



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:25 AM UTC

PDB ID : 1M54 / pdb_00001m54
Title : CYSTATHIONINE-BETA SYNTHASE: REDUCED VICINAL THIOLS
Authors : Taoka, S.; Lepore, B.W.; Kabil, O.; Ojha, S.; Ringe, D.; Banerjee, R.
Deposited on : 2002-07-08
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

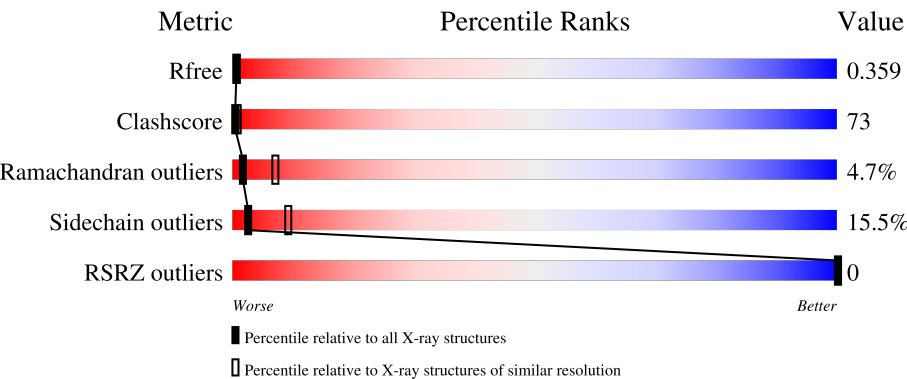
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	363	24%51%16%6%.
1	B	363	27%51%15%. .
1	C	363	21%58%12%. 5%
1	D	363	20%56%15%. 5%
1	E	363	24%53%14%. .

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Mol	Chain	Length	Quality of chain
1	F	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	D	1410	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16403 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	352	Total	C	N	O	S	0	0	0
			2698	1692	471	518	17			
1	B	347	Total	C	N	O	S	0	0	0
			2660	1667	467	509	17			
1	C	346	Total	C	N	O	S	0	0	0
			2651	1664	464	506	17			
1	D	346	Total	C	N	O	S	0	0	0
			2651	1664	464	506	17			
1	E	347	Total	C	N	O	S	0	0	0
			2654	1665	464	508	17			
1	F	344	Total	C	N	O	S	0	0	0
			2637	1655	464	501	17			

There are 6 discrepancies between the modelled and reference sequences:

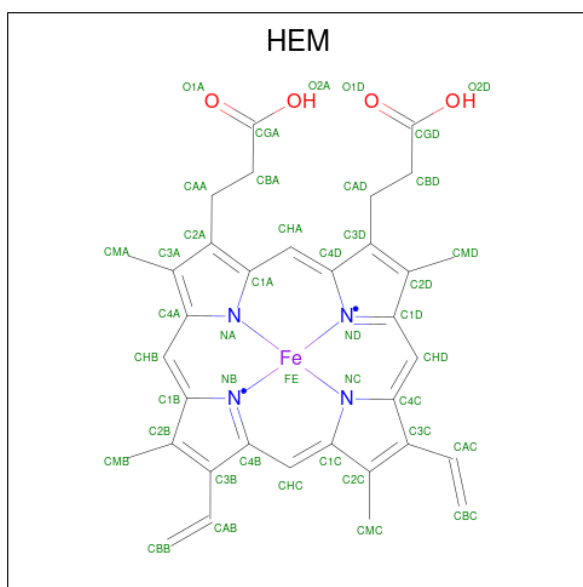
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	ILE	engineered mutation	UNP P35520
B	44	MET	ILE	engineered mutation	UNP P35520
C	44	MET	ILE	engineered mutation	UNP P35520
D	44	MET	ILE	engineered mutation	UNP P35520
E	44	MET	ILE	engineered mutation	UNP P35520
F	44	MET	ILE	engineered mutation	UNP P35520

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

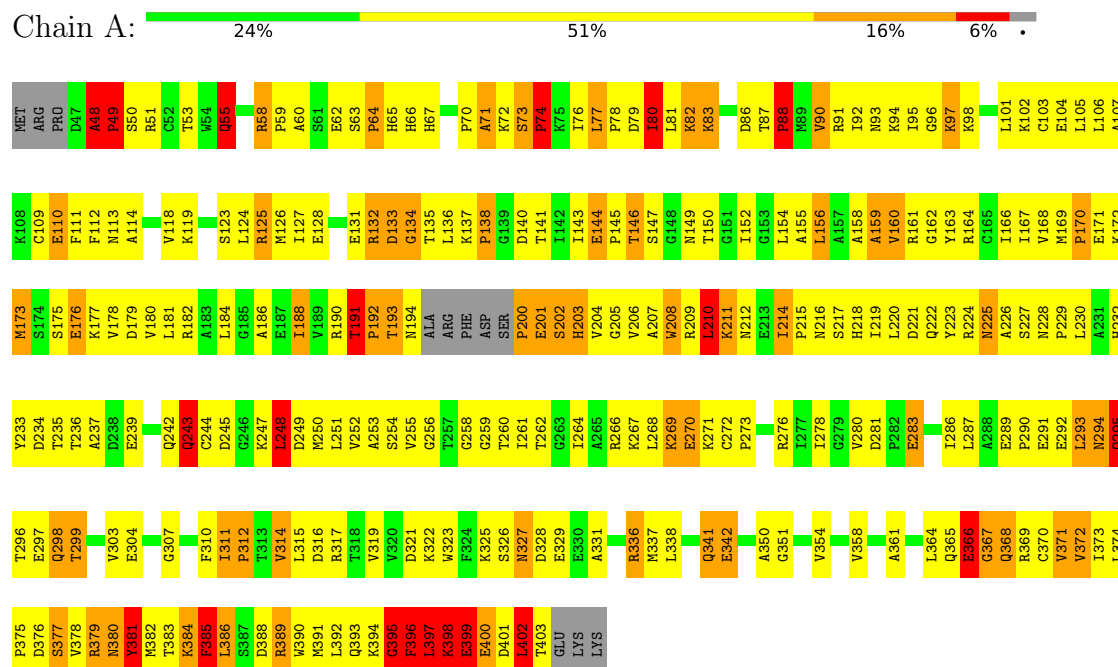
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	12	Total O 12 12	0	0
4	C	14	Total O 14 14	0	0
4	D	26	Total O 26 26	0	0
4	E	24	Total O 24 24	0	0
4	F	16	Total O 16 16	0	0

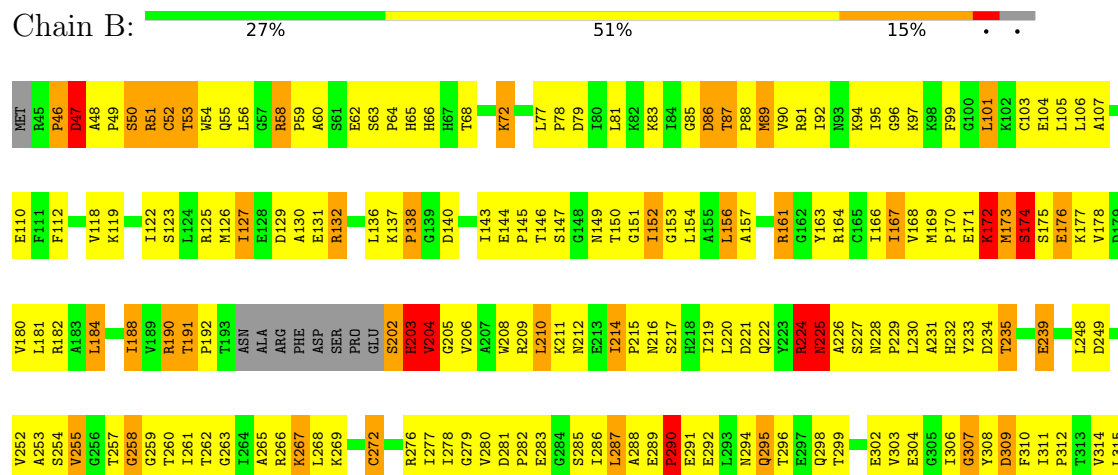
3 Residue-property plots

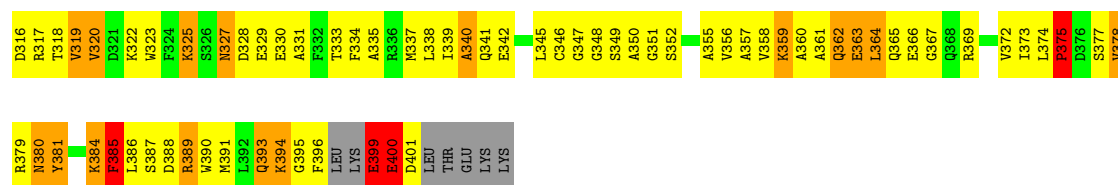
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CYSTATHIONINE BETA-SYNTASE



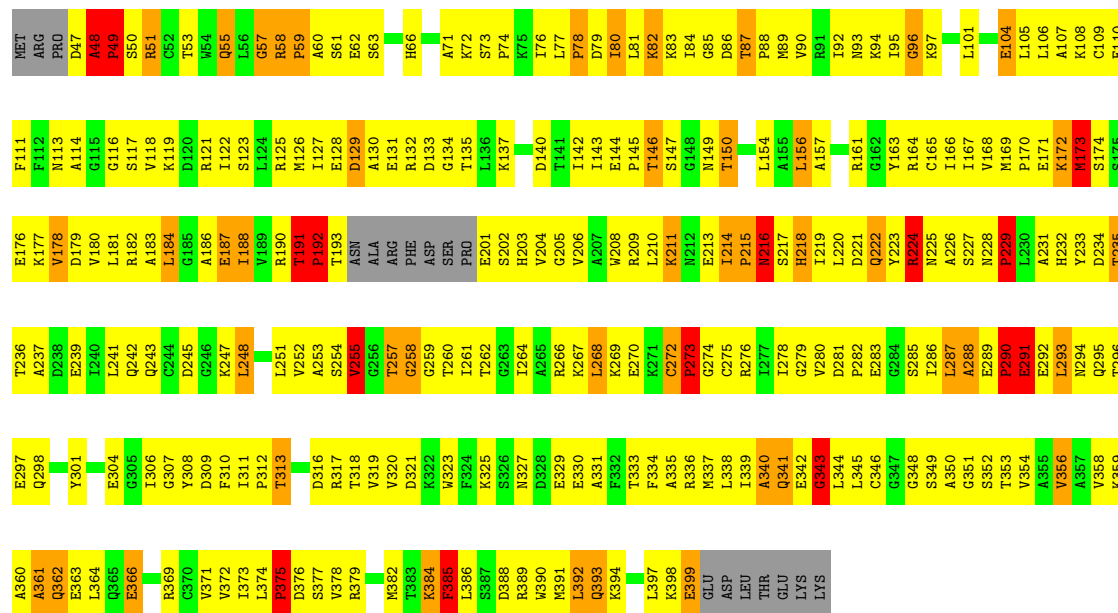
• Molecule 1: CYSTATHIONINE BETA-SYNTASE





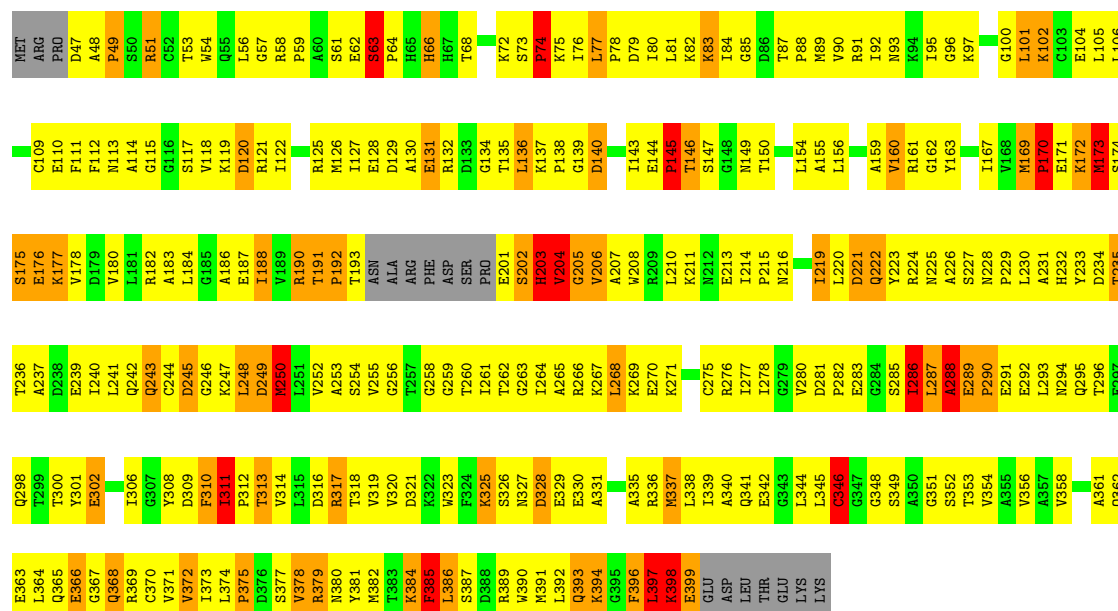
• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain C: 21% 58% 12% 5%

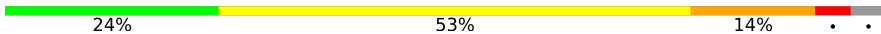
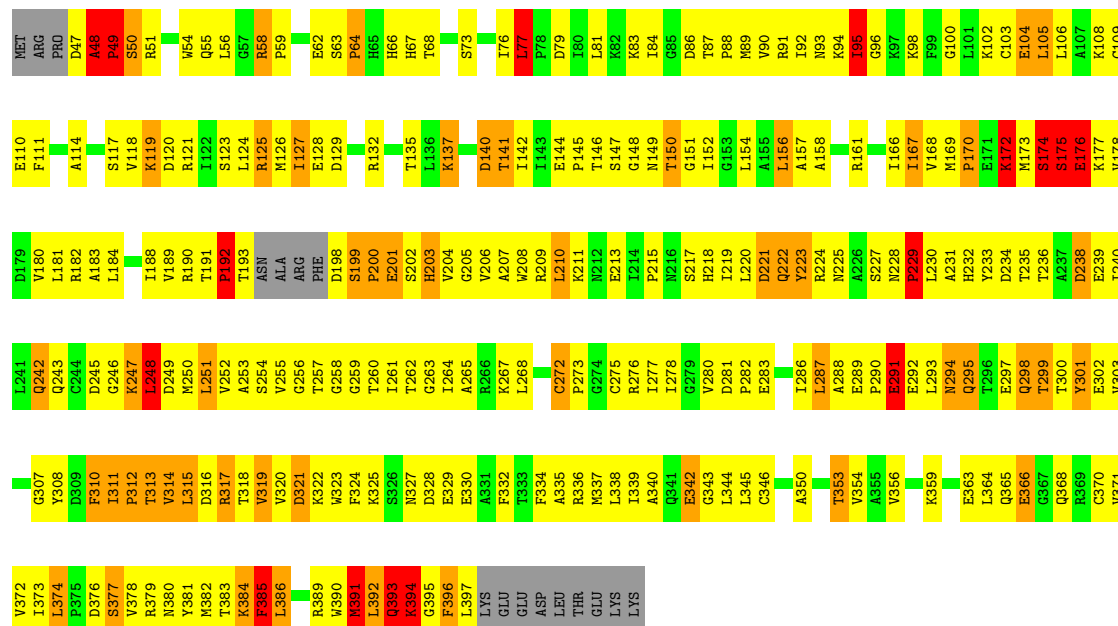


• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

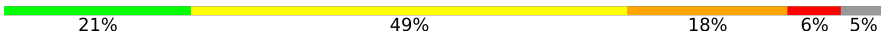
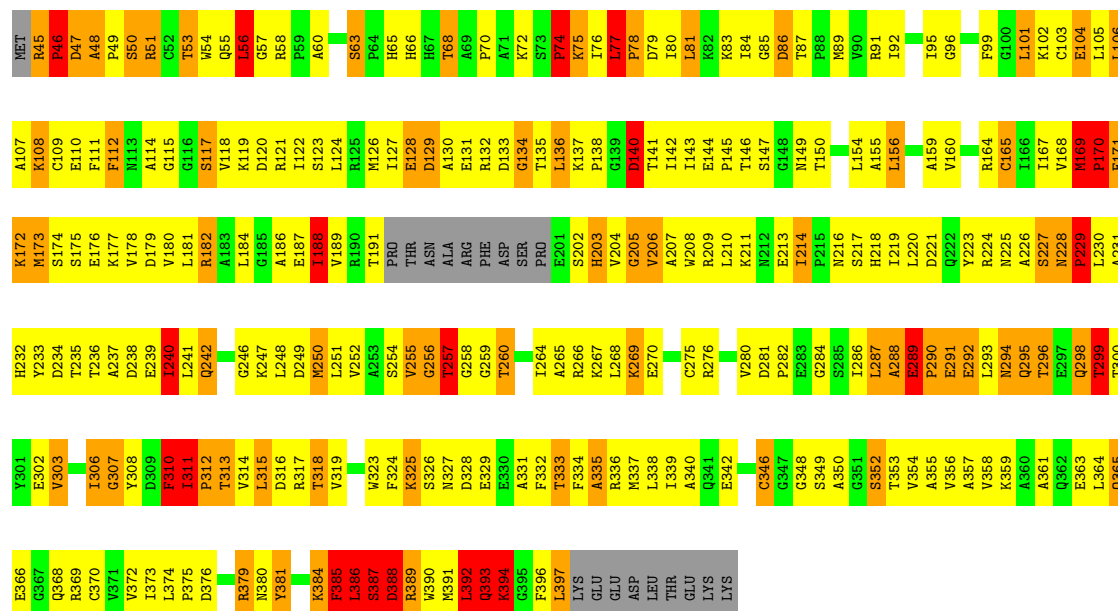
Chain D: 20% 56% 15% 5%



● Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain E:  24% 53% 14%

● Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain F:  21% 49% 18% 6% 5%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.74Å 85.63Å 97.08Å 102.01° 101.53° 112.60°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.3 (50.00-2.90) 89.8 (50.00-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.365 0.274 , 0.359	Depositor DCC
R_{free} test set	8143 reflections (8.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16403	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4977e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PLP, 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	1.11	19/2744 (0.7%)	1.71	85/3709 (2.3%)
1	B	2.26	6/2705 (0.2%)	2.11	60/3655 (1.6%)
1	C	0.99	4/2696 (0.1%)	2.17	73/3643 (2.0%)
1	D	0.87	6/2696 (0.2%)	1.68	85/3643 (2.3%)
1	E	0.99	8/2700 (0.3%)	1.67	70/3651 (1.9%)
1	F	0.90	7/2682 (0.3%)	2.09	84/3624 (2.3%)
All	All	1.28	50/16223 (0.3%)	1.92	457/21925 (2.1%)

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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	ASN	N-CA	83.19	2.53	1.46
1	B	401	ASP	C-O	72.69	2.69	1.23
1	C	173	MET	N-CA	28.98	1.83	1.46
1	A	367	GLY	N-CA	23.52	1.79	1.45
1	E	176	GLU	N-CA	21.01	1.73	1.46

The worst 5 of 457 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	45	ARG	CA-C-N	46.77	178.30	119.84
1	F	45	ARG	C-N-CA	46.77	178.30	119.84
1	B	289	GLU	CA-C-N	46.26	177.66	119.84
1	B	289	GLU	C-N-CA	46.26	177.66	119.84
1	C	48	ALA	CA-C-N	43.15	173.78	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLU	Peptide
1	B	400	GLU	Mainchain
1	C	224	ARG	Mainchain

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	2698	0	2721	383	0
1	B	2660	0	2678	345	0
1	C	2651	0	2678	427	0
1	D	2651	0	2679	460	1
1	E	2654	0	2676	468	1
1	F	2637	0	2668	414	0
2	A	15	0	7	2	0
2	B	15	0	7	2	0
2	C	15	0	7	4	0
2	D	15	0	7	6	0
2	E	15	0	7	2	0
2	F	15	0	7	2	0
3	A	43	0	30	6	0
3	B	43	0	30	6	0
3	C	43	0	30	9	0
3	D	43	0	30	8	0
3	E	43	0	30	6	0
3	F	43	0	30	10	0
4	A	12	0	0	1	0
4	B	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	14	0	0	2	0
4	D	26	0	0	1	0
4	E	24	0	0	0	0
4	F	16	0	0	4	0
All	All	16403	0	16322	2395	1

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 73.

The worst 5 of 2395 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:HIS:CE1	1:D:204:VAL:CG1	1.87	1.56
1:E:176:GLU:N	1:E:176:GLU:CA	1.73	1.49
1:D:203:HIS:CE1	1:D:204:VAL:HG12	1.47	1.46
1:A:367:GLY:N	1:A:367:GLY:CA	1.79	1.44
1:D:173:MET:CE	1:D:173:MET:HA	1.49	1.42

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:GLU:CD	1:E:173:MET:O[1_554]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	348/363 (96%)	271 (78%)	62 (18%)	15 (4%)	2 8
1	B	341/363 (94%)	276 (81%)	54 (16%)	11 (3%)	3 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	342/363 (94%)	284 (83%)	43 (13%)	15 (4%)	2	8
1	D	342/363 (94%)	274 (80%)	52 (15%)	16 (5%)	2	7
1	E	343/363 (94%)	271 (79%)	54 (16%)	18 (5%)	1	5
1	F	340/363 (94%)	268 (79%)	50 (15%)	22 (6%)	1	3
All	All	2056/2178 (94%)	1644 (80%)	315 (15%)	97 (5%)	2	7

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	A	134	GLY
1	A	295	GLN
1	A	299	THR
1	A	385	PHE

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	294/304 (97%)	246 (84%)	48 (16%)	2	8
1	B	289/304 (95%)	243 (84%)	46 (16%)	2	8
1	C	288/304 (95%)	254 (88%)	34 (12%)	5	17
1	D	288/304 (95%)	245 (85%)	43 (15%)	3	10
1	E	289/304 (95%)	245 (85%)	44 (15%)	3	9
1	F	286/304 (94%)	232 (81%)	54 (19%)	1	5
All	All	1734/1824 (95%)	1465 (84%)	269 (16%)	2	9

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	156	LEU
1	F	209	ARG

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Mol	Chain	Res	Type
1	F	385	PHE
1	C	78	PRO
1	C	49	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	149	ASN
1	F	218	HIS
1	E	242	GLN
1	F	66	HIS
1	F	295	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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	D	1410	1	15,15,16	1.66	4 (26%)	21,22,23	1.42	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	C	1310	1	15,15,16	1.61	4 (26%)	21,22,23	1.25	2 (9%)
2	PLP	E	1510	1	15,15,16	1.68	4 (26%)	21,22,23	1.35	3 (14%)
3	HEM	F	1620	1	50,50,50	1.85	13 (26%)	67,82,82	1.06	6 (8%)
2	PLP	F	1610	1	15,15,16	1.42	3 (20%)	21,22,23	1.14	3 (14%)
3	HEM	D	1420	1	50,50,50	1.91	13 (26%)	67,82,82	1.03	3 (4%)
2	PLP	B	1210	1	15,15,16	2.56	6 (40%)	21,22,23	2.17	10 (47%)
3	HEM	B	1220	1	50,50,50	1.82	10 (20%)	67,82,82	0.94	3 (4%)
3	HEM	C	1320	1	50,50,50	1.98	15 (30%)	67,82,82	1.03	3 (4%)
2	PLP	A	1110	1	15,15,16	1.56	3 (20%)	21,22,23	1.20	2 (9%)
3	HEM	A	1120	1	50,50,50	1.93	16 (32%)	67,82,82	0.99	4 (5%)
3	HEM	E	1520	1	50,50,50	1.89	12 (24%)	67,82,82	1.00	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	D	1410	1	-	2/6/6/8	0/1/1/1
2	PLP	C	1310	1	-	1/6/6/8	0/1/1/1
2	PLP	E	1510	1	-	2/6/6/8	0/1/1/1
3	HEM	F	1620	1	-	9/14/54/54	-
2	PLP	F	1610	1	-	0/6/6/8	0/1/1/1
3	HEM	D	1420	1	-	8/14/54/54	-
2	PLP	B	1210	1	-	0/6/6/8	0/1/1/1
3	HEM	B	1220	1	-	6/14/54/54	-
3	HEM	C	1320	1	-	2/14/54/54	-
2	PLP	A	1110	1	-	2/6/6/8	0/1/1/1
3	HEM	A	1120	1	-	2/14/54/54	-
3	HEM	E	1520	1	-	6/14/54/54	-

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	PLP	C3-C2	-5.78	1.35	1.41
3	C	1320	HEM	CBB-CAB	5.29	1.55	1.30
3	A	1120	HEM	CBB-CAB	5.27	1.55	1.30
3	B	1220	HEM	CBB-CAB	5.10	1.54	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1520	HEM	CBB-CAB	5.08	1.54	1.30

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1210	PLP	C3-C4-C5	5.61	125.31	118.59
2	D	1410	PLP	O4P-C5A-C5	4.17	117.17	109.36
2	C	1310	PLP	O4P-C5A-C5	3.76	116.40	109.36
2	E	1510	PLP	O4P-C5A-C5	3.70	116.28	109.36
2	B	1210	PLP	C5-C6-N1	-3.66	117.88	123.83

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1110	PLP	C4-C5-C5A-O4P
2	D	1410	PLP	C4-C5-C5A-O4P
2	D	1410	PLP	C6-C5-C5A-O4P
2	E	1510	PLP	C4-C5-C5A-O4P
2	E	1510	PLP	C6-C5-C5A-O4P

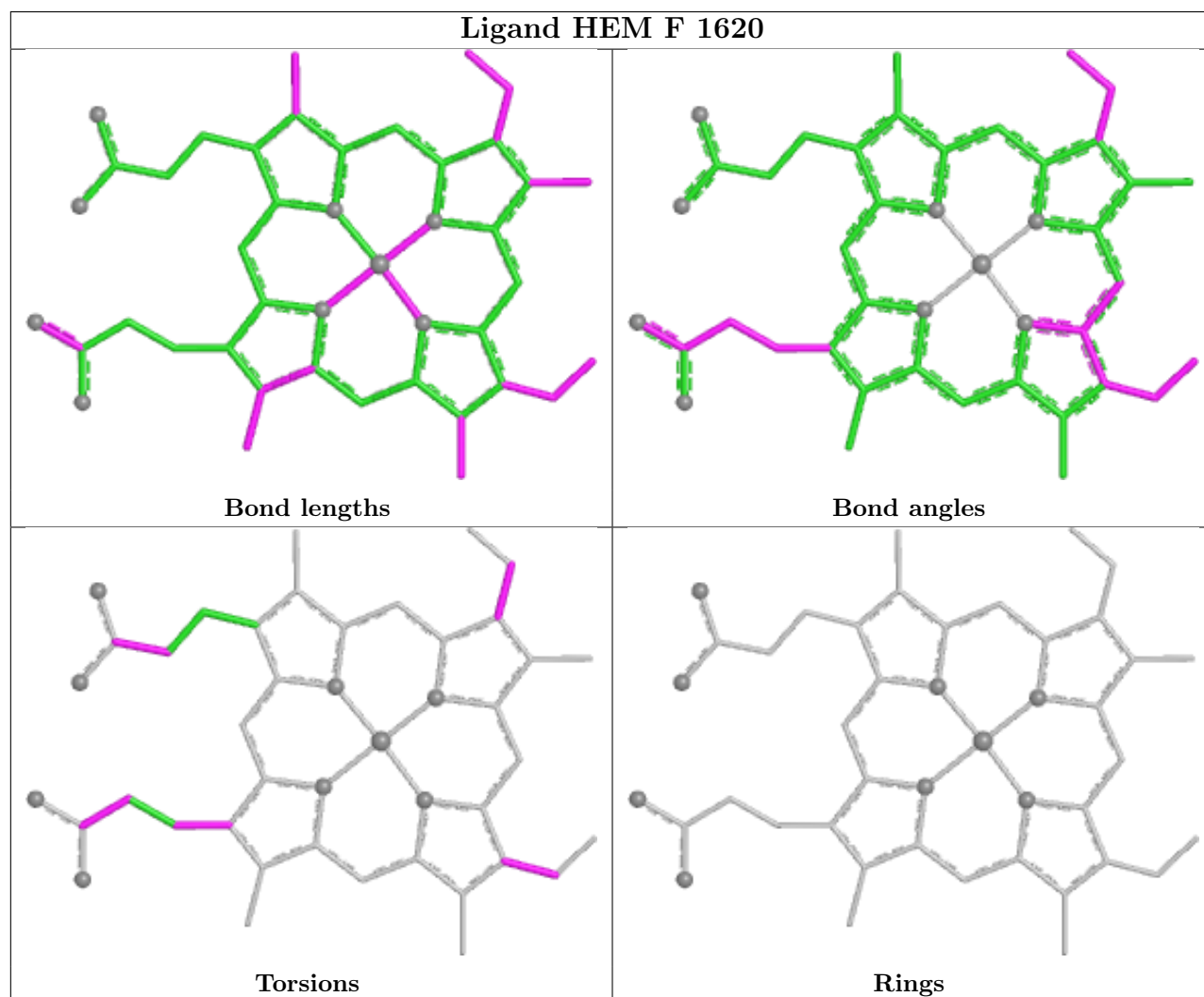
There are no ring outliers.

12 monomers are involved in 63 short contacts:

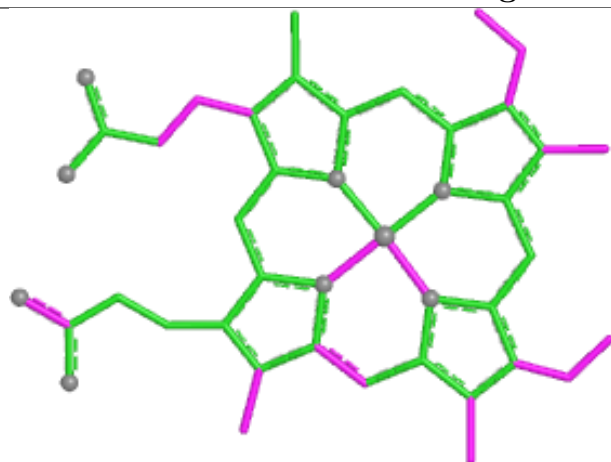
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1410	PLP	6	0
2	C	1310	PLP	4	0
2	E	1510	PLP	2	0
3	F	1620	HEM	10	0
2	F	1610	PLP	2	0
3	D	1420	HEM	8	0
2	B	1210	PLP	2	0
3	B	1220	HEM	6	0
3	C	1320	HEM	9	0
2	A	1110	PLP	2	0
3	A	1120	HEM	6	0
3	E	1520	HEM	6	0

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

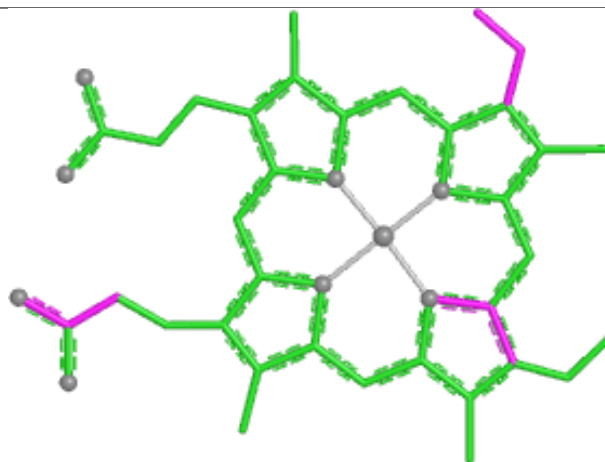
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



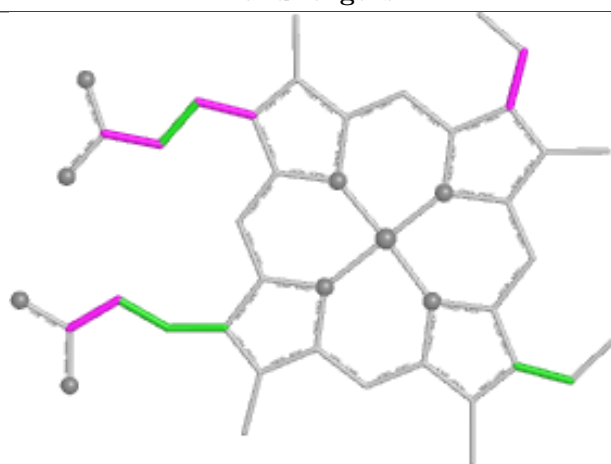
Ligand HEM D 1420



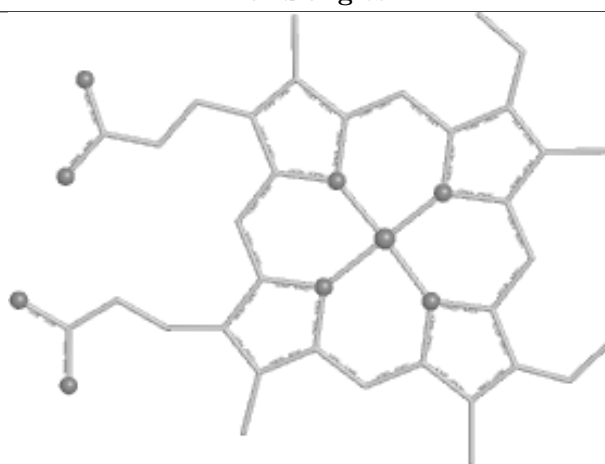
Bond lengths



Bond angles

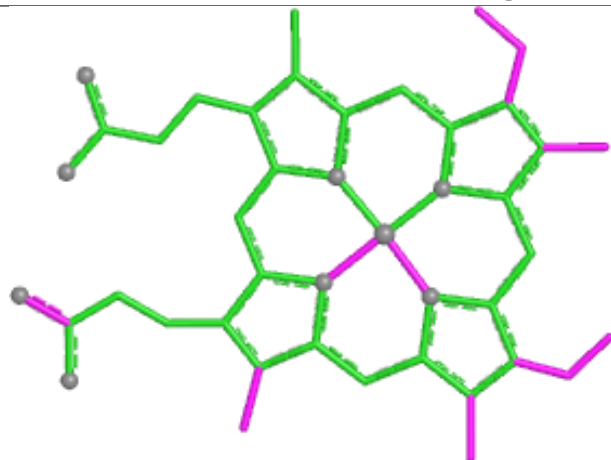


Torsions

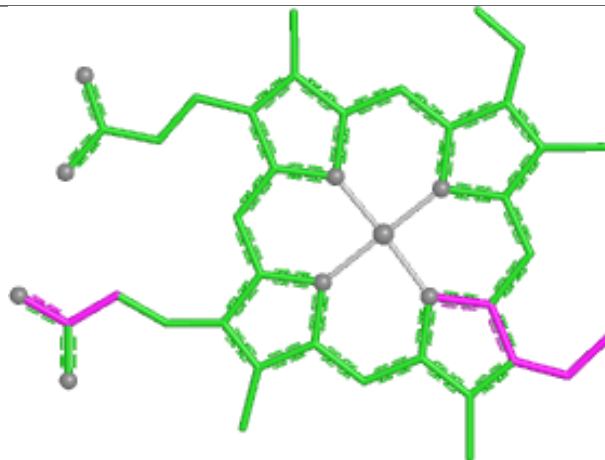


Rings

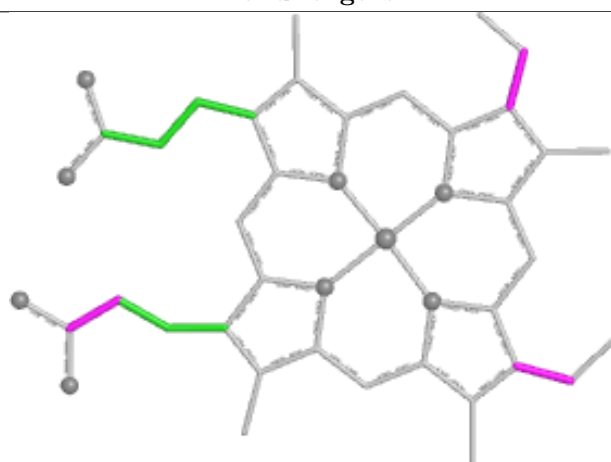
Ligand HEM B 1220



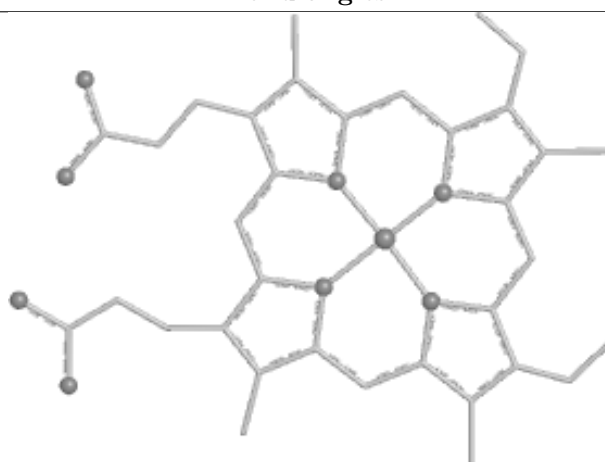
Bond lengths



Bond angles

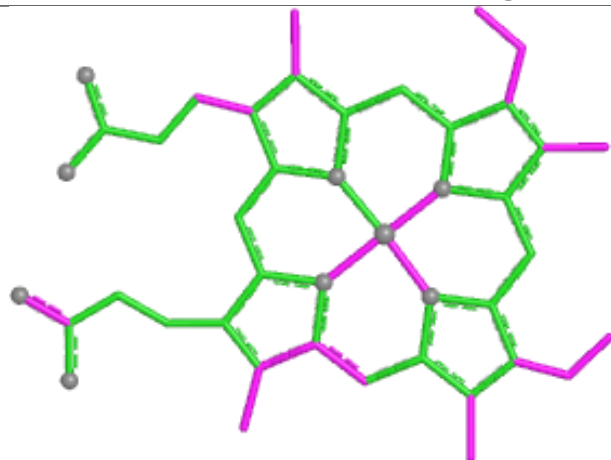


Torsions

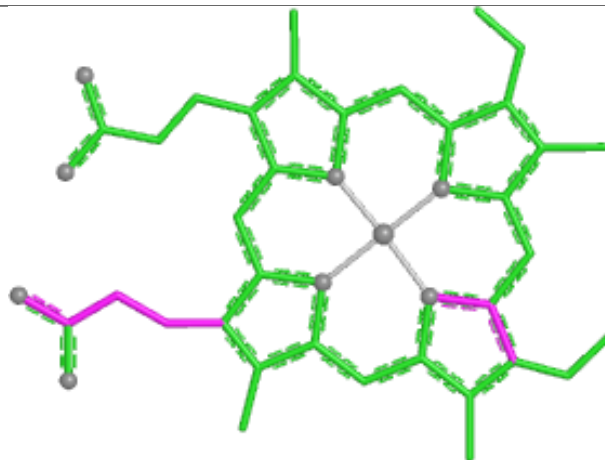


Rings

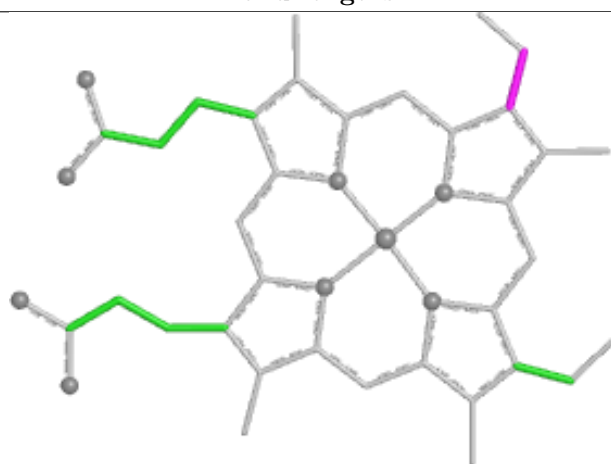
Ligand HEM C 1320



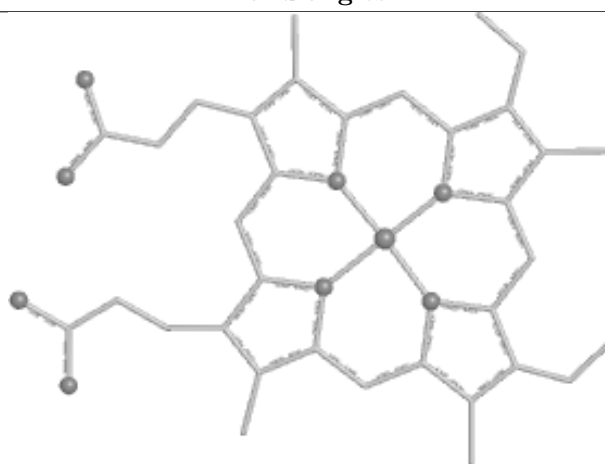
Bond lengths



Bond angles

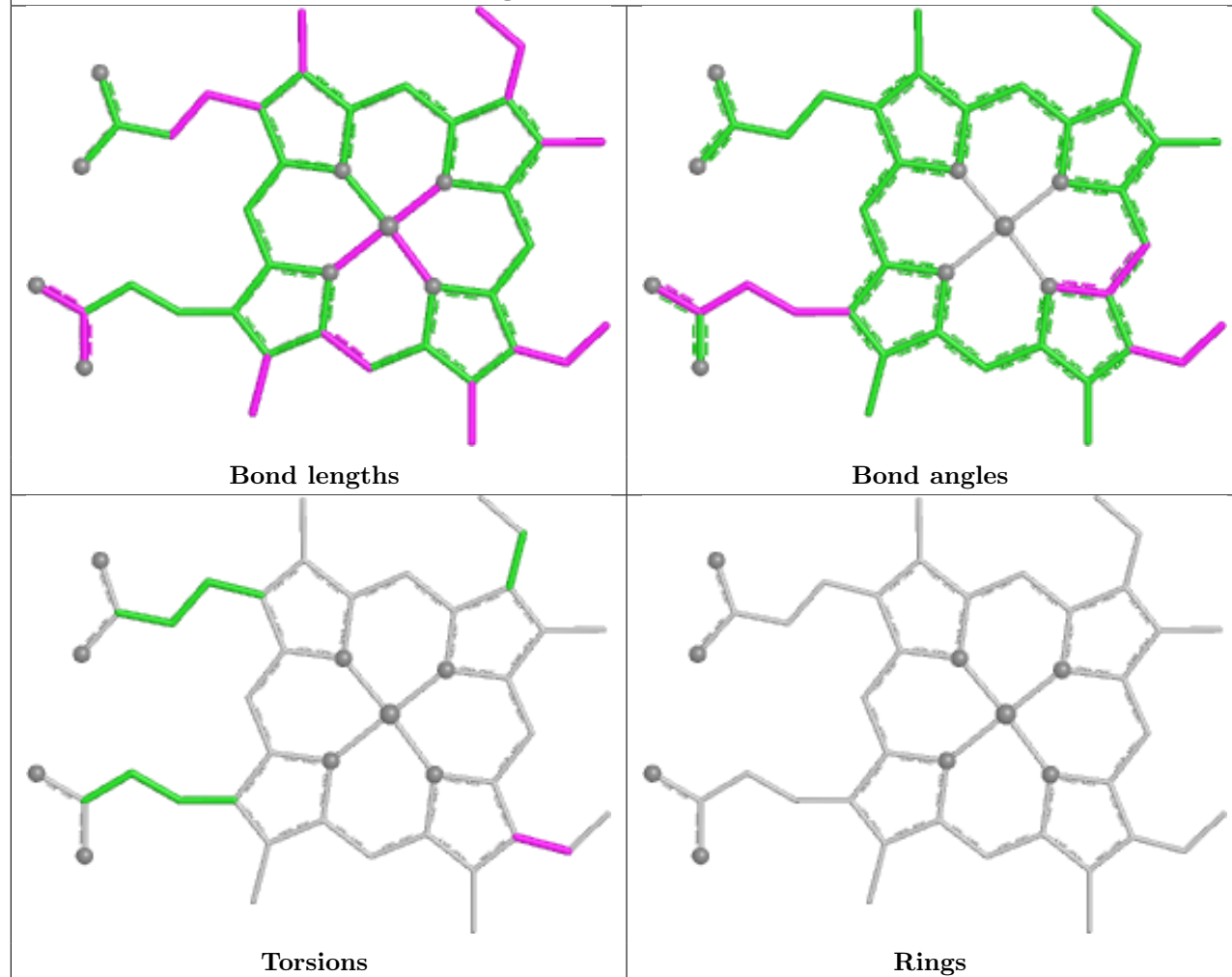


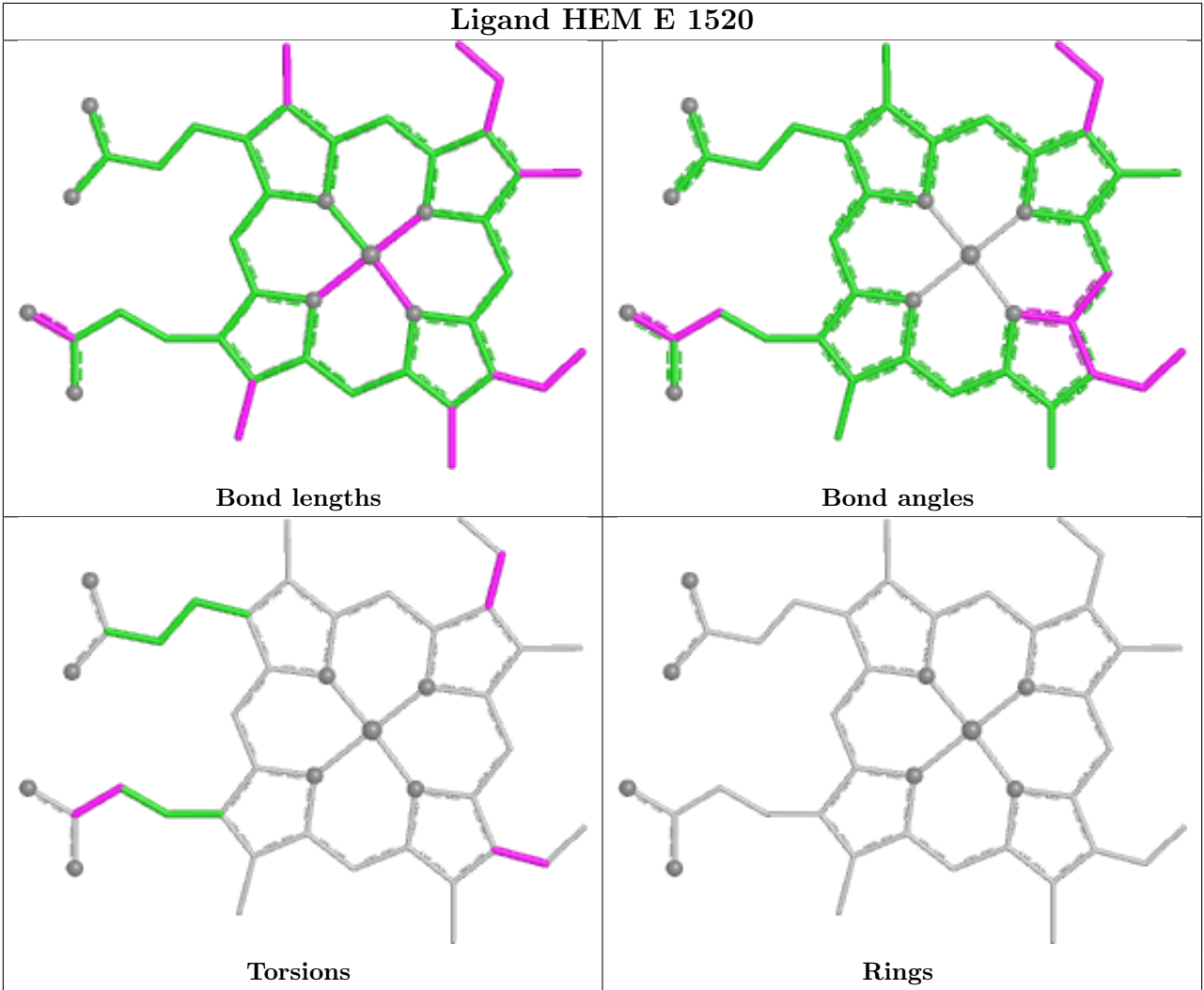
Torsions



Rings

Ligand HEM A 1120





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	159:ALA	C	160:VAL	N	1.19

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	352/363 (96%)	-1.50	0 100 100	8, 24, 44, 61	0
1	B	347/363 (95%)	-1.54	0 100 100	9, 23, 44, 74	0
1	C	346/363 (95%)	-1.52	0 100 100	10, 24, 46, 60	0
1	D	346/363 (95%)	-1.51	0 100 100	10, 24, 44, 59	0
1	E	347/363 (95%)	-1.49	0 100 100	8, 26, 47, 61	0
1	F	344/363 (94%)	-1.49	0 100 100	8, 26, 53, 70	0
All	All	2082/2178 (95%)	-1.51	0 100 100	8, 24, 46, 74	0

There are no RSRZ outliers to report.

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
2	PLP	B	1210	15/16	0.99	0.04	14,21,22,22	0

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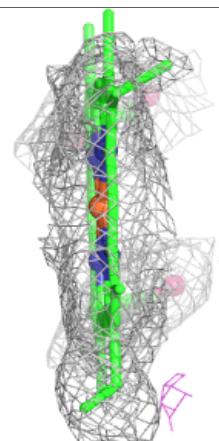
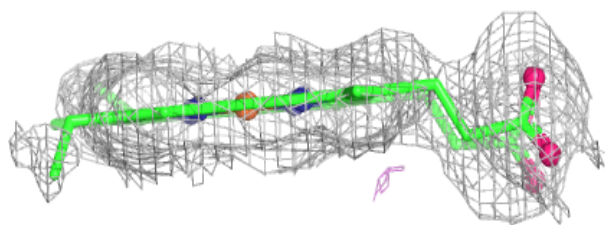
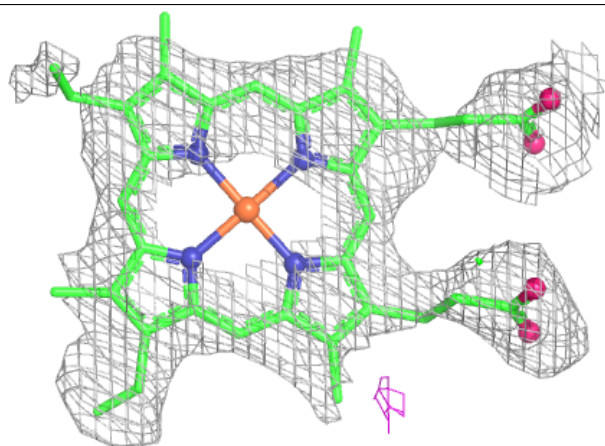
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	C	1310	15/16	0.99	0.03	17,19,23,24	0
2	PLP	E	1510	15/16	0.99	0.04	20,23,26,27	0
3	HEM	A	1120	43/43	0.99	0.04	20,38,40,42	0
3	HEM	B	1220	43/43	0.99	0.04	27,35,38,40	0
3	HEM	C	1320	43/43	0.99	0.04	28,35,39,39	0
3	HEM	D	1420	43/43	0.99	0.04	27,32,34,35	0
3	HEM	E	1520	43/43	0.99	0.04	36,44,46,46	0
3	HEM	F	1620	43/43	0.99	0.04	30,36,38,40	0
2	PLP	D	1410	15/16	1.00	0.04	20,22,24,27	0
2	PLP	A	1110	15/16	1.00	0.03	14,19,23,23	0
2	PLP	F	1610	15/16	1.00	0.03	11,14,17,18	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.

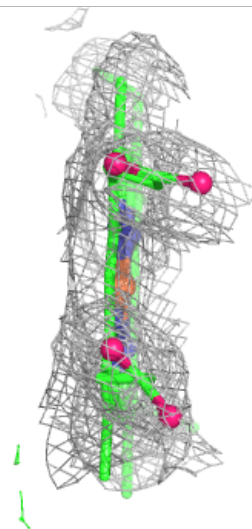
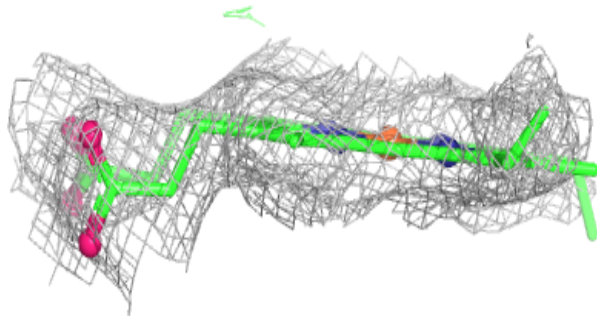
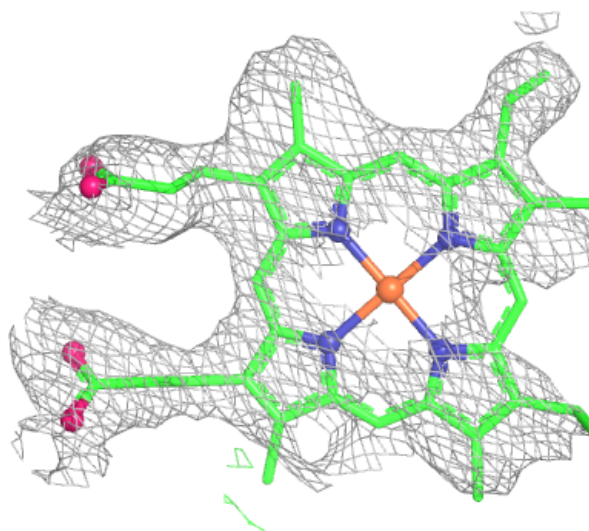
Electron density around HEM A 1120:

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



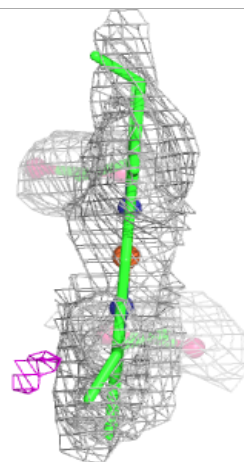
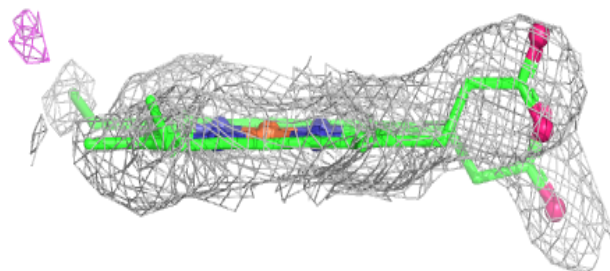
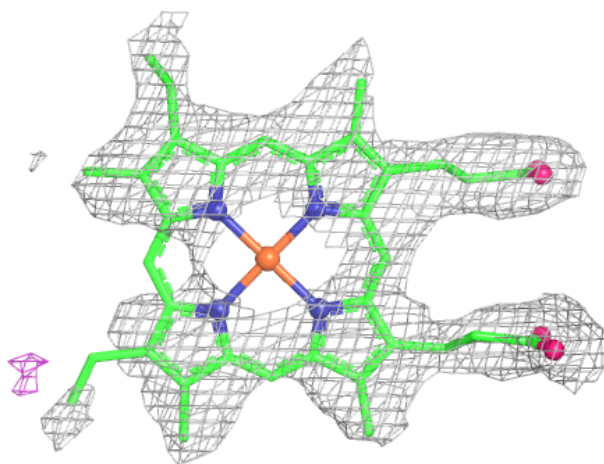
Electron density around HEM B 1220:

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



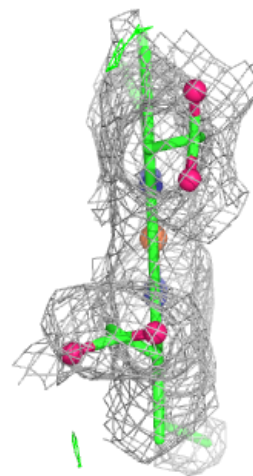
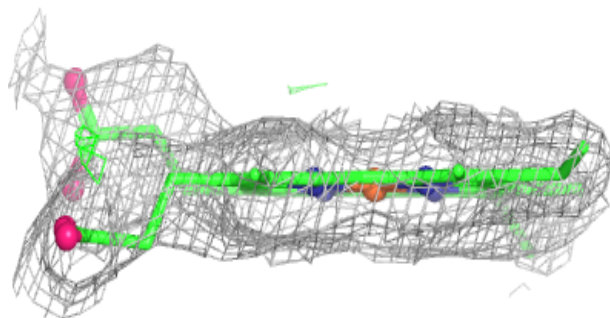
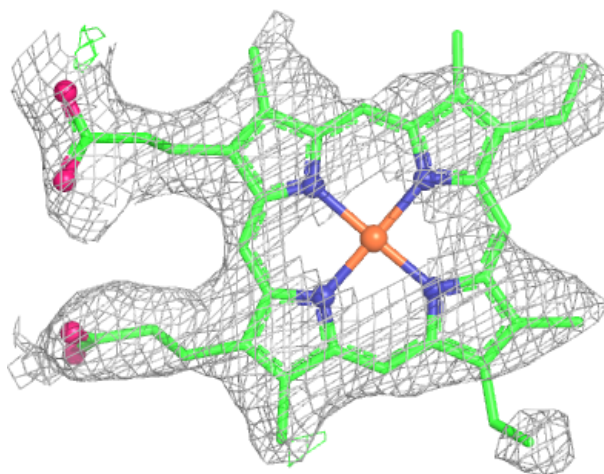
Electron density around HEM C 1320:

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



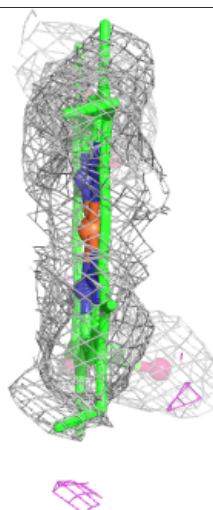
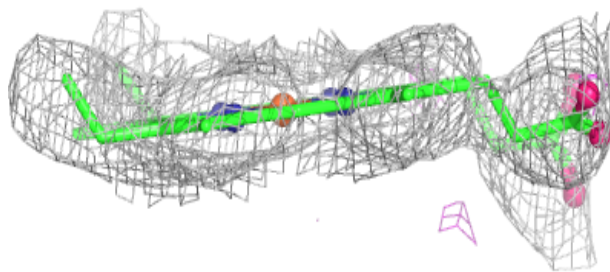
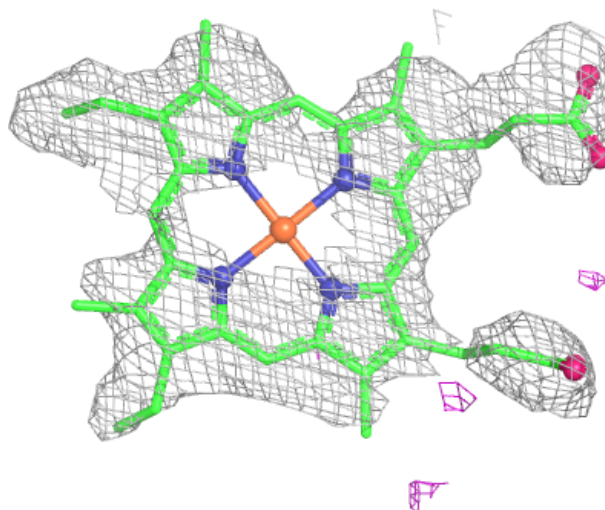
Electron density around HEM D 1420:

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



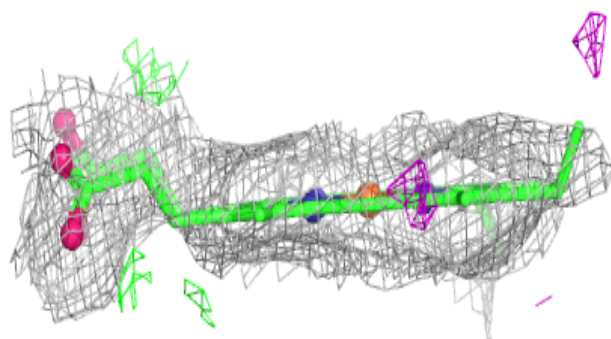
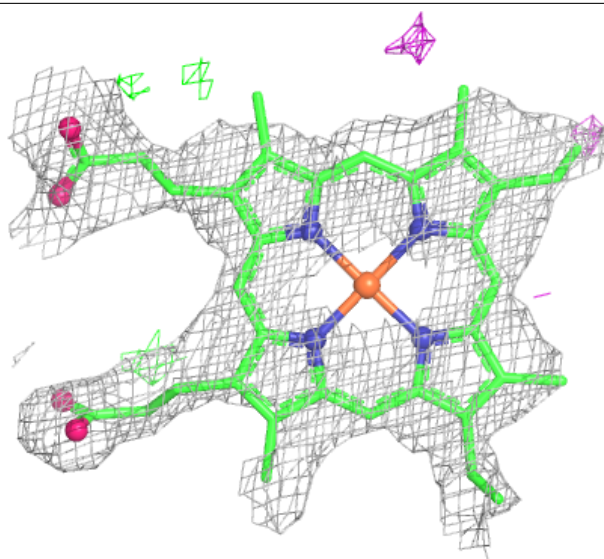
Electron density around HEM E 1520:

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



Electron density around HEM F 1620:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.