wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 10:21 PM EDT

PDB ID	:	4KLR / pdb_00004klr
Title	:	E343Q variant of human ferrochelatase
Authors	:	Lanzilotta, W.N.; Medlock, A.E.
Deposited on	:	2013-05-07
Resolution	:	2.18 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:

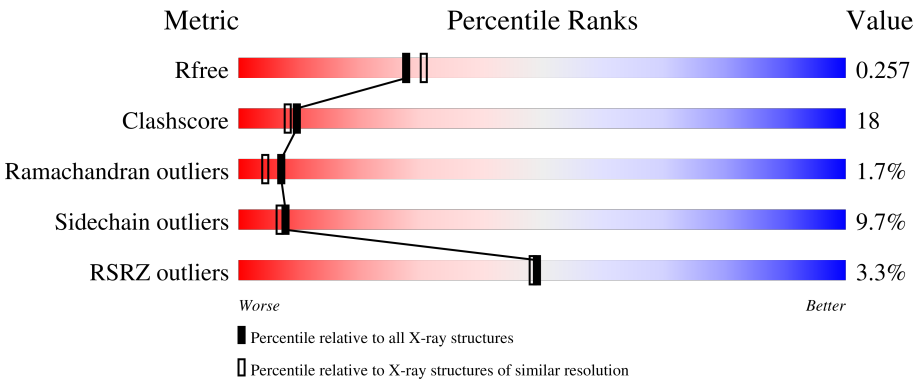
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	370	3% 65% 24% 7% • •
1	B	370	3% 68% 22% 5% • •

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
3	BCT	A	502	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6456 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.

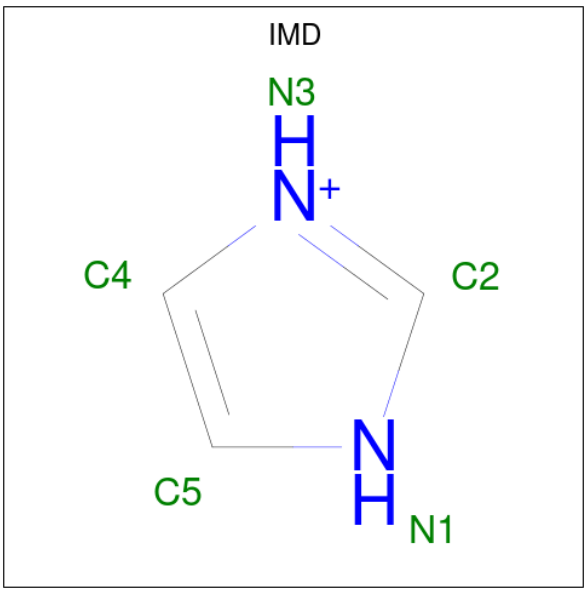
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2917	1858	510	531	18	0	4	0
1	B	359	2928	1864	510	534	20	0	6	0

There are 24 discrepancies between the modelled and reference sequences:

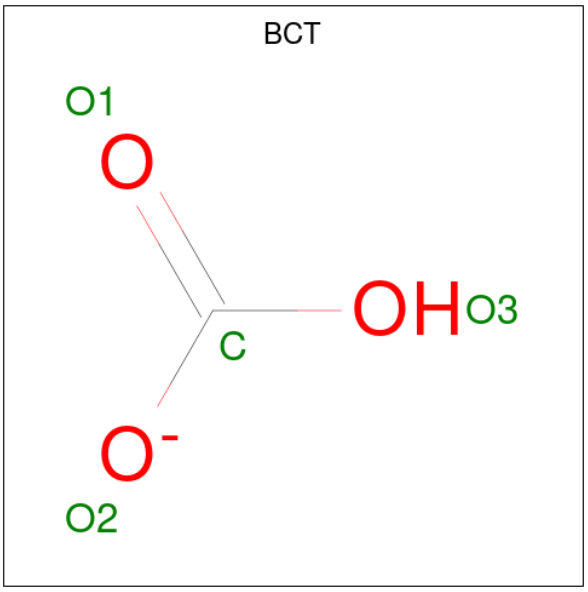
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	expression tag	UNP P22830
A	55	GLY	-	expression tag	UNP P22830
A	56	GLY	-	expression tag	UNP P22830
A	57	SER	-	expression tag	UNP P22830
A	58	HIS	-	expression tag	UNP P22830
A	59	HIS	-	expression tag	UNP P22830
A	60	HIS	-	expression tag	UNP P22830
A	61	HIS	-	expression tag	UNP P22830
A	62	HIS	-	expression tag	UNP P22830
A	63	HIS	-	expression tag	UNP P22830
A	64	GLY	-	expression tag	UNP P22830
A	343	GLN	GLU	engineered mutation	UNP P22830
B	54	MET	-	expression tag	UNP P22830
B	55	GLY	-	expression tag	UNP P22830
B	56	GLY	-	expression tag	UNP P22830
B	57	SER	-	expression tag	UNP P22830
B	58	HIS	-	expression tag	UNP P22830
B	59	HIS	-	expression tag	UNP P22830
B	60	HIS	-	expression tag	UNP P22830
B	61	HIS	-	expression tag	UNP P22830
B	62	HIS	-	expression tag	UNP P22830
B	63	HIS	-	expression tag	UNP P22830
B	64	GLY	-	expression tag	UNP P22830
B	343	GLN	GLU	engineered mutation	UNP P22830

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	5	3	2	0	0
2	B	1	5	3	2	0	0

- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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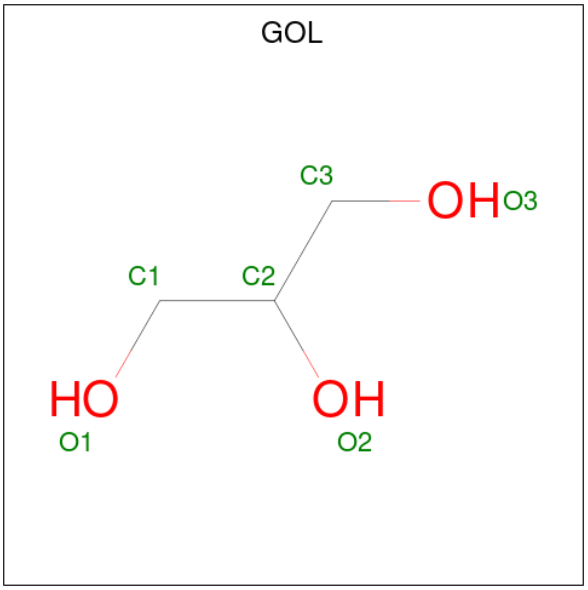
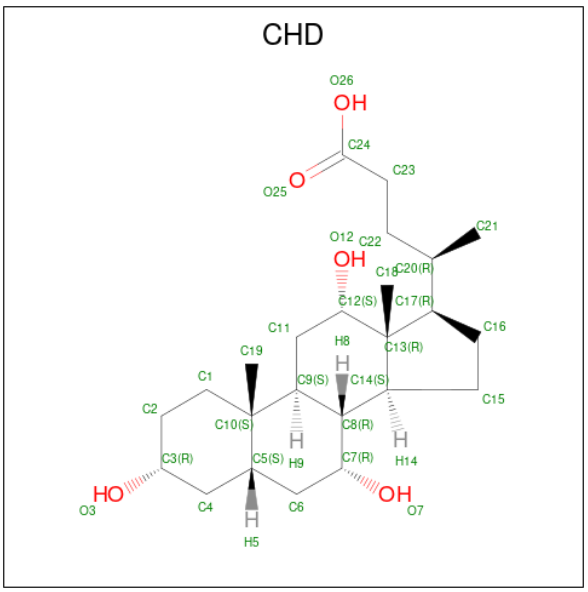
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	4	1	3	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	12	6	6	0	1

- Molecule 5 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).

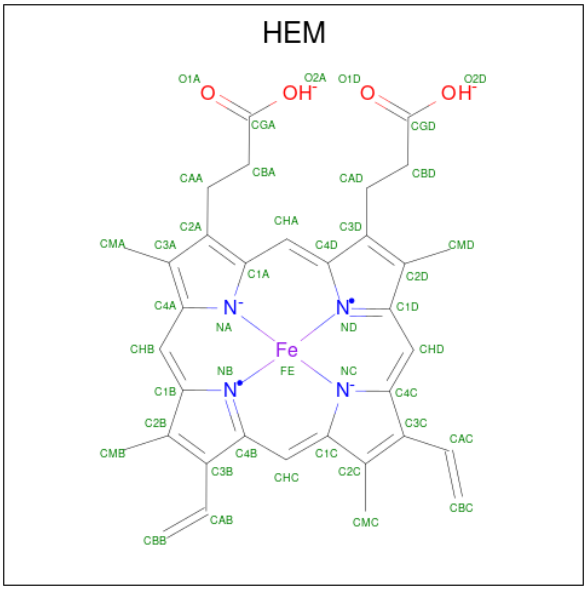


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			29	24	5			
5	A	1	Total	C	O		0	0
			29	24	5			
5	B	1	Total	C	O		0	0
			29	24	5			
5	B	1	Total	C	O		0	0
			29	24	5			
5	B	1	Total	C	O		0	0
			29	24	5			

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

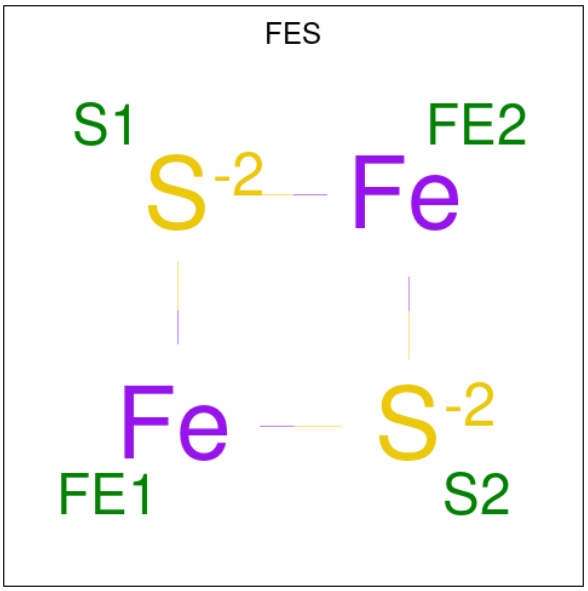
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	A	1	4	2	2	0	0
			Total	Fe	S		
8	B	1	4	2	2	0	0

- Molecule 9 is water.

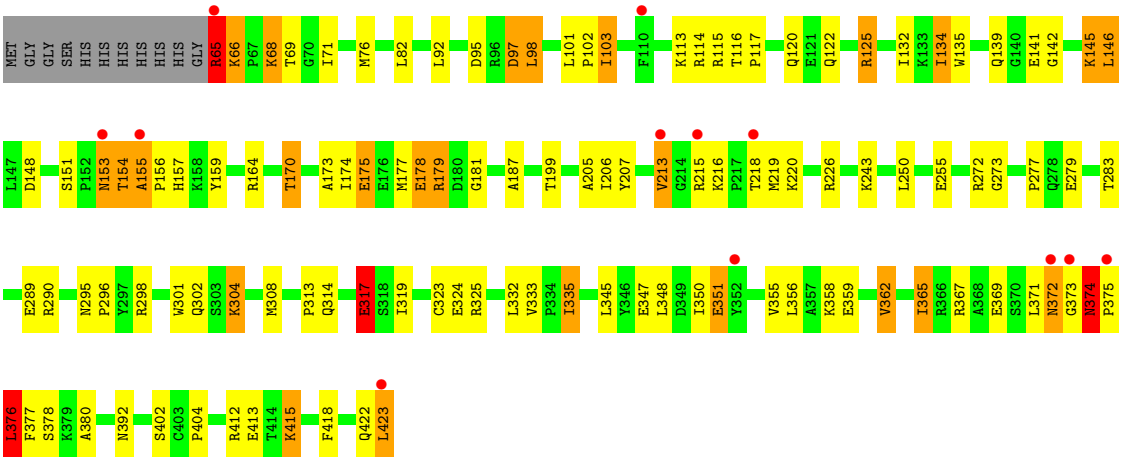
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	170	170	170	0	0
			Total	O		
9	B	171	171	171	0	0

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.

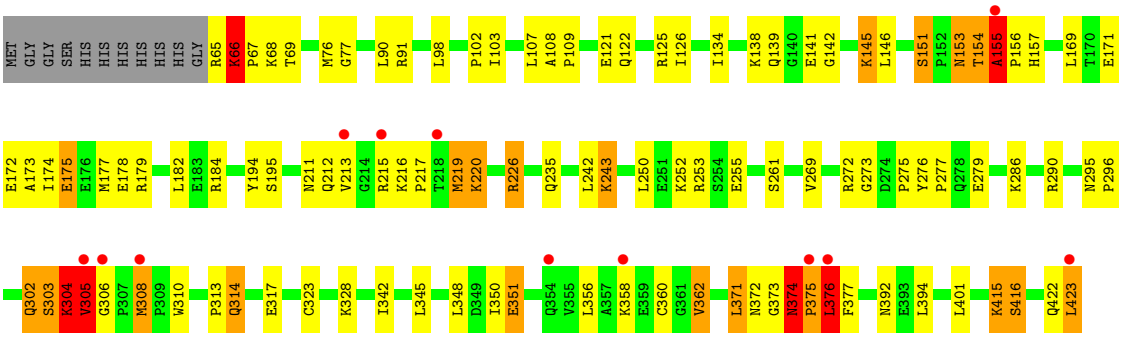
• Molecule 1: Ferrochelatase, mitochondrial

Chain A:



• Molecule 1: Ferrochelatase, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.13Å 92.56Å 109.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.18 70.62 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.71-2.18) 99.9 (70.62-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.200 , 0.258 0.198 , 0.257	Depositor DCC
R_{free} test set	2605 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6456	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 41.42 % 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 2.3685e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CL, GOL, HEM, BCT, CHD, FES, IMD

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	1.31	8/2996 (0.3%)	1.27	12/4056 (0.3%)
1	B	1.32	6/3010 (0.2%)	1.27	16/4076 (0.4%)
All	All	1.32	14/6006 (0.2%)	1.27	28/8132 (0.3%)

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	3
1	B	0	1
All	All	0	4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	305	VAL	CA-CB	8.53	1.66	1.54
1	B	172	GLU	CA-C	-6.49	1.44	1.52
1	B	174	ILE	CA-C	6.08	1.60	1.52
1	A	179	ARG	N-CA	5.63	1.53	1.46
1	B	269	VAL	CA-C	5.62	1.59	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	155	ALA	CA-C-N	-9.55	108.37	120.79
1	B	155	ALA	C-N-CA	-9.55	108.37	120.79
1	B	374	ASN	CA-C-N	8.34	130.26	119.84
1	B	374	ASN	C-N-CA	8.34	130.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	418	PHE	N-CA-C	7.78	119.54	111.14

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	THR	Peptide
1	A	371	LEU	Peptide
1	A	65	ARG	Peptide
1	B	154	THR	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	2917	0	2939	114	0
1	B	2928	0	2946	102	1
2	A	5	0	4	0	0
2	B	5	0	4	1	0
3	A	4	0	0	2	0
3	B	4	0	0	1	0
4	A	12	0	16	4	0
5	A	58	0	78	4	0
5	B	87	0	115	6	0
6	A	1	0	0	0	0
7	A	43	0	30	2	0
7	B	43	0	30	2	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
9	A	170	0	0	9	0
9	B	171	0	0	8	1
All	All	6456	0	6162	218	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 18.

The worst 5 of 218 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:A:125[A]:ARG:HB3	1:A:125[A]:ARG:NH1	1.53	1.23
1:A:304:LYS:CE	1:A:314[A]:GLN:HG2	1.79	1.11
1:A:155:ALA:HB1	1:A:156:PRO:HD2	1.16	1.10
1:A:125[A]:ARG:HH11	1:A:125[A]:ARG:CB	1.72	1.02
1:A:304:LYS:HE3	1:A:314[A]:GLN:HG2	1.02	1.01

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:B:125[A]:ARG:NH1	9:B:741:HOH:O[3_655]	2.02	0.18

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	361/370 (98%)	340 (94%)	17 (5%)	4 (1%)	11 9
1	B	363/370 (98%)	343 (94%)	11 (3%)	9 (2%)	4 2
All	All	724/740 (98%)	683 (94%)	28 (4%)	13 (2%)	7 4

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA
1	A	374	ASN
1	B	155	ALA
1	B	375	PRO
1	B	376	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	328/332 (99%)	292 (89%)	36 (11%)	6 5
1	B	330/332 (99%)	298 (90%)	32 (10%)	8 7
All	All	658/664 (99%)	590 (90%)	68 (10%)	8 6

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314[A]	GLN
1	B	345	LEU
1	B	415	LYS
1	A	317	GLU
1	A	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	GLN
1	B	421	GLN
1	A	374	ASN
1	A	421	GLN
1	B	122	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CHD	B	505	-	32,32,32	1.62	4 (12%)	51,51,51	2.61	19 (37%)
5	CHD	B	503	1	32,32,32	0.95	1 (3%)	51,51,51	2.28	20 (39%)
3	BCT	A	502	7	3,3,3	0.43	0	2,3,3	0.38	0
5	CHD	B	504	-	32,32,32	1.48	5 (15%)	51,51,51	4.12	29 (56%)
4	GOL	A	503[B]	-	5,5,5	0.27	0	5,5,5	1.01	0
2	IMD	B	501	7	5,5,5	0.80	0	5,5,5	1.67	2 (40%)
8	FES	A	508	1	0,4,4	-	-	-		
8	FES	B	507	1	0,4,4	-	-	-		
7	HEM	A	507	3,2	50,50,50	1.86	14 (28%)	67,82,82	1.58	10 (14%)
7	HEM	B	506	3,2	50,50,50	1.75	10 (20%)	67,82,82	1.48	12 (17%)
3	BCT	B	502	7	3,3,3	0.74	0	2,3,3	1.66	1 (50%)
5	CHD	A	504	-	32,32,32	0.91	0	51,51,51	1.88	15 (29%)
4	GOL	A	503[A]	-	5,5,5	0.19	0	5,5,5	1.08	0
2	IMD	A	501	7	5,5,5	0.45	0	5,5,5	0.86	0
5	CHD	A	505	-	32,32,32	0.79	0	51,51,51	1.71	12 (23%)

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
5	CHD	B	505	-	-	7/9/74/74	0/4/4/4
5	CHD	B	503	1	-	7/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHD	B	504	-	-	4/9/74/74	0/4/4/4
4	GOL	A	503[B]	-	-	1/4/4/4	-
2	IMD	B	501	7	-	-	0/1/1/1
8	FES	A	508	1	-	-	0/1/1/1
8	FES	B	507	1	-	-	0/1/1/1
7	HEM	A	507	3,2	-	3/14/54/54	-
7	HEM	B	506	3,2	-	4/14/54/54	-
5	CHD	A	504	-	-	6/9/74/74	0/4/4/4
4	GOL	A	503[A]	-	-	4/4/4/4	-
2	IMD	A	501	7	-	-	0/1/1/1
5	CHD	A	505	-	-	9/9/74/74	0/4/4/4

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	CHD	C16-C15	7.66	1.74	1.54
7	B	506	HEM	C3D-C2D	6.10	1.49	1.36
7	A	507	HEM	C3D-C2D	5.43	1.48	1.36
7	A	507	HEM	FE-NA	4.38	2.09	1.95
5	B	504	CHD	C10-C9	-3.88	1.49	1.56

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	504	CHD	C14-C8-C9	-10.26	95.43	109.75
5	B	504	CHD	C14-C13-C12	8.37	115.06	107.42
5	B	504	CHD	C17-C13-C14	-8.31	91.78	100.11
5	B	504	CHD	C1-C10-C5	7.83	118.99	107.75
5	B	504	CHD	C9-C11-C12	-7.72	104.20	114.29

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503[A]	GOL	O1-C1-C2-C3
4	A	503[A]	GOL	C1-C2-C3-O3
5	A	505	CHD	C21-C20-C22-C23
5	B	505	CHD	C16-C17-C20-C21
5	B	505	CHD	C13-C17-C20-C21

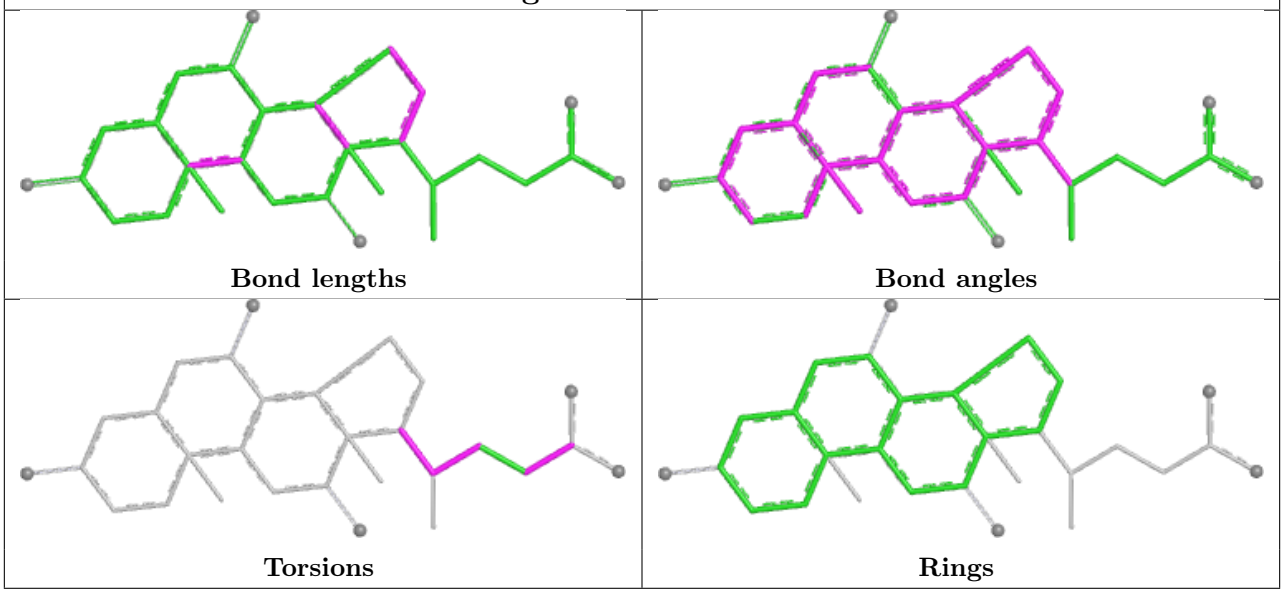
There are no ring outliers.

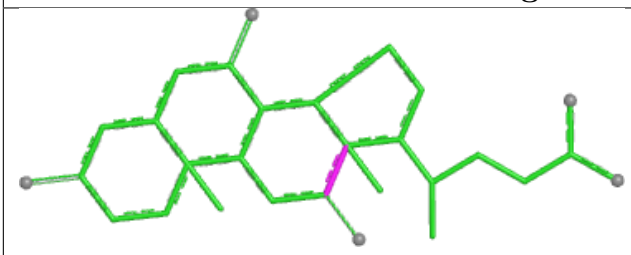
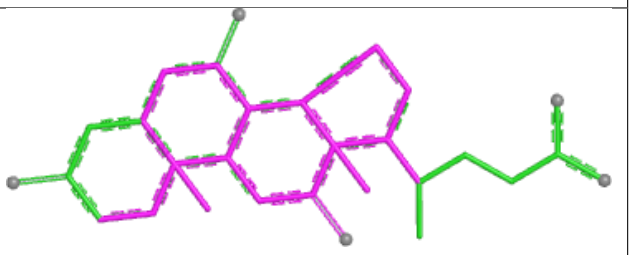
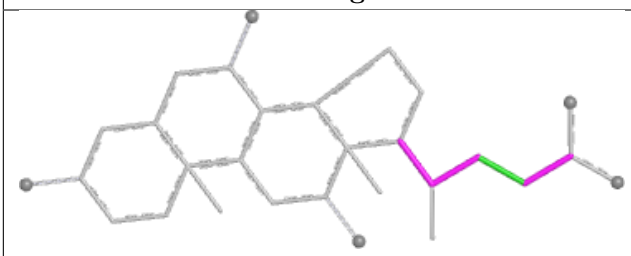
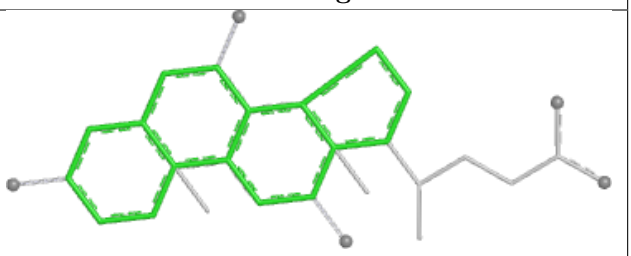
11 monomers are involved in 22 short contacts:

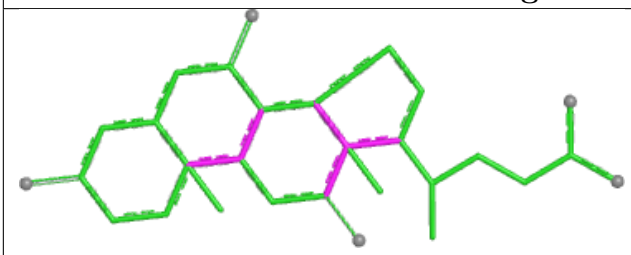
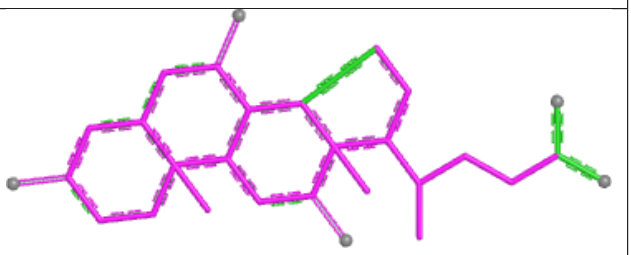
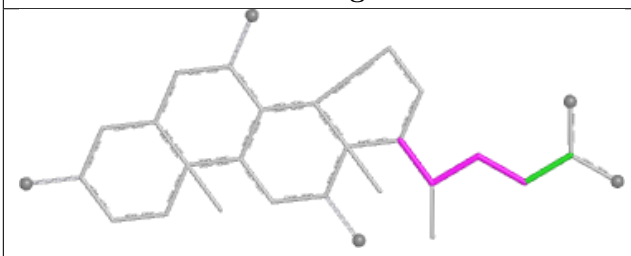
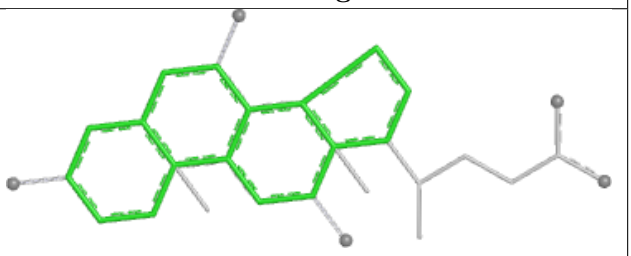
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	CHD	1	0
5	B	503	CHD	5	0
3	A	502	BCT	2	0
4	A	503[B]	GOL	1	0
2	B	501	IMD	1	0
7	A	507	HEM	2	0
7	B	506	HEM	2	0
3	B	502	BCT	1	0
5	A	504	CHD	3	0
4	A	503[A]	GOL	3	0
5	A	505	CHD	1	0

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

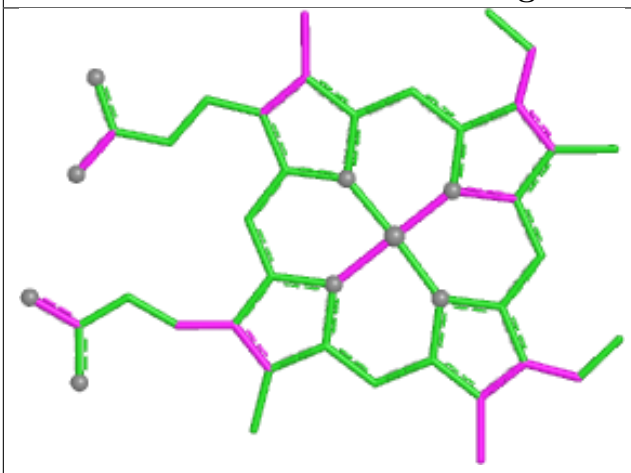
Ligand CHD B 505



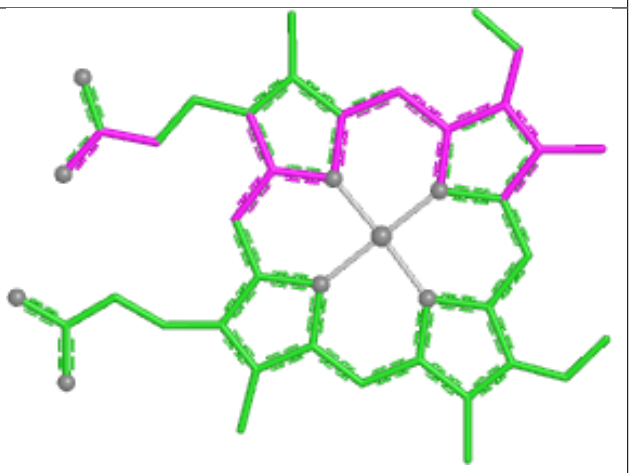
Ligand CHD B 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD B 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

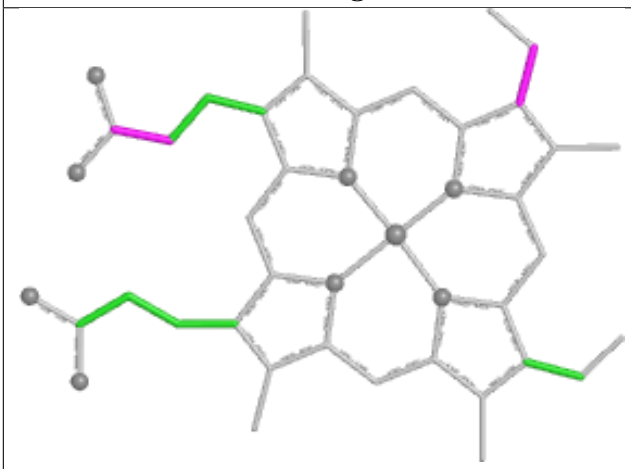
Ligand HEM A 507



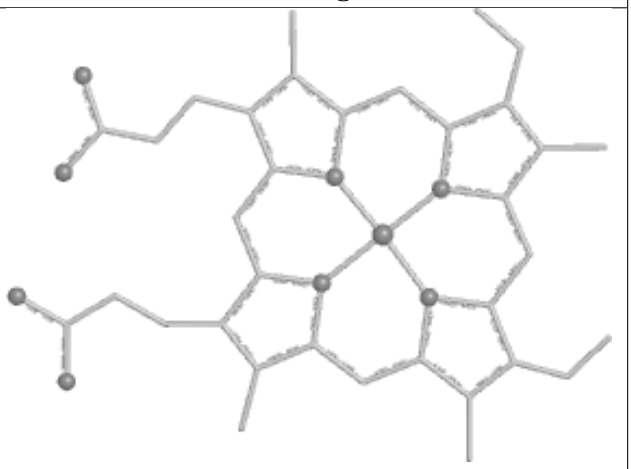
Bond lengths



Bond angles

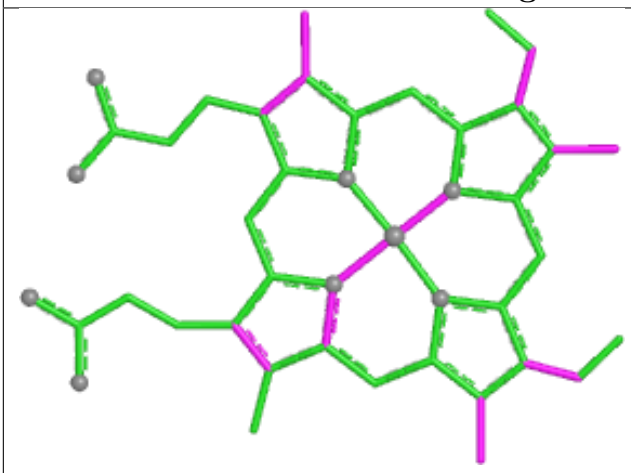


Torsions

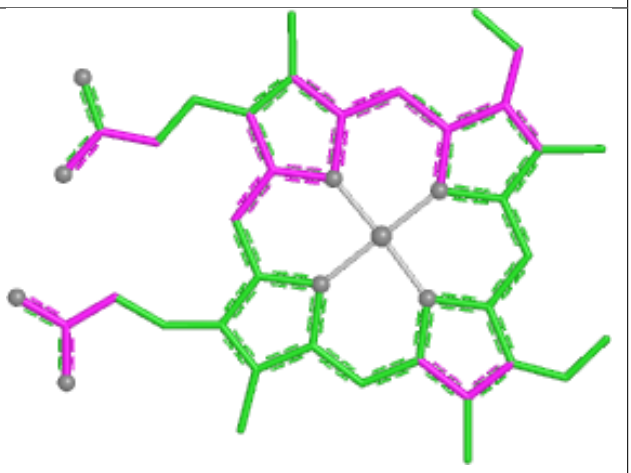


Rings

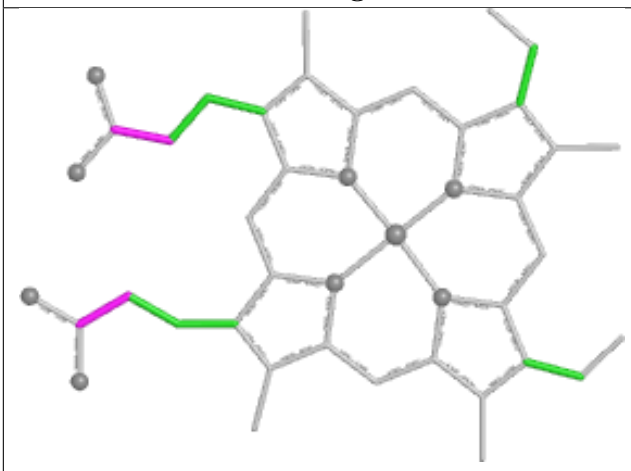
Ligand HEM B 506



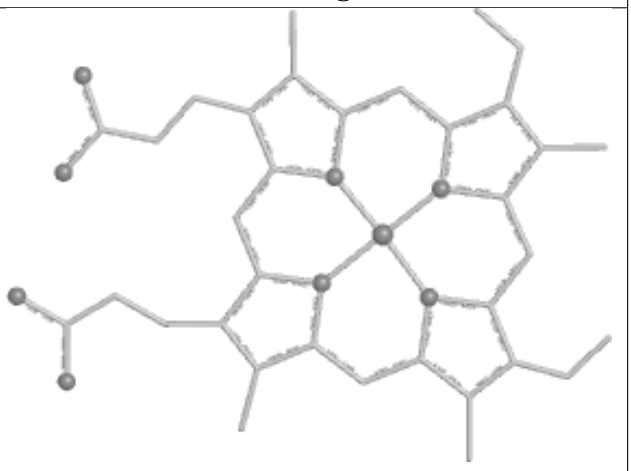
Bond lengths



Bond angles

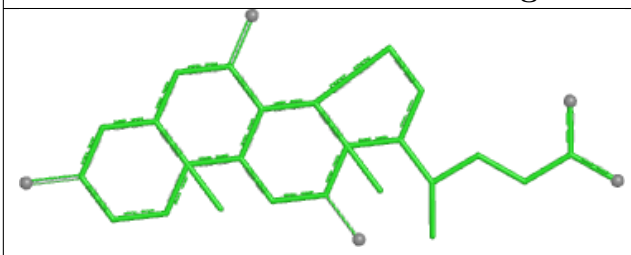


Torsions

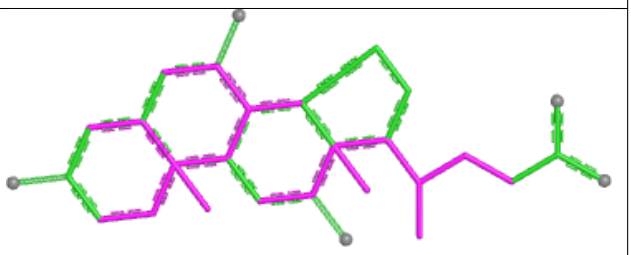


Rings

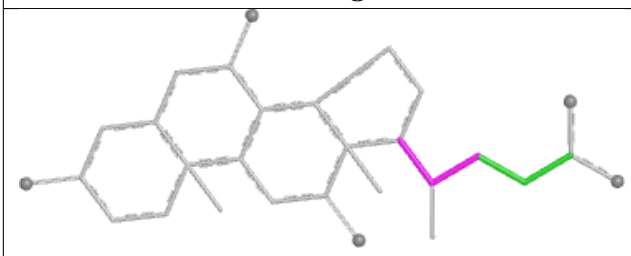
Ligand CHD A 504



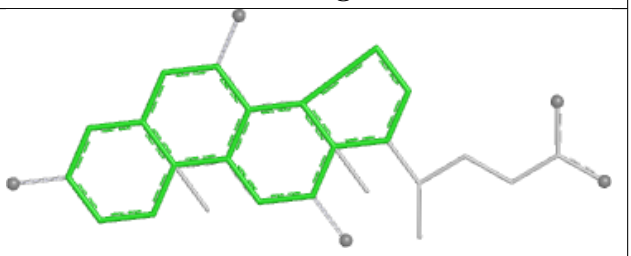
Bond lengths



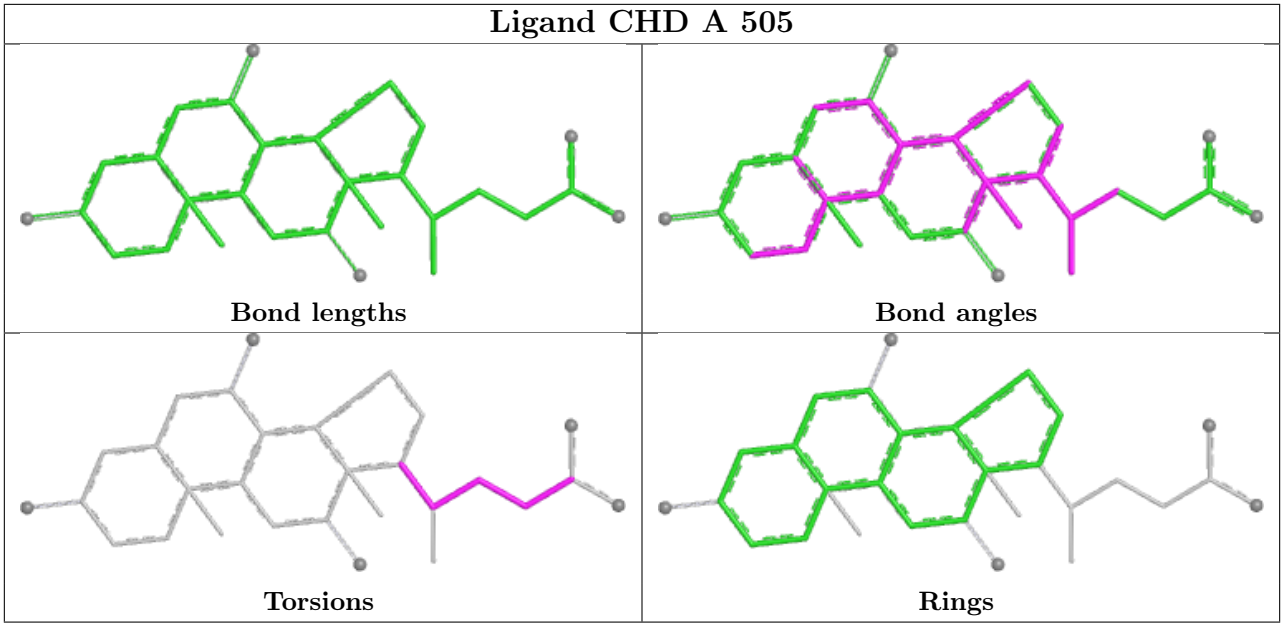
Bond angles



Torsions



Rings



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	359/370 (97%)	0.20	12 (3%)	49	48	9, 30, 52, 61	4 (1%)
1	B	359/370 (97%)	0.14	12 (3%)	49	48	8, 29, 51, 62	6 (1%)
All	All	718/740 (97%)	0.17	24 (3%)	49	48	8, 29, 51, 62	10 (1%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	4.7
1	B	305	VAL	4.6
1	B	213	VAL	3.8
1	B	308[A]	MET	3.5
1	B	423	LEU	3.4

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)

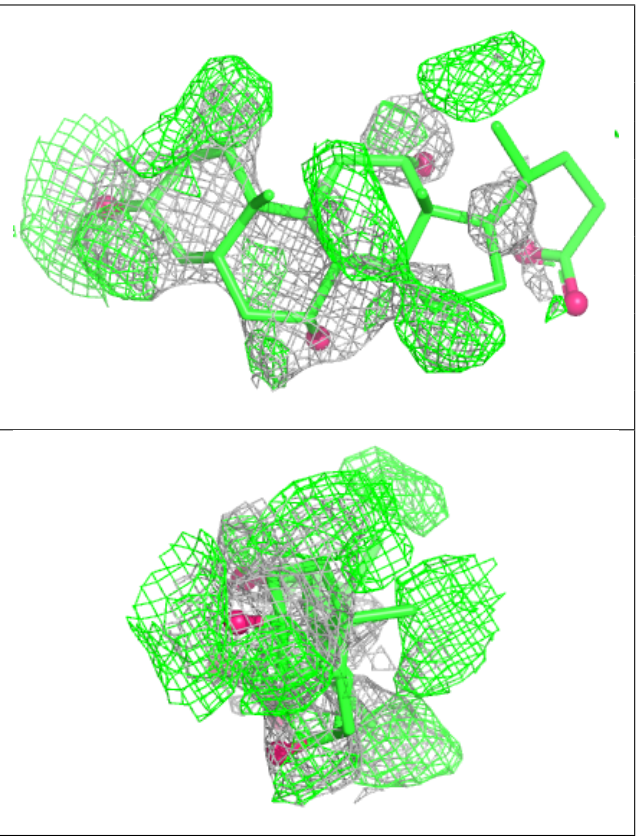
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CHD	B	505	29/29	0.68	0.40	66,68,69,70	29
5	CHD	B	503	29/29	0.73	0.19	69,78,87,88	0
5	CHD	B	504	29/29	0.74	0.36	46,47,50,50	29
5	CHD	A	504	29/29	0.77	0.16	52,58,74,75	0
5	CHD	A	505	29/29	0.81	0.14	62,64,76,76	0
3	BCT	B	502	4/4	0.85	0.14	37,38,39,41	0
3	BCT	A	502	4/4	0.88	0.12	36,36,38,40	0
6	CL	A	506	1/1	0.88	0.23	77,77,77,77	0
2	IMD	B	501	5/5	0.92	0.09	21,23,25,25	0
4	GOL	A	503[A]	6/6	0.93	0.07	10,12,14,16	6
4	GOL	A	503[B]	6/6	0.93	0.07	14,16,19,24	6
2	IMD	A	501	5/5	0.96	0.07	26,26,27,28	0
7	HEM	A	507	43/43	0.98	0.06	9,22,30,35	0
8	FES	A	508	4/4	0.98	0.05	26,26,26,28	0
8	FES	B	507	4/4	0.98	0.05	25,25,25,26	0
7	HEM	B	506	43/43	0.99	0.06	12,19,28,32	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 CHD B 505:

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 CHD B 503:

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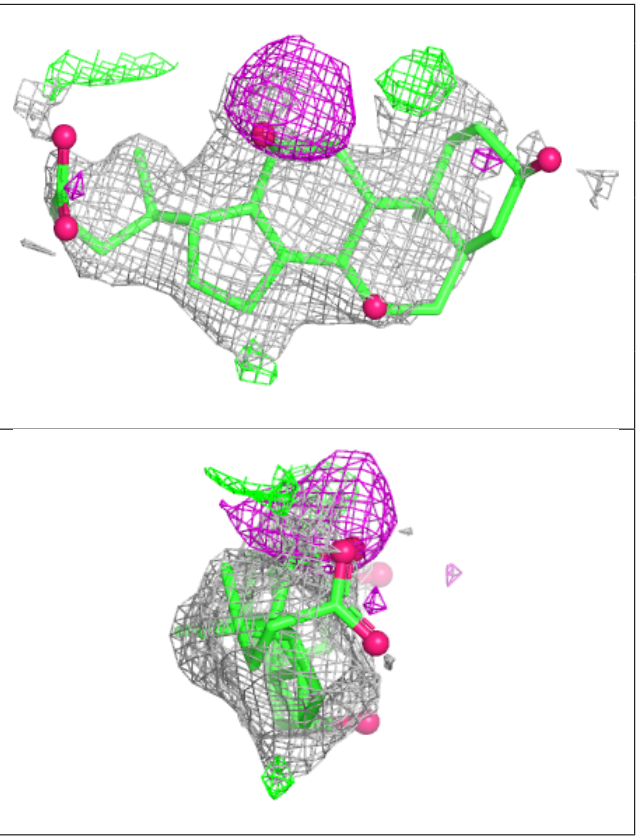
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CHD B 504:

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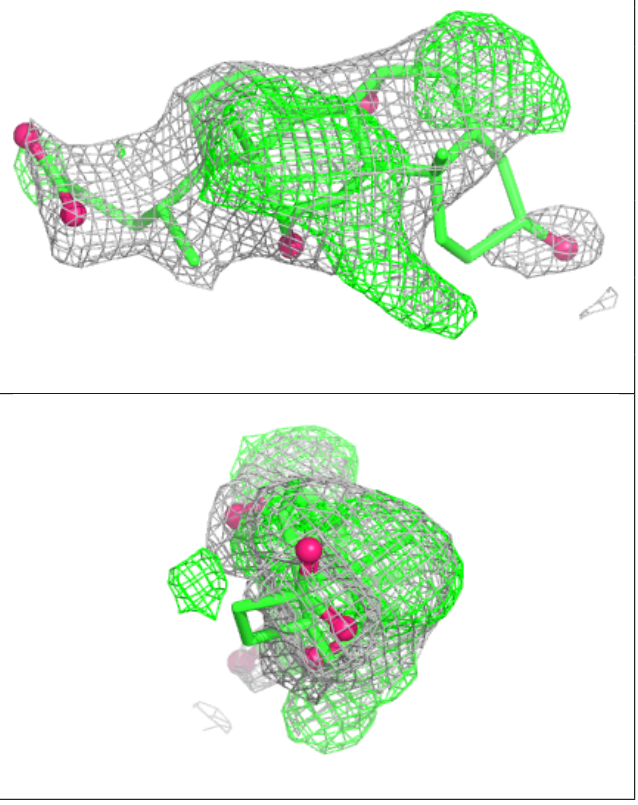
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CHD A 504:

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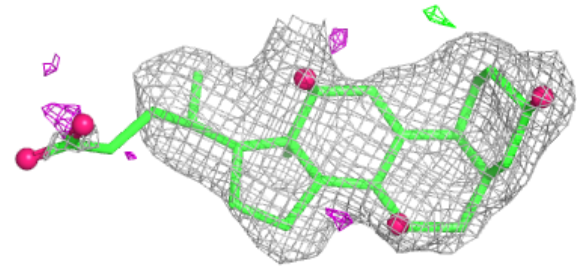
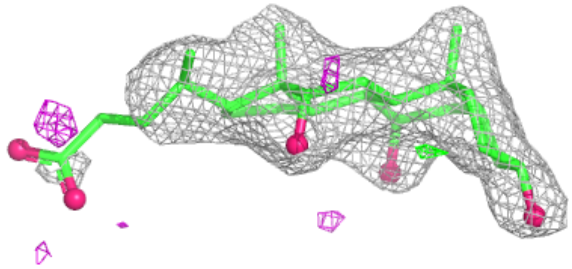
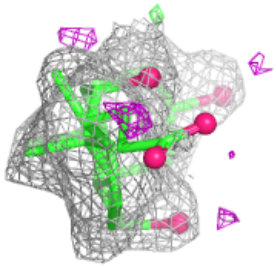
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

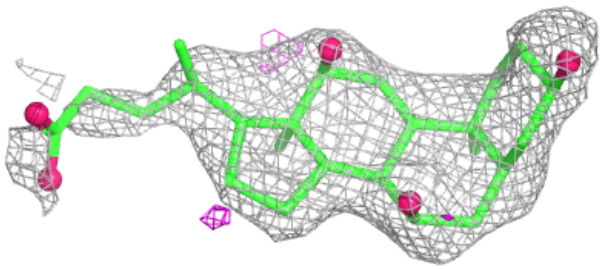


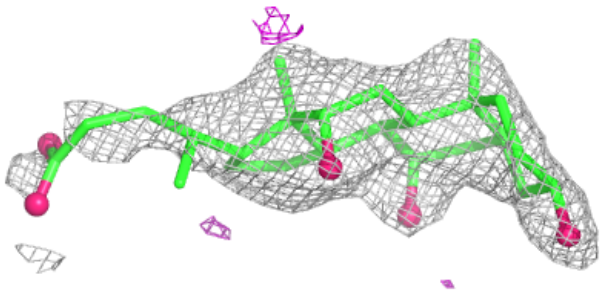


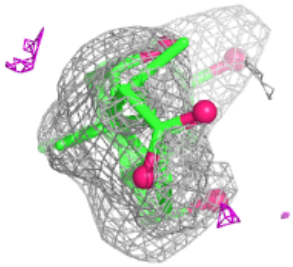


Electron density around CHD A 505:

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

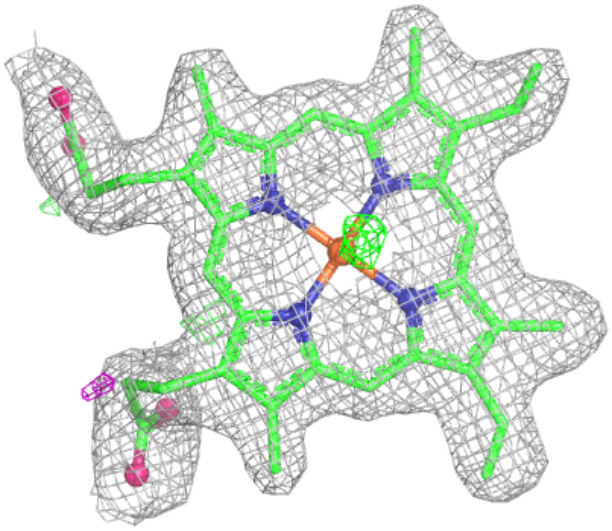


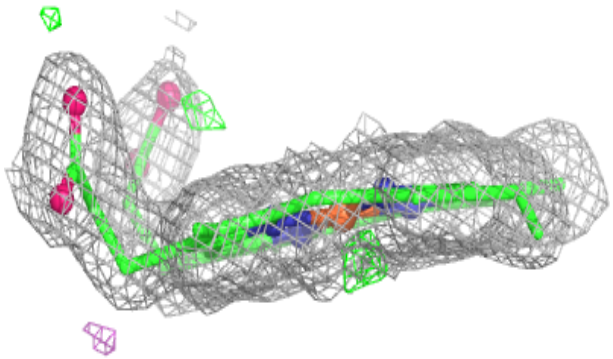




Electron density around HEM A 507:

$2mF_o$-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 506:

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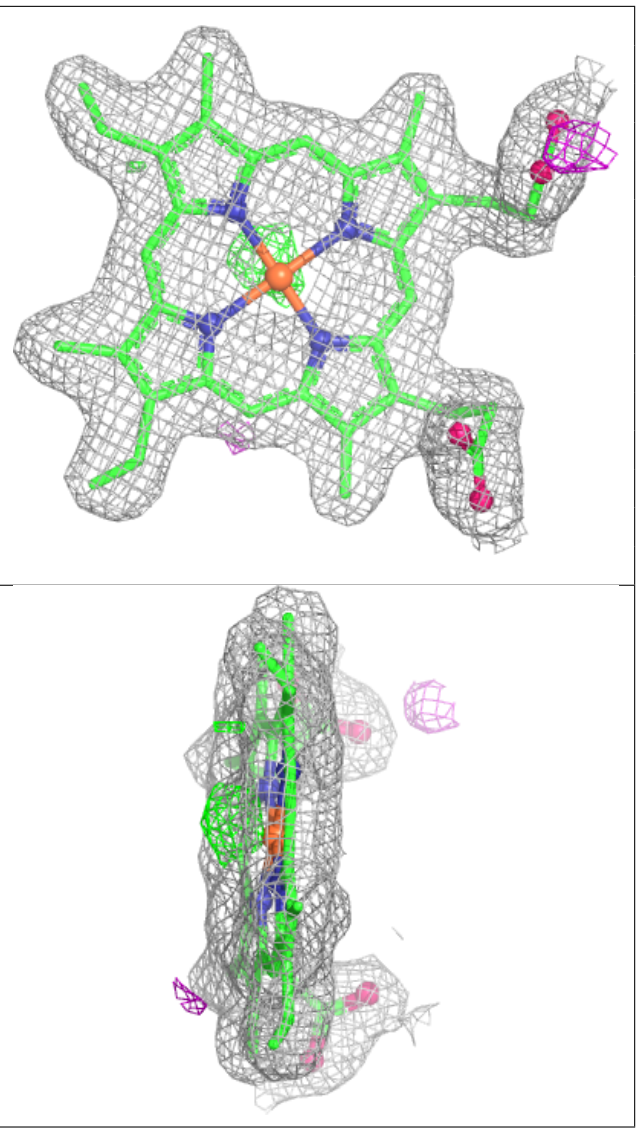
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.