wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 12:51 AM EDT

PDB ID	:	3MZS
Title	:	Crystal Structure of Cytochrome P450 CYP11A1 in complex with 22-hydroxy-cholesterol
Authors	:	Stout, C.D.; Annalora, A.; Mast, N.; Pikuleva, I.
Deposited on	:	2010-05-12
Resolution	:	2.50 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:

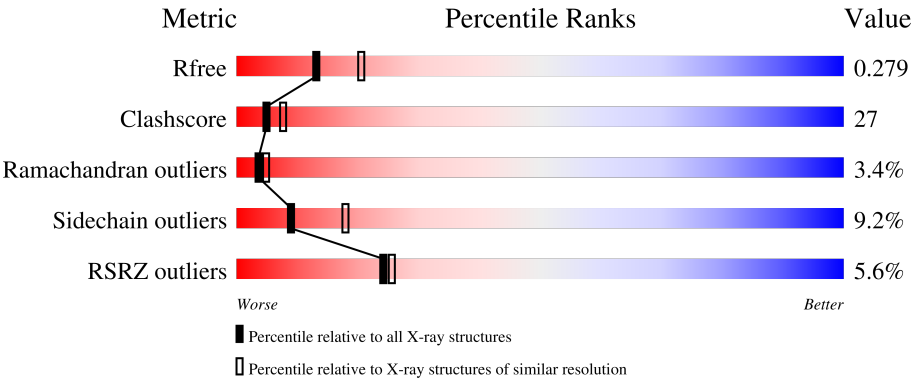
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	486	4% 52% 40%
1	B	486	6% 46% 43% 8%
1	C	486	6% 50% 40% 6%
1	D	486	6% 46% 42% 8%

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
4	IPA	B	502	-	-	X	-
4	IPA	C	502	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16012 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 Cholesterol side-chain cleavage enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			
1	B	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			
1	C	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			
1	D	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P00189
A	2	ALA	-	expression tag	UNP P00189
A	483	HIS	-	expression tag	UNP P00189
A	484	HIS	-	expression tag	UNP P00189
A	485	HIS	-	expression tag	UNP P00189
A	486	HIS	-	expression tag	UNP P00189
B	1	MET	-	expression tag	UNP P00189
B	2	ALA	-	expression tag	UNP P00189
B	483	HIS	-	expression tag	UNP P00189
B	484	HIS	-	expression tag	UNP P00189
B	485	HIS	-	expression tag	UNP P00189
B	486	HIS	-	expression tag	UNP P00189
C	1	MET	-	expression tag	UNP P00189
C	2	ALA	-	expression tag	UNP P00189
C	483	HIS	-	expression tag	UNP P00189
C	484	HIS	-	expression tag	UNP P00189
C	485	HIS	-	expression tag	UNP P00189
C	486	HIS	-	expression tag	UNP P00189
D	1	MET	-	expression tag	UNP P00189
D	2	ALA	-	expression tag	UNP P00189
D	483	HIS	-	expression tag	UNP P00189

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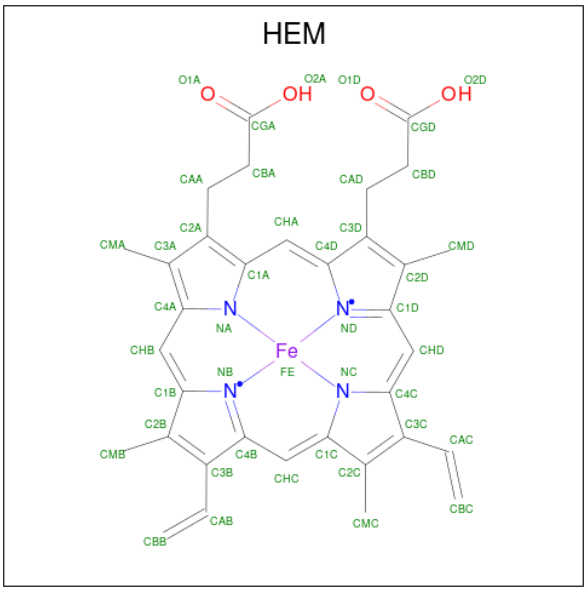
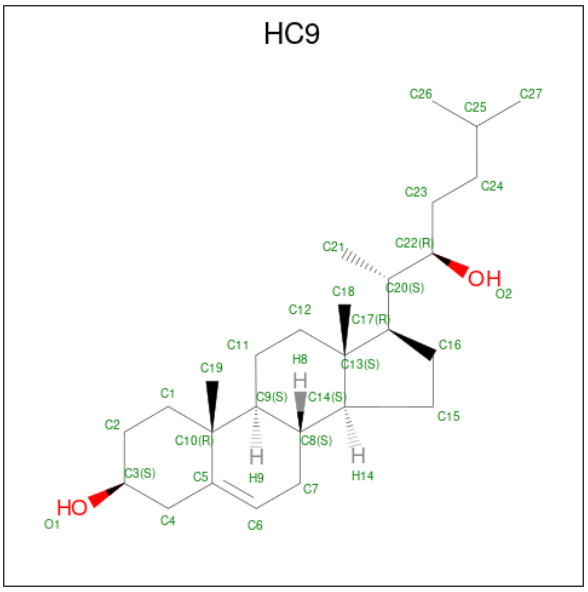
Chain	Residue	Modelled	Actual	Comment	Reference
D	484	HIS	-	expression tag	UNP P00189
D	485	HIS	-	expression tag	UNP P00189
D	486	HIS	-	expression tag	UNP P00189

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



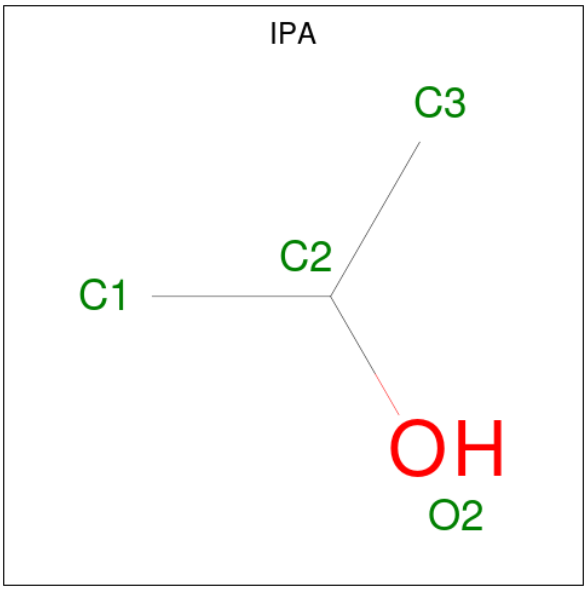
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (3alpha,8alpha,22R)-cholest-5-ene-3,22-diol (three-letter code: HC9) (formula: $C_{27}H_{46}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 29 27 2	0	0
3	B	1	Total C O 29 27 2	0	0
3	C	1	Total C O 29 27 2	0	0
3	D	1	Total C O 29 27 2	0	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

- Molecule 5 is water.

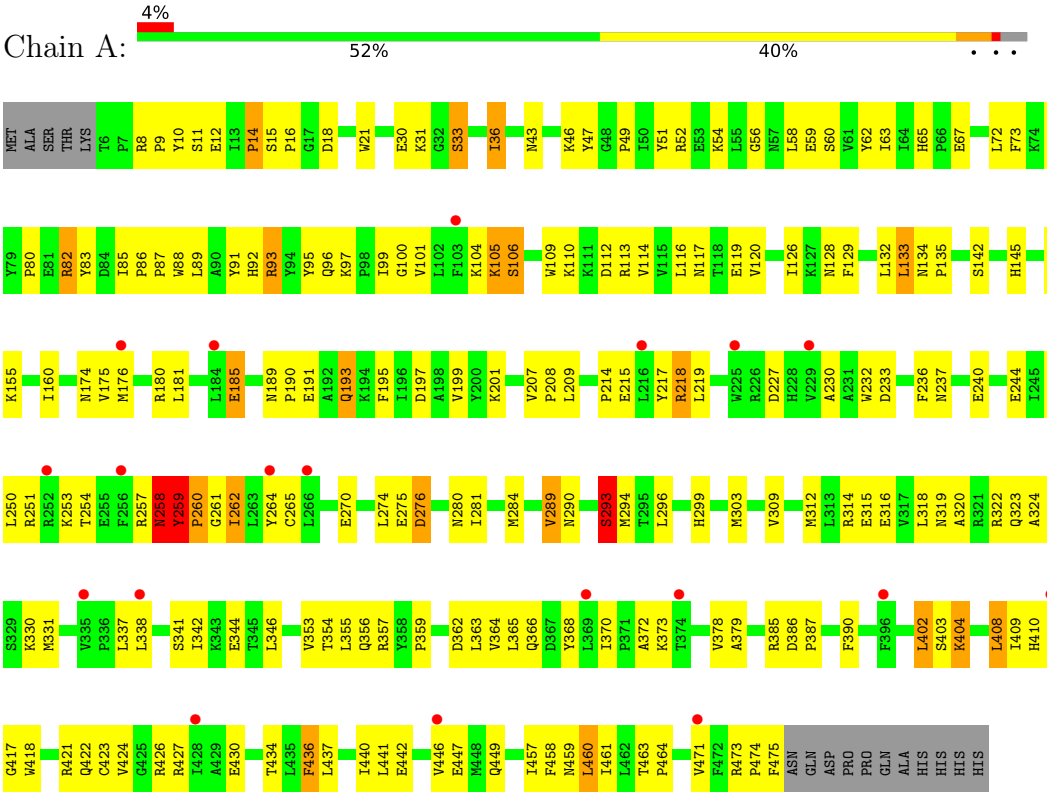
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	B	15	Total O 15 15	0	0
5	C	27	Total O 27 27	0	0
5	D	25	Total O 25 25	0	0

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.

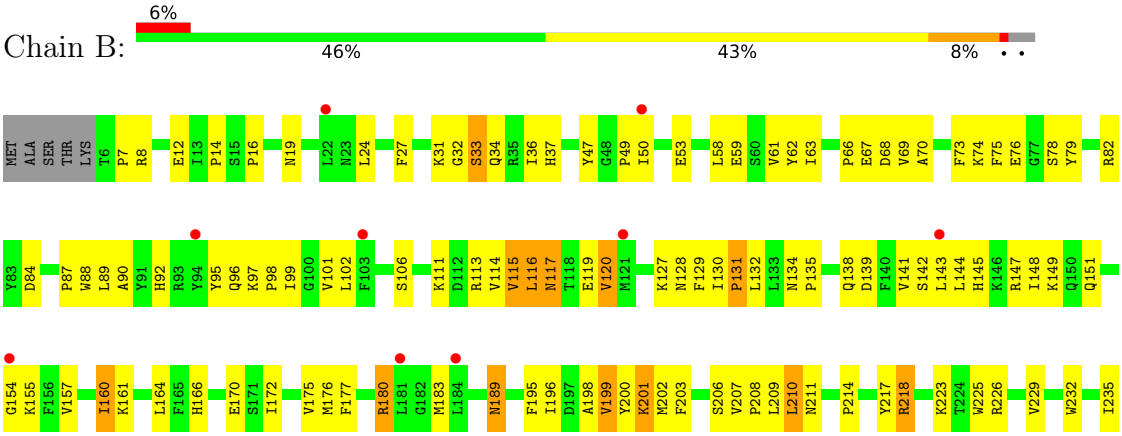
• Molecule 1: Cholesterol side-chain cleavage enzyme

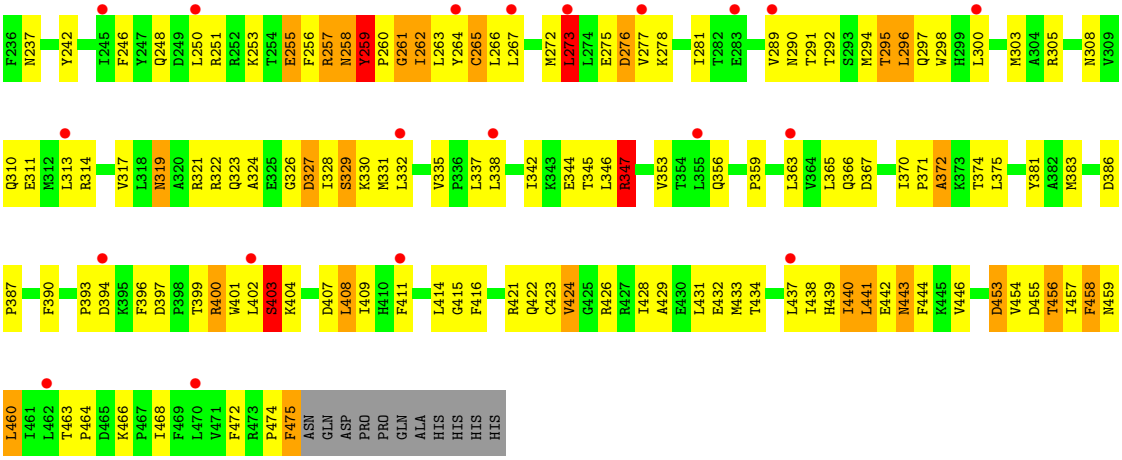
Chain A:



• Molecule 1: Cholesterol side-chain cleavage enzyme

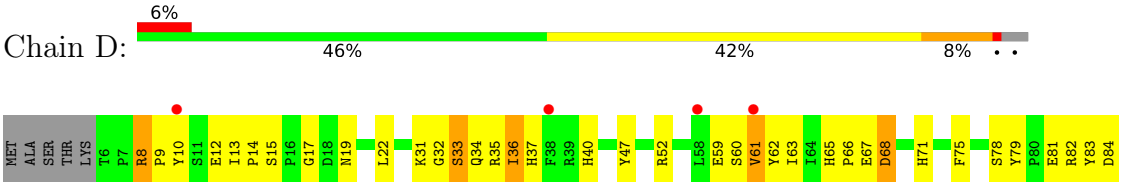
Chain B:

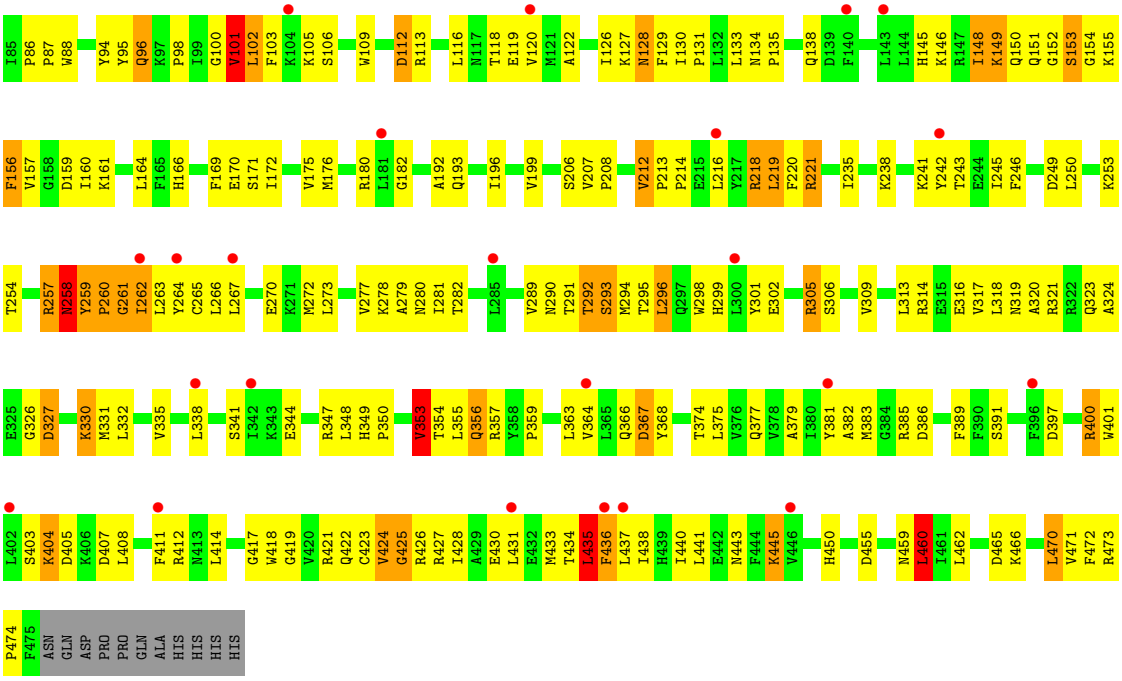




• Molecule 1: Cholesterol side-chain cleavage enzyme

• Molecule 1: Cholesterol side-chain cleavage enzyme




I85 P86 P87 W88 Y94 Y95 Q96 K97 P98 I99 G100 V101 L102 F103 K104 K105 S106 W109 D112 R113 L116 N117 T118 E119 V120 M121 A122 I126 K127 N128 F129 I130 P131 L132 L133 N134 P135 Q138 D139 F140 L143 L144 H145 K146 R147 I148 K149 Q150 Q151 G152 S153 G154 K155
F156 V157 G158 D159 I160 K161 L164 F165 H166 F169 E170 S171 I172 V175 M176 R180 L181 G182 A192 Q193 I196 V199 S206 V207 P208 V212 P213 P214 E215 L216 Y217 R218 L219 F220 R221 I235 K238 K241 Y242 T243 E244 I245 F246 D249 L250 K253
T254 R257 N258 Y259 P260 G261 I262 L263 Y264 C265 L266 L267 E270 R271 M272 L273 V277 K278 A279 N280 I281 T282 L285 V289 N290 T291 T292 S293 M294 T295 L296 Q297 W298 H299 L300 Y301 E302 R305 S306 V309 L313 R314 E315 E316 V317 L318 N319 A320 R321 R322 Q323 A324
E325 G326 D327 K330 M331 L332 V335 L338 S341 I342 K343 E344 R347 L348 H349 P350 V353 T354 L355 Q356 R357 Y358 P359 L363 V364 L365 Q366 D367 Y368 T374 L375 V376 Q377 V378 A379 I380 Y381 A382 M383 G384 R385 D386 F389 F390 S391 F396 D397 R400 W401
L402 S403 K404 D405 K406 D407 L408 F411 R412 N413 L414 G417 W418 G419 V420 R421 Q422 C423 V424 G425 R426 R427 I428 A429 E430 L431 E432 M433 T434 L435 F436 L437 I438 H439 I440 L441 F442 N443 F444 K445 V446 H450 D455 N459 L460 T461 L462 D465 K466 L470 V471 F472 R473
P474 F475 ASN GLN ASP PRO PRO GLN ALA HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.45Å 94.63Å 113.50Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	60.01 – 2.50 60.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (60.01-2.50) 99.3 (60.56-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.266 , 0.281 0.267 , 0.279	Depositor DCC
R_{free} test set	4004 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	84.1	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.276 for h,-k,-l 0.000 for -l,-k,-h	Xtriage
Reported twinning fraction	0.546 for H, K, L 0.454 for -h,-k,l	Depositor
Outliers	1 of 80275 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16012	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, HEM, HC9

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	0.99	5/4014 (0.1%)	0.89	4/5435 (0.1%)
1	B	0.89	1/4014 (0.0%)	0.84	7/5435 (0.1%)
1	C	0.98	2/4014 (0.0%)	0.89	4/5435 (0.1%)
1	D	0.93	2/4014 (0.0%)	0.89	7/5435 (0.1%)
All	All	0.95	10/16056 (0.1%)	0.88	22/21740 (0.1%)

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
1	D	0	1
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	VAL	CA-CB	-9.40	1.35	1.54
1	C	260	PRO	N-CA	7.47	1.59	1.47
1	A	293	SER	CB-OG	7.21	1.51	1.42
1	D	156	PHE	C-N	6.92	1.50	1.34
1	A	458	PHE	CE2-CZ	6.07	1.48	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	156	PHE	CA-C-O	10.56	142.28	120.10
1	D	156	PHE	O-C-N	-9.99	106.71	122.70
1	B	347	ARG	NE-CZ-NH2	8.85	124.73	120.30
1	A	385	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	D	261	GLY	N-CA-C	-7.15	95.23	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	TYR	Peptide
1	B	259	TYR	Peptide
1	C	259	TYR	Peptide
1	D	259	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3904	0	3910	185	0
1	B	3904	0	3910	273	0
1	C	3904	0	3910	207	0
1	D	3904	0	3910	225	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	5	0
3	A	29	0	46	1	0
3	B	29	0	46	2	0
3	C	29	0	45	5	0
3	D	29	0	45	1	0
4	A	4	0	8	1	0
4	B	4	0	8	8	0
4	C	4	0	8	4	0
4	D	4	0	8	2	0
5	A	25	0	0	1	0
5	B	15	0	0	1	0
5	C	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	25	0	0	4	0
All	All	16012	0	15974	875	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 27.

The worst 5 of 875 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:128:ASN:HB3	1:B:260:PRO:CG	1.22	1.61
1:B:128:ASN:HB3	1:B:260:PRO:CD	1.31	1.60
1:B:128:ASN:CB	1:B:260:PRO:CG	1.83	1.55
1:B:128:ASN:CB	1:B:260:PRO:HG2	1.42	1.45
1:D:156:PHE:O	1:D:157:VAL:HG23	1.47	1.12

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	468/486 (96%)	390 (83%)	66 (14%)	12 (3%)	5	8
1	B	468/486 (96%)	391 (84%)	59 (13%)	18 (4%)	3	4
1	C	468/486 (96%)	391 (84%)	59 (13%)	18 (4%)	3	4
1	D	468/486 (96%)	376 (80%)	77 (16%)	15 (3%)	4	5
All	All	1872/1944 (96%)	1548 (83%)	261 (14%)	63 (3%)	3	5

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	404	LYS
1	B	33	SER
1	B	255	GLU
1	B	327	ASP

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	426/440 (97%)	398 (93%)	28 (7%)	16 32
1	B	426/440 (97%)	383 (90%)	43 (10%)	7 14
1	C	426/440 (97%)	389 (91%)	37 (9%)	10 20
1	D	426/440 (97%)	378 (89%)	48 (11%)	6 11
All	All	1704/1760 (97%)	1548 (91%)	156 (9%)	9 18

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	102	LEU
1	D	391	SER
1	D	149	LYS
1	D	262	ILE
1	D	445	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	138	GLN
1	C	459	ASN
1	C	237	ASN
1	C	323	GLN
1	D	45	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 monosaccharides 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	$\#\|Z\| > 2$
3	HC9	A	501	2	32,32,32	1.16	2 (6%)	49,50,50	1.79	10 (20%)
2	HEM	B	500	3,1	41,50,50	2.82	18 (43%)	45,82,82	2.63	13 (28%)
4	IPA	B	502	-	3,3,3	0.72	0	3,3,3	0.88	0
2	HEM	A	500	3,1	41,50,50	2.98	20 (48%)	45,82,82	2.57	10 (22%)
3	HC9	D	501	2	32,32,32	1.29	6 (18%)	49,50,50	2.37	17 (34%)
3	HC9	B	501	2	32,32,32	0.89	0	49,50,50	1.69	8 (16%)
3	HC9	C	501	2	32,32,32	0.93	1 (3%)	49,50,50	1.75	14 (28%)
4	IPA	A	502	-	3,3,3	0.88	0	3,3,3	0.52	0
4	IPA	C	502	-	3,3,3	0.66	0	3,3,3	0.53	0
4	IPA	D	502	-	3,3,3	0.73	0	3,3,3	0.62	0
2	HEM	C	500	3,1	41,50,50	2.94	18 (43%)	45,82,82	2.56	13 (28%)
2	HEM	D	500	3,1	41,50,50	3.01	20 (48%)	45,82,82	2.77	12 (26%)

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	HC9	A	501	2	-	2/13/71/71	0/4/4/4
2	HEM	B	500	3,1	-	2/12/54/54	-
2	HEM	A	500	3,1	-	0/12/54/54	-
3	HC9	D	501	2	-	1/13/71/71	0/4/4/4
3	HC9	B	501	2	-	5/13/71/71	0/4/4/4
3	HC9	C	501	2	-	1/13/71/71	0/4/4/4
2	HEM	C	500	3,1	-	2/12/54/54	-
2	HEM	D	500	3,1	-	5/12/54/54	-

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3C-C2C	7.24	1.50	1.40
2	D	500	HEM	C3B-C2B	7.19	1.51	1.37
2	C	500	HEM	C3C-C2C	6.60	1.49	1.40
2	B	500	HEM	C3B-C2B	6.44	1.50	1.37
2	A	500	HEM	C3B-C2B	6.42	1.50	1.37

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	HEM	C4B-C3B-C2B	-9.63	99.47	107.11
2	B	500	HEM	C4B-C3B-C2B	-9.13	99.86	107.11
2	A	500	HEM	C4B-C3B-C2B	-9.02	99.96	107.11
2	D	500	HEM	CHC-C4B-C3B	-8.90	110.94	124.57
2	A	500	HEM	CHC-C4B-C3B	-8.85	111.02	124.57

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

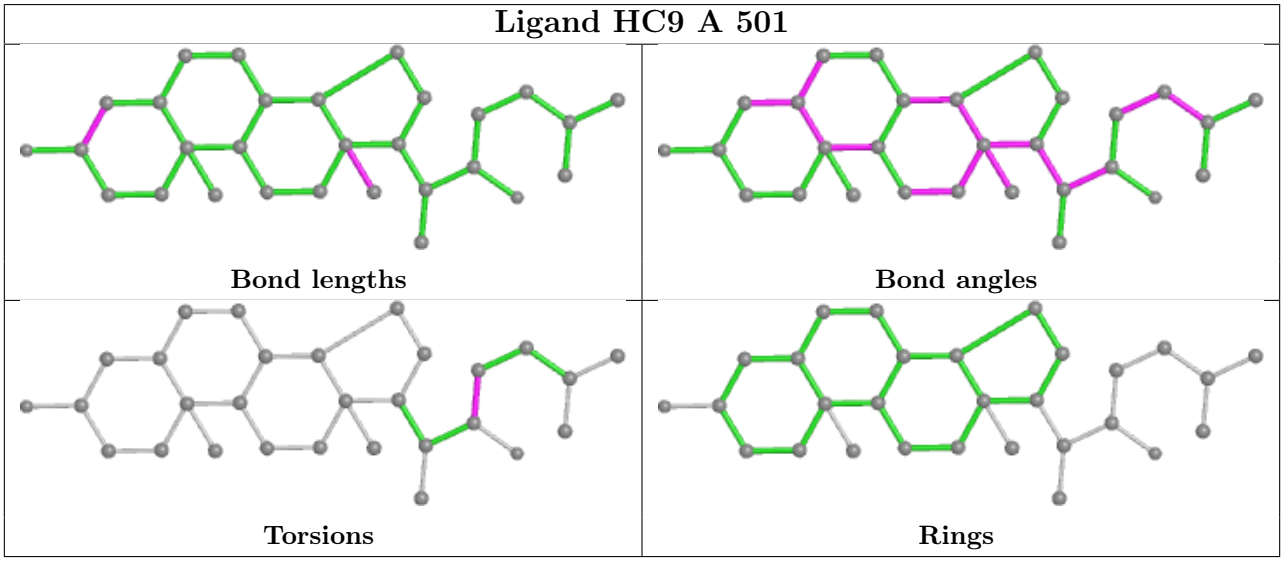
Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C1A-C2A-CAA-CBA
2	D	500	HEM	C3A-C2A-CAA-CBA
3	B	501	HC9	C20-C22-C23-C24
3	C	501	HC9	C17-C20-C22-O2
3	B	501	HC9	C22-C23-C24-C25

There are no ring outliers.

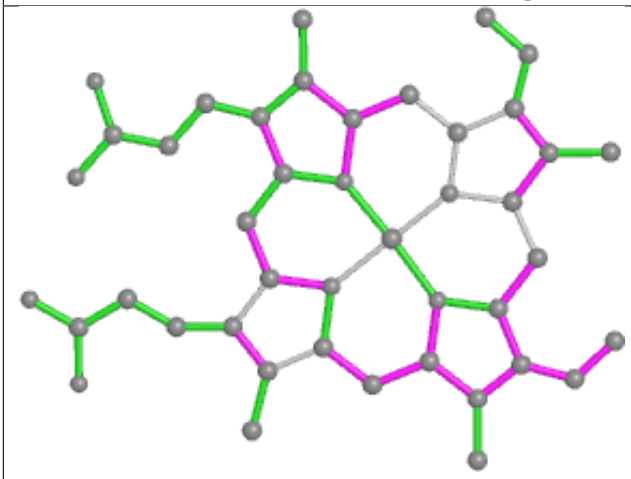
12 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HC9	1	0
2	B	500	HEM	4	0
4	B	502	IPA	8	0
2	A	500	HEM	4	0
3	D	501	HC9	1	0
3	B	501	HC9	2	0
3	C	501	HC9	5	0
4	A	502	IPA	1	0
4	C	502	IPA	4	0
4	D	502	IPA	2	0
2	C	500	HEM	5	0
2	D	500	HEM	5	0

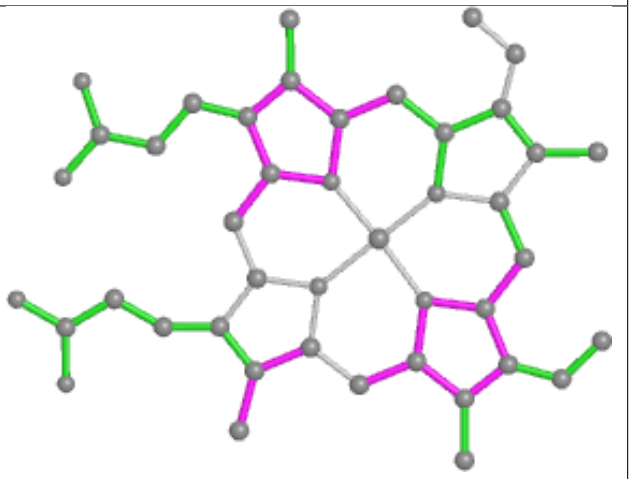
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



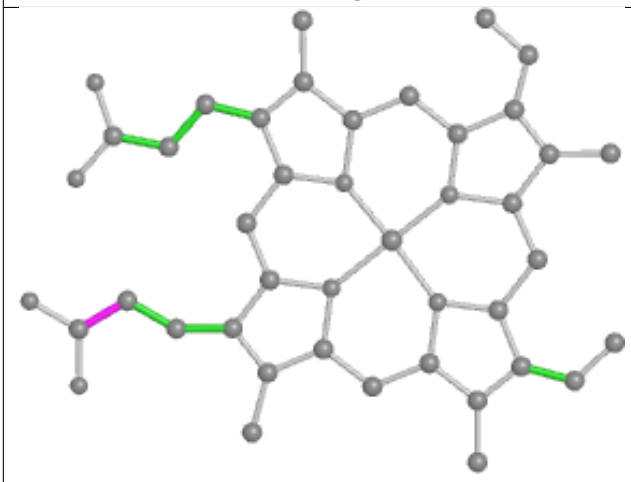
Ligand HEM B 500



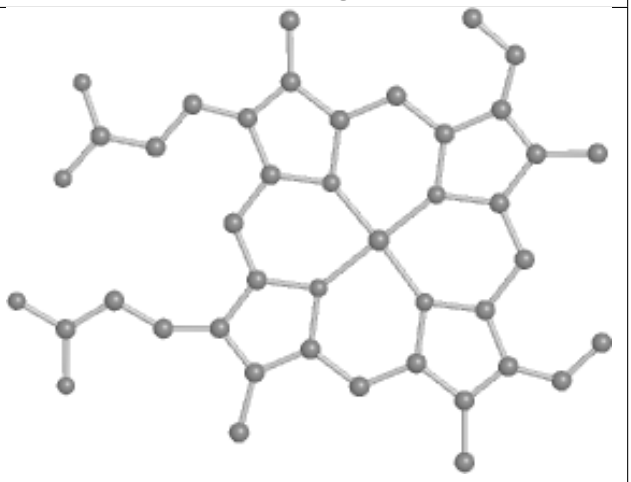
Bond lengths



Bond angles

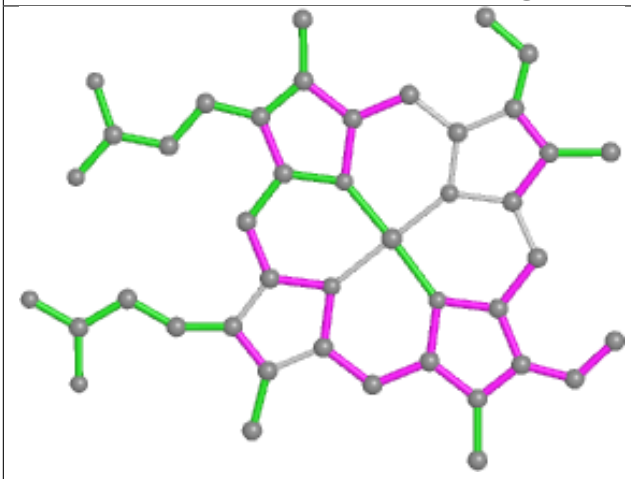


Torsions



Rings

Ligand HEM A 500



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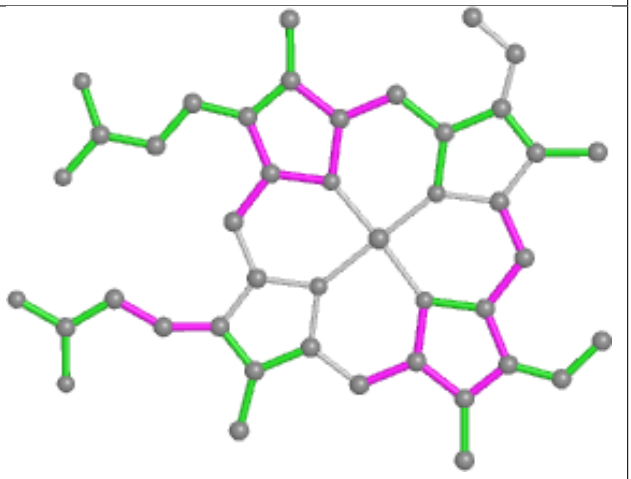
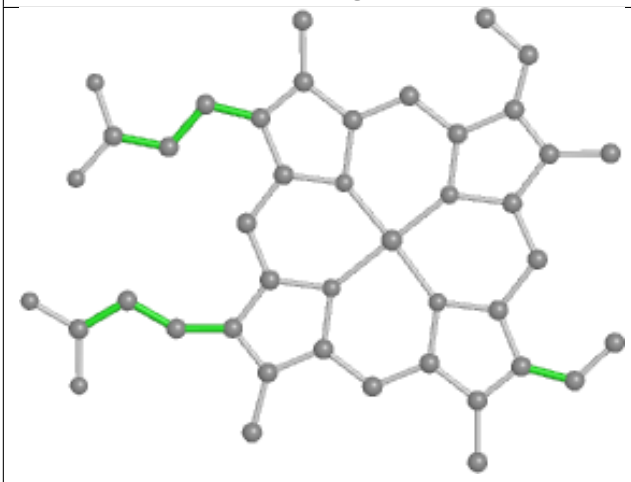
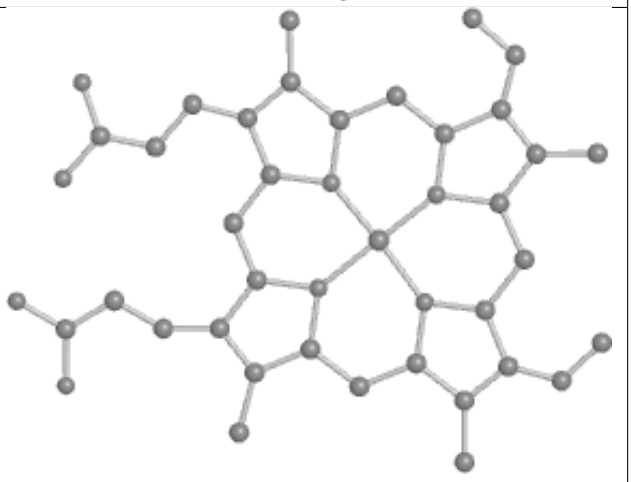


Bond angles

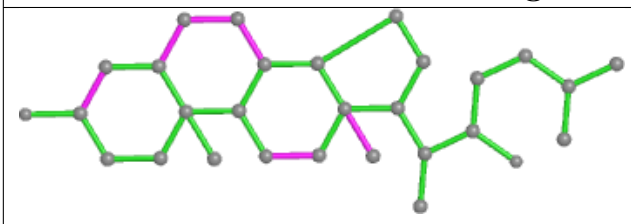


Torsions

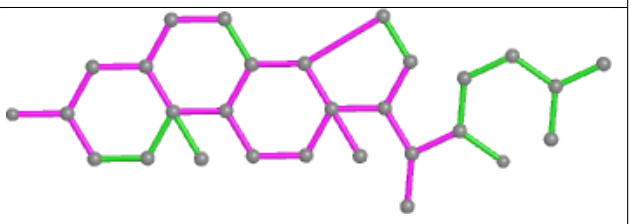


Rings

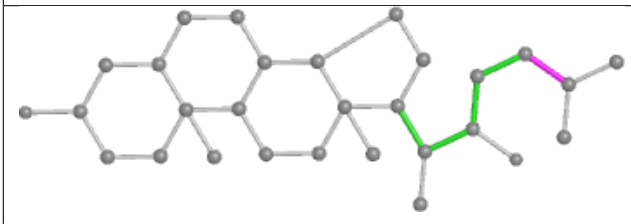
Ligand HC9 D 501



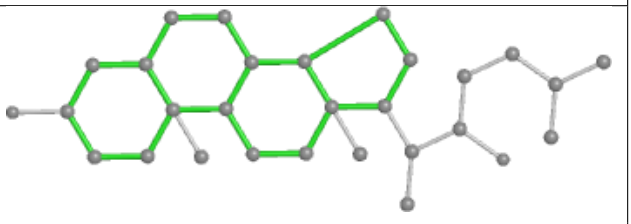
Bond lengths



Bond angles

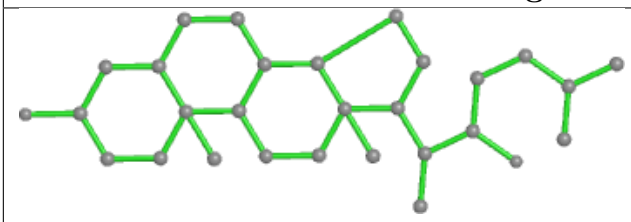


Torsions

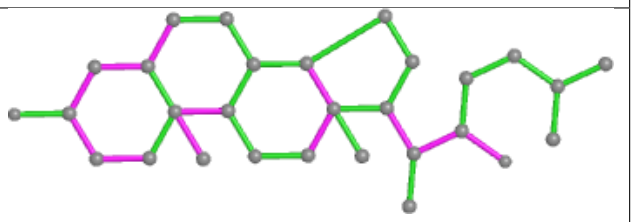


Rings

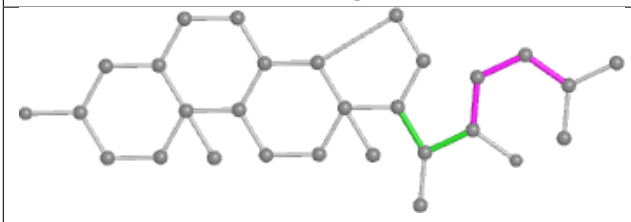
Ligand HC9 B 501



Bond lengths



Bond angles



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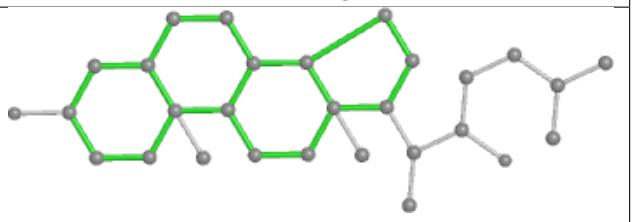
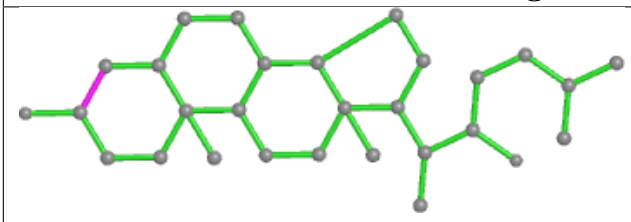


Rings

Ligand HC9 C 501



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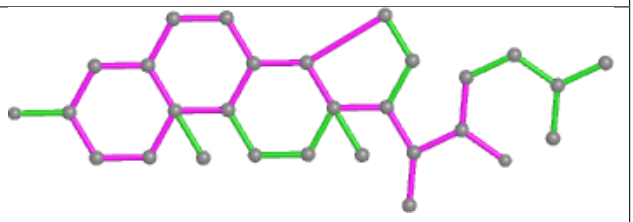
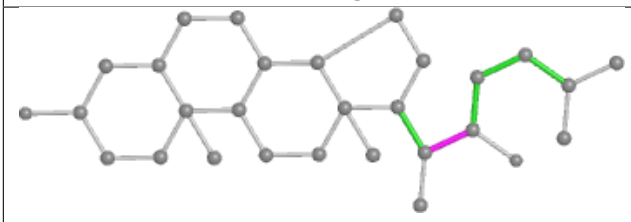


Bond angles



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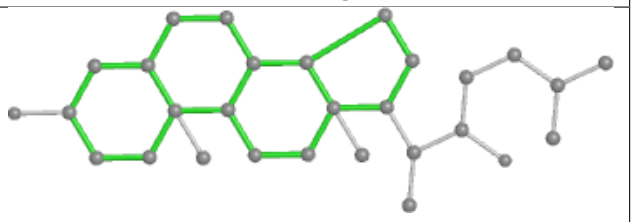
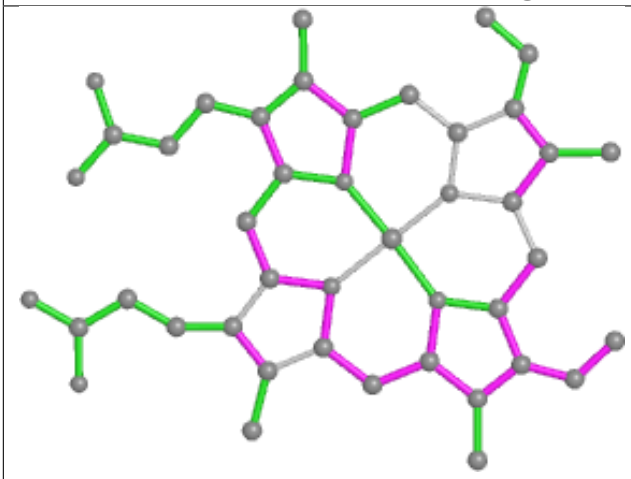


Rings

Ligand HEM C 500



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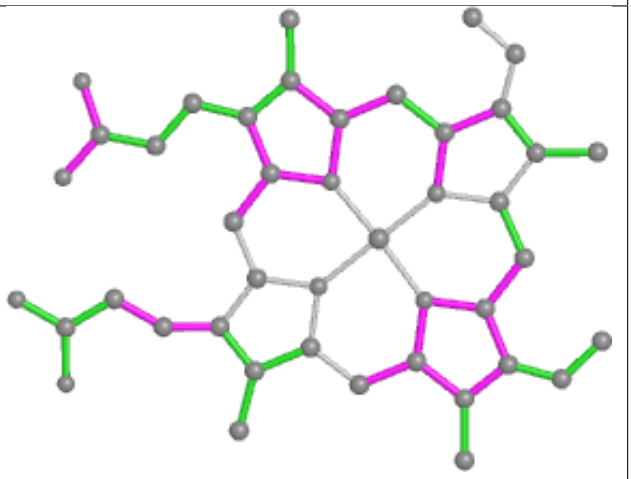
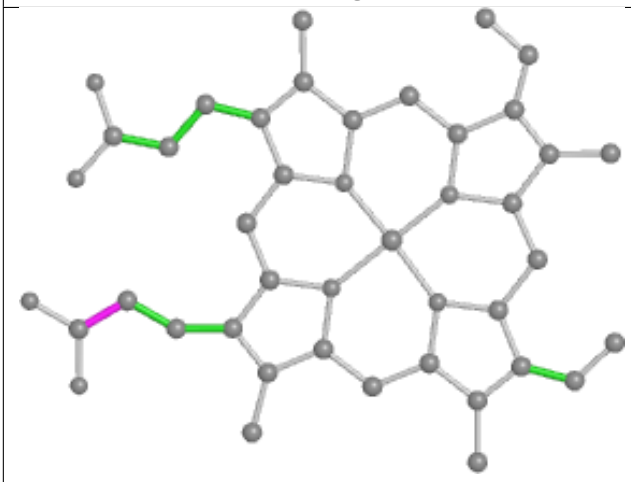
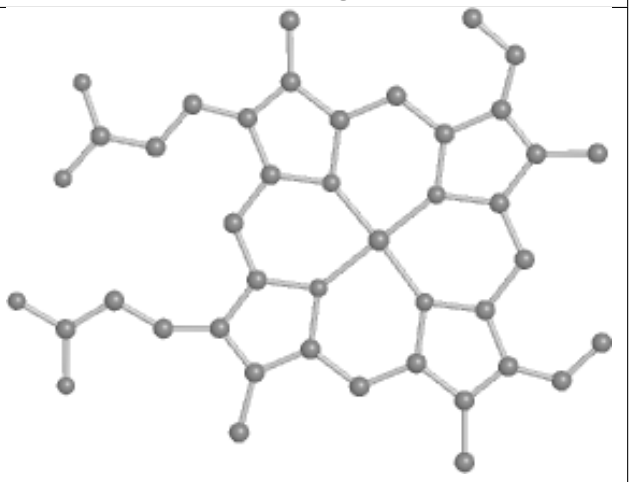


Bond angles

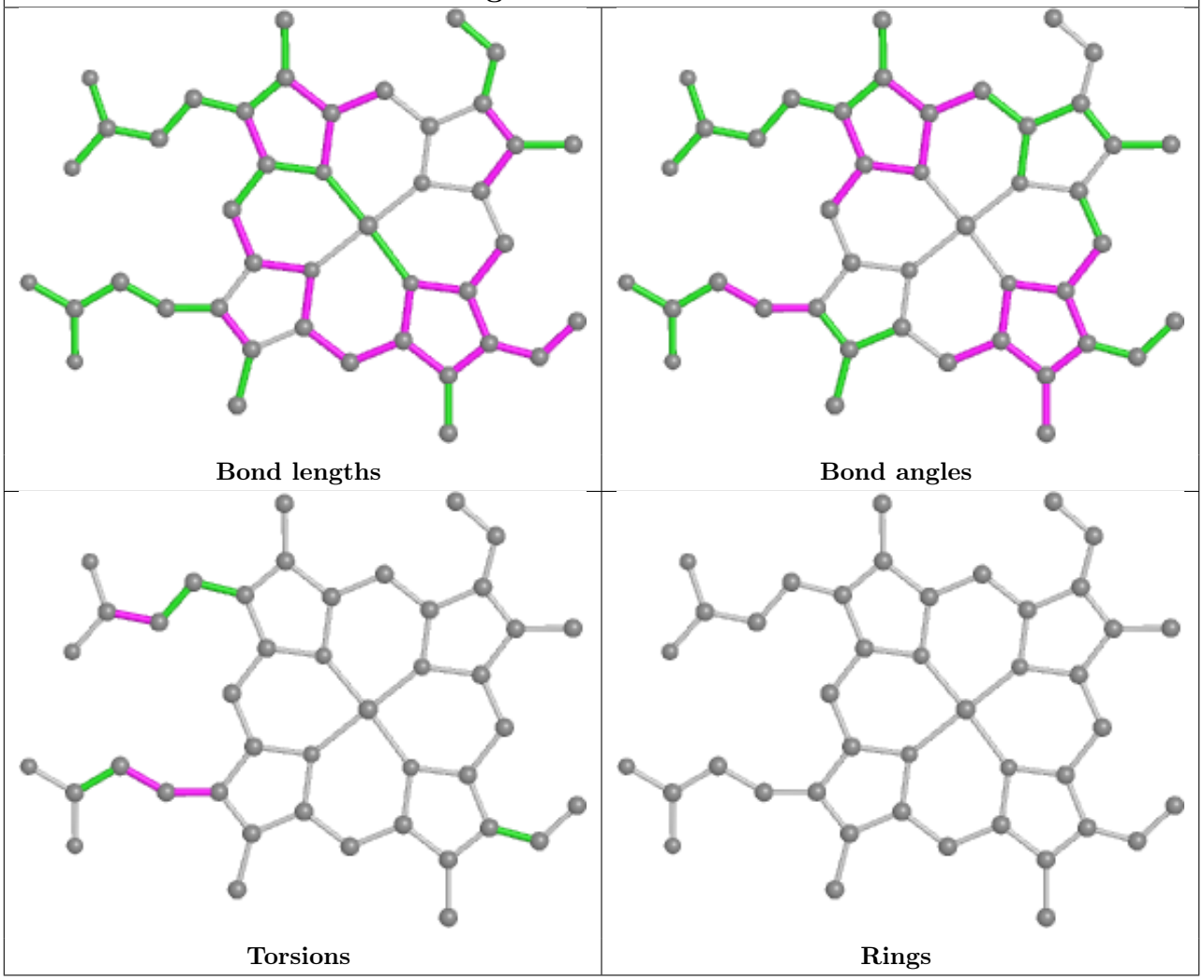


Torsions



Rings

Ligand HEM D 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	470/486 (96%)	0.43	19 (4%)	38	41	34, 65, 84, 96	0
1	B	470/486 (96%)	0.51	29 (6%)	20	21	39, 67, 87, 97	0
1	C	470/486 (96%)	0.46	31 (6%)	18	19	35, 65, 84, 93	0
1	D	470/486 (96%)	0.47	27 (5%)	23	25	32, 67, 86, 94	0
All	All	1880/1944 (96%)	0.47	106 (5%)	24	25	32, 66, 85, 97	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	266	LEU	5.8
1	C	263	LEU	5.2
1	B	184	LEU	4.1
1	B	154	GLY	4.1
1	A	446	VAL	3.6

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

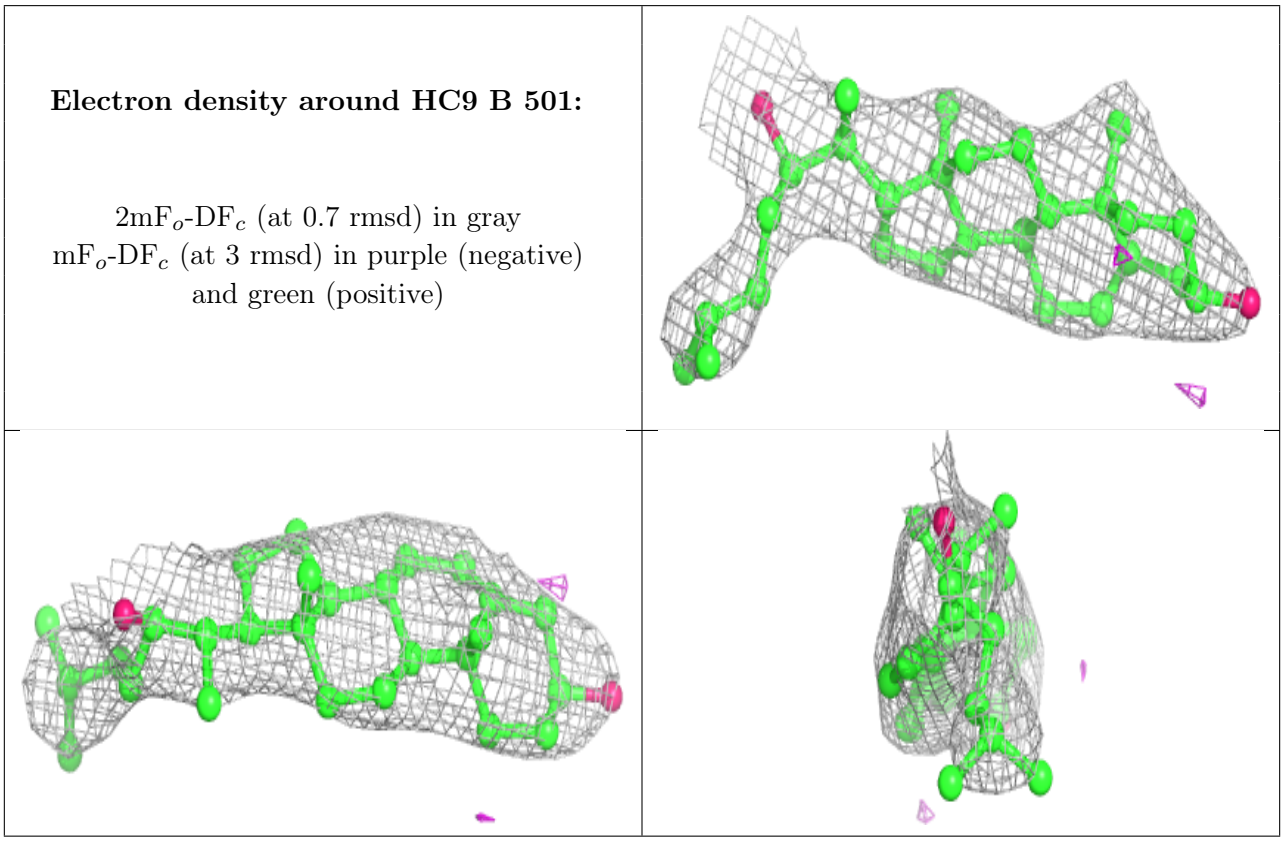
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	IPA	D	502	4/4	0.89	0.40	59,59,61,65	0
4	IPA	A	502	4/4	0.94	0.52	49,49,50,51	0
4	IPA	B	502	4/4	0.94	0.52	60,61,62,63	0
3	HC9	B	501	29/29	0.94	0.27	44,53,64,68	0
3	HC9	A	501	29/29	0.95	0.27	41,49,58,60	0
3	HC9	D	501	29/29	0.96	0.23	39,48,56,61	0
4	IPA	C	502	4/4	0.96	0.51	60,61,61,63	0
2	HEM	B	500	43/43	0.96	0.16	34,47,55,60	0
3	HC9	C	501	29/29	0.97	0.23	44,54,61,66	0
2	HEM	C	500	43/43	0.97	0.18	37,50,56,59	0
2	HEM	D	500	43/43	0.97	0.18	18,41,56,62	0
2	HEM	A	500	43/43	0.98	0.16	25,43,54,57	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.

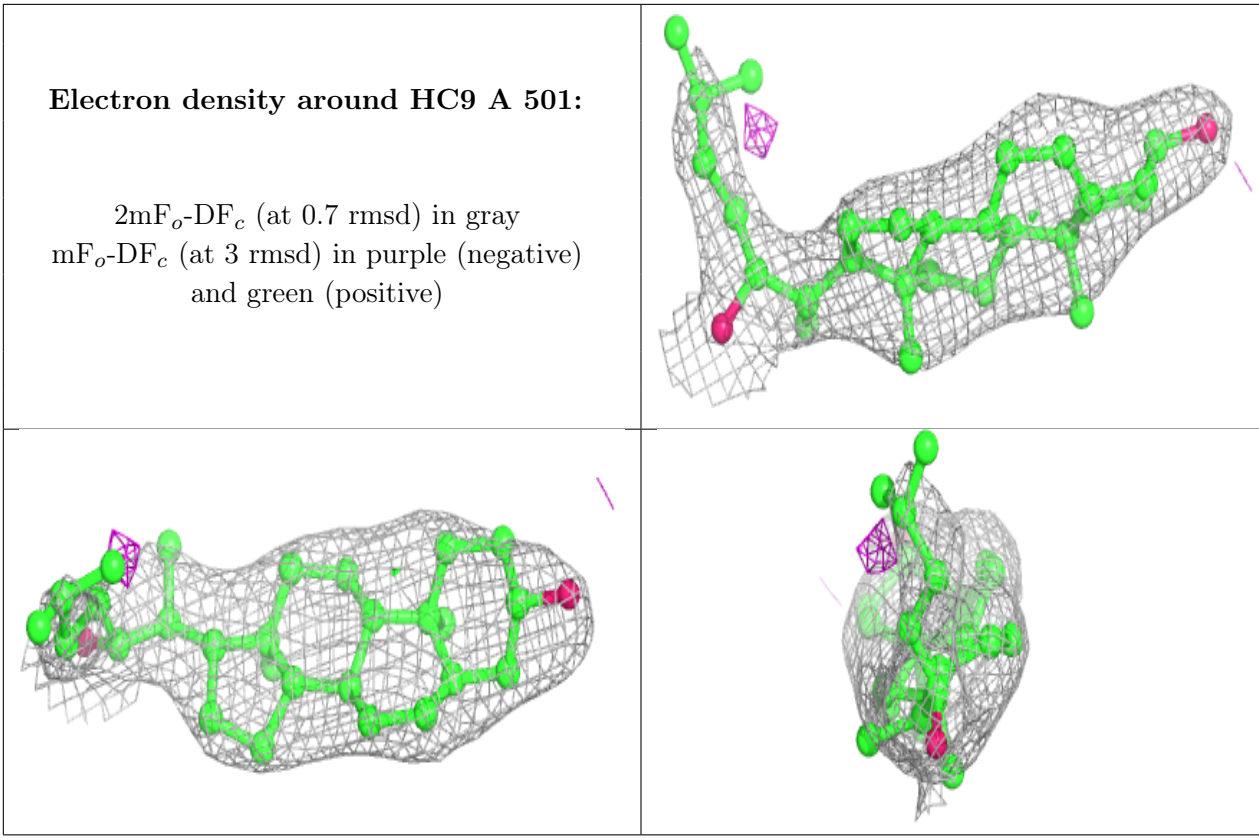
Electron density around HC9 B 501:

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



Electron density around HC9 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)



Electron density around HC9 D 501:

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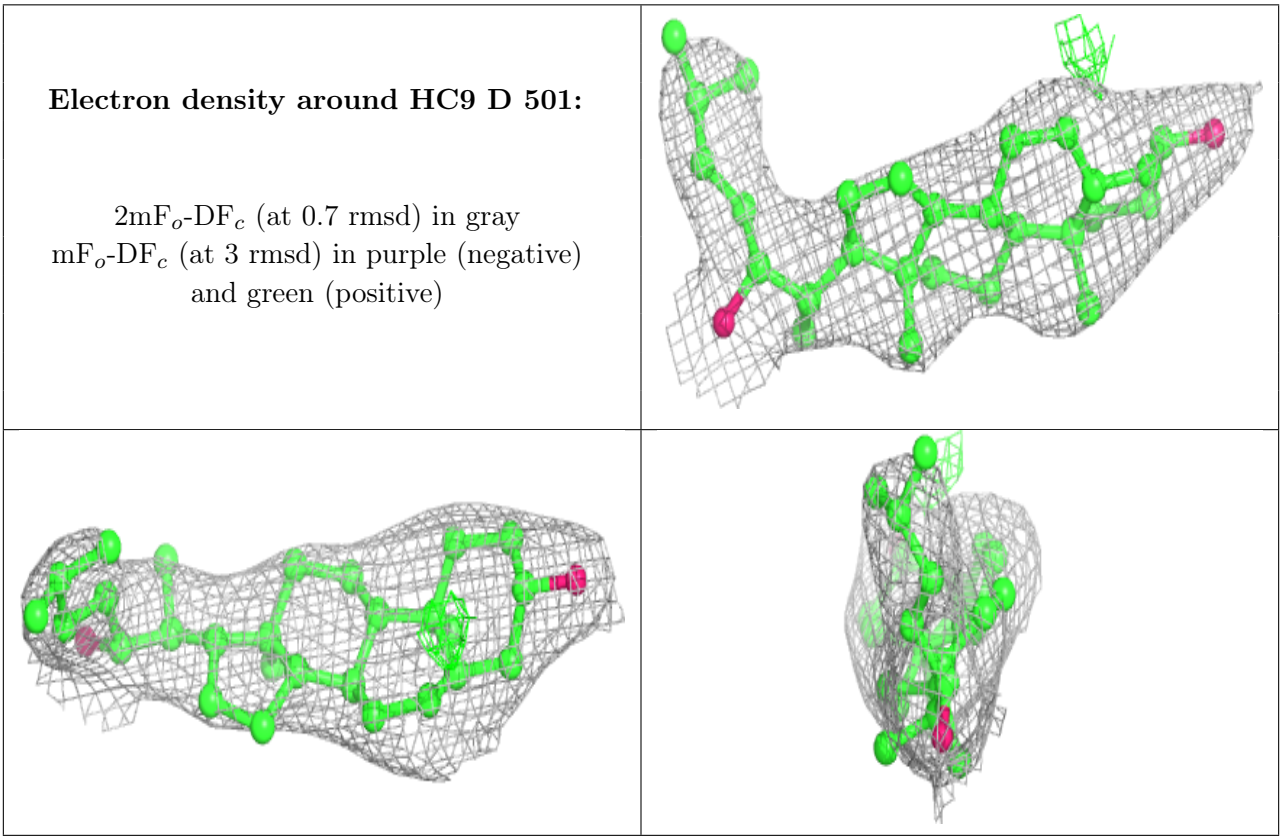
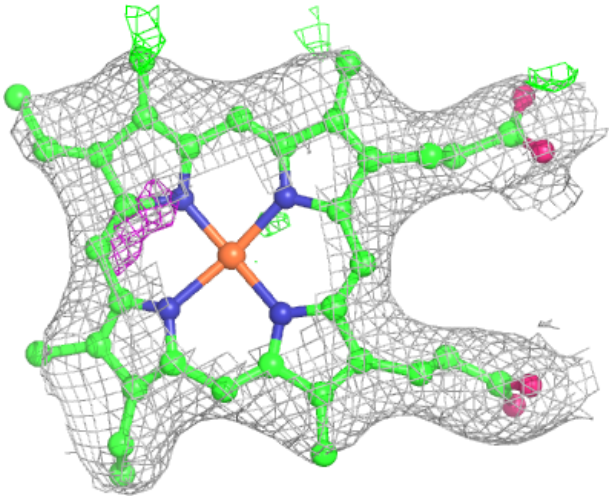
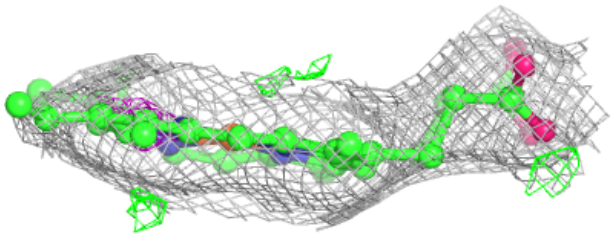
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

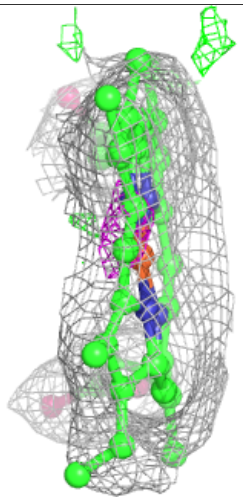


Electron density around HEM B 500:

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

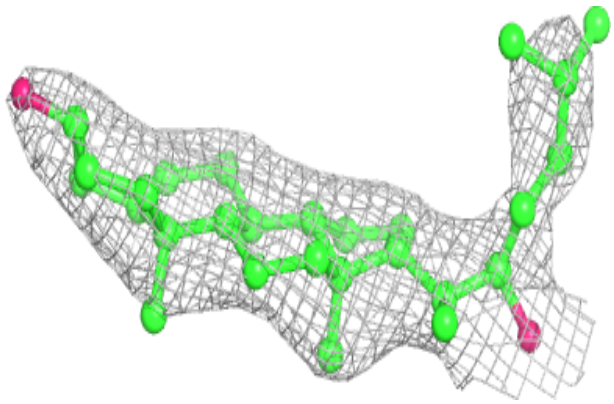


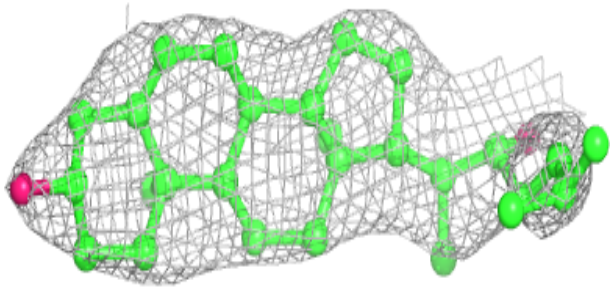


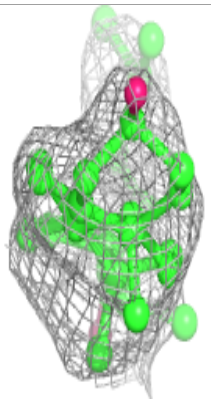


Electron density around HC9 C 501:

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

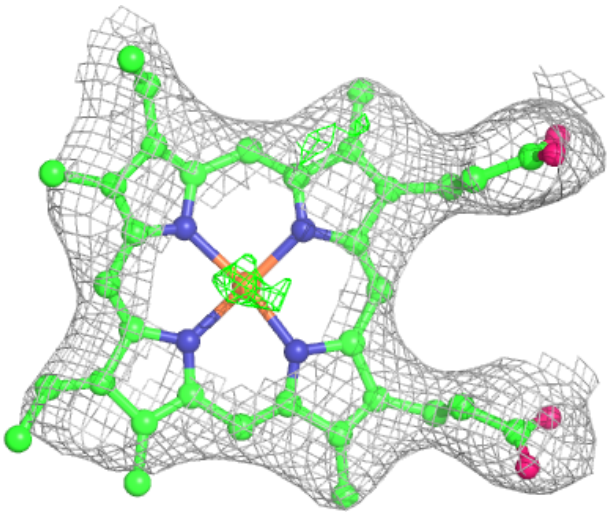


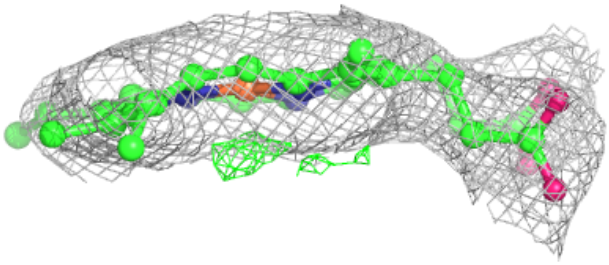


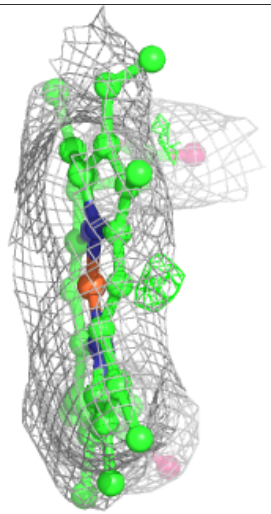


Electron density around HEM C 500:

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

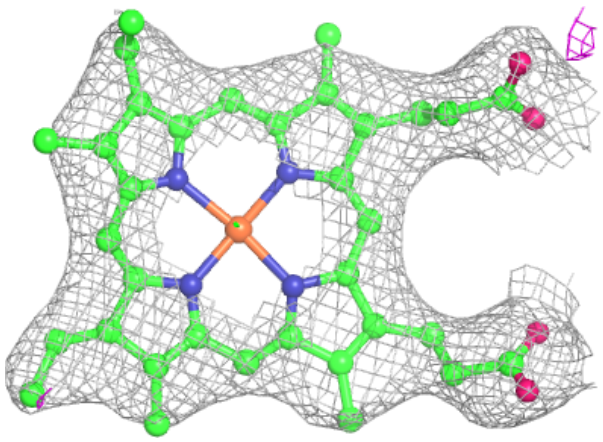


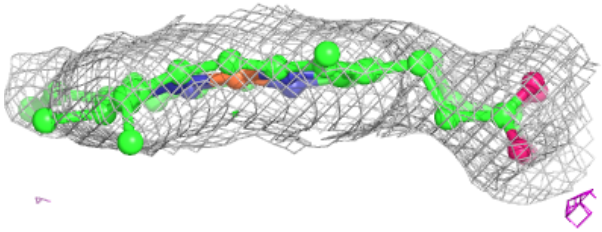


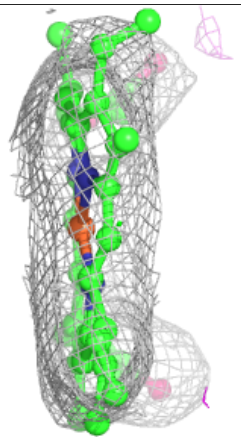


Electron density around HEM D 500:

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

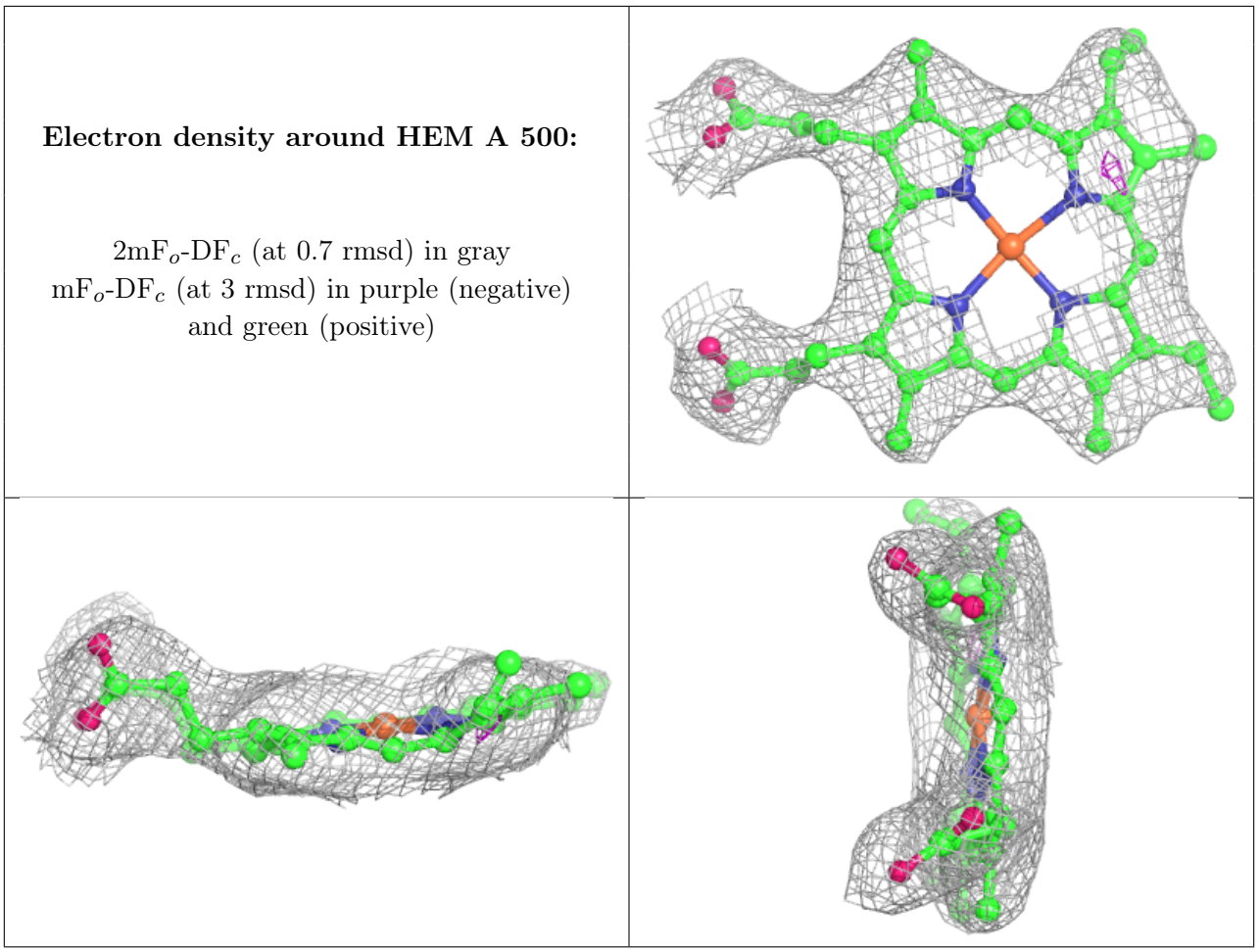






Electron density around HEM A 500:

$2mF_o$-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.