Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2026 – 09:25 PM EDT

PDB ID	:	1FSX / pdb_00001fsx
Title	:	THE X-RAY STRUCTURE DETERMINATION OF BOVINE CARBON-MONOXY HB AT 2.1 A RESOLUTION AND ITS RELATIONSHIP TO THE QUATERNARY STRUCTURE OF OTHER HB CRYSTAL FORMS
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Deposited on	:	2000-09-11
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

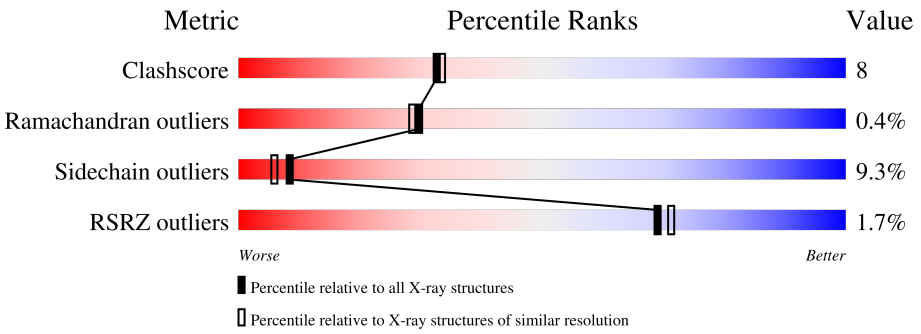
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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

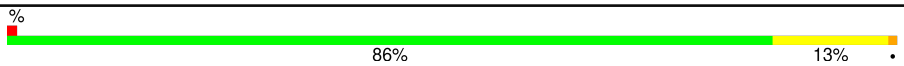
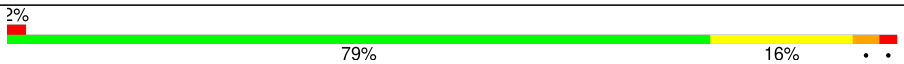
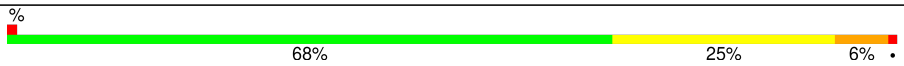
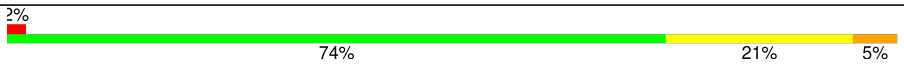
The reported resolution of this entry is 2.10 Å.

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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	141	
1	C	141	
2	B	145	
2	D	145	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4702 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.

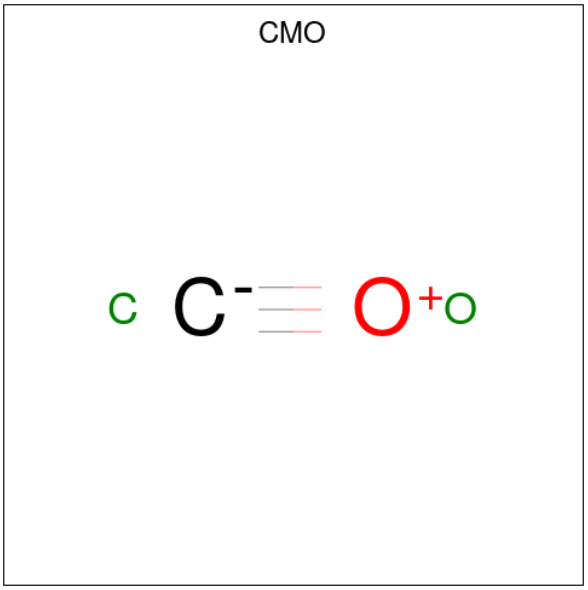
- Molecule 1 is a protein called HEMOGLOBIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1066	683	186	196	1	0	0	0
1	C	141	1066	683	186	196	1	0	0	0

- Molecule 2 is a protein called HEMOGLOBIN BETA CHAIN.

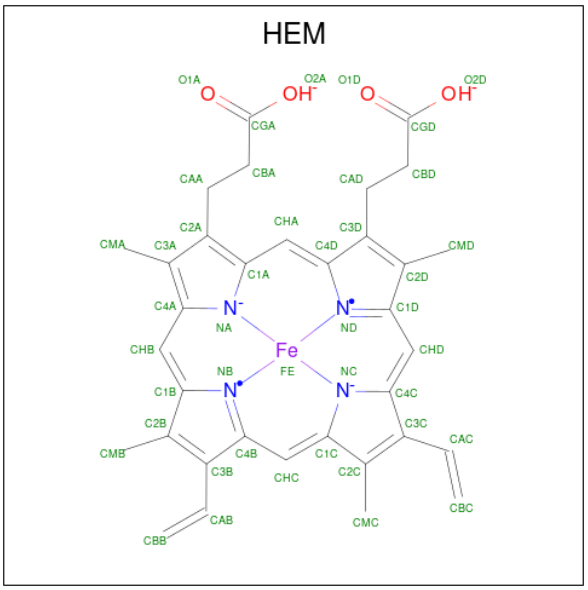
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	145	1127	726	194	203	4	0	0	0
2	D	145	1127	726	194	203	4	0	0	0

- Molecule 3 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 4 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		
4	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	D	1	43	34	1	4	4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	43	43	43	0	0

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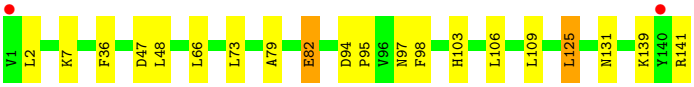
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	26	26	26	0	0
			Total	O		
5	C	38	38	38	0	0
			Total	O		
5	D	29	29	29	0	0

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.

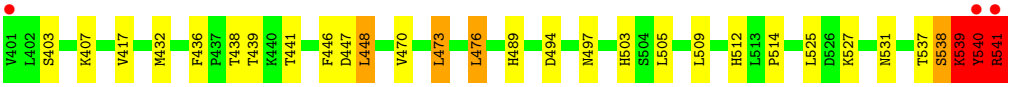
• Molecule 1: HEMOGLOBIN ALPHA CHAIN

Chain A:



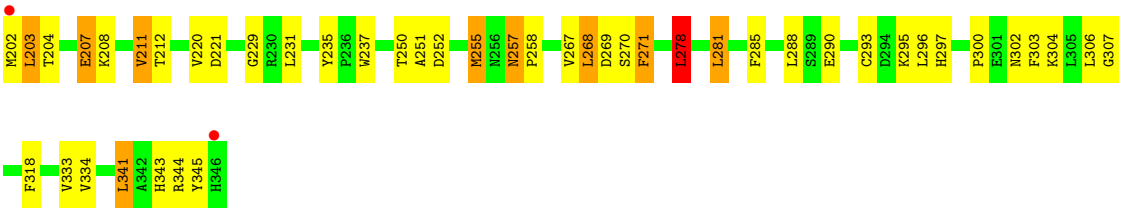
• Molecule 1: HEMOGLOBIN ALPHA CHAIN

Chain C:



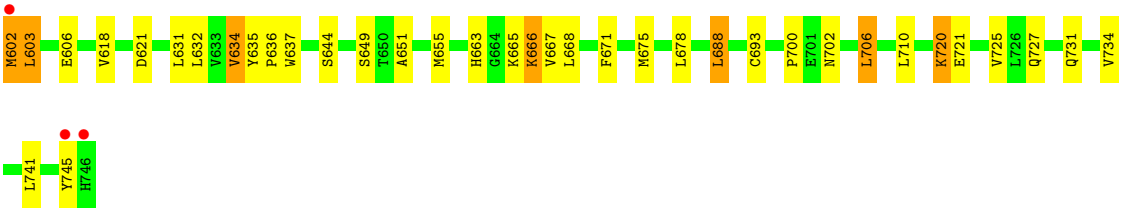
• Molecule 2: HEMOGLOBIN BETA CHAIN

Chain B:



• Molecule 2: HEMOGLOBIN BETA CHAIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.41Å 110.63Å 65.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.50 – 2.10 64.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.50-2.10) 95.4 (64.50-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 1.94Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.205 , 0.254 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4702	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.82% 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, CMO

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	0.64	0/1093	1.05	4/1483 (0.3%)
1	C	0.65	0/1093	1.07	10/1483 (0.7%)
2	B	0.63	1/1152 (0.1%)	1.05	8/1556 (0.5%)
2	D	0.61	0/1152	1.04	5/1556 (0.3%)
All	All	0.63	1/4490 (0.0%)	1.05	27/6078 (0.4%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	255	MET	SD-CE	-6.89	1.62	1.79

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	540	TYR	N-CA-C	7.70	127.21	110.80
1	C	447	ASP	N-CA-C	-7.26	97.42	108.96
1	A	47	ASP	N-CA-C	-7.13	96.01	108.20
2	D	649	SER	N-CA-C	7.03	121.48	112.34
2	D	618	VAL	N-CA-C	6.76	118.55	108.54
2	B	207	GLU	N-CA-C	-6.70	103.90	111.14
1	C	539	LYS	CA-C-N	6.68	134.29	121.54
1	C	539	LYS	C-N-CA	6.68	134.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	436	PHE	CA-C-N	6.46	126.97	119.47
1	C	436	PHE	C-N-CA	6.46	126.97	119.47
2	D	635	TYR	CA-C-N	6.34	127.76	119.84
2	D	635	TYR	C-N-CA	6.34	127.76	119.84
1	A	36	PHE	CA-C-N	6.23	126.69	119.47
1	A	36	PHE	C-N-CA	6.23	126.69	119.47
2	B	235	TYR	CA-C-N	6.13	127.50	119.84
2	B	235	TYR	C-N-CA	6.13	127.50	119.84
1	C	494	ASP	CA-C-N	6.06	126.50	119.47
1	C	494	ASP	C-N-CA	6.06	126.50	119.47
2	B	269	ASP	N-CA-C	-5.91	104.92	111.36
2	B	293	CYS	N-CA-C	5.70	118.59	111.24
1	A	79	ALA	N-CA-C	5.57	118.28	111.82
2	D	634	VAL	N-CA-C	5.34	116.11	110.72
1	C	538	SER	N-CA-C	5.29	118.89	112.23
1	C	417	VAL	N-CA-C	-5.28	105.35	110.42
2	B	257	ASN	CA-C-N	5.05	124.66	119.05
2	B	257	ASN	C-N-CA	5.05	124.66	119.05
2	B	318	PHE	N-CA-C	5.03	119.56	113.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	541	ARG	Sidechain

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	1066	0	1069	9	0
1	C	1066	0	1066	18	0
2	B	1127	0	1129	25	0
2	D	1127	0	1129	22	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	1	0
4	C	43	0	30	0	0
4	D	43	0	30	2	0
5	A	43	0	0	1	0
5	B	26	0	0	0	0
5	C	38	0	0	1	0
5	D	29	0	0	2	0
All	All	4702	0	4513	72	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 8.

All (72) 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:C:541:ARG:HD2	5:C:809:HOH:O	1.57	1.02
1:C:541:ARG:HG3	1:C:541:ARG:NH1	1.75	0.99
1:C:541:ARG:HG3	1:C:541:ARG:HH11	1.23	0.98
2:D:693:CYS:SG	2:D:745:TYR:CE2	2.67	0.87
1:C:537:THR:O	1:C:541:ARG:O	1.97	0.82
2:D:602:MET:SD	2:D:603:LEU:N	2.55	0.80
2:B:229:GLY:C	2:B:255:MET:HE1	2.11	0.74
2:D:666:LYS:HD3	4:D:748:HEM:HBA2	1.73	0.70
2:D:693:CYS:SG	2:D:745:TYR:CD2	2.82	0.70
1:C:539:LYS:O	1:C:539:LYS:HG3	1.93	0.68
2:B:203:LEU:HD12	2:B:207:GLU:HB3	1.80	0.64
2:D:721:GLU:HG2	5:D:849:HOH:O	1.97	0.64
2:D:621:ASP:HA	2:D:665:LYS:HD3	1.81	0.63
2:D:688:LEU:HD21	4:D:748:HEM:HMA1	1.82	0.62
1:A:82:GLU:H	1:A:82:GLU:CD	2.05	0.62
1:A:141:ARG:HE	1:C:527:LYS:HD3	1.68	0.58
2:B:290:GLU:HG2	2:B:344:ARG:HE	1.68	0.57
2:B:203:LEU:HD12	2:B:207:GLU:CB	2.35	0.56
1:C:438:THR:O	1:C:441:THR:HB	2.06	0.55
1:C:538:SER:C	1:C:540:TYR:H	2.15	0.54
2:D:631:LEU:HD22	2:D:706:LEU:HG	1.91	0.53
1:C:503:HIS:HE1	2:D:731:GLN:OE1	1.93	0.52
2:B:285:PHE:HD2	2:B:288:LEU:HD12	1.75	0.52
1:C:541:ARG:HH11	1:C:541:ARG:CG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:LEU:HB2	2:B:207:GLU:OE2	2.09	0.52
1:C:470:VAL:HA	1:C:473:LEU:HD13	1.91	0.51
1:A:103:HIS:HD2	5:A:838:HOH:O	1.93	0.51
1:C:489:HIS:HB2	1:C:539:LYS:HD3	1.94	0.50
1:A:139:LYS:O	1:A:139:LYS:HD3	2.11	0.50
1:C:446:PHE:HB3	1:C:448:LEU:HD13	1.94	0.49
2:D:651:ALA:O	2:D:655:MET:HG2	2.12	0.49
2:D:720:LYS:NZ	2:D:720:LYS:HA	2.27	0.49
2:B:267:VAL:O	2:B:270:SER:HB3	2.13	0.49
2:D:637:TRP:HE1	2:D:702:ASN:HD21	1.61	0.49
2:B:237:TRP:HE1	2:B:302:ASN:HD21	1.60	0.48
2:B:231:LEU:HD22	2:B:306:LEU:HD23	1.94	0.48
2:B:307:GLY:HA3	2:B:334:VAL:HG13	1.95	0.48
2:D:663:HIS:O	2:D:667:VAL:HG23	2.14	0.47
2:B:220:VAL:HG13	2:B:268:LEU:CB	2.46	0.46
2:B:300:PRO:HA	2:B:303:PHE:CE2	2.50	0.46
1:C:512:HIS:C	1:C:514:PRO:HD3	2.40	0.46
2:D:700:PRO:HG3	2:D:745:TYR:CD2	2.50	0.46
2:D:671:PHE:O	2:D:675:MET:HG2	2.15	0.46
2:B:208:LYS:HE3	2:B:208:LYS:HB2	1.75	0.45
1:A:125:LEU:HD13	1:A:125:LEU:HA	1.78	0.45
2:B:220:VAL:HG13	2:B:268:LEU:HB3	1.98	0.45
2:D:666:LYS:HA	2:D:666:LYS:HE2	2.00	0.43
2:B:250:THR:HG22	2:B:252:ASP:H	1.84	0.43
1:C:403:SER:O	1:C:407:LYS:HG3	2.18	0.43
1:A:2:LEU:O	1:A:7:LYS:HE3	2.18	0.43
1:A:106:LEU:HD21	1:A:125:LEU:HB3	2.00	0.43
1:A:94:ASP:HB3	1:A:97:ASN:ND2	2.34	0.43
2:B:278:LEU:HD12	2:B:278:LEU:HA	1.86	0.43
2:B:296:LEU:O	2:B:297:HIS:HB2	2.19	0.43
2:B:251:ALA:O	2:B:255:MET:HG2	2.19	0.43
2:D:720:LYS:HA	2:D:720:LYS:HZ2	1.82	0.43
2:D:727:GLN:O	2:D:731:GLN:HG2	2.18	0.43
2:B:204:THR:OG1	2:B:207:GLU:HG3	2.18	0.43
1:C:439:THR:HG22	1:C:497:ASN:OD1	2.18	0.42
2:B:211:VAL:HG12	2:B:212:THR:N	2.35	0.42
2:D:634:VAL:C	2:D:636:PRO:HD3	2.43	0.42
2:B:302:ASN:HB3	4:B:348:HEM:HMC1	2.02	0.42
2:B:257:ASN:HA	2:B:258:PRO:HD3	1.91	0.42
1:C:432:MET:HE2	1:C:432:MET:HB3	1.89	0.42
2:D:688:LEU:HD12	2:D:688:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:678:LEU:HD23	2:D:678:LEU:HA	1.88	0.41
1:C:476:LEU:HD12	1:C:476:LEU:HA	1.89	0.41
2:D:725:VAL:HG22	5:D:899:HOH:O	2.21	0.41
1:A:95:PRO:HA	1:A:98:PHE:HD2	1.85	0.41
2:B:285:PHE:HB3	2:B:341:LEU:HD22	2.03	0.41
2:B:281:LEU:HD12	2:B:281:LEU:HA	1.94	0.40
2:B:268:LEU:HA	2:B:271:PHE:HB2	2.02	0.40

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	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	C	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
2	B	143/145 (99%)	140 (98%)	2 (1%)	1 (1%)	18	15
2	D	143/145 (99%)	139 (97%)	3 (2%)	1 (1%)	18	15
All	All	564/572 (99%)	551 (98%)	11 (2%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	278	LEU
2	D	603	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	112/112 (100%)	105 (94%)	7 (6%)	16 14
1	C	112/112 (100%)	102 (91%)	10 (9%)	9 6
2	B	118/118 (100%)	104 (88%)	14 (12%)	5 3
2	D	118/118 (100%)	106 (90%)	12 (10%)	7 4
All	All	460/460 (100%)	417 (91%)	43 (9%)	8 6

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	66	LEU
1	A	73	LEU
1	A	82	GLU
1	A	109	LEU
1	A	125	LEU
1	A	131	ASN
2	B	202	MET
2	B	203	LEU
2	B	211	VAL
2	B	221	ASP
2	B	268	LEU
2	B	271	PHE
2	B	278	LEU
2	B	281	LEU
2	B	295	LYS
2	B	304	LYS
2	B	333	VAL
2	B	341	LEU
2	B	343	HIS
2	B	345	TYR
1	C	448	LEU
1	C	473	LEU
1	C	476	LEU
1	C	505	LEU
1	C	509	LEU
1	C	525	LEU
1	C	531	ASN
1	C	539	LYS
1	C	540	TYR

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Mol	Chain	Res	Type
1	C	541	ARG
2	D	602	MET
2	D	606	GLU
2	D	632	LEU
2	D	644	SER
2	D	666	LYS
2	D	668	LEU
2	D	688	LEU
2	D	706	LEU
2	D	710	LEU
2	D	720	LYS
2	D	734	VAL
2	D	741	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
2	B	263	HIS
2	B	273	ASN
2	B	302	ASN
2	B	339	ASN
1	C	409	ASN
1	C	472	HIS
1	C	503	HIS
2	D	673	ASN
2	D	702	ASN
2	D	746	HIS

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)

8 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	CMO	D	747	-	0,1,1	-	-	-		
4	HEM	D	748	2	50,50,50	1.52	10 (20%)	67,82,82	1.24	6 (8%)
3	CMO	B	347	-	0,1,1	-	-	-		
4	HEM	C	543	1	50,50,50	1.73	8 (16%)	67,82,82	1.12	7 (10%)
3	CMO	A	142	-	0,1,1	-	-	-		
4	HEM	A	143	1	50,50,50	1.78	13 (26%)	67,82,82	1.26	8 (11%)
3	CMO	C	542	-	0,1,1	-	-	-		
4	HEM	B	348	2	50,50,50	1.65	13 (26%)	67,82,82	1.27	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	D	748	2	-	5/14/54/54	-
4	HEM	C	543	1	-	6/14/54/54	-
4	HEM	A	143	1	-	4/14/54/54	-
4	HEM	B	348	2	-	6/14/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	543	HEM	FE-NC	5.85	2.14	1.95
4	C	543	HEM	FE-NB	5.74	2.12	1.94
4	A	143	HEM	FE-ND	5.65	2.12	1.94
4	B	348	HEM	FE-NA	4.13	2.08	1.95
4	D	748	HEM	FE-NB	3.94	2.07	1.94
4	A	143	HEM	C3C-C2C	3.87	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	543	HEM	CAB-C3B	-3.81	1.37	1.47
4	B	348	HEM	FE-NC	3.62	2.07	1.95
4	A	143	HEM	CBC-CAC	3.38	1.46	1.30
4	B	348	HEM	CBB-CAB	3.35	1.46	1.30
4	D	748	HEM	CBB-CAB	3.29	1.46	1.30
4	B	348	HEM	CBC-CAC	3.27	1.46	1.30
4	C	543	HEM	CAC-C3C	-3.23	1.38	1.47
4	D	748	HEM	CBC-CAC	3.15	1.45	1.30
4	D	748	HEM	CAC-C3C	-3.04	1.39	1.47
4	D	748	HEM	FE-ND	2.97	2.04	1.94
4	A	143	HEM	FE-NA	2.92	2.04	1.95
4	A	143	HEM	CMC-C2C	2.92	1.56	1.50
4	A	143	HEM	CBB-CAB	2.83	1.44	1.30
4	B	348	HEM	CAC-C3C	-2.76	1.40	1.47
4	B	348	HEM	CMD-C2D	2.72	1.56	1.50
4	C	543	HEM	CBC-CAC	2.59	1.42	1.30
4	D	748	HEM	C4A-C3A	2.51	1.49	1.43
4	A	143	HEM	C1C-C2C	2.49	1.50	1.45
4	B	348	HEM	CHD-C4C	2.43	1.43	1.38
4	A	143	HEM	CHD-C4C	2.42	1.43	1.38
4	B	348	HEM	CMB-C2B	2.41	1.55	1.50
4	A	143	HEM	CHA-C1A	2.37	1.44	1.39
4	B	348	HEM	C4A-NA	2.32	1.44	1.39
4	D	748	HEM	C1C-C2C	-2.30	1.40	1.45
4	B	348	HEM	C1C-NC	-2.27	1.35	1.39
4	D	748	HEM	C2A-C3A	-2.26	1.33	1.38
4	B	348	HEM	CAB-C3B	-2.26	1.41	1.47
4	A	143	HEM	CAB-C3B	-2.23	1.41	1.47
4	C	543	HEM	C1D-ND	2.21	1.43	1.38
4	D	748	HEM	C3C-C4C	-2.20	1.42	1.46
4	C	543	HEM	C1A-C2A	2.19	1.49	1.44
4	D	748	HEM	CAB-C3B	-2.14	1.41	1.47
4	A	143	HEM	CHA-C4D	2.13	1.42	1.38
4	A	143	HEM	C4C-NC	2.10	1.43	1.39
4	B	348	HEM	C1B-NB	2.05	1.43	1.40
4	C	543	HEM	CHC-C1C	2.03	1.42	1.38
4	A	143	HEM	C4D-C3D	2.01	1.48	1.45
4	B	348	HEM	C3B-C4B	2.00	1.48	1.44

All (26) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	348	HEM	C1D-C2D-C3D	-3.90	102.88	106.98
4	B	348	HEM	CMD-C2D-C1D	3.80	130.98	125.03
4	D	748	HEM	CMA-C3A-C4A	3.34	130.51	125.42
4	A	143	HEM	C2B-C1B-NB	3.25	113.57	109.84
4	A	143	HEM	C3B-C4B-NB	2.93	111.57	109.47
4	A	143	HEM	C3C-C2C-C1C	-2.83	104.37	107.05
4	C	543	HEM	CBA-CAA-C2A	-2.81	104.75	112.53
4	A	143	HEM	CHC-C1C-NC	-2.78	121.42	124.45
4	D	748	HEM	C2B-C1B-NB	2.74	112.99	109.84
4	C	543	HEM	C1D-C2D-C3D	-2.67	104.18	106.98
4	A	143	HEM	CHD-C4C-C3C	-2.66	120.72	125.21
4	B	348	HEM	C4D-C3D-C2D	2.59	110.67	106.89
4	D	748	HEM	CMD-C2D-C1D	2.56	129.03	125.03
4	D	748	HEM	CMB-C2B-C1B	2.51	128.96	125.03
4	B	348	HEM	CHC-C1C-NC	-2.50	121.73	124.45
4	A	143	HEM	CHD-C4C-NC	2.49	127.17	124.45
4	A	143	HEM	C3B-C2B-C1B	-2.42	104.59	106.41
4	D	748	HEM	CHC-C4B-NB	-2.35	121.89	124.42
4	D	748	HEM	CHD-C1D-ND	-2.27	121.97	124.42
4	C	543	HEM	C1C-CHC-C4B	2.10	130.48	126.02
4	C	543	HEM	CHA-C4D-ND	-2.09	121.78	124.37
4	A	143	HEM	CHB-C1B-C2B	-2.06	121.08	126.95
4	C	543	HEM	C3B-C2B-C1B	2.06	107.96	106.41
4	C	543	HEM	C4A-C3A-C2A	-2.04	104.47	106.82
4	C	543	HEM	CMA-C3A-C4A	2.03	128.50	125.42
4	B	348	HEM	C2B-C1B-NB	2.01	112.15	109.84

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	543	HEM	C2C-C3C-CAC-CBC
4	C	543	HEM	C4C-C3C-CAC-CBC
4	D	748	HEM	C2C-C3C-CAC-CBC
4	D	748	HEM	C4C-C3C-CAC-CBC
4	C	543	HEM	C2B-C3B-CAB-CBB
4	A	143	HEM	C2C-C3C-CAC-CBC
4	B	348	HEM	C2B-C3B-CAB-CBB
4	B	348	HEM	C4B-C3B-CAB-CBB
4	C	543	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	D	748	HEM	C4B-C3B-CAB-CBB
4	B	348	HEM	CAD-CBD-CGD-O1D
4	B	348	HEM	CAD-CBD-CGD-O2D
4	C	543	HEM	CAD-CBD-CGD-O1D
4	B	348	HEM	CAA-CBA-CGA-O1A
4	C	543	HEM	CAD-CBD-CGD-O2D
4	D	748	HEM	CAA-CBA-CGA-O1A
4	A	143	HEM	CAA-CBA-CGA-O1A
4	A	143	HEM	CAA-CBA-CGA-O2A
4	B	348	HEM	CAA-CBA-CGA-O2A
4	D	748	HEM	CAA-CBA-CGA-O2A
4	A	143	HEM	C4C-C3C-CAC-CBC

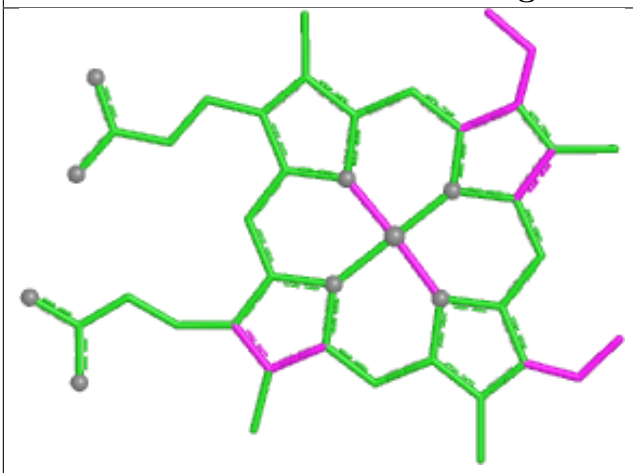
There are no ring outliers.

2 monomers are involved in 3 short contacts:

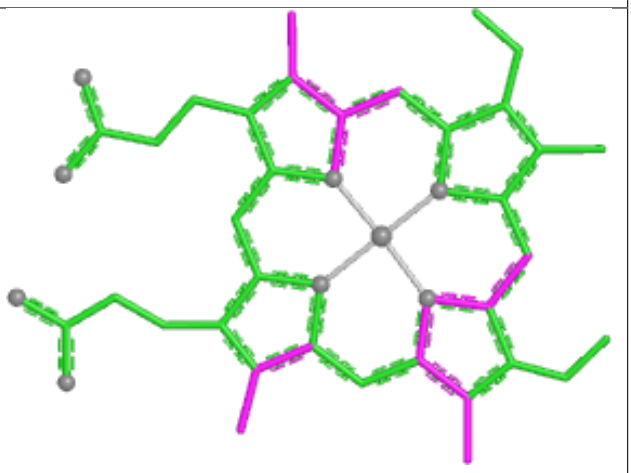
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	748	HEM	2	0
4	B	348	HEM	1	0

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

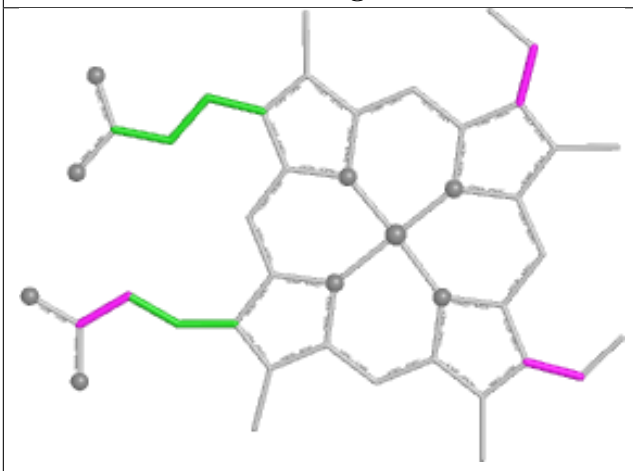
Ligand HEM D 748



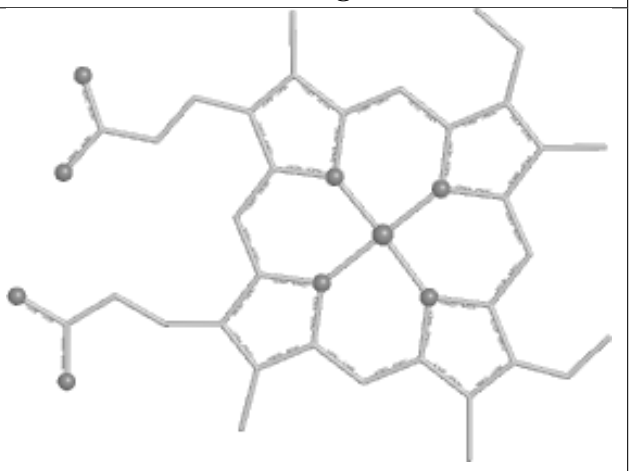
Bond lengths



Bond angles

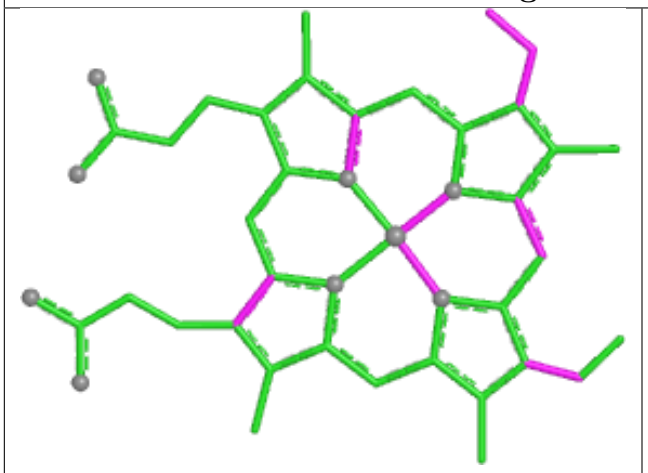


Torsions

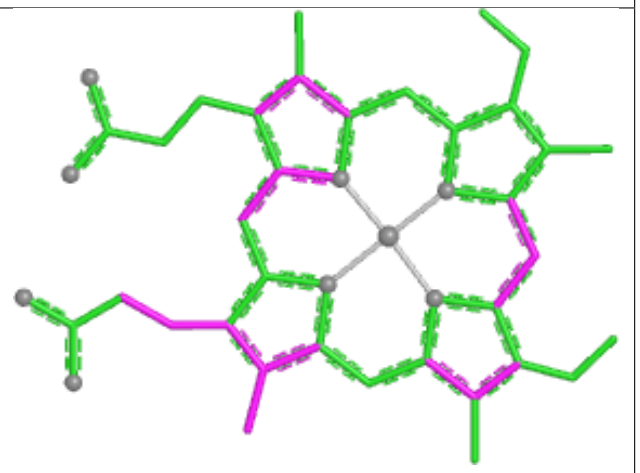


Rings

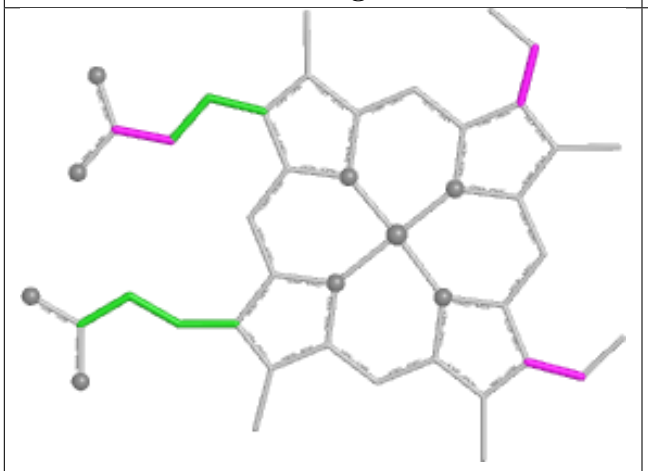
Ligand HEM C 543



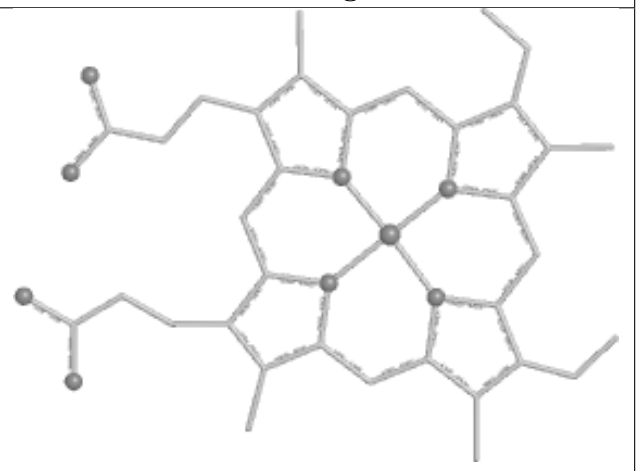
Bond lengths



Bond angles

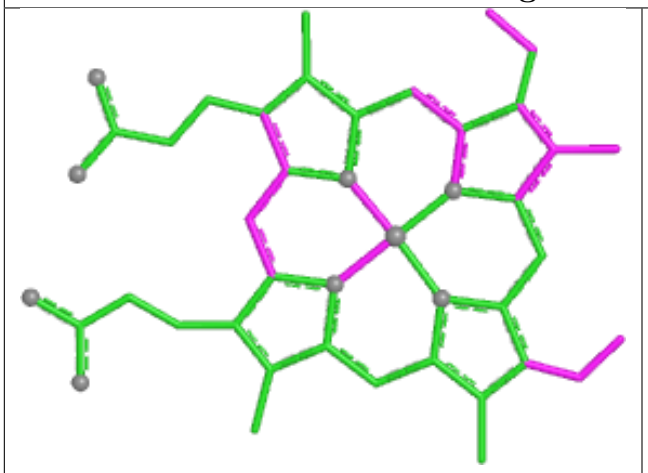


Torsions

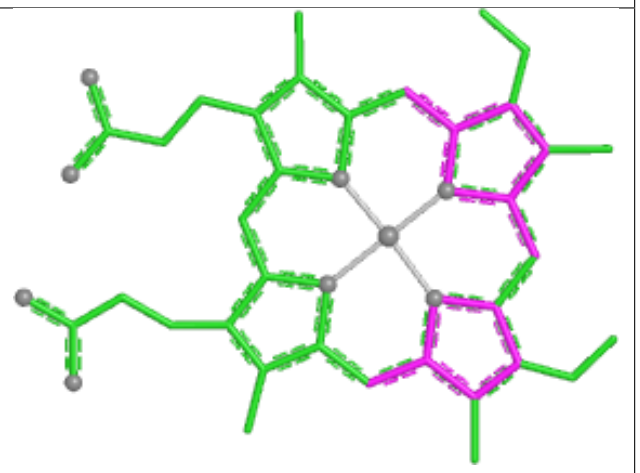


Rings

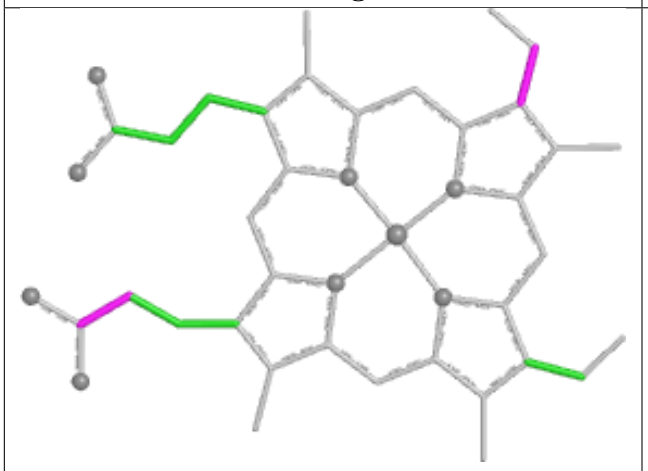
Ligand HEM A 143



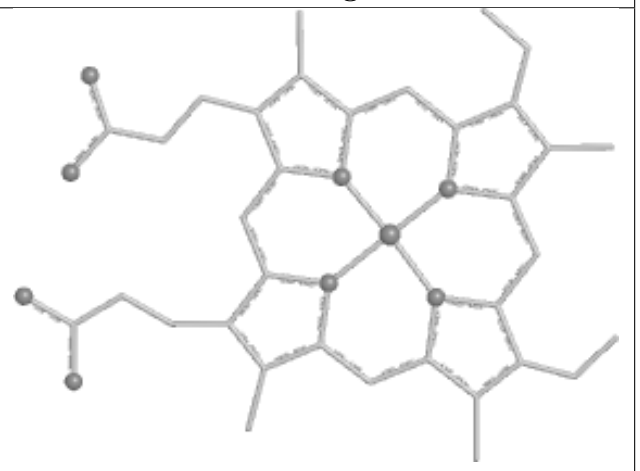
Bond lengths



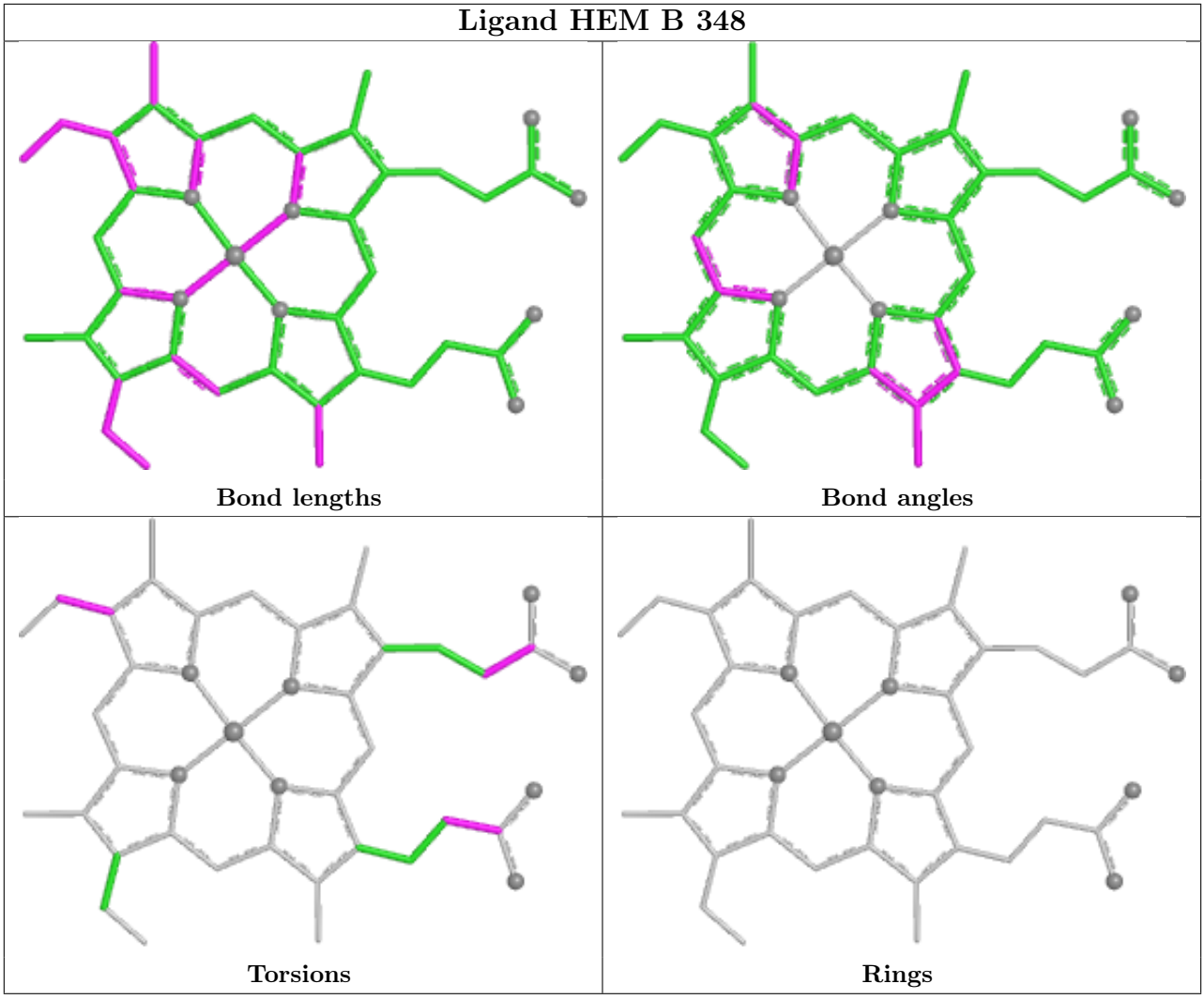
Bond angles



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	141/141 (100%)	-0.02	2 (1%)	73	75	22, 33, 51, 70	0
1	C	141/141 (100%)	-0.02	3 (2%)	63	66	20, 33, 53, 71	0
2	B	145/145 (100%)	0.16	2 (1%)	73	75	22, 39, 58, 78	0
2	D	145/145 (100%)	0.06	3 (2%)	63	66	22, 37, 54, 70	0
All	All	572/572 (100%)	0.05	10 (1%)	69	71	20, 36, 56, 78	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	541	ARG	5.0
1	C	540	TYR	3.8
1	A	1	VAL	3.6
1	A	140	TYR	3.4
2	B	346	HIS	3.1
2	D	745	TYR	3.0
1	C	401	VAL	2.8
2	B	202	MET	2.8
2	D	602	MET	2.6
2	D	746	HIS	2.2

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)

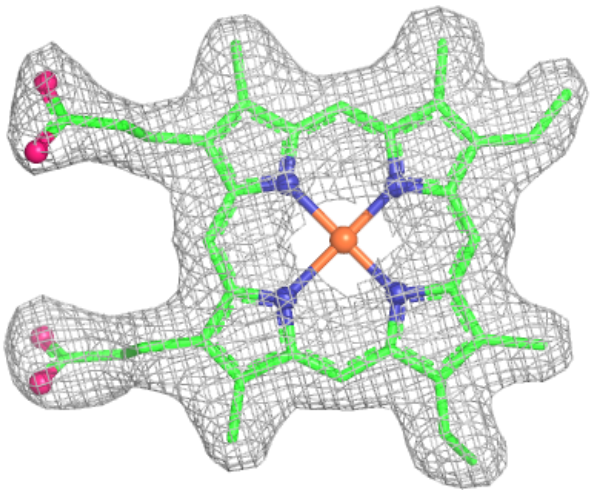
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

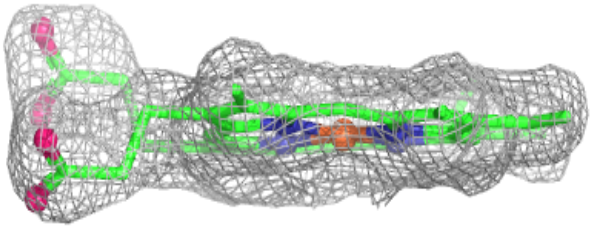
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CMO	B	347	2/2	0.94	0.09	33,33,33,38	0
3	CMO	A	142	2/2	0.95	0.10	27,27,27,33	0
3	CMO	D	747	2/2	0.96	0.09	32,32,32,40	0
3	CMO	C	542	2/2	0.97	0.06	27,27,27,31	0
4	HEM	A	143	43/43	0.97	0.07	22,33,50,56	0
4	HEM	B	348	43/43	0.97	0.08	24,35,56,61	0
4	HEM	C	543	43/43	0.97	0.07	24,33,51,54	0
4	HEM	D	748	43/43	0.97	0.08	21,34,55,62	0

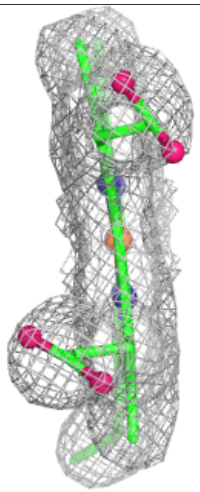
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 143:

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

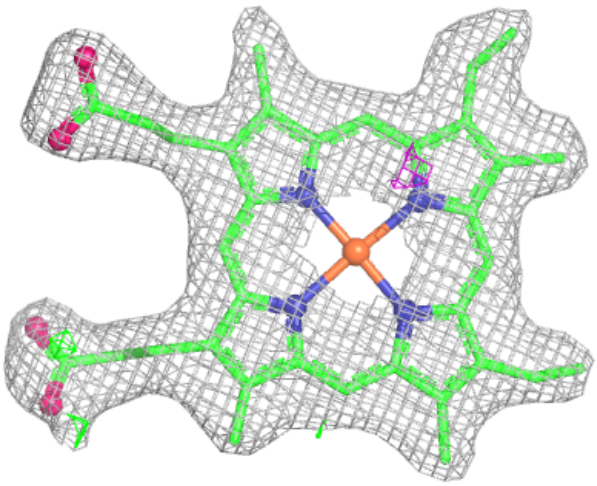


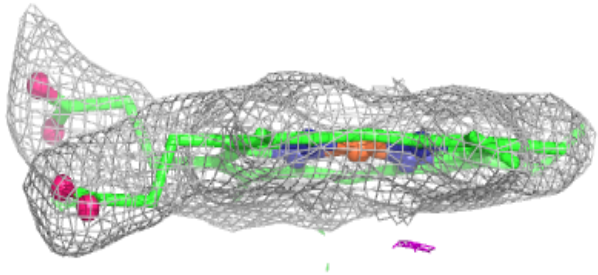


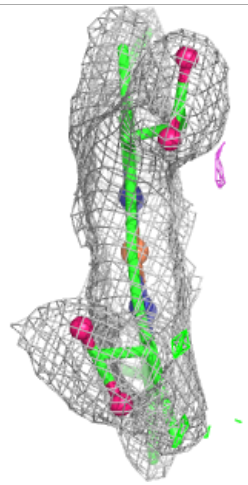


Electron density around HEM B 348:

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

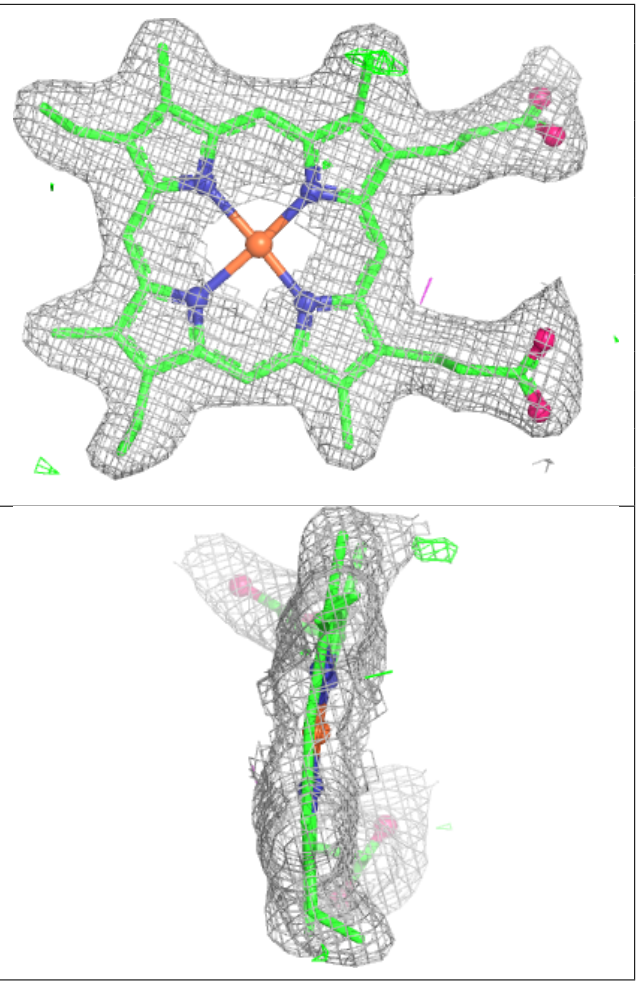






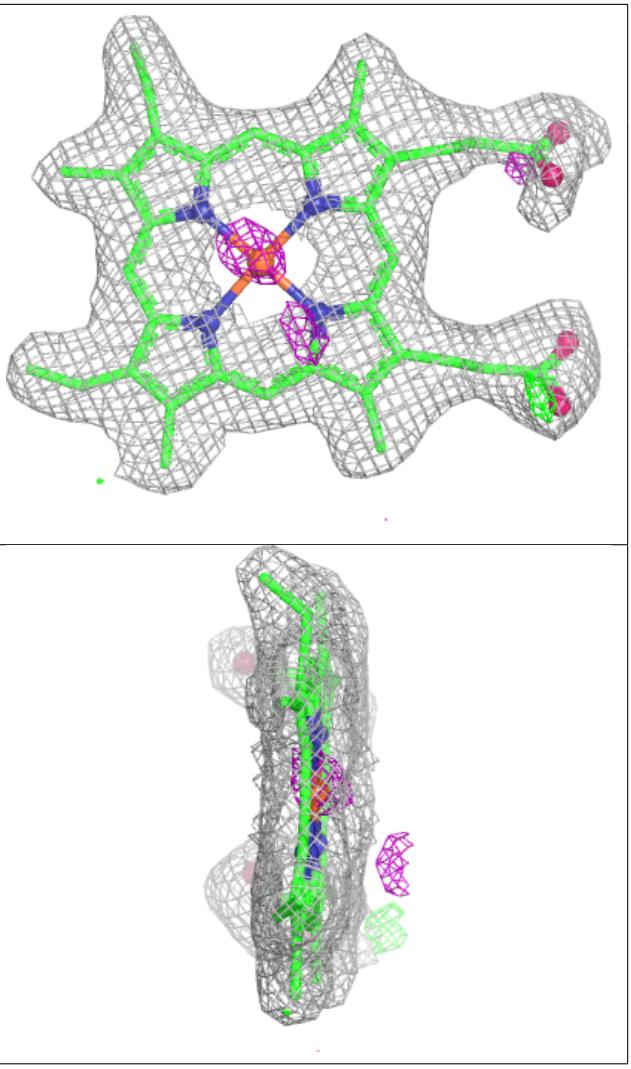
Electron density around HEM C 543:

$2mF_o$-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 748:

$2mF_o$-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.