



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:51 pm BST

PDB ID : 5MMS
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.; Bandedeiras, 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 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 : 2.11
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) : 2.11

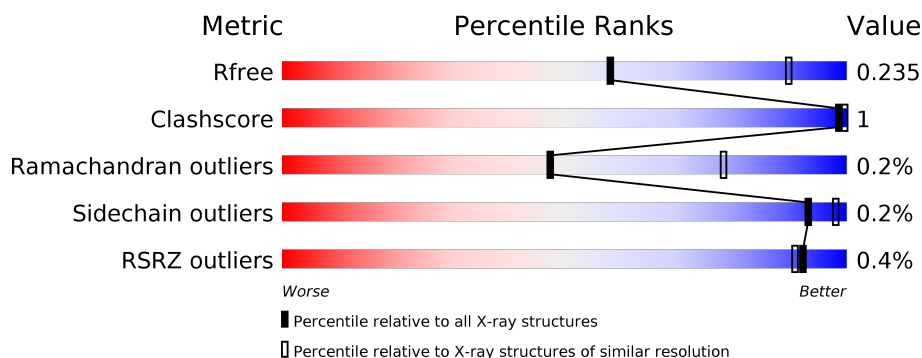
1 Overall quality at a glance ⓘ

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	<div> <div>82%</div> <div>17%</div> </div>
1	B	408	<div> <div>83%</div> <div>15%</div> </div>
1	C	408	<div> <div>82%</div> <div>16%</div> </div>
1	D	408	<div> <div>86%</div> <div>13%</div> </div>
1	E	408	<div> <div>84%</div> <div>14%</div> </div>
1	F	408	<div> <div>82%</div> <div>16%</div> </div>

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 (three-letter code: 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 (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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 (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

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

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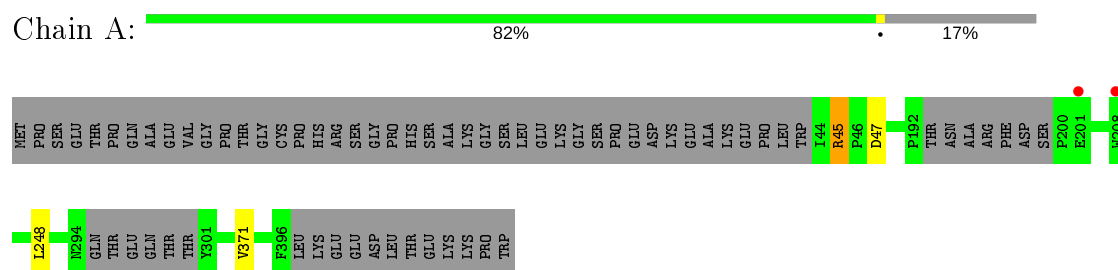
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	30	Total 30	O 30	0	0
5	C	22	Total 22	O 22	0	0
5	D	32	Total 32	O 32	0	0
5	E	38	Total 38	O 38	0	0
5	F	37	Total 37	O 37	0	0

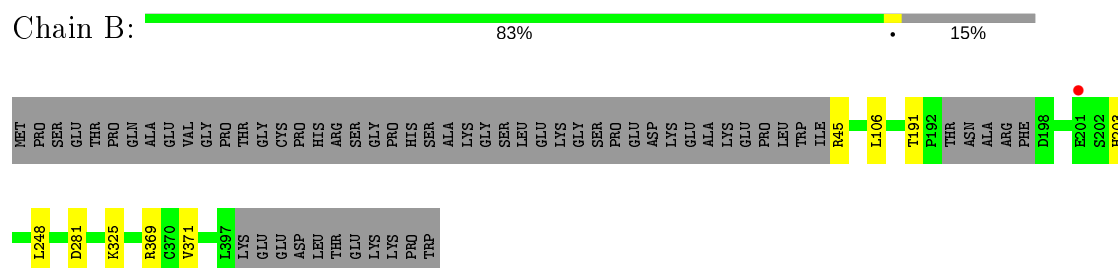
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

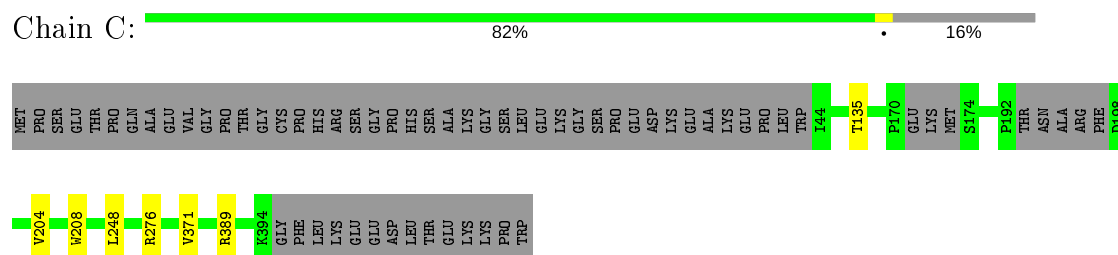
• Molecule 1: Cystathionine beta-synthase



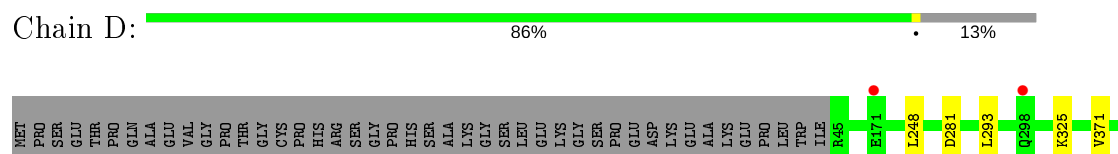
• Molecule 1: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase

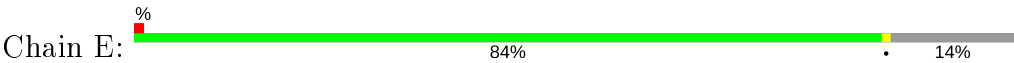


• Molecule 1: Cystathionine beta-synthase



E400
ASP
LEU
THR
GLU
LYS
LYS
PRO
TRP

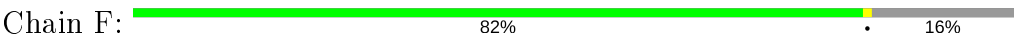
• Molecule 1: Cystathionine beta-synthase



MET PRO SER GLU THR PRO GLN ALA VAL GLY PRO THR GLY CYS PRO HIS ARG SER GLY PRO HIS SER SER LYS GLY SER LEU GLU LYS GLY SER PRO GLU LYS GLU ALA LYS LEU TRP I44 R45 H66 H67 T68 K172 P192 E201 L248 N294 GLN

THR GLU GLN THR T300 V371 L397 LYS GLU GLU ASP LEU THR PRO LYS LYS LYS PRO TRP

• Molecule 1: Cystathionine beta-synthase



MET PRO SER GLU THR PRO GLN ALA VAL GLY PRO THR GLY CYS PRO HIS ARG SER GLY PRO HIS SER SER LYS GLY SER LEU GLU LYS GLY SER PRO GLU LYS GLU ALA LYS LEU TRP I44 P170 GLU LYS MET S174 T191 PRO THR ASN ALA ARG PHE ASP SER

PRO GLU S202 W208 L248 D281 K325 D328 F332 V371 L397 LYS GLU GLU ASP LEU THR GLU LYS LYS PRO TRP

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 76.34 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (76.35-2.80) 98.5 (76.34-2.80)	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 0.194 , 0.235	Depositor DCC
R_{free} test set	2836 reflections (4.82%)	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 , 58.1	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	0.92	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.48	0/2649	0.65	0/3577
1	B	0.50	0/2712	0.66	0/3666
1	C	0.48	0/2669	0.65	0/3609
1	D	0.49	0/2783	0.65	0/3762
1	E	0.49	0/2722	0.67	0/3679
1	F	0.49	0/2654	0.65	0/3586
All	All	0.49	0/16189	0.66	0/21879

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	1	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
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	17	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 (17) 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: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:HMC2	2:D:1001:HEM:HBC2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41	72
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%)	17	46
1	F	335/408 (82%)	323 (96%)	12 (4%)	0	100	100
All	All	2049/2448 (84%)	1980 (97%)	65 (3%)	4 (0%)	47	78

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 [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	282/341 (83%)	282 (100%)	0	100	100
1	B	290/341 (85%)	289 (100%)	1 (0%)	92	98
1	C	286/341 (84%)	284 (99%)	2 (1%)	84	95
1	D	297/341 (87%)	296 (100%)	1 (0%)	92	98
1	E	290/341 (85%)	290 (100%)	0	100	100
1	F	283/341 (83%)	283 (100%)	0	100	100
All	All	1728/2046 (84%)	1724 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	ARG
1	C	135	THR
1	C	389	ARG
1	D	293	LEU

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

Mol	Chain	Res	Type
1	E	341	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	D	1002	1	15,15,16	0.91	1 (6%)	20,22,23	0.85	0
2	HEM	B	1001	1	27,50,50	1.19	2 (7%)	17,82,82	1.52	3 (17%)
2	HEM	A	1001	1	27,50,50	1.31	2 (7%)	17,82,82	1.64	4 (23%)
2	HEM	D	1001	1	27,50,50	1.97	10 (37%)	17,82,82	2.59	7 (41%)
2	HEM	C	1001	1	27,50,50	1.43	4 (14%)	17,82,82	1.76	2 (11%)
2	HEM	E	502	1	27,50,50	1.30	4 (14%)	17,82,82	2.05	5 (29%)
3	PLP	E	503	1	15,15,16	0.92	2 (13%)	20,22,23	0.87	0
3	PLP	F	503	1	15,15,16	1.03	0	20,22,23	0.78	0
2	HEM	F	502	1	27,50,50	1.15	1 (3%)	17,82,82	1.51	4 (23%)
3	PLP	B	1002	1	15,15,16	0.87	1 (6%)	20,22,23	0.87	0
3	PLP	C	1002	1	15,15,16	0.94	1 (6%)	20,22,23	0.85	0
3	PLP	A	1002	1	15,15,16	0.98	1 (6%)	20,22,23	0.76	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	D	1002	1	-	0/6/6/8	0/1/1/1
2	HEM	B	1001	1	-	0/6/54/54	-
2	HEM	A	1001	1	-	0/6/54/54	-
2	HEM	D	1001	1	-	2/6/54/54	-
2	HEM	C	1001	1	-	0/6/54/54	-
2	HEM	E	502	1	-	0/6/54/54	-
3	PLP	E	503	1	-	0/6/6/8	0/1/1/1
3	PLP	F	503	1	-	0/6/6/8	0/1/1/1
2	HEM	F	502	1	-	0/6/54/54	-
3	PLP	B	1002	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	C	1002	1	-	0/6/6/8	0/1/1/1
3	PLP	A	1002	1	-	0/6/6/8	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	HEM	CAD-C3D	4.37	1.59	1.52
2	D	1001	HEM	C4B-NB	-4.04	1.27	1.36
2	D	1001	HEM	C3B-CAB	3.24	1.54	1.47
2	C	1001	HEM	C3B-C2B	-3.08	1.36	1.40
2	E	502	HEM	CAA-C2A	-3.05	1.47	1.52
2	D	1001	HEM	C3B-C2B	-3.02	1.36	1.40
2	D	1001	HEM	CMD-C2D	-2.62	1.46	1.51
2	D	1001	HEM	C1D-ND	-2.59	1.30	1.36
2	A	1001	HEM	C3C-C2C	2.49	1.43	1.40
3	B	1002	PLP	C4A-C4	-2.45	1.46	1.51
3	A	1002	PLP	C4A-C4	-2.41	1.46	1.51
3	E	503	PLP	C4A-C4	-2.38	1.46	1.51
2	E	502	HEM	C4D-C3D	2.38	1.48	1.42
3	D	1002	PLP	C4A-C4	-2.37	1.46	1.51
2	B	1001	HEM	C3B-C2B	-2.36	1.37	1.40
2	D	1001	HEM	C2A-C3A	-2.35	1.30	1.37
2	D	1001	HEM	C4A-CHB	-2.33	1.34	1.41
2	C	1001	HEM	C1D-ND	-2.33	1.31	1.36
2	D	1001	HEM	C4D-C3D	2.33	1.47	1.42
3	C	1002	PLP	C4A-C4	-2.33	1.46	1.51
2	E	502	HEM	C3C-C2C	-2.27	1.37	1.40
2	D	1001	HEM	CAA-C2A	-2.12	1.48	1.52
2	A	1001	HEM	C3B-C2B	-2.12	1.37	1.40
3	E	503	PLP	P-O4P	2.11	1.67	1.60
2	C	1001	HEM	CMA-C3A	2.10	1.56	1.51
2	F	502	HEM	C3B-C2B	-2.06	1.37	1.40
2	C	1001	HEM	CAD-C3D	2.05	1.55	1.52
2	E	502	HEM	C3B-CAB	2.04	1.52	1.47
2	B	1001	HEM	CMC-C2C	2.00	1.56	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	HEM	CBA-CAA-C2A	5.45	122.53	112.49
2	D	1001	HEM	CAA-CBA-CGA	-5.44	103.54	112.67
2	C	1001	HEM	CAA-CBA-CGA	-5.03	104.23	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	502	HEM	CAA-CBA-CGA	-4.62	104.92	112.67
2	E	502	HEM	C4A-C3A-C2A	-4.39	103.94	107.00
2	D	1001	HEM	C3B-C4B-NB	4.12	114.54	109.21
2	A	1001	HEM	C4A-C3A-C2A	-3.78	104.36	107.00
2	B	1001	HEM	C4A-C3A-C2A	-3.58	104.51	107.00
2	D	1001	HEM	C4A-C3A-C2A	-3.40	104.63	107.00
2	C	1001	HEM	C4A-C3A-C2A	-3.03	104.89	107.00
2	D	1001	HEM	CMC-C2C-C3C	3.01	130.30	124.68
2	E	502	HEM	CBA-CAA-C2A	2.95	117.93	112.49
2	F	502	HEM	CAA-CBA-CGA	-2.95	107.73	112.67
2	A	1001	HEM	C4C-C3C-C2C	-2.91	104.87	106.90
2	A	1001	HEM	CAA-CBA-CGA	-2.87	107.85	112.67
2	B	1001	HEM	C4C-C3C-C2C	-2.79	104.95	106.90
2	E	502	HEM	C1D-C2D-C3D	-2.67	105.14	107.00
2	F	502	HEM	C4A-C3A-C2A	-2.67	105.14	107.00
2	F	502	HEM	C4C-C3C-C2C	-2.58	105.10	106.90
2	E	502	HEM	CMA-C3A-C2A	2.47	129.60	124.94
2	F	502	HEM	C3B-C4B-NB	2.41	112.32	109.21
2	B	1001	HEM	C3B-C4B-NB	2.21	112.07	109.21
2	A	1001	HEM	C1D-C2D-C3D	-2.17	105.49	107.00
2	D	1001	HEM	CAA-C2A-C3A	2.11	133.30	127.25
2	D	1001	HEM	CMD-C2D-C1D	2.00	131.54	128.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1001	HEM	C1A-C2A-CAA-CBA
2	D	1001	HEM	C3A-C2A-CAA-CBA

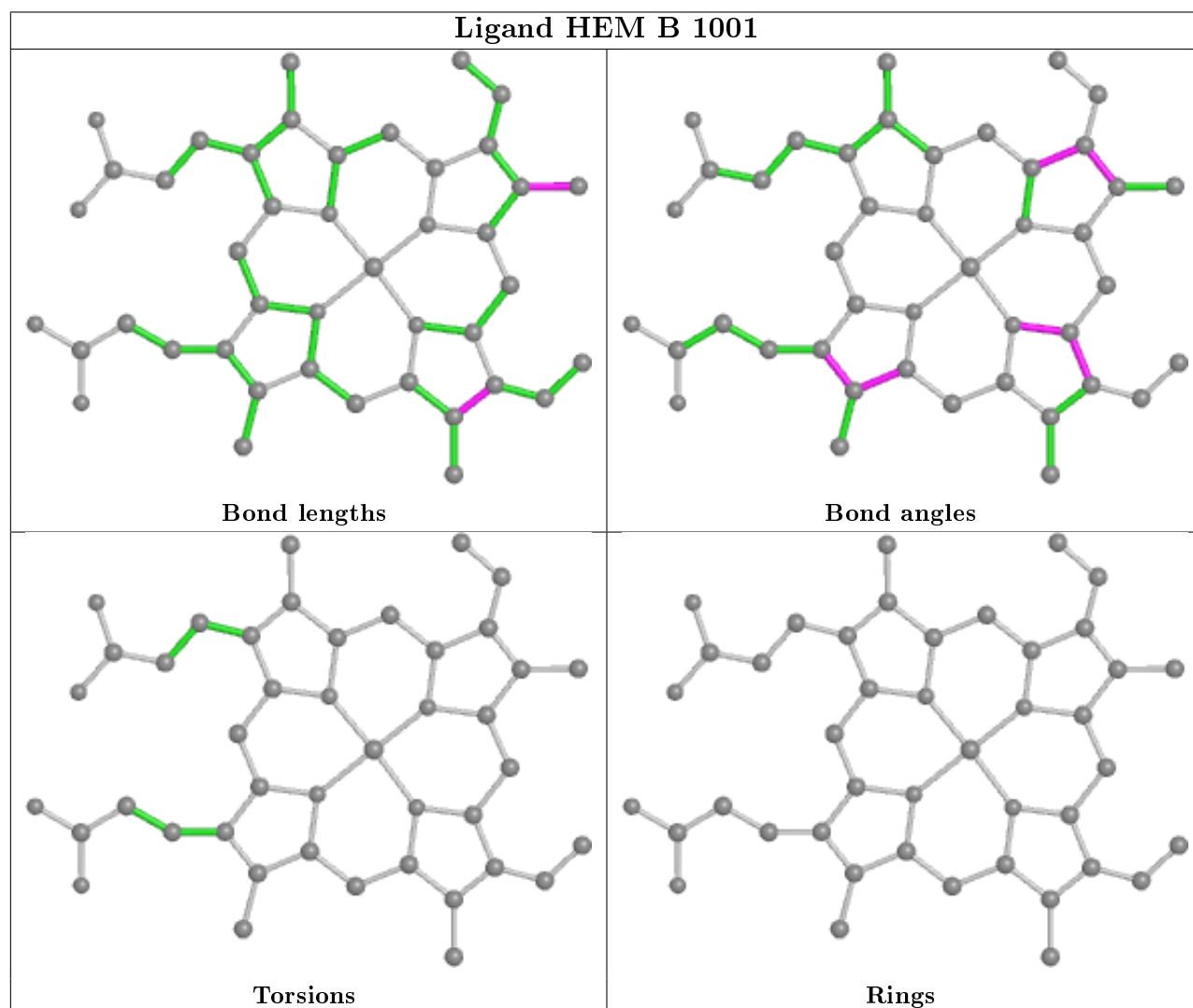
There are no ring outliers.

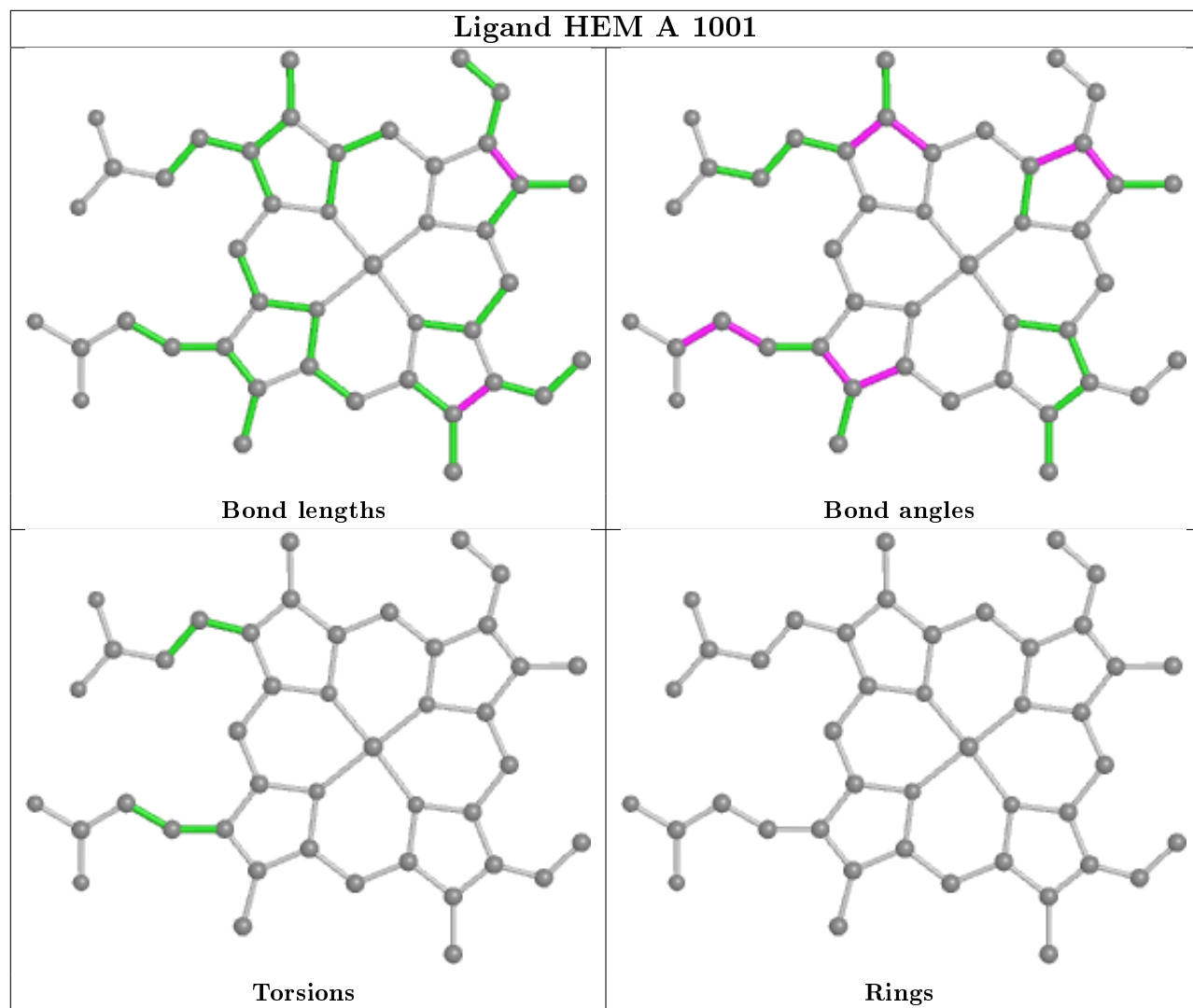
1 monomer is involved in 1 short contact:

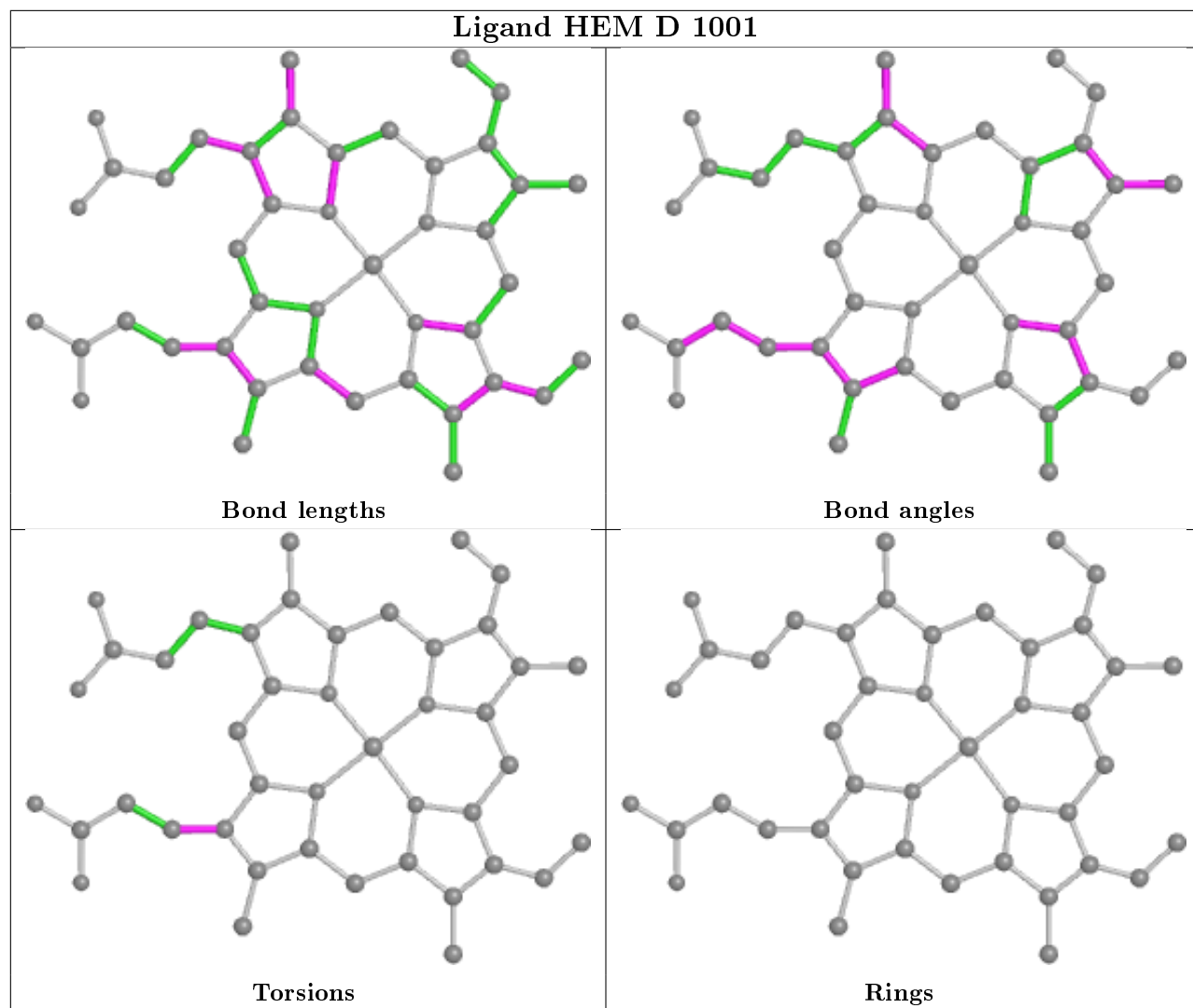
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	HEM	1	0

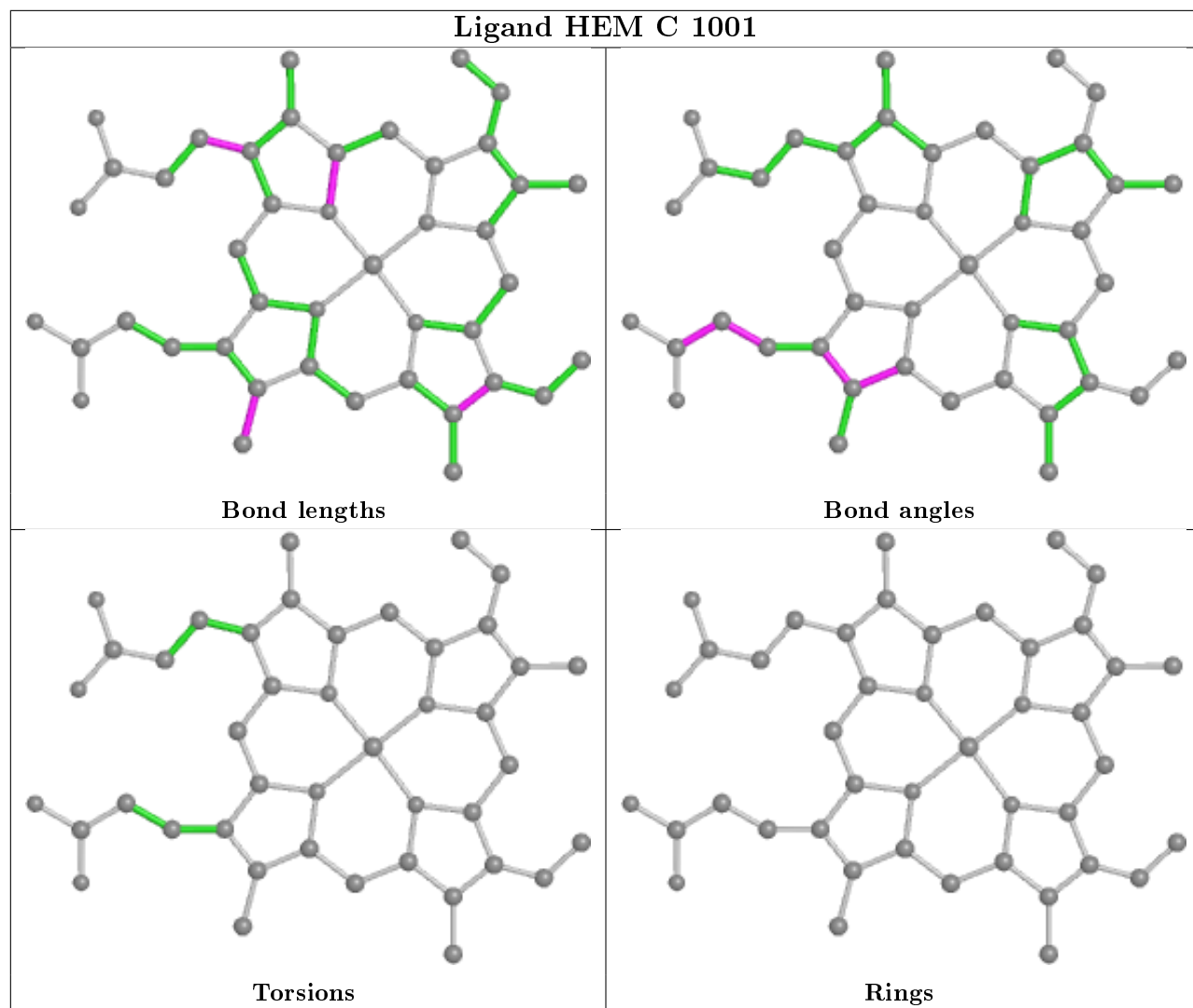
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

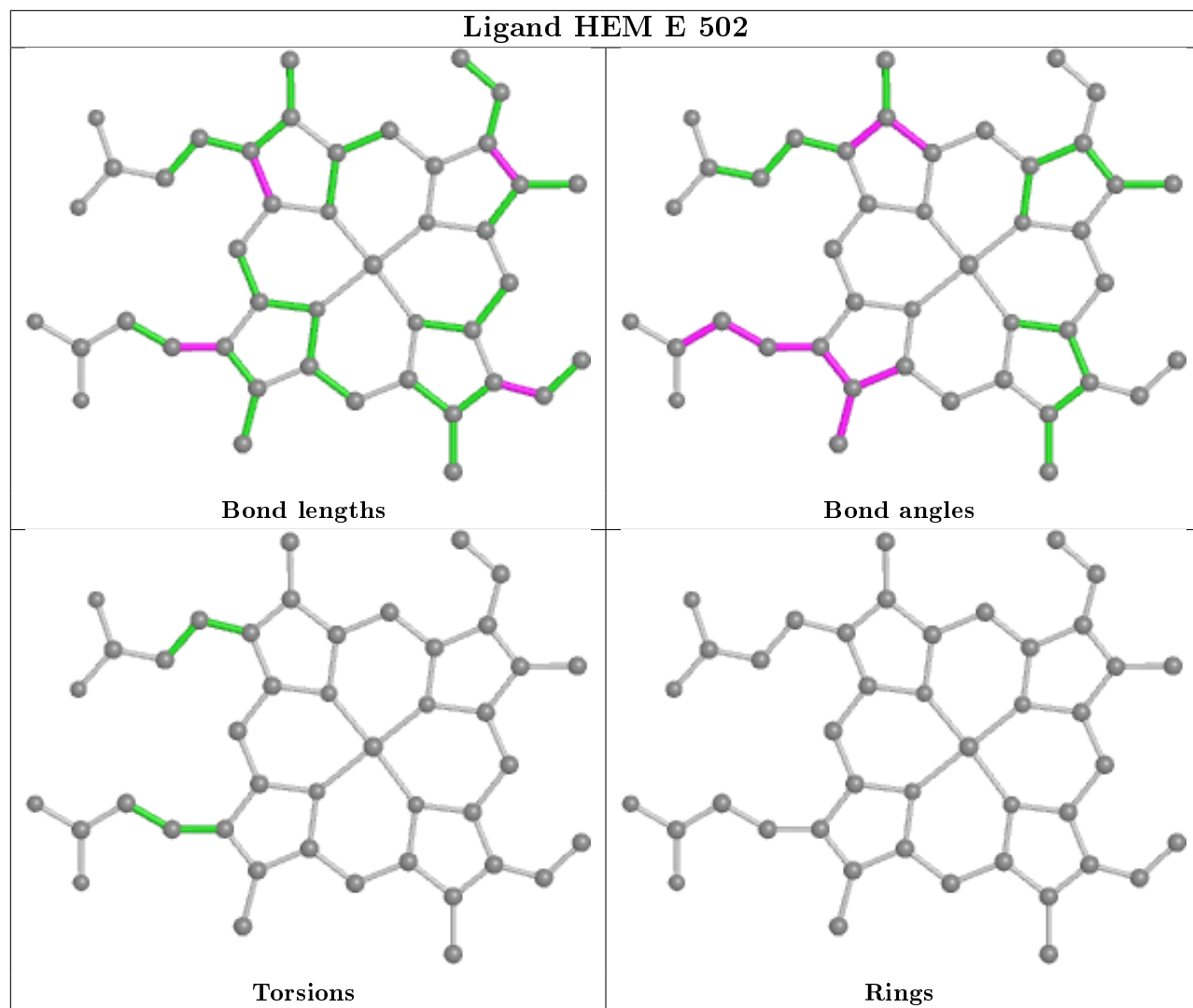
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

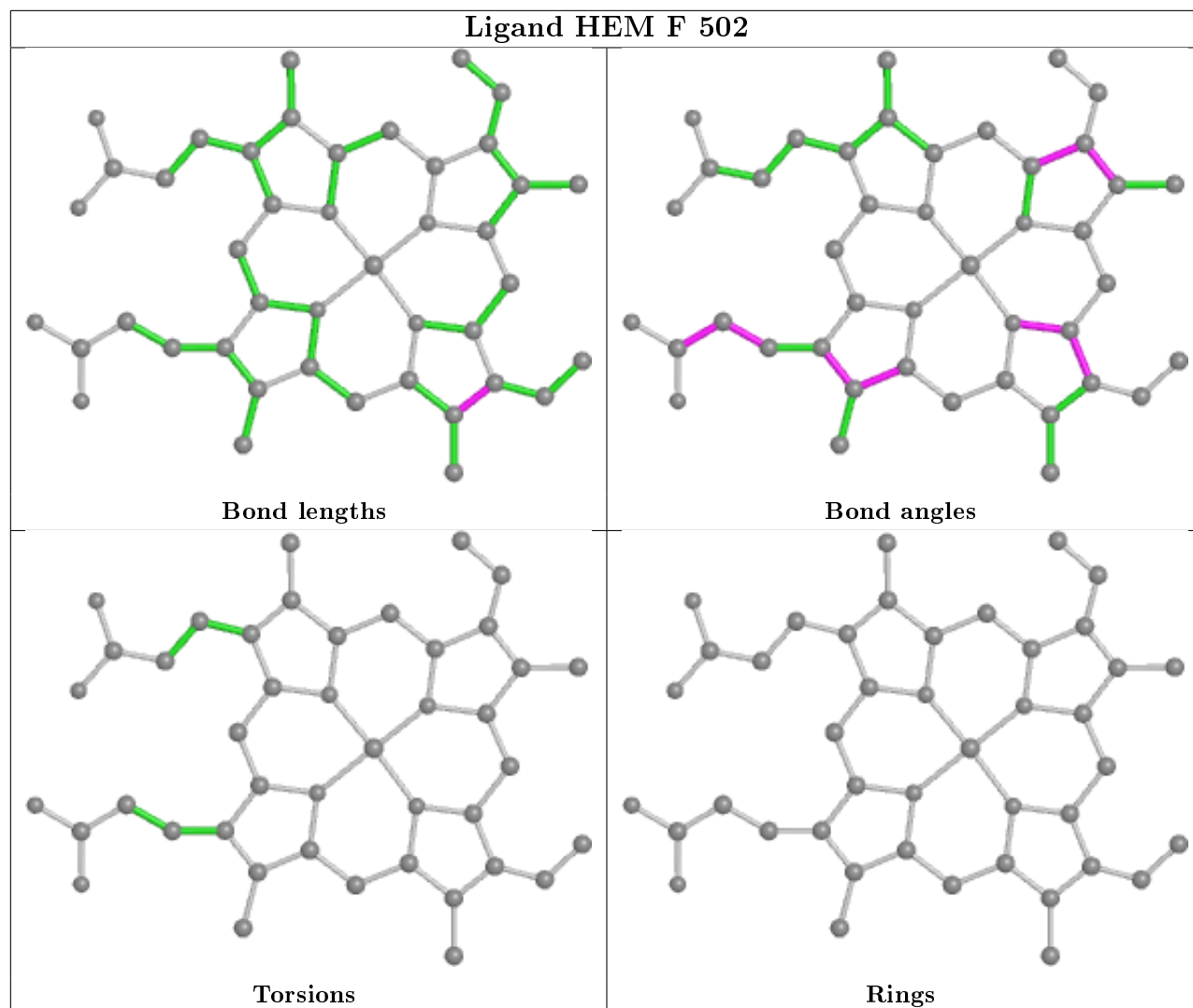












5.7 Other polymers [i](#)

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	340/408 (83%)	-0.36	2 (0%) 89 86	27, 44, 69, 99	0
1	B	348/408 (85%)	-0.41	1 (0%) 94 93	22, 40, 67, 88	0
1	C	343/408 (84%)	-0.37	0 100 100	25, 44, 73, 116	0
1	D	356/408 (87%)	-0.43	2 (0%) 89 86	24, 40, 69, 91	0
1	E	349/408 (85%)	-0.30	3 (0%) 84 80	26, 42, 79, 108	0
1	F	341/408 (83%)	-0.38	1 (0%) 94 93	25, 41, 67, 100	0
All	All	2077/2448 (84%)	-0.37	9 (0%) 92 91	22, 42, 71, 116	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	GLU	6.2
1	E	201	GLU	3.5
1	B	201	GLU	3.4
1	E	68	THR	2.5
1	D	171	GLU	2.3
1	D	298	GLN	2.3
1	E	66	HIS	2.2
1	F	208	TRP	2.2
1	A	208	TRP	2.1

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 carbohydrates in this entry.

6.4 Ligands

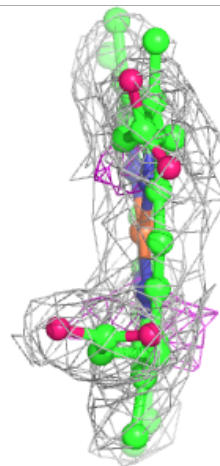
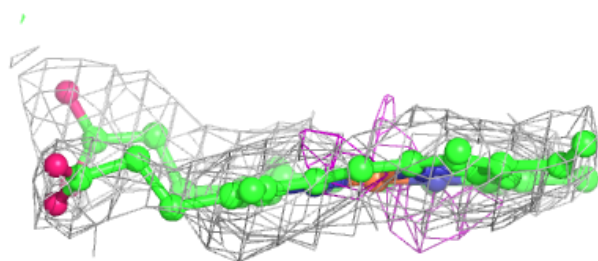
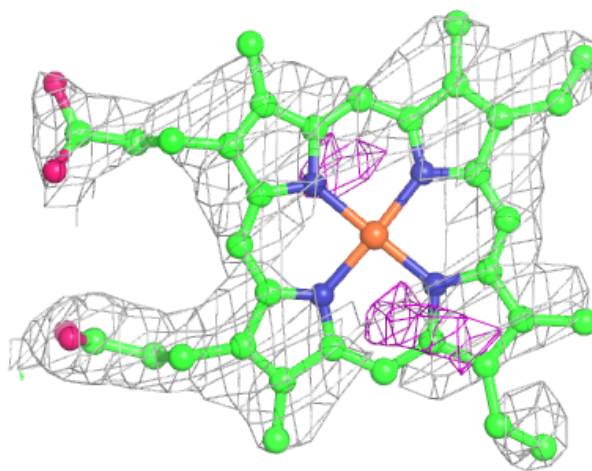
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	E	501	1/1	0.91	0.17	40,40,40,40	0
4	NA	E	504	1/1	0.91	0.13	33,33,33,33	0
2	HEM	A	1001	43/43	0.94	0.23	45,48,54,58	0
2	HEM	B	1001	43/43	0.95	0.19	39,42,48,52	0
3	PLP	F	503	15/16	0.96	0.15	13,29,37,40	0
2	HEM	E	502	43/43	0.96	0.19	40,43,50,52	0
2	HEM	F	502	43/43	0.96	0.21	37,40,48,50	0
3	PLP	E	503	15/16	0.97	0.18	34,42,46,50	0
2	HEM	D	1001	43/43	0.97	0.14	39,42,47,51	0
2	HEM	C	1001	43/43	0.97	0.16	31,33,40,42	0
4	NA	F	501	1/1	0.97	0.14	30,30,30,30	0
3	PLP	C	1002	15/16	0.97	0.15	25,37,46,46	0
3	PLP	A	1002	15/16	0.97	0.19	28,38,46,47	0
3	PLP	D	1002	15/16	0.98	0.13	23,27,30,37	0
3	PLP	B	1002	15/16	0.98	0.16	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.

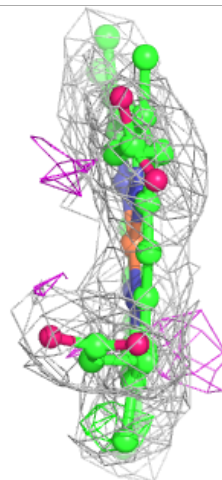
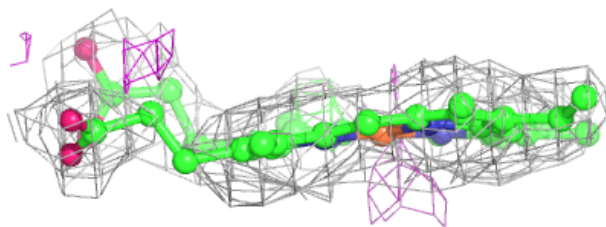
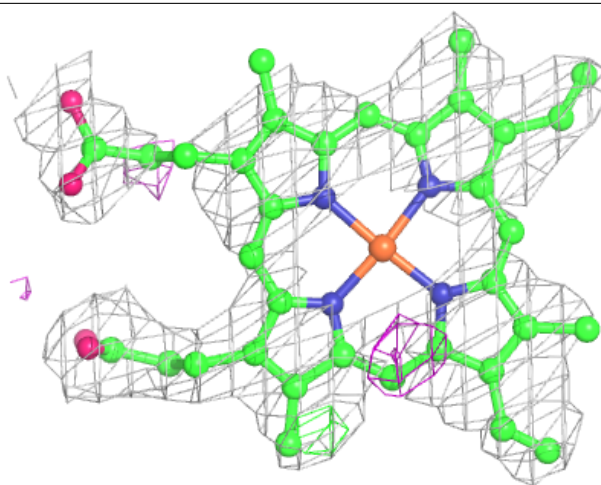
Electron density around HEM A 1001:

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



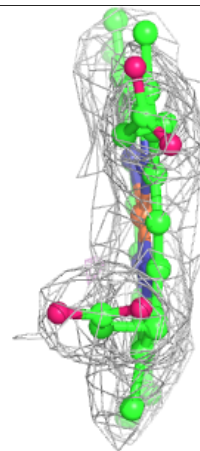
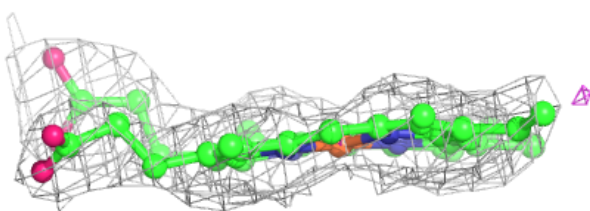
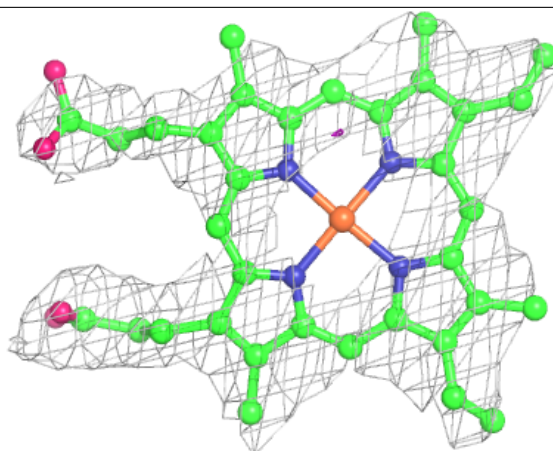
Electron density around HEM B 1001:

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



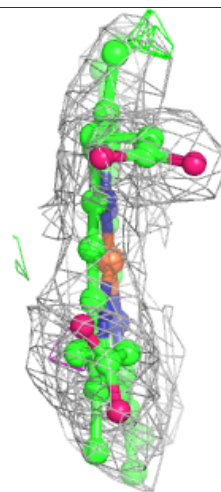
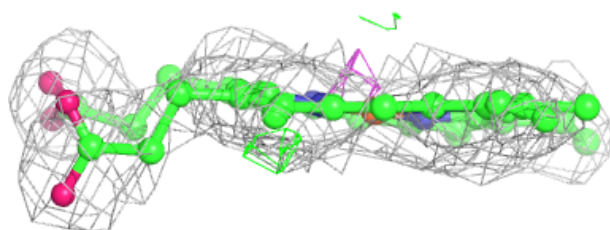
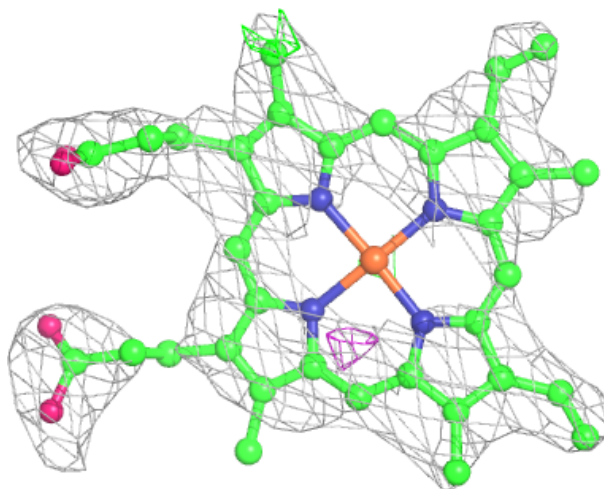
Electron density around HEM E 502:

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



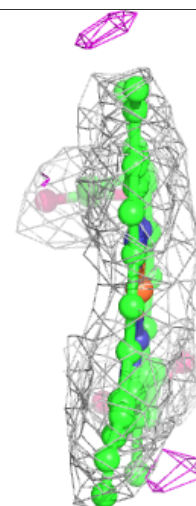
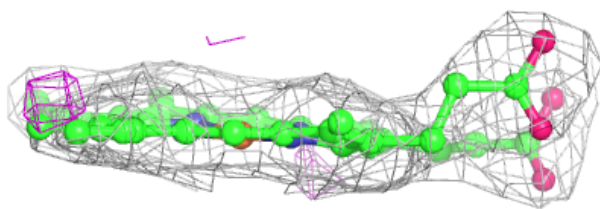
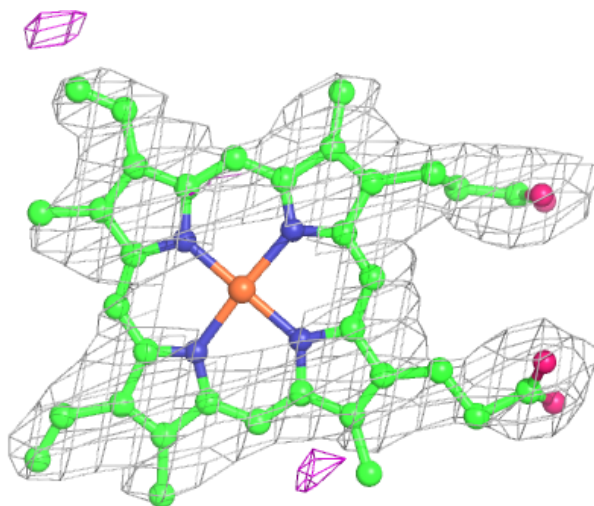
Electron density around HEM F 502:

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



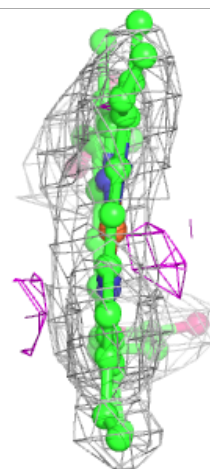
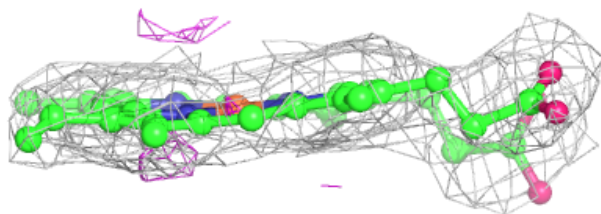
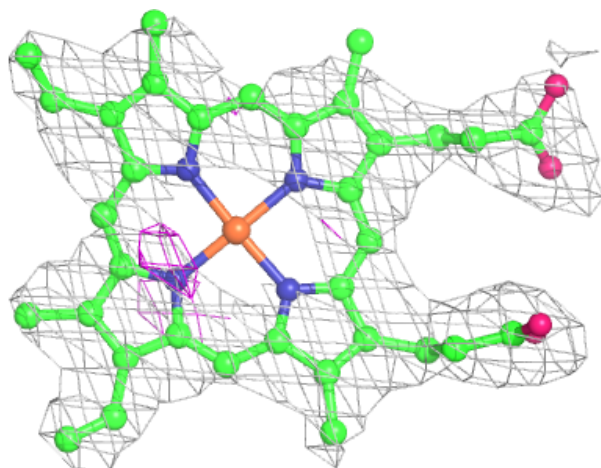
Electron density around HEM D 1001:

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



Electron density around HEM 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.