wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2026 – 10:21 pm BST

PDB ID	:	9U2X / pdb_00009u2x
Title	:	Crystal structure of N244L variant from Bacillus subtilis
Authors	:	Borges, P.T.; Martins, L.O.
Deposited on	:	2026-01-30
Resolution	:	2.67 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 (i) symbol.

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

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

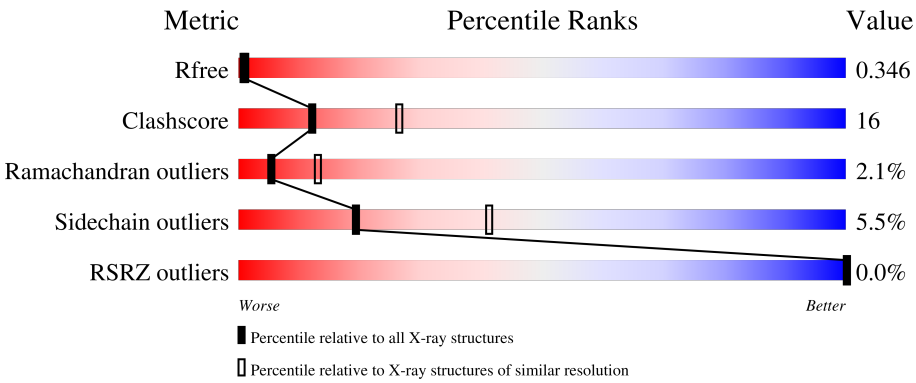
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	359	65% 31% • •
1	B	359	67% 29% • •
1	C	359	65% 31% • •
1	D	359	66% 29% • •
1	E	359	66% 28% 5% •

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Mol	Chain	Length	Quality of chain
1	F	359	59% 35%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16847 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.

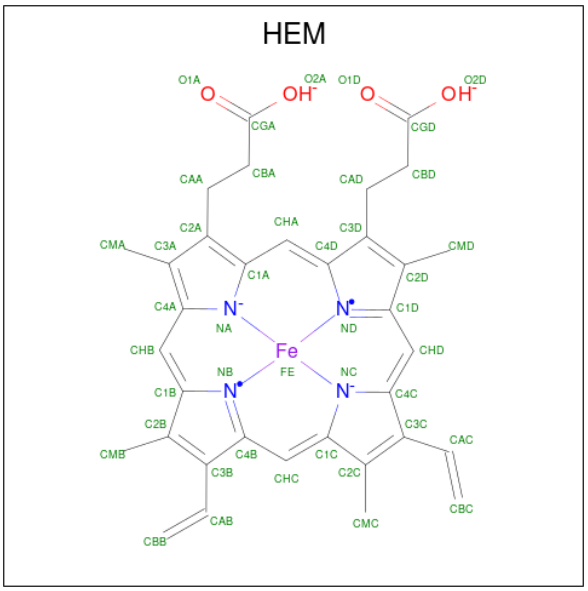
- Molecule 1 is a protein called Deferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2754	1743	474	524	13	0	0	0
1	B	354	2754	1743	474	524	13	0	0	0
1	C	354	2754	1743	474	524	13	0	0	0
1	D	353	2743	1737	470	523	13	0	0	0
1	E	354	2754	1743	474	524	13	0	0	0
1	F	354	2754	1743	474	524	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	LEU	ASN	variant	UNP P39597
B	244	LEU	ASN	variant	UNP P39597
C	244	LEU	ASN	variant	UNP P39597
D	244	LEU	ASN	variant	UNP P39597
E	244	LEU	ASN	variant	UNP P39597
F	244	LEU	ASN	variant	UNP P39597

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



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

- Molecule 3 is water.

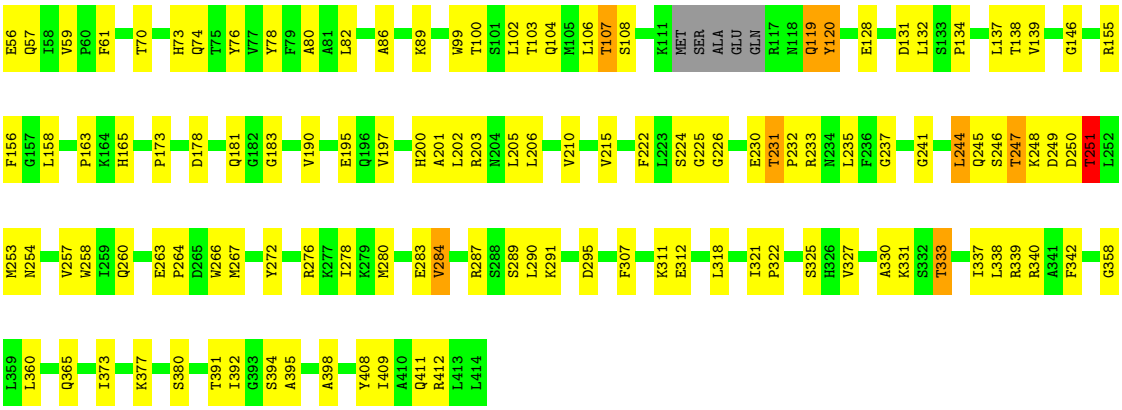
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	7	7	7	0	0
			Total	O		
3	B	9	9	9	0	0
			Total	O		
3	C	15	15	15	0	0
			Total	O		
3	D	12	12	12	0	0
			Total	O		
3	E	13	13	13	0	0
			Total	O		
3	F	20	20	20	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

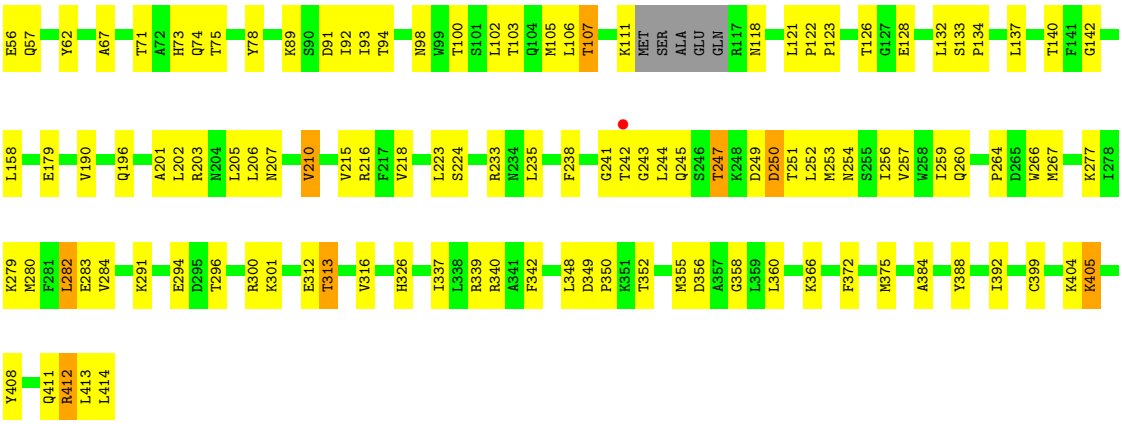
- Molecule 1: Deferrochelatase

Chain A:



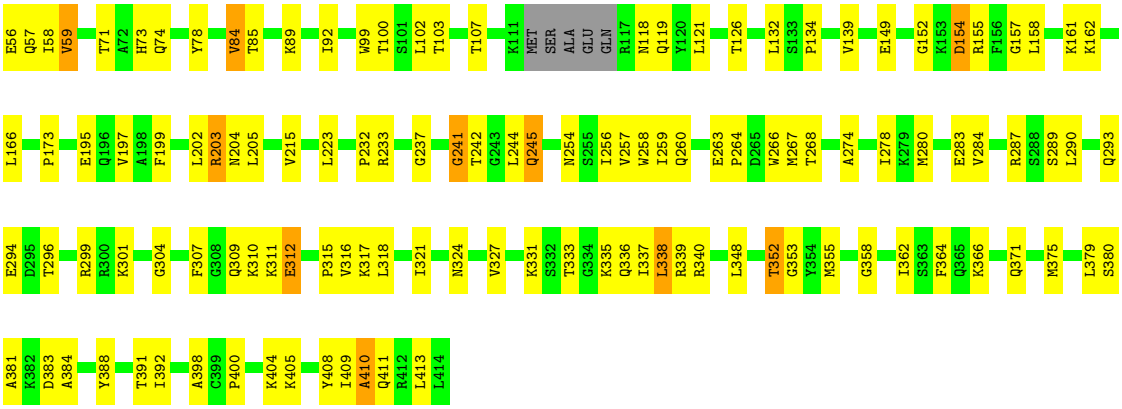
- Molecule 1: Deferrochelatase

Chain B:



- Molecule 1: Deferrochelatase

Chain C:

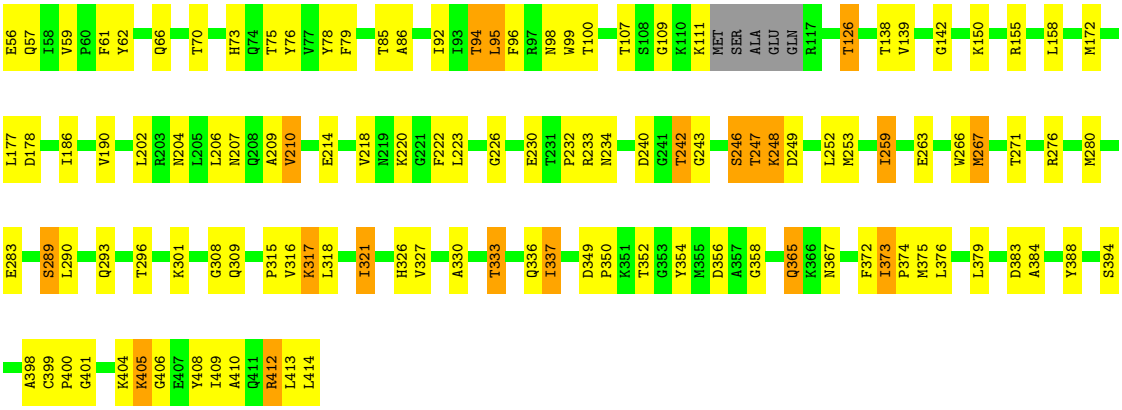


- Molecule 1: Deferrochelatase

Chain D:

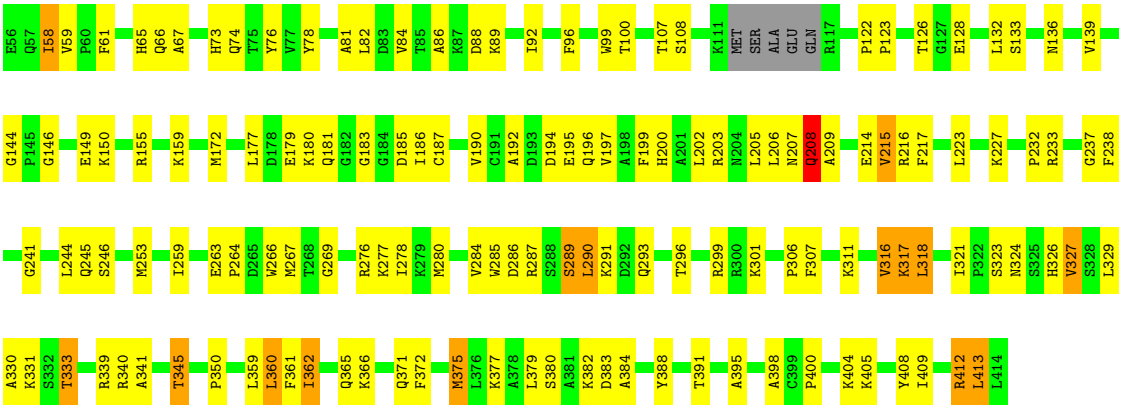
- Molecule 1: Deferrochelatase

Chain E:



- Molecule 1: Deferrochelatase

Chain F:


E56 Q57 I58 V59 P60 F61 H65 Q66 A67 H73 Q74 T75 Y76 V77 Y78 A81 L82 D83 V84 T85 A86 K87 D88 K89 I92 F96 W99 T100 T107 S108 K111 MET SER ALA GLU GLN R117 P122 P123 T126 G127 E128 L132 S133 N136 V139
G144 P145 G146 E149 K150 R155 K159 M172 L177 D178 E179 K180 Q181 G182 G183 G184 D185 I186 C187 V190 C191 A192 D193 D194 E195 Q196 V197 A198 F199 H200 A201 L202 R203 N204 L205 L206 N207 Q208 A209 E214 V215 R216 F217 L223 K227 P232 R233 G237 F238
G241 L244 Q245 S246 M253 I259 E263 P264 D265 W266 M267 T268 G269 R276 K277 I278 K279 M280 V284 W285 D286 R287 S288 S289 L290 K291 D292 Q293 T296 R299 R300 K301 P306 F307 K311 V316 K317 L318 I321 P322 S323 N324 S325 H326 V327 S328 L329
A330 K331 S332 T333 R339 R340 A341 T345 P350 L359 L360 F361 I362 Q365 K366 Q371 F372 M375 L376 K377 A378 L379 S380 A381 K382 D383 A384 Y388 T391 A395 A398 C399 P400 K404 K405 Y408 I409 R412 L413 L414

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	351.93Å 73.88Å 127.23Å 90.00° 110.74° 90.00°	Depositor
Resolution (Å)	83.41 – 2.67 83.41 – 2.67	Depositor EDS
% Data completeness (in resolution range)	47.6 (83.41-2.67) 47.7 (83.41-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.297 , 0.348 0.298 , 0.346	Depositor DCC
R_{free} test set	2060 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16847	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.15	0/2813	0.45	0/3791
1	B	0.15	0/2813	0.45	0/3791
1	C	0.15	0/2813	0.46	0/3791
1	D	0.15	0/2802	0.47	0/3777
1	E	0.16	0/2813	0.45	0/3791
1	F	0.24	0/2813	0.53	0/3791
All	All	0.17	0/16867	0.47	0/22732

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	2754	0	2722	82	0
1	B	2754	0	2722	85	0
1	C	2754	0	2719	85	1
1	D	2743	0	2709	70	2
1	E	2754	0	2722	83	1
1	F	2754	0	2722	123	0
2	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	8	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	4	0
2	F	43	0	30	6	0
3	A	7	0	0	0	0
3	B	9	0	0	0	0
3	C	15	0	0	3	0
3	D	12	0	0	3	0
3	E	13	0	0	1	0
3	F	20	0	0	5	0
All	All	16847	0	16496	518	2

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 16.

The worst 5 of 518 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:57:GLN:HE22	1:B:133:SER:HB3	1.13	1.04
1:F:61:PHE:HZ	1:F:409:ILE:HD11	1.26	0.98
1:F:244:LEU:HD21	1:F:339:ARG:H	1.30	0.95
1:F:244:LEU:HD21	1:F:339:ARG:N	1.81	0.94
1:E:375:MET:HE2	2:E:501:HEM:HAC	1.49	0.91

All (2) 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:194:ASP:O	1:E:76:TYR:OH[1_565]	2.09	0.11
1:C:324:ASN:ND2	1:D:120:TYR:O[4_547]	2.19	0.01

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	350/359 (98%)	321 (92%)	23 (7%)	6 (2%)	7	17
1	B	350/359 (98%)	326 (93%)	21 (6%)	3 (1%)	14	31
1	C	350/359 (98%)	330 (94%)	12 (3%)	8 (2%)	5	11
1	D	349/359 (97%)	322 (92%)	17 (5%)	10 (3%)	3	8
1	E	350/359 (98%)	321 (92%)	21 (6%)	8 (2%)	5	11
1	F	350/359 (98%)	316 (90%)	25 (7%)	9 (3%)	4	9
All	All	2099/2154 (97%)	1936 (92%)	119 (6%)	44 (2%)	5	13

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	THR
1	A	250	ASP
1	B	250	ASP
1	D	86	ALA
1	D	177	LEU

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	296/300 (99%)	280 (95%)	16 (5%)	20	42
1	B	296/300 (99%)	285 (96%)	11 (4%)	30	56
1	C	296/300 (99%)	286 (97%)	10 (3%)	32	59
1	D	295/300 (98%)	277 (94%)	18 (6%)	17	37
1	E	296/300 (99%)	275 (93%)	21 (7%)	13	30
1	F	296/300 (99%)	275 (93%)	21 (7%)	13	30
All	All	1775/1800 (99%)	1678 (94%)	97 (6%)	19	41

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	95	LEU
1	E	333	THR
1	E	206	LEU
1	E	259	ILE
1	E	412	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	189	GLN
1	F	136	ASN
1	F	200	HIS
1	F	57	GLN
1	C	219	ASN

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)

6 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	HEM	E	501	1	50,50,50	1.41	8 (16%)	66,82,82	1.20	7 (10%)
2	HEM	F	501	1	50,50,50	1.59	10 (20%)	66,82,82	1.36	9 (13%)
2	HEM	A	501	1	50,50,50	1.38	8 (16%)	66,82,82	1.18	4 (6%)
2	HEM	B	501	1	50,50,50	1.52	8 (16%)	66,82,82	1.43	6 (9%)
2	HEM	D	501	1	50,50,50	1.38	7 (14%)	66,82,82	1.23	7 (10%)
2	HEM	C	501	1	50,50,50	1.44	8 (16%)	66,82,82	1.16	6 (9%)

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	HEM	E	501	1	-	4/14/54/54	-
2	HEM	F	501	1	-	4/14/54/54	-
2	HEM	A	501	1	-	4/14/54/54	-
2	HEM	B	501	1	-	4/14/54/54	-
2	HEM	D	501	1	-	4/14/54/54	-
2	HEM	C	501	1	-	4/14/54/54	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	HEM	FE-ND	5.16	2.10	1.94
2	F	501	HEM	FE-NB	4.59	2.09	1.94
2	B	501	HEM	FE-NB	4.24	2.08	1.94
2	B	501	HEM	FE-ND	3.77	2.06	1.94
2	C	501	HEM	FE-NB	3.70	2.06	1.94

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CAD-CBD-CGD	-7.48	97.50	113.60
2	F	501	HEM	C4C-NC-C1C	4.24	109.50	105.35
2	F	501	HEM	CHD-C1D-C2D	3.32	130.16	124.98
2	D	501	HEM	C4D-ND-C1D	3.13	108.30	105.07
2	D	501	HEM	C4C-NC-C1C	3.10	108.38	105.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O1D
2	E	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAA-CBA-CGA-O1A
2	F	501	HEM	CAD-CBD-CGD-O1D

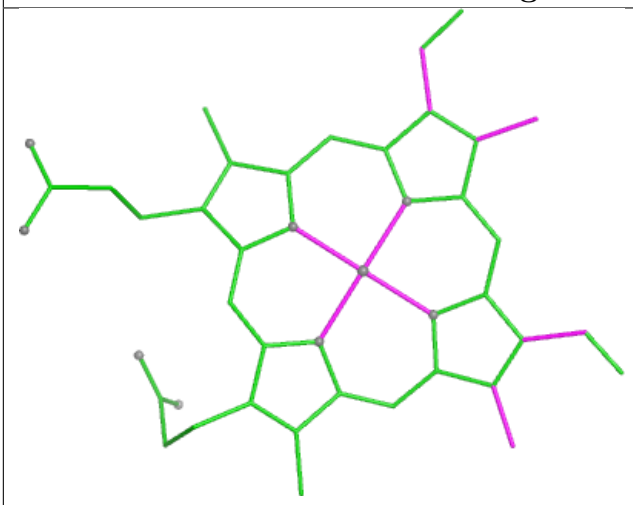
There are no ring outliers.

6 monomers are involved in 25 short contacts:

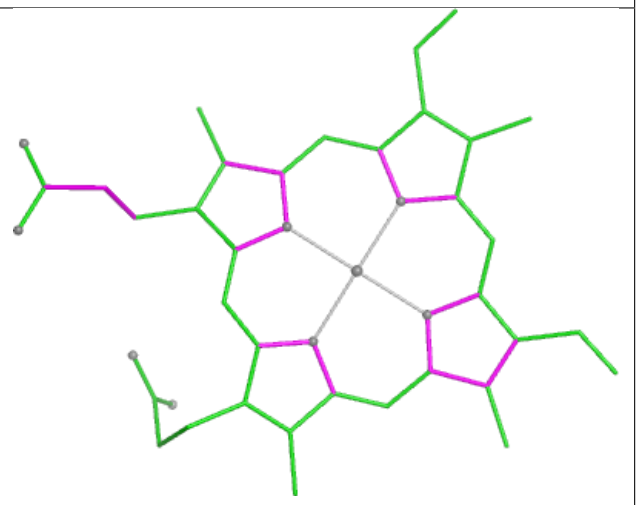
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	HEM	4	0
2	F	501	HEM	6	0
2	A	501	HEM	2	0
2	B	501	HEM	8	0
2	D	501	HEM	3	0
2	C	501	HEM	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

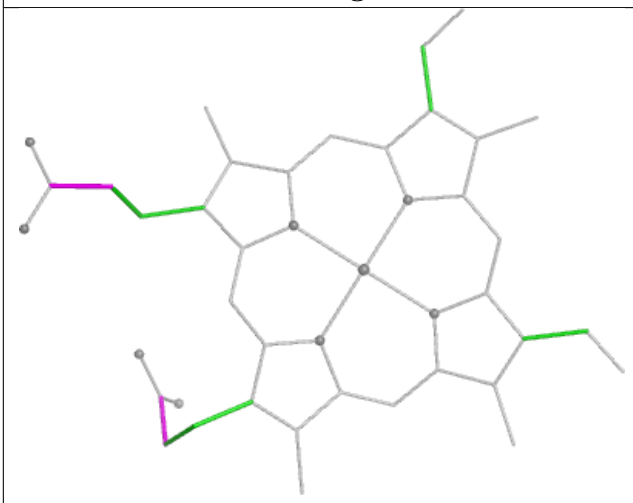
Ligand HEM E 501



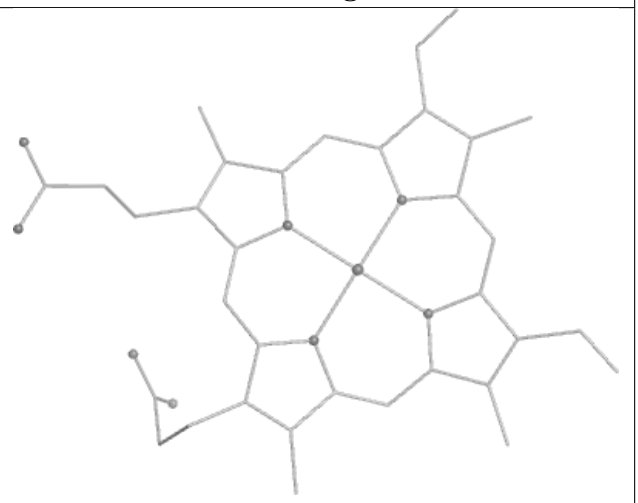
Bond lengths



Bond angles

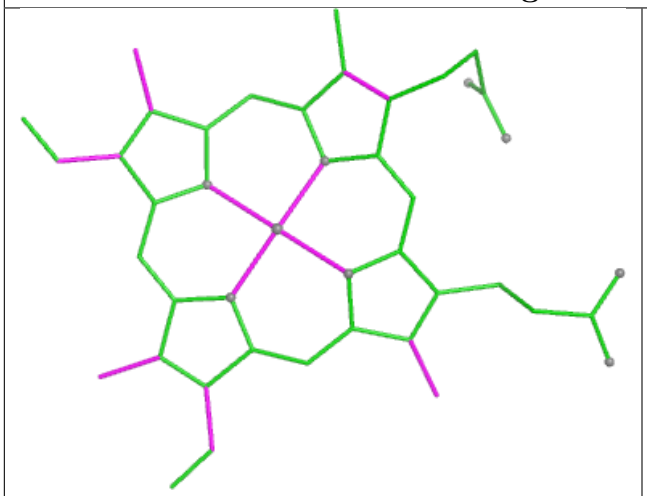


Torsions

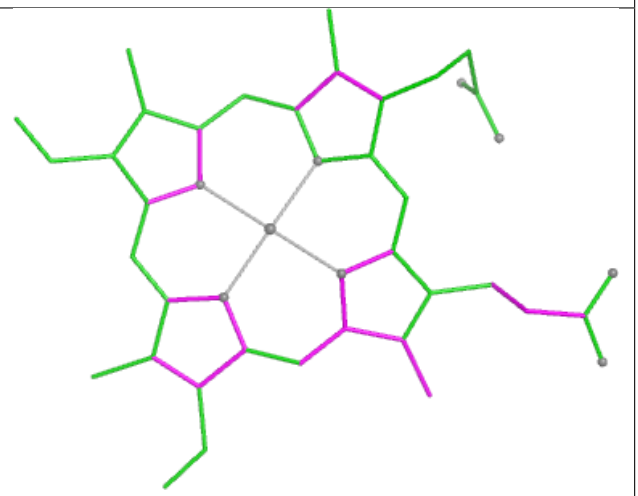


Rings

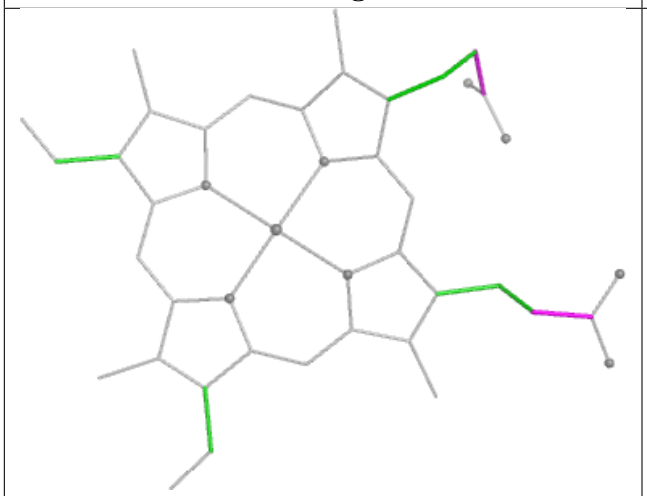
Ligand HEM F 501



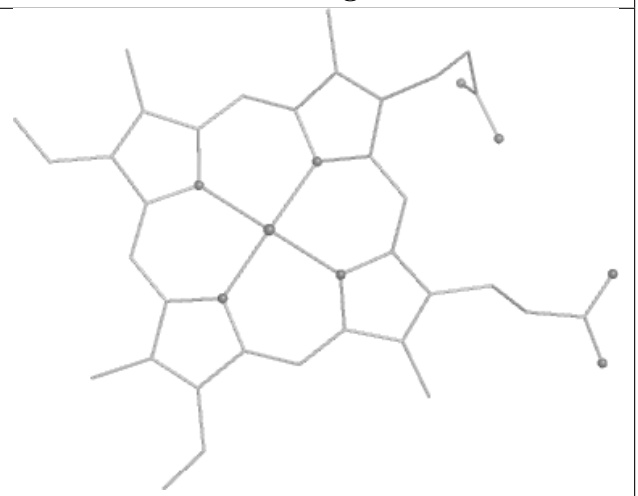
Bond lengths



Bond angles

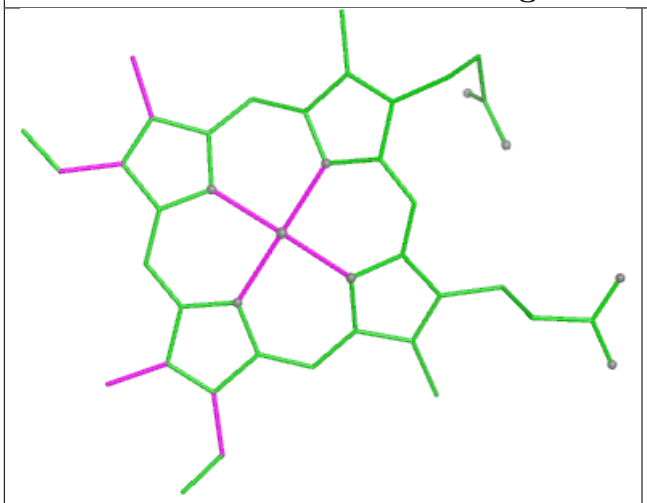


Torsions

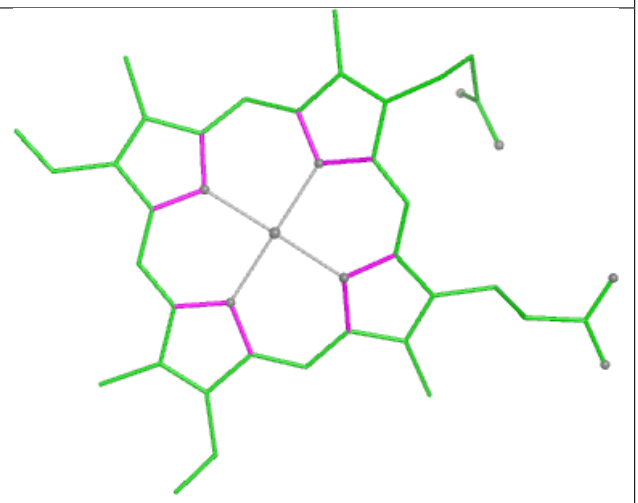


Rings

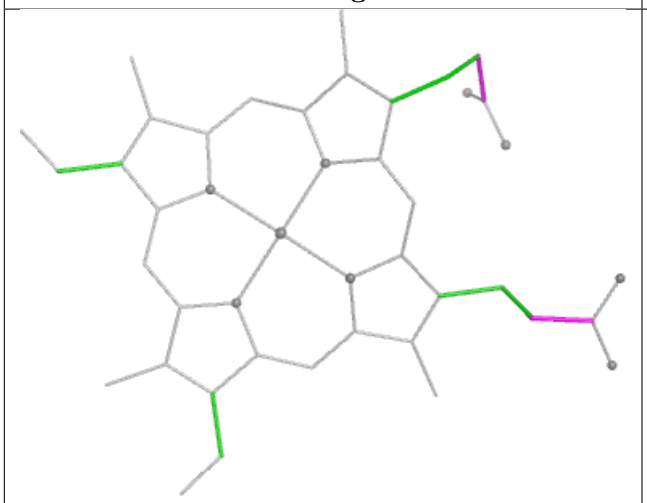
Ligand HEM A 501



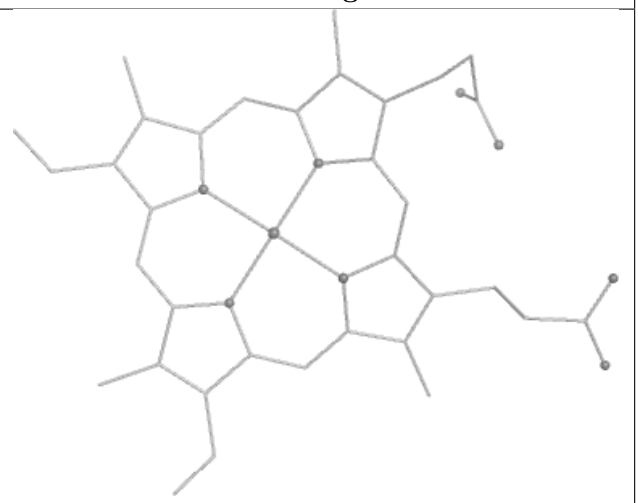
Bond lengths



Bond angles

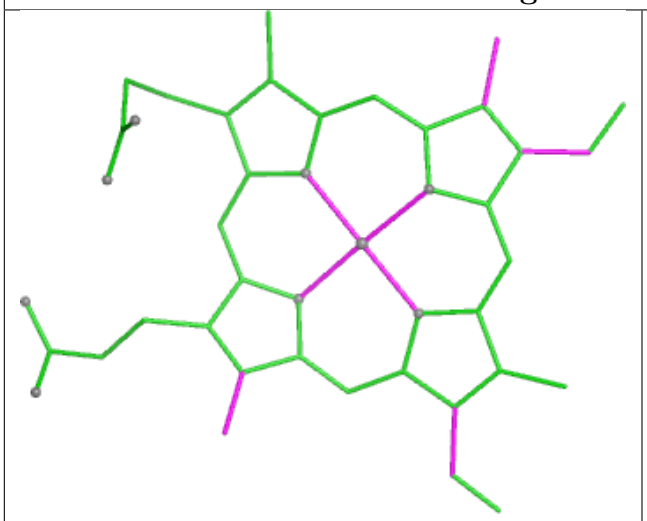


Torsions

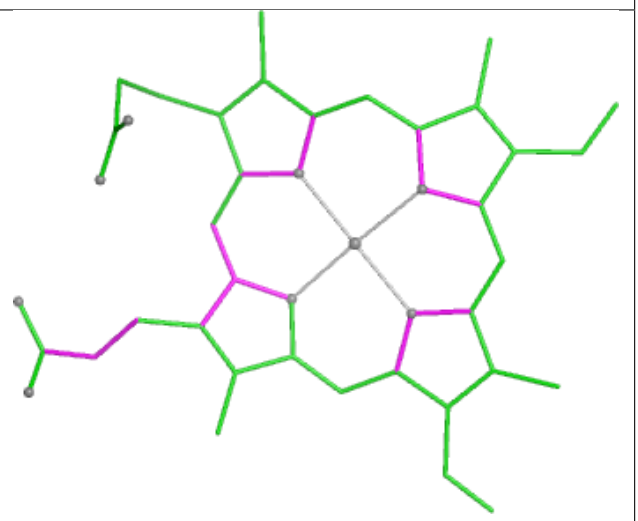


Rings

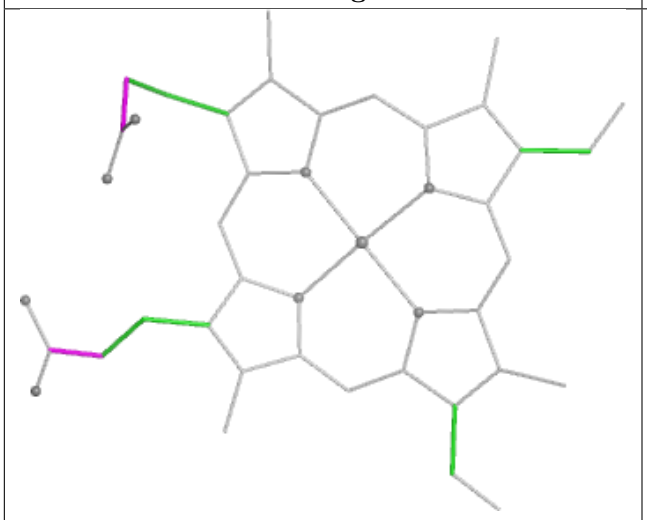
Ligand HEM B 501



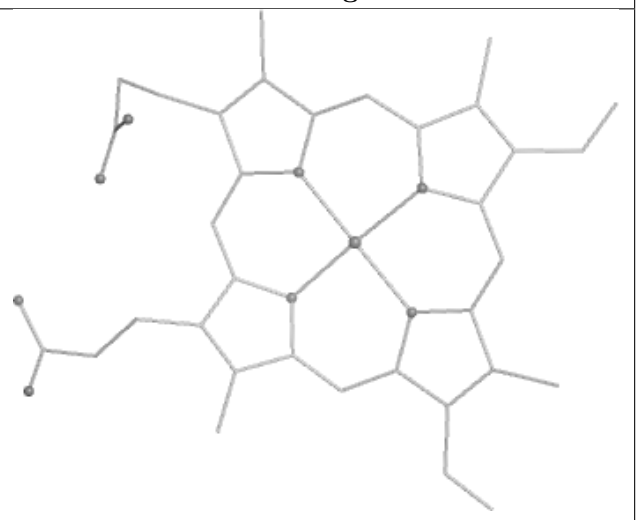
Bond lengths



Bond angles

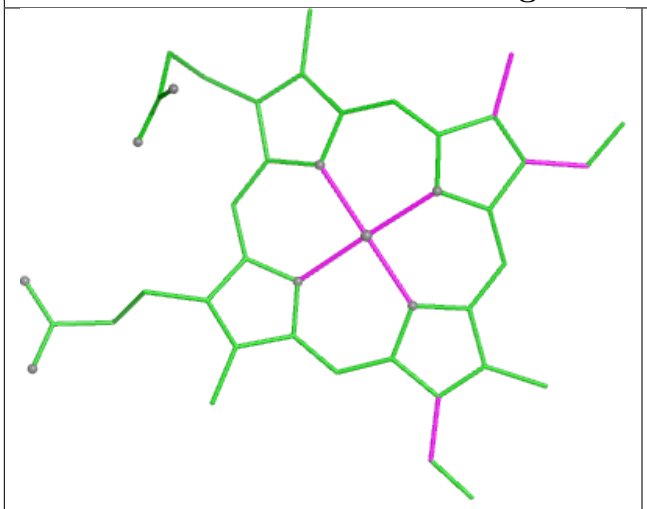


Torsions

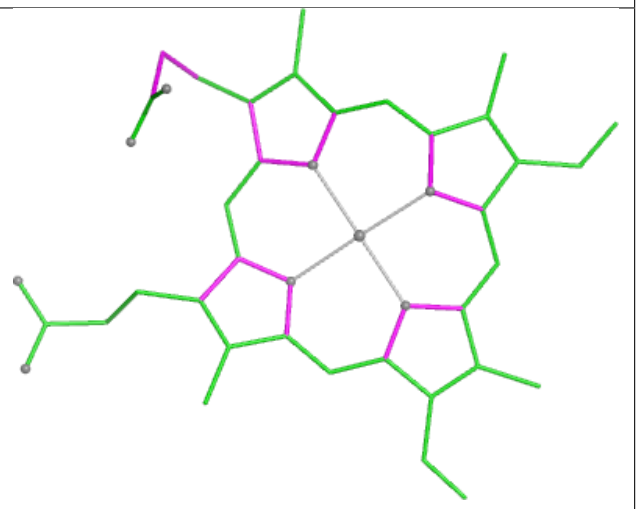


Rings

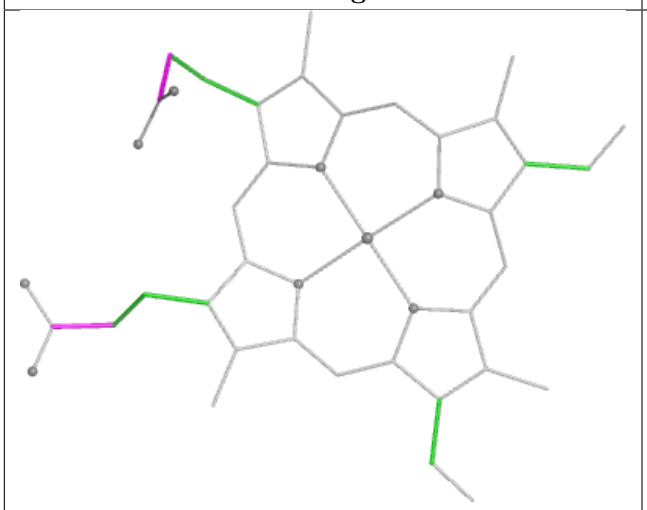
Ligand HEM D 501



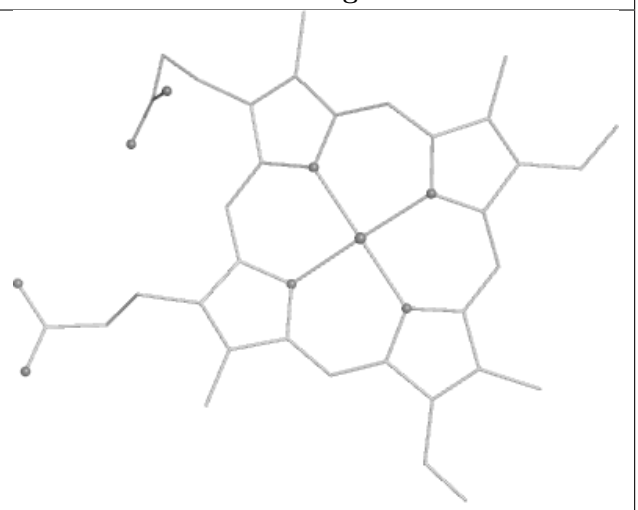
Bond lengths



Bond angles

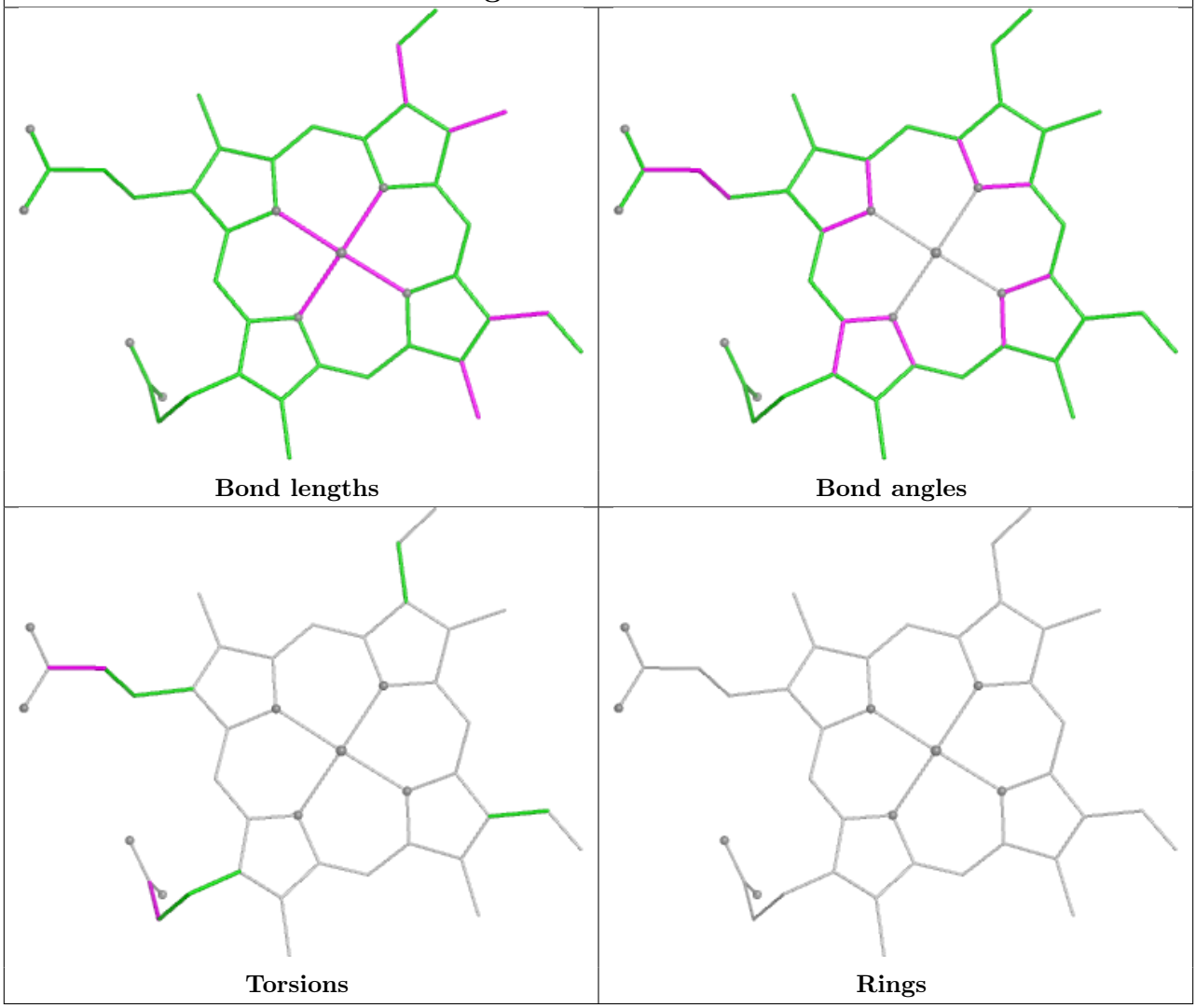


Torsions



Rings

Ligand HEM C 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	354/359 (98%)	-1.14	0 100 100	26, 61, 96, 125	0
1	B	354/359 (98%)	-1.02	1 (0%) 90 89	19, 63, 100, 148	0
1	C	354/359 (98%)	-1.02	0 100 100	34, 65, 101, 120	0
1	D	353/359 (98%)	-0.84	0 100 100	35, 69, 92, 127	0
1	E	354/359 (98%)	-0.74	0 100 100	50, 75, 101, 138	0
1	F	354/359 (98%)	-0.87	0 100 100	46, 82, 107, 135	0
All	All	2123/2154 (98%)	-0.94	1 (0%) 100 100	19, 70, 102, 148	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	THR	2.7

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)

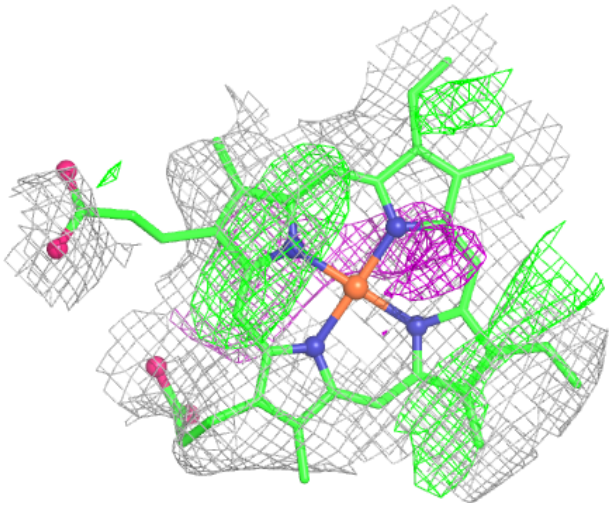
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

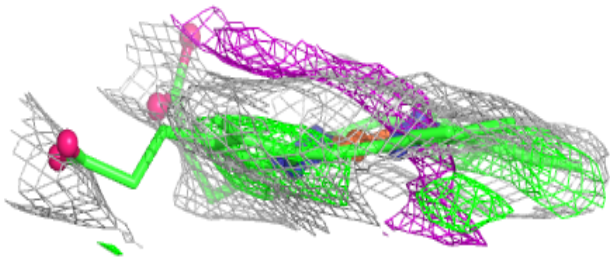
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	F	501	43/43	0.98	0.09	56,101,118,125	0
2	HEM	B	501	43/43	0.99	0.05	32,56,97,119	0
2	HEM	C	501	43/43	0.99	0.06	61,77,101,113	0
2	HEM	D	501	43/43	0.99	0.05	32,65,80,88	0
2	HEM	E	501	43/43	0.99	0.03	23,41,79,95	0
2	HEM	A	501	43/43	0.99	0.05	26,60,72,79	0

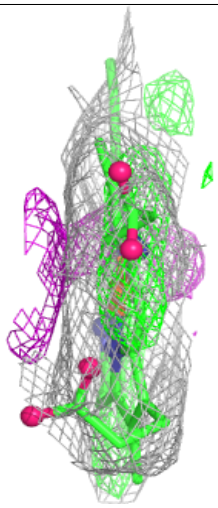
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM F 501:

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

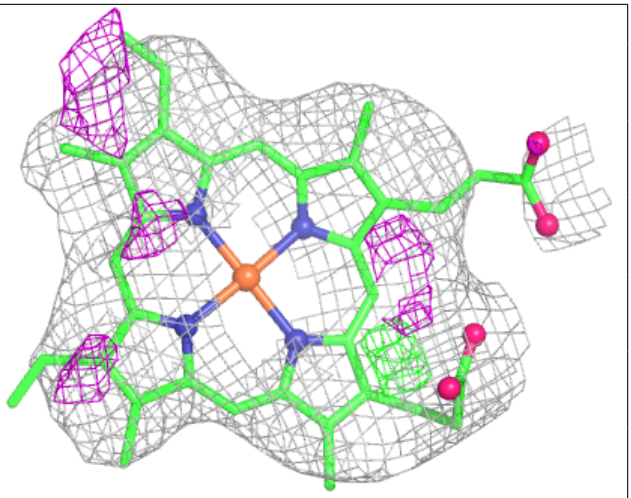


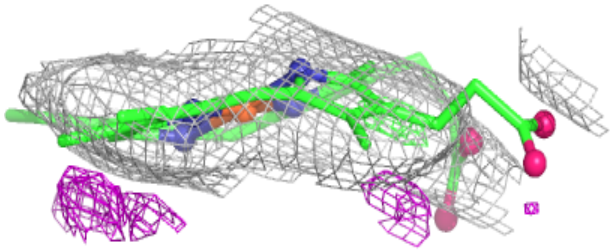


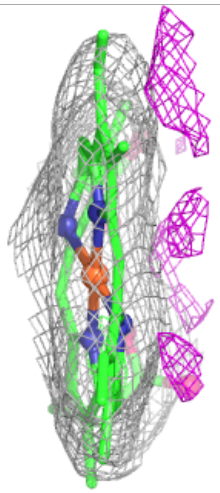


Electron density around HEM B 501:

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

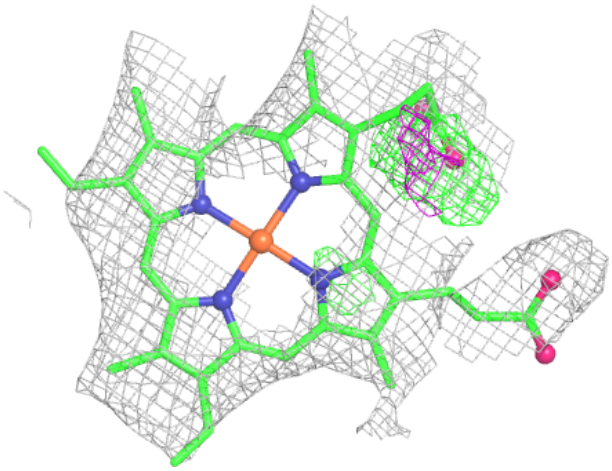


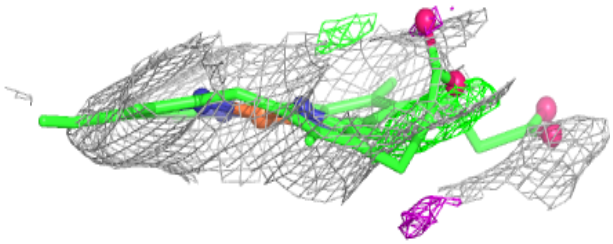


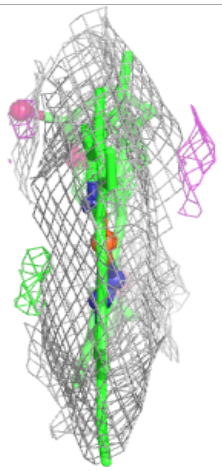


Electron density around HEM C 501:

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

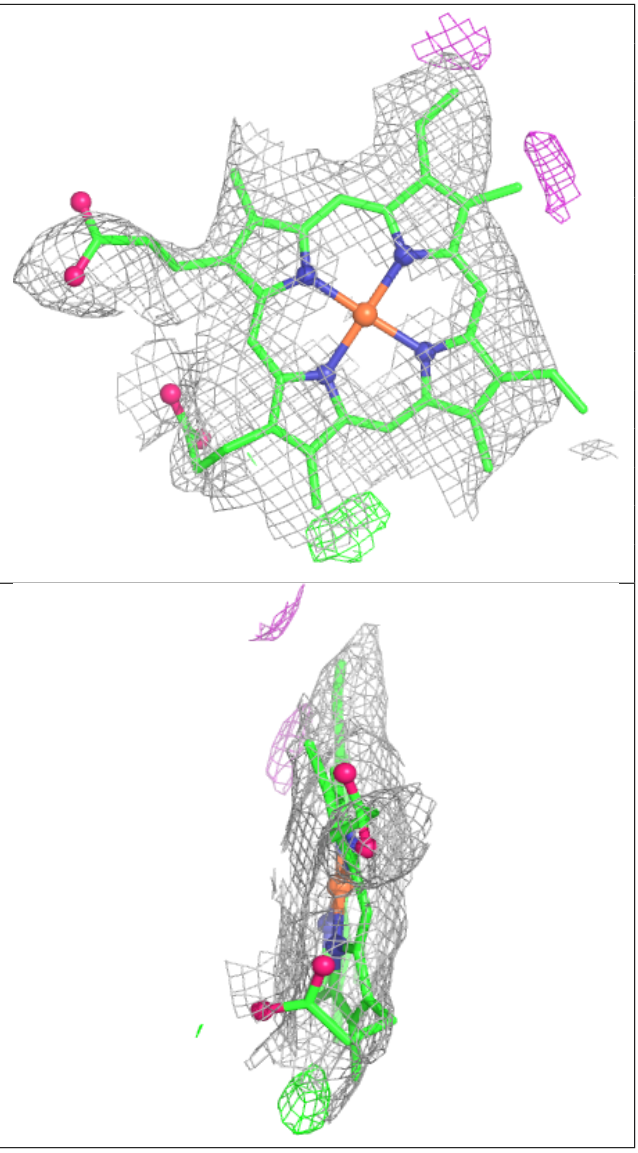






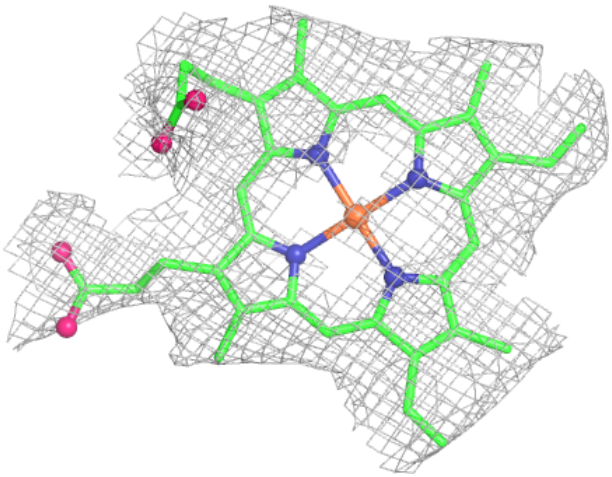
Electron density around HEM D 501:

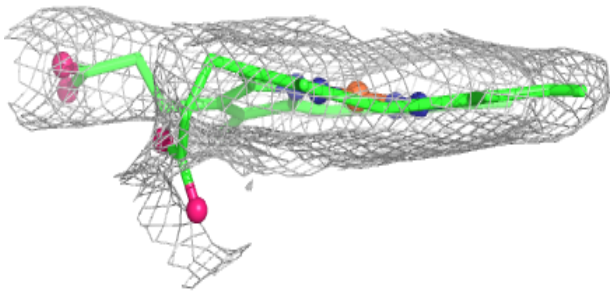
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

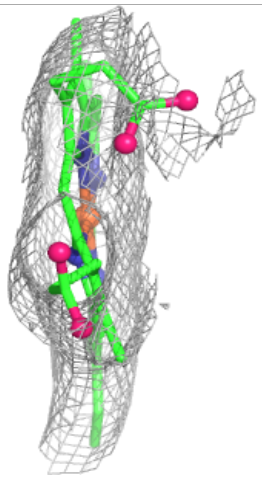


Electron density around HEM E 501:

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

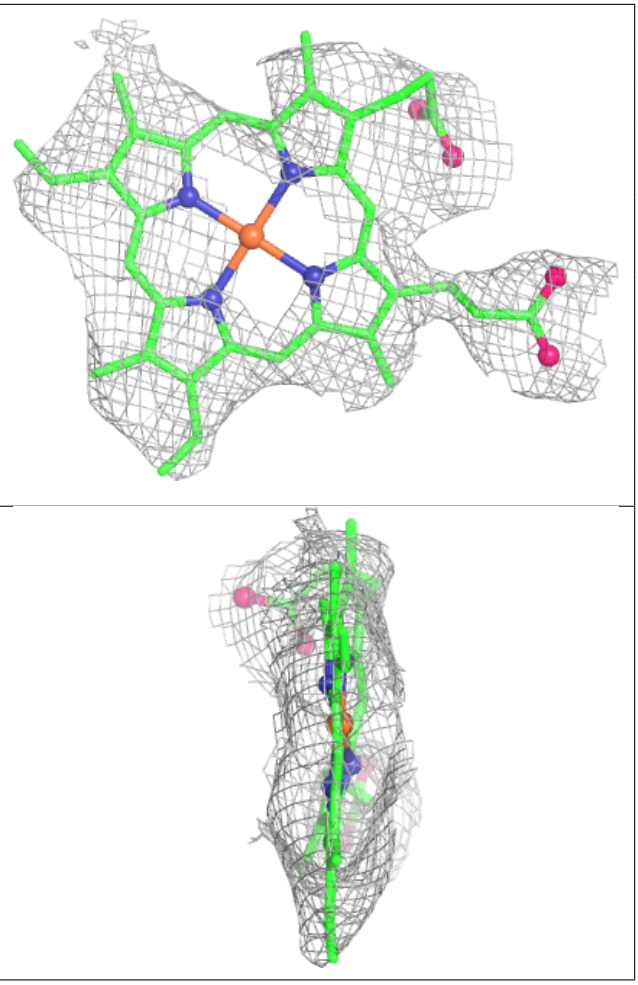






Electron density around HEM A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.