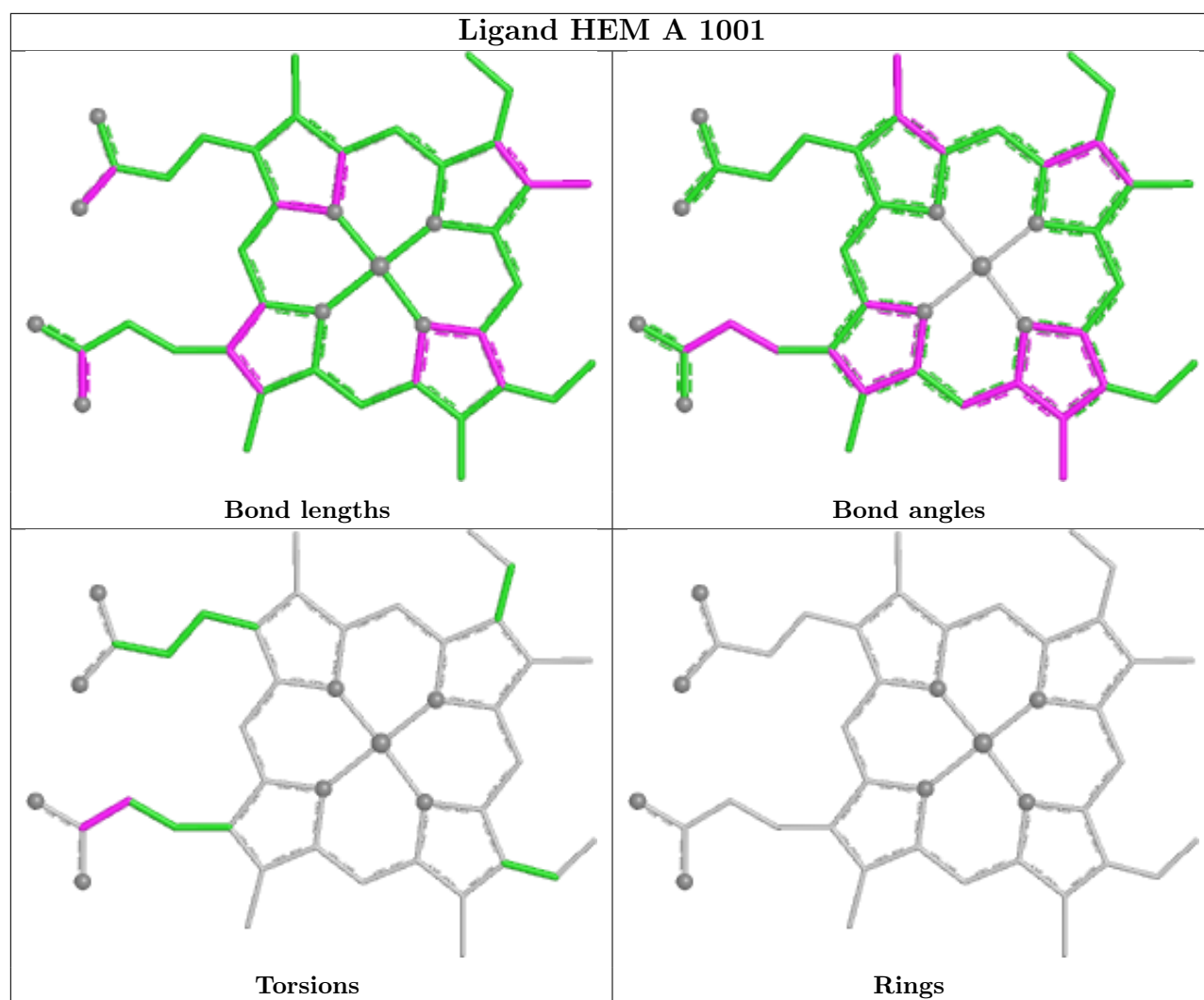




Ligand HEM B 1001







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/408 (83%)	0.07	3 (0%) 81 74	27, 44, 69, 99	0
1	B	348/408 (85%)	-0.00	2 (0%) 85 80	22, 40, 67, 88	0
1	C	343/408 (84%)	0.11	6 (1%) 69 60	25, 44, 73, 116	0
1	D	356/408 (87%)	0.07	3 (0%) 82 75	24, 40, 69, 91	0
1	E	349/408 (85%)	0.09	5 (1%) 73 64	26, 42, 79, 108	0
1	F	341/408 (83%)	0.09	5 (1%) 72 63	25, 41, 67, 100	0
All	All	2077/2448 (84%)	0.07	24 (1%) 76 68	22, 42, 71, 116	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	299	THR	4.1
1	A	44	ILE	4.0
1	D	172	LYS	3.5
1	C	44	ILE	3.1
1	F	174	SER	3.1
1	C	170	PRO	3.0
1	E	44	ILE	2.9
1	B	199	SER	2.8
1	E	173	MET	2.6
1	F	208	TRP	2.6
1	E	60	ALA	2.6
1	A	201	GLU	2.6
1	E	68	THR	2.5
1	B	201	GLU	2.5
1	C	174	SER	2.4
1	D	400	GLU	2.4
1	A	71	ALA	2.4
1	F	191	THR	2.2
1	E	197	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	294	ASN	2.1
1	F	170	PRO	2.1
1	D	171	GLU	2.1
1	C	192	PRO	2.0
1	F	53	THR	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.

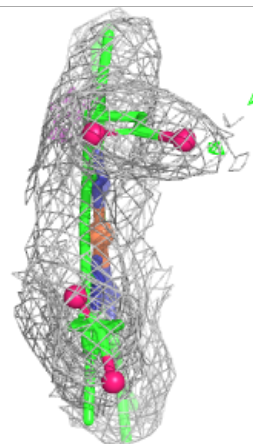
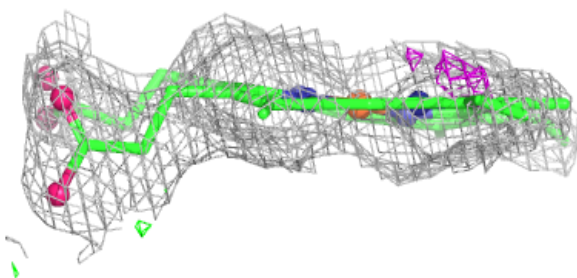
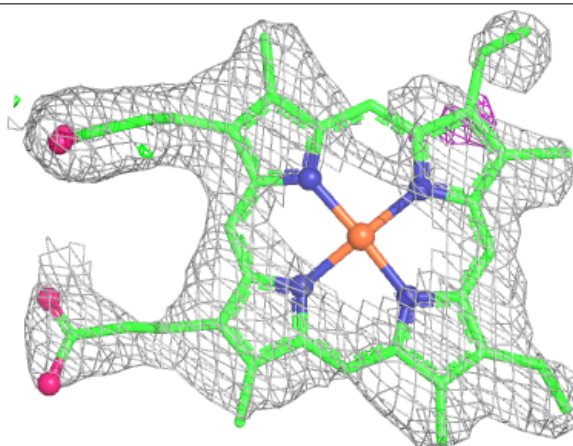
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	E	501	1/1	0.89	0.16	40,40,40,40	0
4	NA	F	501	1/1	0.92	0.07	30,30,30,30	0
4	NA	E	504	1/1	0.93	0.09	33,33,33,33	0
2	HEM	A	1001	43/43	0.95	0.10	45,48,54,58	0
2	HEM	B	1001	43/43	0.95	0.10	39,42,48,52	0
3	PLP	E	503	15/16	0.95	0.10	34,42,46,50	0
2	HEM	D	1001	43/43	0.96	0.09	39,42,47,51	0
3	PLP	F	503	15/16	0.96	0.10	13,29,37,40	0
2	HEM	E	502	43/43	0.96	0.10	40,43,50,52	0
2	HEM	F	502	43/43	0.96	0.09	37,40,48,50	0
3	PLP	A	1002	15/16	0.96	0.09	28,38,46,47	0
3	PLP	D	1002	15/16	0.97	0.07	23,27,30,37	0
2	HEM	C	1001	43/43	0.97	0.08	31,33,40,42	0
3	PLP	C	1002	15/16	0.97	0.08	25,37,46,46	0
3	PLP	B	1002	15/16	0.98	0.07	25,33,37,40	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.

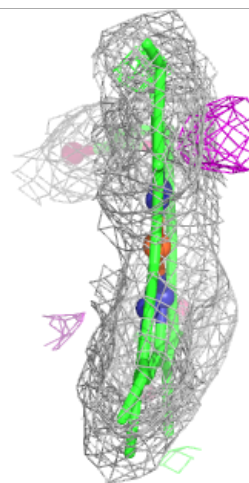
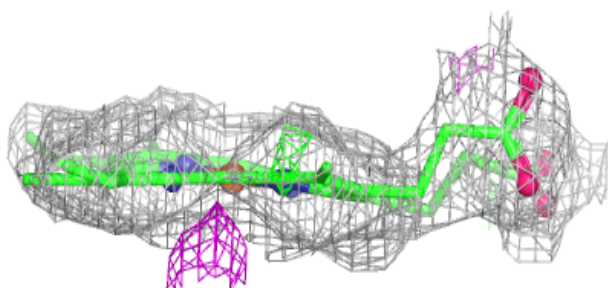
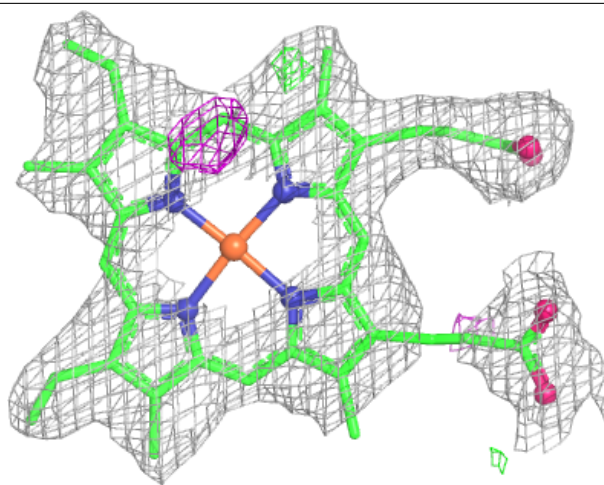
Electron density around HEM A 1001:

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



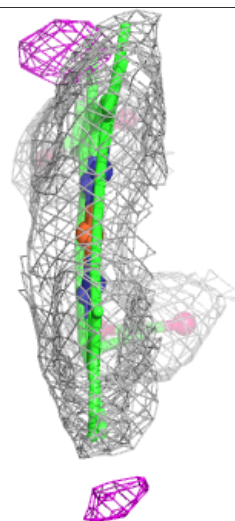
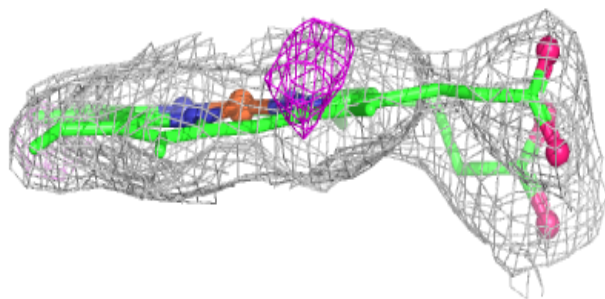
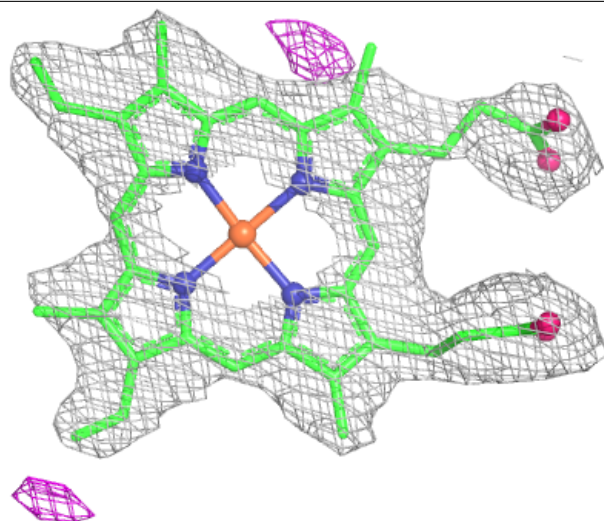
Electron density around HEM B 1001:

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



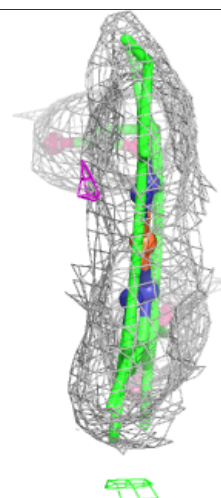
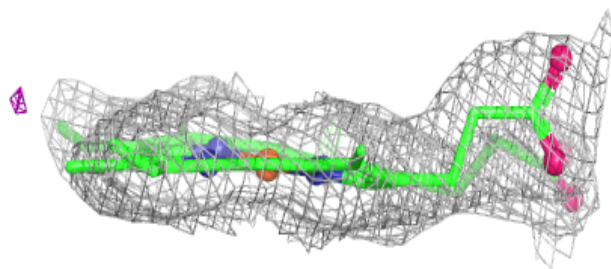
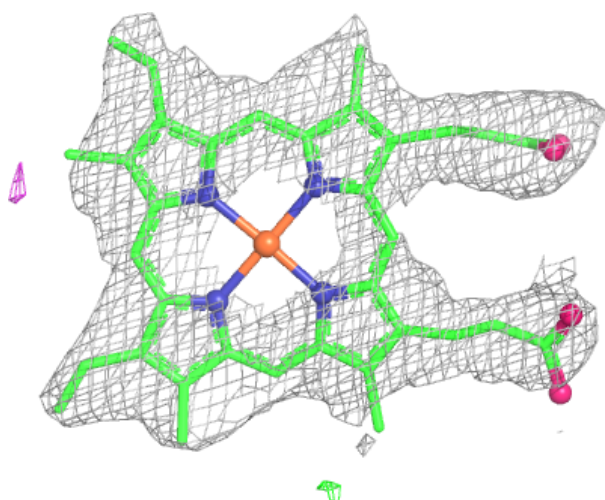
Electron density around HEM D 1001:

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



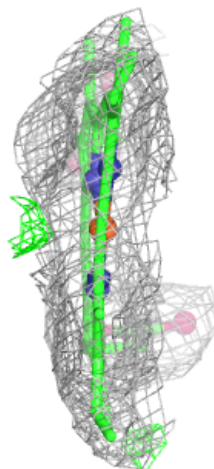
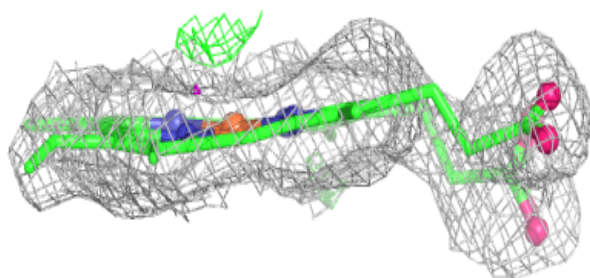
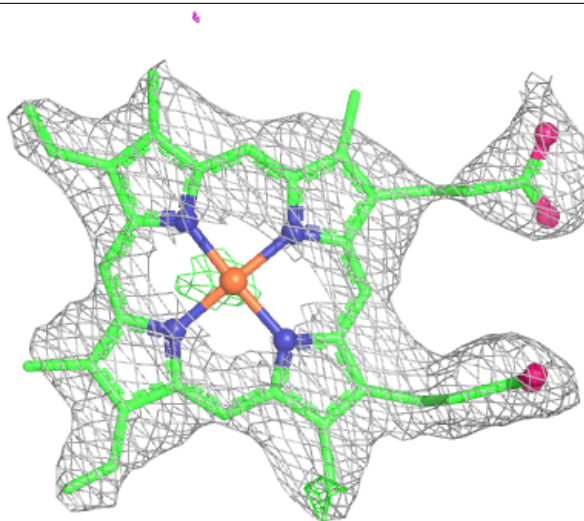
Electron density around HEM E 502:

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



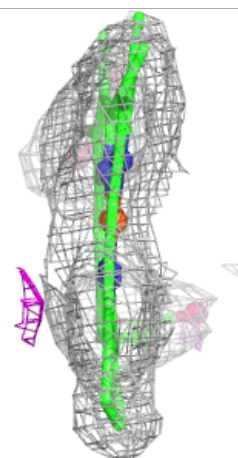
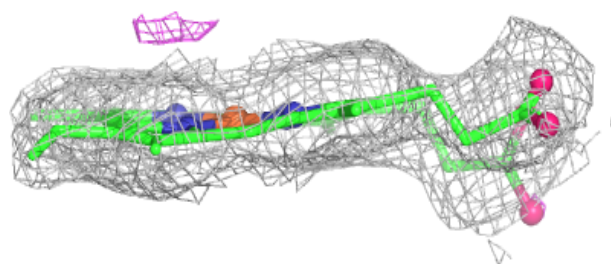
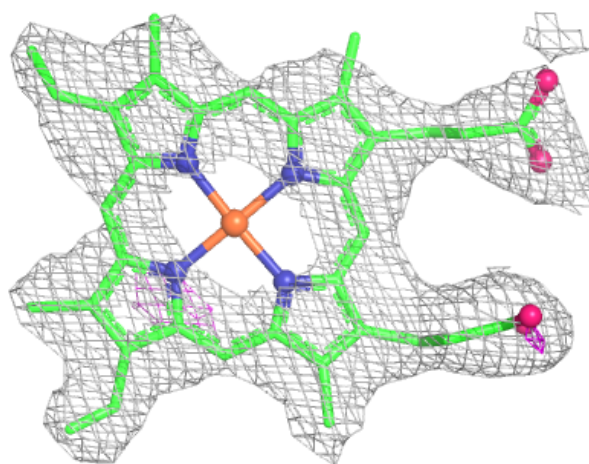
Electron density around HEM F 502:

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



Electron density around HEM C 1001:

$2mF_o-DF_c$ (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.