Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 07:22 PM EDT

PDB ID	:	1GBU
Title	:	DEOXY (BETA-(C93A,C112G)) HUMAN HEMOGLOBIN
Authors	:	Vasquez, G.B.; Ji, X.; Fronticelli, C.; Gilliland, G.L.
Deposited on	:	1996-01-04
Resolution	:	1.80 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 (1)) were used in the production of this report:

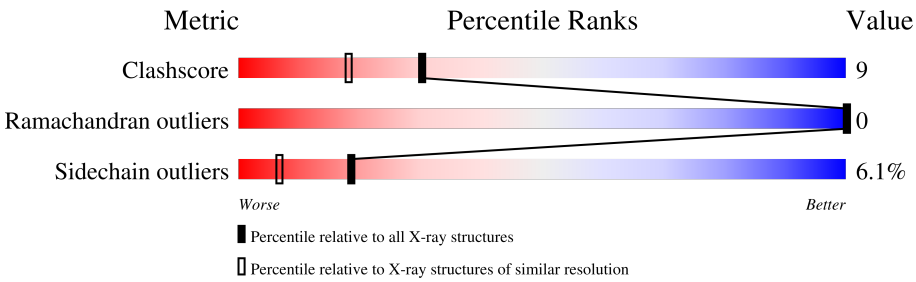
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	71% 22% 6% •
1	C	141	69% 25% 5% •
2	B	146	71% 26% • •
2	D	146	74% 19% 7%

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	SO4	B	147	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5012 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1069	685	187	194	3	0	0	0
1	C	141	1069	685	187	194	3	0	0	0

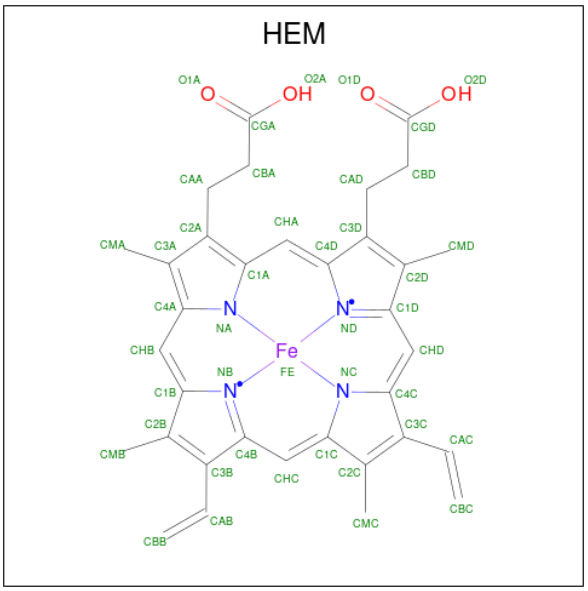
- Molecule 2 is a protein called HEMOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1120	723	195	201	1	0	0	0
2	D	146	1120	723	195	201	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

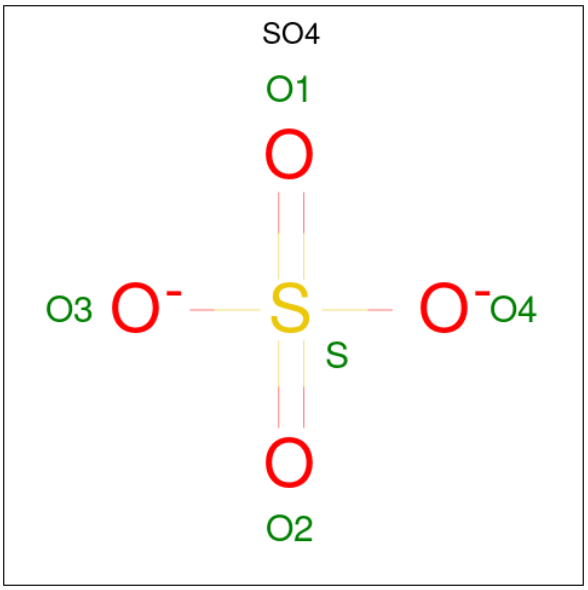
Chain	Residue	Modelled	Actual	Comment	Reference
B	93	ALA	CYS	engineered mutation	UNP P68871
B	112	GLY	CYS	engineered mutation	UNP P68871
D	93	ALA	CYS	engineered mutation	UNP P68871
D	112	GLY	CYS	engineered mutation	UNP P68871

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	122	122	122	0	0
			Total	O		
5	B	94	94	94	0	0
			Total	O		
5	C	125	125	125	0	0
			Total	O		
5	D	111	111	111	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. 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. 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.

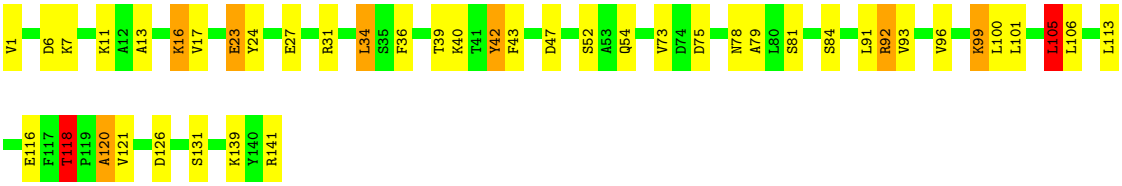
Note EDS was not executed.

• Molecule 1: HEMOGLOBIN

Chain A:

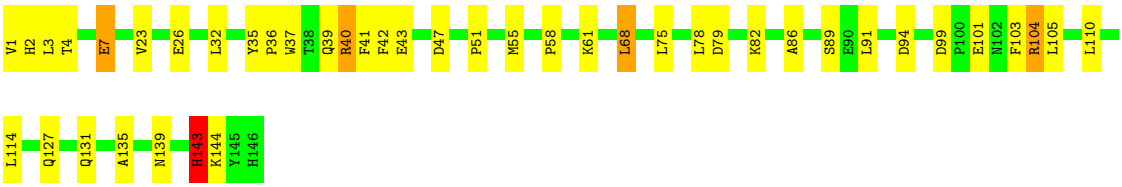
• Molecule 1: HEMOGLOBIN

Chain C:



• Molecule 2: HEMOGLOBIN

Chain B:



• Molecule 2: HEMOGLOBIN

Chain D:

Q127
Q131
N139
Y145
H146

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.02Å 82.94Å 53.83Å 90.00° 99.16° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80	Depositor
% Data completeness (in resolution range)	82.7 (6.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	PROLSQ, GPRLSA	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5012	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

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: SO4, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.14	0/1097	1.97	32/1491 (2.1%)
1	C	1.23	2/1097 (0.2%)	2.01	31/1491 (2.1%)
2	B	1.14	0/1150	1.81	25/1562 (1.6%)
2	D	1.17	0/1150	1.89	28/1562 (1.8%)
All	All	1.17	2/4494 (0.0%)	1.92	116/6106 (1.9%)

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
2	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	ARG	CZ-NH2	6.91	1.42	1.33
1	C	40	LYS	N-CA	5.29	1.56	1.46

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	141	ARG	NE-CZ-NH1	18.53	129.56	120.30
1	A	92	ARG	NE-CZ-NH2	-16.04	112.28	120.30
1	C	92	ARG	NE-CZ-NH2	-13.95	113.32	120.30
1	A	141	ARG	NE-CZ-NH2	-13.15	113.72	120.30
2	D	40	ARG	NE-CZ-NH1	13.08	126.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	40	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	C	92	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	A	6	ASP	CB-CG-OD2	-12.50	107.05	118.30
2	D	30	ARG	NE-CZ-NH2	-12.41	114.10	120.30
2	B	99	ASP	CB-CG-OD2	-11.89	107.60	118.30
1	A	137	THR	OG1-CB-CG2	10.70	134.61	110.00
1	C	141	ARG	NE-CZ-NH2	-10.29	115.15	120.30
2	B	79	ASP	CB-CG-OD1	9.79	127.12	118.30
2	B	32	LEU	CB-CG-CD1	9.40	126.98	111.00
1	A	141	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	47	ASP	CB-CG-OD1	9.16	126.55	118.30
1	C	6	ASP	CB-CG-OD1	9.06	126.46	118.30
2	B	143	HIS	CA-CB-CG	8.96	128.83	113.60
1	C	6	ASP	CB-CG-OD2	-8.94	110.26	118.30
1	C	105	LEU	CA-CB-CG	8.81	135.56	115.30
1	C	36	PHE	CB-CG-CD1	-8.80	114.64	120.80
1	C	118	THR	N-CA-CB	-8.27	94.59	110.30
1	A	105	LEU	CA-CB-CG	8.01	133.72	115.30
1	C	96	VAL	CA-CB-CG2	7.97	122.86	110.90
2	D	21	ASP	CB-CG-OD1	7.62	125.16	118.30
2	B	35	TYR	CB-CG-CD1	-7.42	116.55	121.00
2	D	73	ASP	CB-CG-OD1	7.39	124.95	118.30
2	B	99	ASP	OD1-CG-OD2	7.36	137.28	123.30
1	C	42	TYR	O-C-N	7.27	134.33	122.70
1	C	31	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	36	PHE	O-C-N	7.14	134.67	121.10
2	D	84	THR	CA-CB-CG2	7.08	122.31	112.40
1	C	75	ASP	CB-CG-OD2	-7.07	111.94	118.30
2	D	60	VAL	CA-CB-CG2	7.05	121.47	110.90
1	A	92	ARG	CD-NE-CZ	-6.92	113.91	123.60
1	A	128	PHE	CB-CG-CD2	-6.91	115.96	120.80
2	B	103	PHE	O-C-N	6.76	133.52	122.70
2	B	43	GLU	OE1-CD-OE2	6.74	131.39	123.30
2	D	43	GLU	CG-CD-OE1	6.73	131.76	118.30
1	A	65	ALA	CB-CA-C	6.68	120.12	110.10
1	A	137	THR	N-CA-CB	-6.68	97.62	110.30
1	A	54	GLN	O-C-N	6.64	133.32	122.70
1	A	29	LEU	CB-CG-CD2	-6.64	99.72	111.00
2	D	114	LEU	O-C-N	6.63	133.31	122.70
1	C	43	PHE	CB-CG-CD2	-6.60	116.18	120.80
2	D	30	ARG	NH1-CZ-NH2	6.55	126.61	119.40
1	A	31	ARG	NE-CZ-NH1	6.54	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	47	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	54	GLN	O-C-N	6.49	133.08	122.70
2	D	145	TYR	CB-CG-CD2	-6.42	117.14	121.00
1	C	34	LEU	O-C-N	6.42	132.97	122.70
1	A	92	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	43	PHE	CB-CG-CD1	6.40	125.28	120.80
2	D	90	GLU	OE1-CD-OE2	6.28	130.84	123.30
1	C	40	LYS	CA-CB-CG	6.20	127.04	113.40
1	A	94	ASP	CB-CG-OD1	-6.18	112.74	118.30
2	B	94	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	52	SER	CA-C-O	6.11	132.94	120.10
2	D	65	LYS	CA-CB-CG	6.06	126.74	113.40
2	D	145	TYR	CB-CG-CD1	6.06	124.64	121.00
1	A	38	THR	CA-CB-CG2	-6.05	103.93	112.40
2	B	47	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	C	118	THR	CA-CB-CG2	6.05	120.87	112.40
1	A	122	HIS	CA-CB-CG	6.01	123.82	113.60
2	D	21	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	D	109	VAL	CA-CB-CG1	-5.94	101.99	110.90
2	B	40	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	B	26	GLU	CA-CB-CG	5.92	126.43	113.40
2	D	22	GLU	CB-CG-CD	5.90	130.14	114.20
1	C	131	SER	O-C-N	5.89	132.12	122.70
1	A	121	VAL	CA-CB-CG2	-5.82	102.17	110.90
1	C	42	TYR	CB-CG-CD1	-5.82	117.51	121.00
2	B	42	PHE	CG-CD1-CE1	5.81	127.19	120.80
1	C	23	GLU	CB-CG-CD	5.78	129.82	114.20
2	D	127	GLN	N-CA-CB	5.72	120.89	110.60
1	A	21	ALA	CB-CA-C	5.70	118.65	110.10
2	D	139	ASN	CA-CB-CG	-5.66	100.95	113.40
2	B	105	LEU	O-C-N	5.66	131.75	122.70
2	B	94	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	C	47	ASP	O-C-N	5.66	131.75	122.70
2	D	127	GLN	CA-C-O	5.64	131.94	120.10
2	D	26	GLU	CG-CD-OE2	-5.60	107.11	118.30
1	C	120	ALA	O-C-N	5.59	131.65	122.70
1	A	6	ASP	CB-CG-OD1	5.58	123.33	118.30
2	B	101	GLU	CG-CD-OE2	-5.57	107.17	118.30
2	B	131	GLN	N-CA-CB	5.56	120.61	110.60
2	B	7	GLU	CG-CD-OE2	-5.53	107.24	118.30
2	B	110	LEU	N-CA-CB	5.52	121.43	110.40
2	D	131	GLN	CB-CG-CD	5.52	125.94	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	ASP	CB-CG-OD1	5.47	123.22	118.30
2	D	22	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	A	36	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	C	39	THR	O-C-N	5.34	131.25	122.70
1	A	116	GLU	CG-CD-OE1	5.33	128.96	118.30
1	A	116	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	A	128	PHE	CD1-CG-CD2	5.32	125.21	118.30
1	C	120	ALA	N-CA-CB	5.30	117.52	110.10
2	B	103	PHE	N-CA-CB	5.27	120.08	110.60
2	D	22	GLU	CG-CD-OE1	5.26	128.83	118.30
2	D	90	GLU	CG-CD-OE2	-5.25	107.79	118.30
2	B	103	PHE	CB-CG-CD2	-5.23	117.14	120.80
2	B	41	PHE	O-C-N	5.22	131.05	122.70
1	A	104	CYS	CB-CA-C	5.21	120.83	110.40
2	B	35	TYR	O-C-N	5.18	130.94	121.10
1	A	135	VAL	O-C-N	5.17	130.98	122.70
2	D	41	PHE	CB-CG-CD1	-5.15	117.19	120.80
1	A	47	ASP	O-C-N	5.13	130.90	122.70
1	A	124	SER	O-C-N	5.09	130.84	122.70
2	D	32	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	30	GLU	OE1-CD-OE2	5.07	129.39	123.30
1	C	126	ASP	CB-CG-OD1	5.05	122.84	118.30
2	B	114	LEU	O-C-N	5.05	130.77	122.70
2	D	35	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	A	37	PRO	N-CD-CG	5.03	110.74	103.20
1	C	27	GLU	CG-CD-OE2	-5.02	108.27	118.30
2	B	7	GLU	CG-CD-OE1	5.01	128.32	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	ARG	Sidechain
2	D	40	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	1069	0	1073	17	0
1	C	1069	0	1073	29	0
2	B	1120	0	1116	26	0
2	D	1120	0	1116	14	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
3	C	43	0	30	0	0
3	D	43	0	30	3	0
4	B	5	0	0	2	0
4	D	5	0	0	0	0
5	A	122	0	0	2	0
5	B	94	0	0	2	0
5	C	125	0	0	4	0
5	D	111	0	0	2	0
All	All	5012	0	4498	84	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 9.

All (84) 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:118:THR:HG22	1:C:121:VAL:H	1.29	0.96
1:C:113:LEU:HB3	1:C:116:GLU:HG2	1.54	0.89
2:D:104:ARG:H	2:D:104:ARG:HD2	1.49	0.77
2:D:24:GLY:HA2	2:D:68:LEU:HD13	1.70	0.73
2:D:104:ARG:HD2	2:D:104:ARG:N	2.04	0.72
2:B:4:THR:OG1	2:B:7:GLU:HG3	1.90	0.71
1:A:84:SER:HB2	1:A:139:LYS:HE3	1.72	0.69
3:D:148:HEM:HBB2	3:D:148:HEM:HHC	1.73	0.69
1:A:30:GLU:O	1:A:34:LEU:HD13	1.93	0.69
1:C:118:THR:HG22	1:C:121:VAL:N	2.07	0.66
1:A:7:LYS:O	1:A:11:LYS:HG3	1.98	0.63
1:C:16:LYS:HE2	1:C:116:GLU:OE1	2.00	0.62
2:B:37:TRP:HA	1:C:92:ARG:HD3	1.82	0.61
2:B:1:VAL:CG2	2:B:3:LEU:HG	2.31	0.61
2:D:146:HIS:CD2	2:D:146:HIS:H	2.19	0.60
2:B:1:VAL:HG22	2:B:3:LEU:HG	1.83	0.60
1:C:118:THR:CG2	1:C:121:VAL:H	2.09	0.60
2:B:23:VAL:HG12	2:B:68:LEU:HD11	1.85	0.58
2:B:75:LEU:HD23	2:B:78:LEU:HD21	1.85	0.58
1:C:84:SER:HB3	1:C:139:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:HIS:H	2:B:2:HIS:CD2	2.21	0.58
1:A:137:THR:HG21	5:A:176:HOH:O	2.05	0.56
2:B:86:ALA:HA	2:B:143:HIS:CE1	2.40	0.56
1:C:99:LYS:HD3	1:C:100:LEU:HD23	1.88	0.55
1:C:113:LEU:HD22	1:C:116:GLU:HG3	1.89	0.55
1:C:113:LEU:CB	1:C:116:GLU:HG2	2.34	0.55
1:C:16:LYS:NZ	1:C:16:LYS:HB2	2.22	0.54
2:B:104:ARG:HH12	2:B:135:ALA:HA	1.72	0.54
1:A:7:LYS:NZ	1:A:74:ASP:OD1	2.26	0.52
2:D:94:ASP:OD1	2:D:146:HIS:NE2	2.43	0.51
1:A:84:SER:CB	1:A:139:LYS:HE3	2.40	0.51
1:C:99:LYS:HD3	1:C:100:LEU:CD2	2.41	0.51
2:B:86:ALA:HA	2:B:143:HIS:HE1	1.75	0.50
1:C:13:ALA:O	1:C:16:LYS:HB3	2.11	0.50
2:B:82:LYS:HZ2	2:B:82:LYS:HB2	1.77	0.49
2:B:82:LYS:NZ	4:B:147:SO4:O3	2.44	0.49
1:C:11:LYS:HE3	1:C:73:VAL:HG11	1.94	0.49
1:C:42:TYR:CE2	1:C:93:VAL:HA	2.47	0.49
1:C:99:LYS:NZ	5:C:211:HOH:O	2.46	0.49
1:C:79:ALA:HA	5:C:218:HOH:O	2.12	0.48
2:B:82:LYS:N	4:B:147:SO4:O4	2.42	0.48
1:A:51:GLY:HA2	1:A:56:LYS:HE3	1.96	0.47
2:D:75:LEU:O	2:D:78:LEU:HD22	2.15	0.47
2:B:51:PRO:HD2	5:B:166:HOH:O	2.15	0.47
2:B:104:ARG:NH2	2:B:139:ASN:OD1	2.48	0.47
2:B:40:ARG:NH2	1:C:91:LEU:O	2.34	0.47
2:B:51:PRO:O	2:B:55:MET:HG2	2.15	0.47
3:D:148:HEM:HHC	3:D:148:HEM:CBB	2.42	0.46
1:A:90:LYS:HD3	1:A:90:LYS:N	2.31	0.46
1:C:17:VAL:HG22	1:C:24:TYR:CE2	2.51	0.46
3:D:148:HEM:HBC2	3:D:148:HEM:HMC2	1.98	0.46
1:A:106:LEU:HD23	5:B:198:HOH:O	2.16	0.45
1:C:113:LEU:HD22	1:C:116:GLU:CG	2.46	0.45
1:A:31:ARG:HD3	2:B:127:GLN:OE1	2.17	0.45
2:D:57:ASN:HA	2:D:58:PRO:HD2	1.82	0.45
2:B:91:LEU:HD21	3:B:148:HEM:HBA2	1.98	0.44
2:D:101:GLU:HA	2:D:104:ARG:HD3	1.99	0.44
2:B:91:LEU:CD2	3:B:148:HEM:HBA2	2.47	0.44
1:C:101:LEU:HG	1:C:105:LEU:HD22	1.99	0.44
1:C:78:ASN:ND2	5:C:227:HOH:O	2.50	0.44
1:A:83:LEU:HD21	3:A:142:HEM:HMA1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:SER:OG	2:B:144:LYS:HB2	2.18	0.43
2:B:36:PRO:O	2:B:39:GLN:HB2	2.19	0.43
2:D:22:GLU:HG2	5:D:188:HOH:O	2.19	0.43
1:A:60:LYS:HG3	5:A:248:HOH:O	2.17	0.43
2:B:58:PRO:HA	2:B:61:LYS:HD2	2.01	0.43
1:C:81:SER:OG	1:C:139:LYS:NZ	2.51	0.43
1:C:16:LYS:HB2	1:C:16:LYS:HZ3	1.83	0.42
1:A:94:ASP:OD1	2:D:101:GLU:HG2	2.19	0.42
2:B:1:VAL:HG23	2:B:2:HIS:N	2.34	0.42
1:C:99:LYS:HG3	5:C:211:HOH:O	2.19	0.42
1:C:16:LYS:HG2	1:C:116:GLU:HG3	2.01	0.42
1:C:118:THR:HG23	1:C:120:ALA:H	1.84	0.42
1:A:38:THR:HB	2:D:100:PRO:HD2	2.01	0.42
2:D:82:LYS:HE2	5:D:215:HOH:O	2.20	0.41
2:B:23:VAL:HG12	2:B:68:LEU:CD1	2.49	0.41
2:D:51:PRO:O	2:D:55:MET:HG2	2.21	0.41
1:A:58:HIS:HE1	3:A:142:HEM:C1A	2.39	0.41
1:A:94:ASP:HA	1:A:95:PRO:HD3	1.92	0.41
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.85	0.41
2:D:117:HIS:HD2	2:D:118:PHE:CZ	2.39	0.41
1:A:13:ALA:O	1:A:16:LYS:HB3	2.22	0.40
2:B:2:HIS:CD2	2:B:2:HIS:N	2.90	0.40
1:C:7:LYS:HG2	1:C:73:VAL:HG21	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%)	134 (96%)	5 (4%)	0	100	100
1	C	139/141 (99%)	137 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
All	All	566/574 (99%)	556 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	113/113 (100%)	105 (93%)	8 (7%)	14	5
1	C	113/113 (100%)	106 (94%)	7 (6%)	18	6
2	B	116/116 (100%)	113 (97%)	3 (3%)	46	32
2	D	116/116 (100%)	106 (91%)	10 (9%)	10	3
All	All	458/458 (100%)	430 (94%)	28 (6%)	18	7

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	52	SER
1	A	90	LYS
1	A	92	ARG
1	A	95	PRO
1	A	105	LEU
1	A	109	LEU
1	A	137	THR
2	B	68	LEU
2	B	104	ARG
2	B	143	HIS
1	C	1	VAL
1	C	16	LYS
1	C	23	GLU

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Mol	Chain	Res	Type
1	C	99	LYS
1	C	105	LEU
1	C	106	LEU
1	C	118	THR
2	D	1	VAL
2	D	21	ASP
2	D	26	GLU
2	D	68	LEU
2	D	78	LEU
2	D	82	LYS
2	D	104	ARG
2	D	120	LYS
2	D	139	ASN
2	D	146	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
2	B	2	HIS
2	B	146	HIS
2	D	19	ASN
2	D	117	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	A	142	1	41,50,50	1.91	12 (29%)	45,82,82	1.56	10 (22%)
3	HEM	C	142	1	41,50,50	1.79	13 (31%)	45,82,82	2.02	14 (31%)
4	SO4	D	147	-	4,4,4	0.65	0	6,6,6	0.35	0
3	HEM	D	148	2	41,50,50	1.70	10 (24%)	45,82,82	1.78	12 (26%)
3	HEM	B	148	2	41,50,50	1.57	8 (19%)	45,82,82	1.92	12 (26%)
4	SO4	B	147	-	4,4,4	0.67	0	6,6,6	0.26	0

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	HEM	B	148	2	-	1/12/54/54	-
3	HEM	D	148	2	-	5/12/54/54	-
3	HEM	C	142	1	-	6/12/54/54	-
3	HEM	A	142	1	-	2/12/54/54	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	C3C-C2C	-5.26	1.33	1.40
3	D	148	HEM	CAA-C2A	4.13	1.58	1.52
3	A	142	HEM	CAA-C2A	4.08	1.58	1.52
3	C	142	HEM	CAB-C3B	3.96	1.58	1.47
3	D	148	HEM	C3C-C2C	-3.87	1.35	1.40
3	C	142	HEM	C3C-C2C	-3.59	1.35	1.40
3	B	148	HEM	C3C-C2C	-3.40	1.35	1.40
3	C	142	HEM	CBD-CGD	3.33	1.58	1.50
3	A	142	HEM	CAD-C3D	3.00	1.59	1.51
3	B	148	HEM	CAB-C3B	2.94	1.55	1.47
3	D	148	HEM	CAB-C3B	2.89	1.55	1.47
3	A	142	HEM	CMC-C2C	2.88	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	148	HEM	C1B-NB	-2.80	1.35	1.40
3	B	148	HEM	CAD-C3D	2.78	1.58	1.51
3	A	142	HEM	C3C-CAC	2.78	1.53	1.47
3	C	142	HEM	CAD-C3D	2.74	1.58	1.51
3	C	142	HEM	C1A-NA	2.72	1.41	1.36
3	B	148	HEM	CAA-C2A	2.70	1.56	1.52
3	C	142	HEM	CMC-C2C	2.57	1.57	1.51
3	D	148	HEM	C1B-C2B	2.54	1.49	1.44
3	A	142	HEM	CAB-C3B	2.54	1.54	1.47
3	C	142	HEM	CAA-C2A	2.53	1.55	1.52
3	B	148	HEM	C1B-C2B	2.48	1.49	1.44
3	C	142	HEM	O2D-CGD	-2.47	1.22	1.30
3	C	142	HEM	CMB-C2B	2.41	1.55	1.50
3	A	142	HEM	C1A-NA	2.34	1.41	1.36
3	D	148	HEM	C1D-C2D	2.32	1.49	1.44
3	A	142	HEM	C3B-C2B	-2.32	1.32	1.37
3	C	142	HEM	C3C-CAC	2.26	1.52	1.47
3	D	148	HEM	CMC-C2C	2.25	1.56	1.51
3	D	148	HEM	CBD-CAD	2.24	1.59	1.52
3	B	148	HEM	CHB-C1B	2.20	1.40	1.35
3	A	142	HEM	FE-NB	2.17	2.07	1.96
3	C	142	HEM	C4D-C3D	-2.16	1.41	1.45
3	C	142	HEM	FE-NB	2.14	2.07	1.96
3	A	142	HEM	CMB-C2B	2.13	1.55	1.50
3	D	148	HEM	C1A-NA	2.12	1.40	1.36
3	A	142	HEM	CBD-CGD	2.07	1.55	1.50
3	C	142	HEM	C3B-C2B	-2.05	1.33	1.37
3	A	142	HEM	CHB-C1B	2.05	1.40	1.35
3	D	148	HEM	CMD-C2D	2.03	1.55	1.50
3	B	148	HEM	C1A-NA	2.02	1.40	1.36
3	D	148	HEM	FE-NB	2.01	2.06	1.96

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	142	HEM	O2D-CGD-O1D	6.22	138.81	123.30
3	B	148	HEM	C4B-CHC-C1C	5.03	129.20	122.56
3	B	148	HEM	CMA-C3A-C4A	-3.91	122.46	128.46
3	B	148	HEM	CMB-C2B-C1B	-3.73	119.36	125.04
3	A	142	HEM	CMA-C3A-C4A	-3.69	122.80	128.46
3	A	142	HEM	O2D-CGD-O1D	3.65	132.39	123.30
3	D	148	HEM	CMA-C3A-C4A	-3.65	122.86	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	148	HEM	O2D-CGD-O1D	3.47	131.96	123.30
3	C	142	HEM	C4B-CHC-C1C	3.43	127.09	122.56
3	C	142	HEM	O1D-CGD-CBD	-3.40	112.16	123.08
3	D	148	HEM	CAA-CBA-CGA	3.36	123.18	113.76
3	C	142	HEM	C2C-C3C-C4C	-3.28	104.61	106.90
3	C	142	HEM	CAD-CBD-CGD	-3.26	106.59	113.60
3	D	148	HEM	CHD-C1D-ND	3.22	127.93	124.43
3	B	148	HEM	CMA-C3A-C2A	3.21	131.00	124.94
3	C	142	HEM	CHD-C1D-ND	3.10	127.80	124.43
3	C	142	HEM	C4B-C3B-C2B	3.05	109.53	107.11
3	D	148	HEM	CBA-CAA-C2A	-3.05	107.42	112.62
3	D	148	HEM	CMA-C3A-C2A	3.02	130.64	124.94
3	D	148	HEM	O1A-CGA-CBA	-2.97	113.53	123.08
3	B	148	HEM	O1D-CGD-CBD	-2.96	113.58	123.08
3	B	148	HEM	C1B-NB-C4B	2.86	108.03	105.07
3	A	142	HEM	CMA-C3A-C2A	2.76	130.15	124.94
3	D	148	HEM	CMB-C2B-C1B	-2.74	120.86	125.04
3	A	142	HEM	CMB-C2B-C1B	-2.66	120.98	125.04
3	C	142	HEM	CHD-C1D-C2D	-2.64	120.85	124.98
3	A	142	HEM	O1D-CGD-CBD	-2.62	114.66	123.08
3	D	148	HEM	C4D-ND-C1D	2.62	107.78	105.07
3	D	148	HEM	C4B-CHC-C1C	2.61	126.01	122.56
3	B	148	HEM	CHD-C1D-ND	2.53	127.17	124.43
3	B	148	HEM	C3D-C4D-ND	-2.49	107.39	110.17
3	A	142	HEM	C2C-C3C-C4C	-2.46	105.18	106.90
3	C	142	HEM	CBB-CAB-C3B	-2.45	115.43	127.62
3	B	148	HEM	CMB-C2B-C3B	2.44	134.29	128.30
3	D	148	HEM	CAD-CBD-CGD	-2.44	108.35	113.60
3	C	142	HEM	C4D-C3D-C2D	2.44	110.45	106.90
3	A	142	HEM	CHC-C4B-NB	2.40	127.04	124.43
3	D	148	HEM	O2A-CGA-CBA	2.39	121.69	114.03
3	C	142	HEM	CMD-C2D-C3D	2.37	132.54	126.12
3	A	142	HEM	CBA-CAA-C2A	2.34	116.62	112.62
3	B	148	HEM	O1A-CGA-CBA	-2.32	115.62	123.08
3	A	142	HEM	CHD-C1D-ND	2.24	126.86	124.43
3	C	142	HEM	CMA-C3A-C4A	-2.19	125.09	128.46
3	D	148	HEM	C4C-CHD-C1D	-2.15	119.73	122.56
3	C	142	HEM	CHC-C4B-C3B	2.11	127.79	124.57
3	B	148	HEM	CHB-C1B-NB	2.08	126.95	124.38
3	A	142	HEM	CAD-C3D-C2D	-2.06	124.05	127.88
3	C	142	HEM	CMD-C2D-C1D	-2.04	121.94	125.04

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	148	HEM	C2A-CAA-CBA-CGA
3	C	142	HEM	C2B-C3B-CAB-CBB
3	C	142	HEM	CAA-CBA-CGA-O1A
3	D	148	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	148	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O2D
3	D	148	HEM	CAA-CBA-CGA-O1A
3	D	148	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	C4B-C3B-CAB-CBB
3	B	148	HEM	CAD-CBD-CGD-O2D

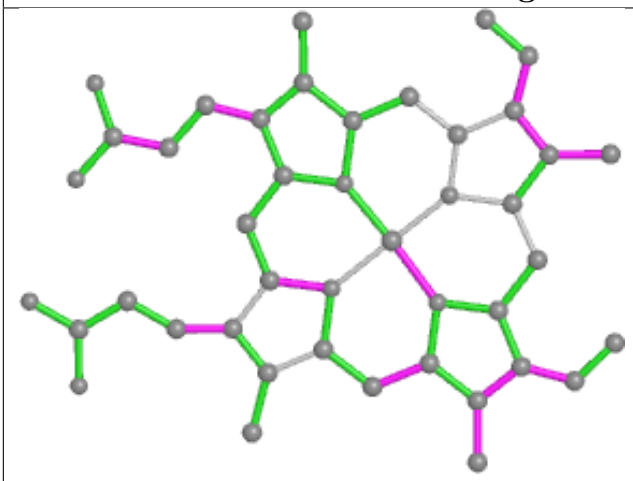
There are no ring outliers.

4 monomers are involved in 9 short contacts:

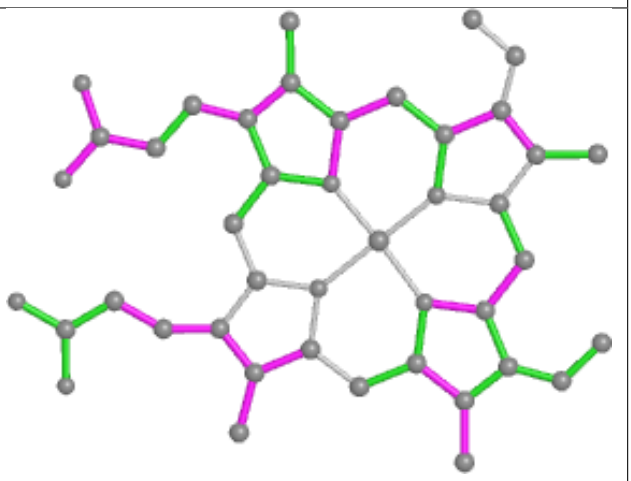
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	HEM	2	0
3	D	148	HEM	3	0
3	B	148	HEM	2	0
4	B	147	SO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

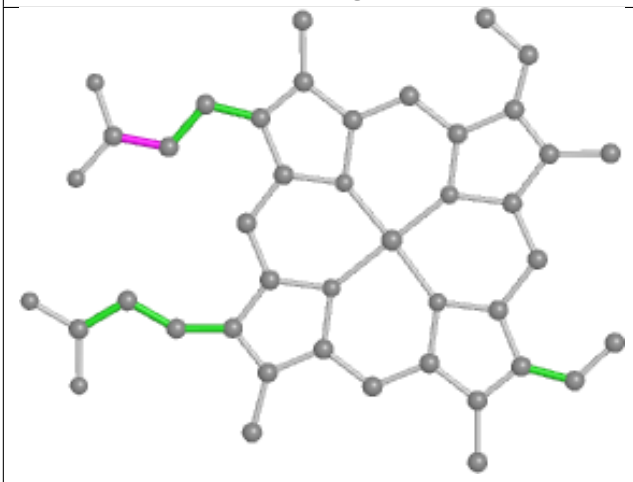
Ligand HEM A 142



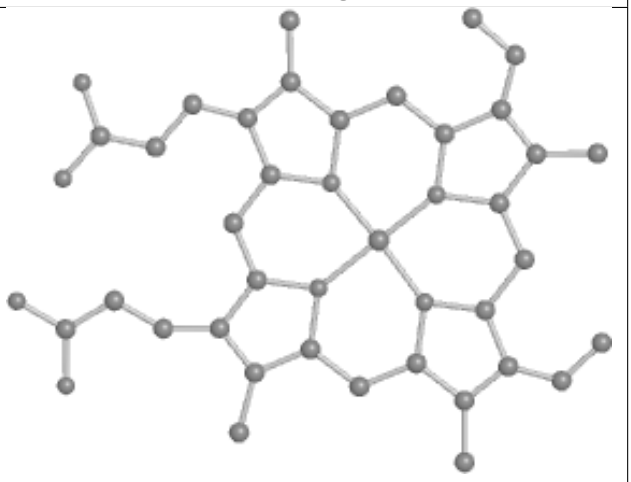
Bond lengths



Bond angles

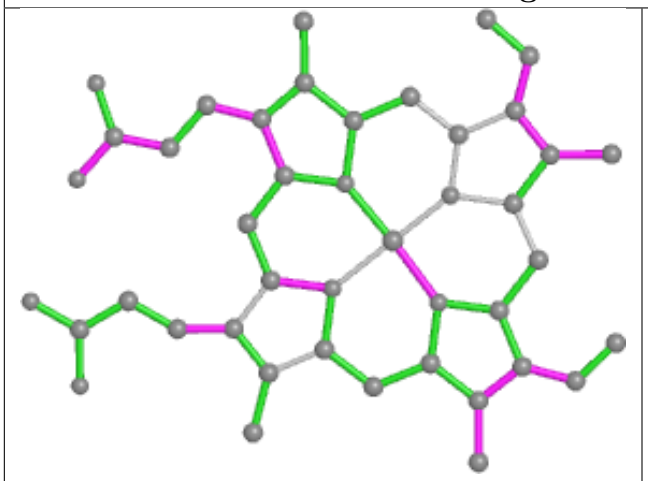


Torsions

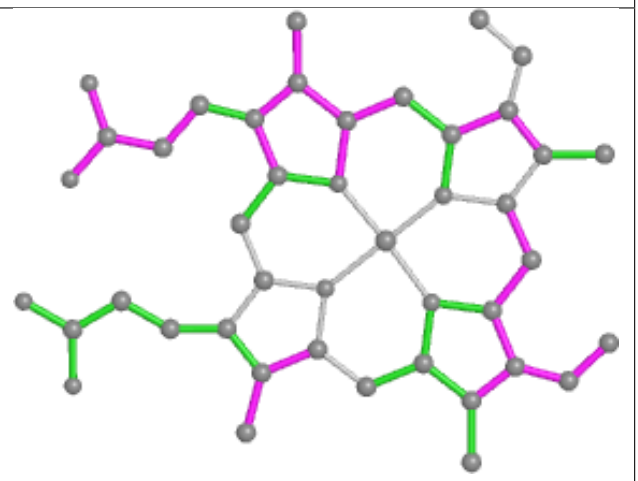


Rings

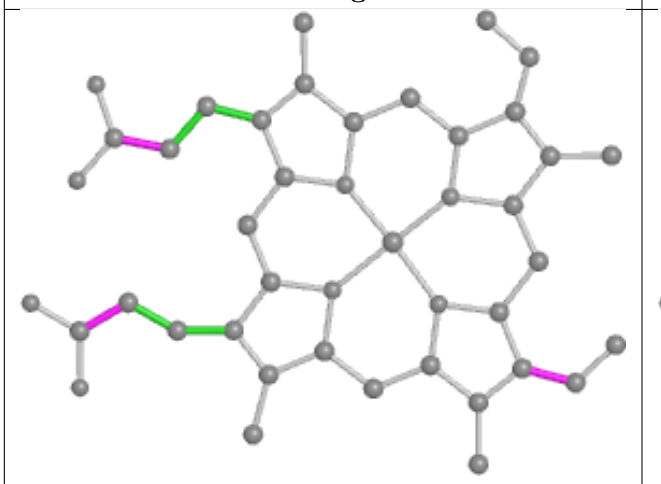
Ligand HEM C 142



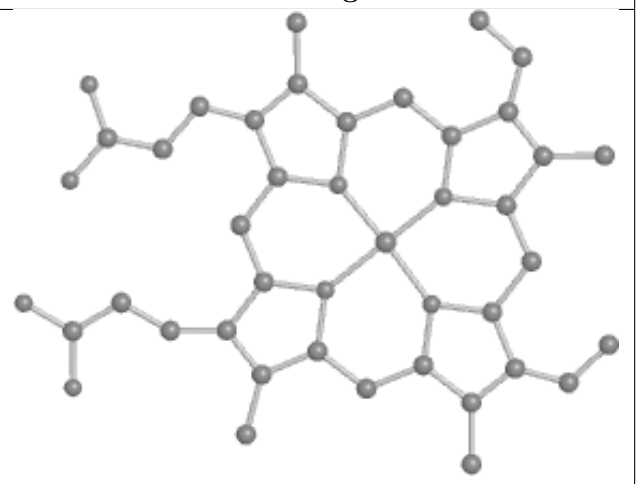
Bond lengths



Bond angles

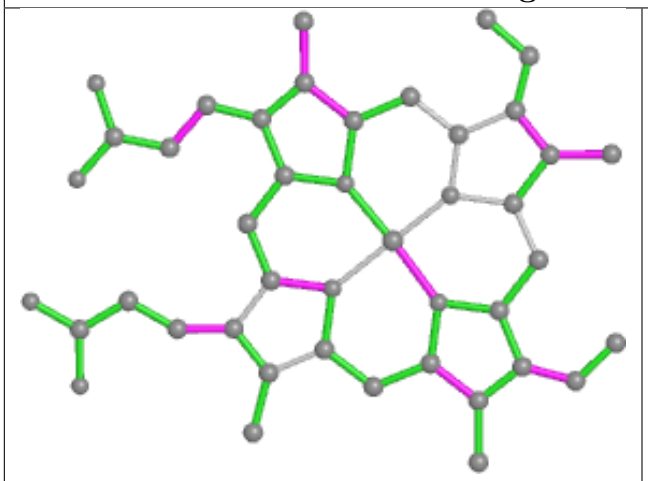


Torsions

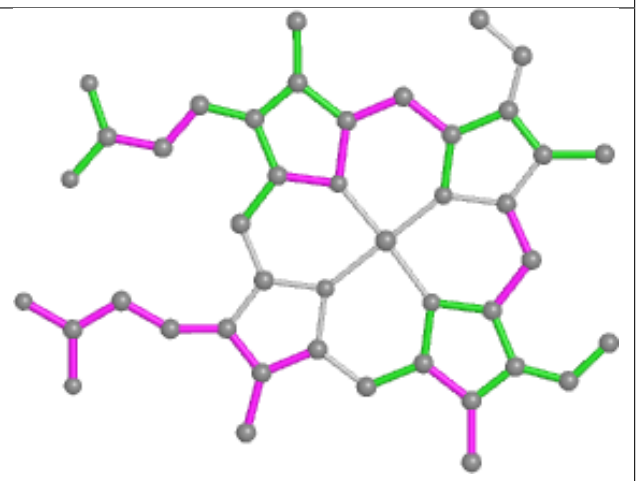


Rings

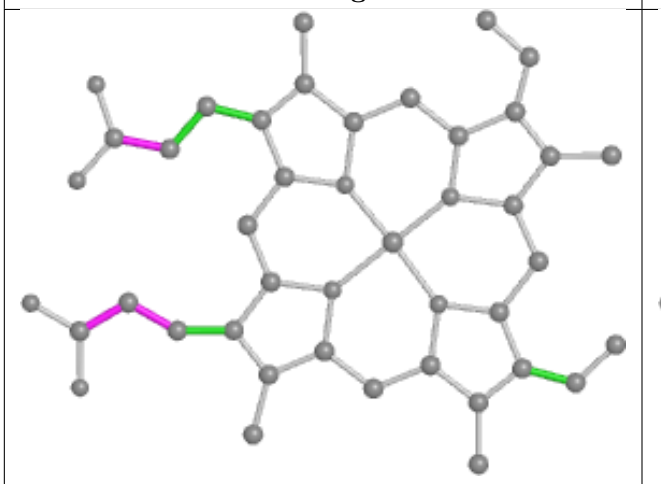
Ligand HEM D 148



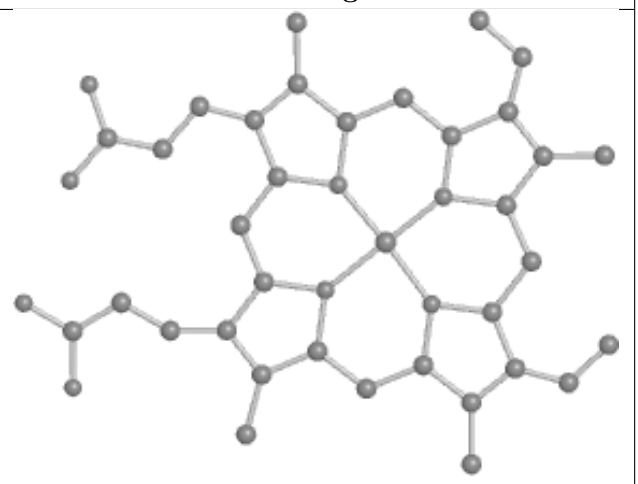
Bond lengths



Bond angles

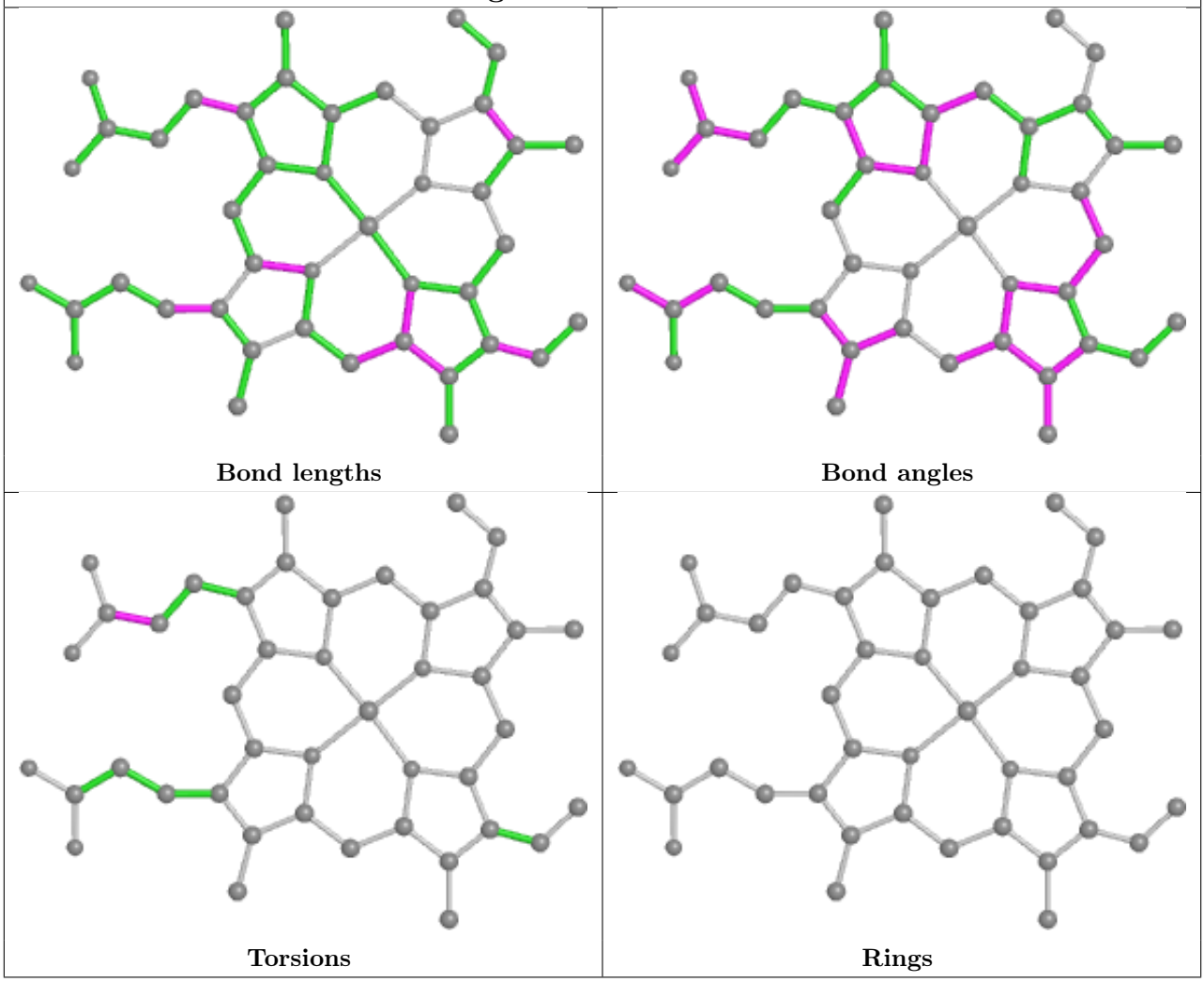


Torsions



Rings

Ligand HEM B 148



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.