Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:27 AM EDT

PDB ID	:	2HHE / pdb_00002hhe
Title	:	OXYGEN AFFINITY MODULATION BY THE N-TERMINI OF THE BETA CHAINS IN HUMAN AND BOVINE HEMOGLOBIN
Authors	:	Gilliland, G.L.; Pechik, I.; Fronticelli, C.; Ji, X.
Deposited on	:	1994-09-29
Resolution	:	2.20 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 ⓘ 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 ⓘ) were used in the production of this report:

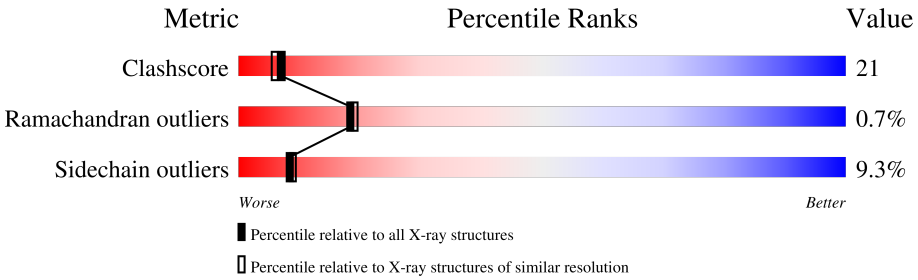
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & 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 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	47% 40% 11%
1	C	141	40% 46% 12%
2	B	145	38% 43% 17%
2	D	145	43% 42% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4972 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.

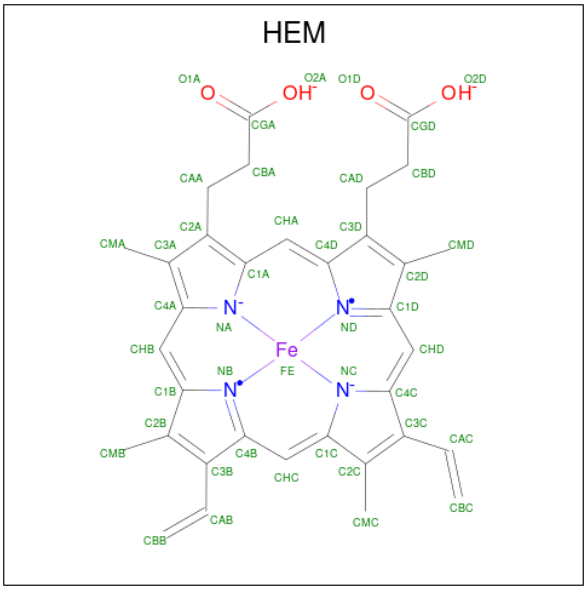
- Molecule 1 is a protein called HEMOGLOBIN (DEOXY) (ALPHA CHAIN).

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

- Molecule 2 is a protein called HEMOGLOBIN (DEOXY) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1114	718	192	200	4			
2	D	145	Total	C	N	O	S	0	0	0
			1114	718	192	200	4			

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	B	107	Total	O	0	0
			107	107		
4	C	117	Total	O	0	0
			117	117		
4	D	118	Total	O	0	0
			118	118		

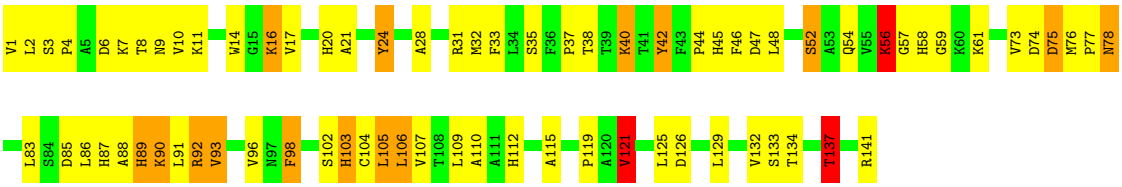
3 Residue-property plots (i)

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.

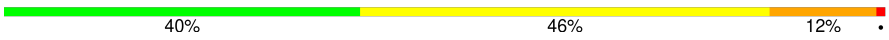
• Molecule 1: HEMOGLOBIN (DEOXY) (ALPHA CHAIN)

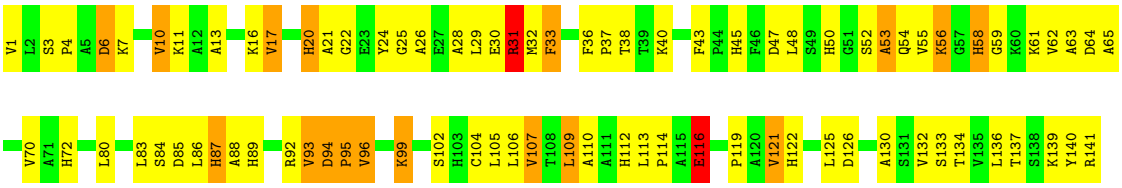
Chain A:



• Molecule 1: HEMOGLOBIN (DEOXY) (ALPHA CHAIN)

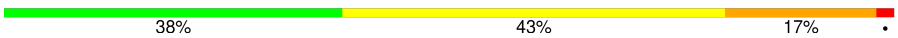
Chain C:





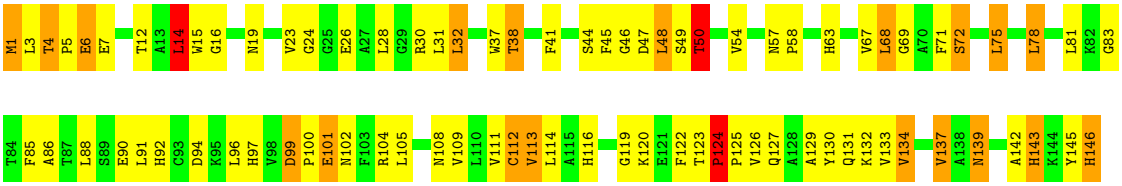
• Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)

Chain B:



• Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)

Chain D:


M1 L3 T4 P5 E6 E7 T12 A13 L14 W15 G16 N19 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 W37 T38 F41 S44 F45 G46 D47 L48 S49 T50 V54 N57 P58 H63 V67 L68 G69 A70 F71 S72 L75 L78 L81 K82 G83
T84 F85 A86 T87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 R104 L105 N108 V109 L110 V111 C112 V113 L114 A115 H116 G119 K120 E121 F122 T123 P124 P125 V126 Q127 A128 A129 Y130 Q131 K132 V133 V134 V137 A138 N139 A142 H143 K144 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	62.71Å 82.38Å 53.58Å 90.00° 99.21° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4972	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.45	1/1097 (0.1%)	2.21	42/1491 (2.8%)
1	C	1.51	3/1097 (0.3%)	2.24	57/1491 (3.8%)
2	B	1.48	1/1143 (0.1%)	2.29	78/1551 (5.0%)
2	D	1.41	3/1143 (0.3%)	2.23	42/1551 (2.7%)
All	All	1.46	8/4480 (0.2%)	2.24	219/6084 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	30	ARG	NE-CZ	-6.33	1.26	1.33
1	C	36	PHE	N-CA	6.12	1.53	1.46
2	D	30	ARG	CD-NE	-5.84	1.38	1.46
2	D	139	ASN	C-O	5.46	1.30	1.24
2	B	33	VAL	CA-CB	5.42	1.60	1.55
1	A	59	GLY	N-CA	5.40	1.52	1.45
1	C	133	SER	C-N	-5.25	1.27	1.33
1	C	121	VAL	C-N	-5.17	1.27	1.33

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	30	ARG	CD-NE-CZ	26.72	161.81	124.40
2	B	63	HIS	CA-CB-CG	-9.52	104.28	113.80
1	C	121	VAL	CA-C-N	9.31	132.55	120.44
1	C	121	VAL	C-N-CA	9.31	132.55	120.44
2	D	124	PRO	CB-CA-C	9.23	122.17	110.92
1	A	47	ASP	N-CA-C	-9.21	95.16	109.25
1	C	20	HIS	CA-CB-CG	-9.18	104.62	113.80
1	A	31	ARG	CD-NE-CZ	9.18	137.25	124.40
2	B	50	THR	O-C-N	8.62	127.23	121.71
1	C	133	SER	CA-C-N	8.32	131.78	120.54
1	C	133	SER	C-N-CA	8.32	131.78	120.54
2	D	101	GLU	CA-C-N	8.13	131.51	120.38
2	D	101	GLU	C-N-CA	8.13	131.51	120.38
2	D	23	VAL	CA-C-N	7.89	128.86	120.03
2	D	23	VAL	C-N-CA	7.89	128.86	120.03
2	D	134	VAL	CB-CA-C	7.70	121.82	111.97
1	A	93	VAL	CA-C-O	-7.68	112.03	120.71
2	B	19	ASN	CA-CB-CG	7.65	120.25	112.60
1	C	10	VAL	O-C-N	7.52	129.69	121.94
1	A	46	PHE	CA-CB-CG	7.51	121.31	113.80
1	A	75	ASP	CA-C-O	-7.49	114.70	121.67
2	B	57	ASN	CA-C-O	7.48	125.99	119.71
1	A	112	HIS	CA-C-O	-7.46	110.69	118.90
2	B	97	HIS	CB-CA-C	-7.28	102.10	111.86
1	C	134	THR	CA-CB-OG1	-7.22	98.78	109.60
2	D	146	HIS	CA-CB-CG	-7.21	106.59	113.80
2	B	105	LEU	O-C-N	7.19	129.51	122.03
2	B	138	ALA	O-C-N	7.17	129.46	122.07
2	D	116	HIS	O-C-N	7.14	129.80	122.09
1	C	29	LEU	CA-C-O	7.13	128.31	120.82
2	B	47	ASP	CA-CB-CG	-7.04	105.56	112.60
1	A	121	VAL	CA-C-N	7.02	130.54	120.79
1	A	121	VAL	C-N-CA	7.02	130.54	120.79
2	B	73	ASP	CA-C-N	6.98	127.73	119.98
2	B	73	ASP	C-N-CA	6.98	127.73	119.98
2	D	23	VAL	CB-CA-C	6.98	121.16	112.02
2	D	99	ASP	CB-CA-C	6.97	121.12	109.69
1	C	122	HIS	N-CA-C	-6.89	103.70	111.07
2	B	57	ASN	CB-CA-C	6.88	120.03	109.50
1	C	89	HIS	CA-CB-CG	-6.86	106.94	113.80
1	A	24	TYR	O-C-N	6.86	131.15	122.23
1	C	17	VAL	CB-CA-C	6.85	121.39	112.14
2	D	69	GLY	N-CA-C	-6.84	104.56	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	24	GLY	CA-C-N	6.81	127.54	119.98
2	B	24	GLY	C-N-CA	6.81	127.54	119.98
1	A	98	PHE	CA-CB-CG	-6.81	106.99	113.80
1	C	109	LEU	N-CA-C	-6.79	103.33	111.69
2	B	68	LEU	CA-C-O	-6.73	112.49	120.10
2	B	60	VAL	O-C-N	6.67	128.42	121.89
1	A	141	ARG	CD-NE-CZ	6.64	133.70	124.40
2	B	137	VAL	CA-C-N	6.61	129.04	120.44
2	B	137	VAL	C-N-CA	6.61	129.04	120.44
1	C	130	ALA	N-CA-C	-6.61	104.16	111.36
2	B	112	CYS	N-CA-C	-6.59	104.02	111.07
2	B	126	VAL	N-CA-C	-6.59	104.07	110.72
2	B	14	LEU	N-CA-C	6.57	119.28	111.33
1	C	17	VAL	N-CA-C	-6.57	103.92	110.62
2	B	97	HIS	CA-CB-CG	-6.49	107.31	113.80
2	B	113	VAL	CA-C-O	-6.48	114.53	121.27
1	C	59	GLY	CA-C-N	6.46	128.84	120.44
1	C	59	GLY	C-N-CA	6.46	128.84	120.44
1	A	109	LEU	CB-CA-C	6.45	120.90	110.96
2	B	30	ARG	NE-CZ-NH1	6.41	127.91	121.50
2	B	86	ALA	CA-C-N	6.37	129.11	120.38
2	B	86	ALA	C-N-CA	6.37	129.11	120.38
1	C	126	ASP	N-CA-C	-6.36	103.97	111.03
2	B	124	PRO	CB-CA-C	6.36	118.68	110.92
1	C	64	ASP	CA-CB-CG	6.35	118.95	112.60
1	C	87	HIS	N-CA-CB	6.33	119.50	110.13
1	A	121	VAL	CB-CA-C	6.30	119.88	111.94
2	D	14	LEU	CB-CA-C	6.29	122.75	110.67
1	C	119	PRO	CA-C-N	6.29	129.22	120.29
1	C	119	PRO	C-N-CA	6.29	129.22	120.29
2	D	94	ASP	N-CA-C	6.27	118.92	111.71
1	A	121	VAL	N-CA-C	-6.26	104.95	111.58
2	B	97	HIS	CA-C-N	-6.24	115.06	122.93
2	B	97	HIS	C-N-CA	-6.24	115.06	122.93
2	D	105	LEU	N-CA-C	-6.24	104.39	111.07
2	D	50	THR	O-C-N	6.23	125.70	121.71
1	A	89	HIS	CA-CB-CG	-6.22	107.58	113.80
2	D	97	HIS	CA-CB-CG	-6.14	107.66	113.80
2	B	134	VAL	CB-CA-C	6.13	120.68	112.22
2	B	142	ALA	CA-C-N	6.11	133.20	121.54
2	B	142	ALA	C-N-CA	6.11	133.20	121.54
2	B	16	GLY	N-CA-C	-6.09	105.44	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	134	THR	CA-CB-OG1	-6.08	100.48	109.60
2	B	129	ALA	O-C-N	6.07	128.40	122.09
1	A	125	LEU	CA-C-N	6.06	128.65	120.65
1	A	125	LEU	C-N-CA	6.06	128.65	120.65
2	D	72	SER	O-C-N	6.06	128.31	122.07
1	A	6	ASP	O-C-N	6.04	128.38	122.09
2	B	117	HIS	CA-CB-CG	6.04	119.84	113.80
1	A	28	ALA	N-CA-C	-6.04	104.61	111.07
2	B	26	GLU	CA-C-N	6.02	128.59	120.65
2	B	26	GLU	C-N-CA	6.02	128.59	120.65
2	B	112	CYS	O-C-N	6.01	128.26	122.07
1	C	59	GLY	CA-C-O	5.98	126.91	120.75
2	B	87	THR	CB-CA-C	-5.98	100.52	110.68
2	B	97	HIS	O-C-N	5.98	129.76	122.58
2	B	13	ALA	CA-C-O	-5.93	114.55	121.07
2	D	139	ASN	CA-C-O	-5.90	114.30	120.55
2	D	94	ASP	CA-C-O	-5.89	113.44	120.10
2	B	122	PHE	CA-CB-CG	-5.83	107.97	113.80
2	B	103	PHE	N-CA-CB	5.80	119.14	110.22
2	B	12	THR	CA-CB-OG1	-5.78	100.93	109.60
2	B	57	ASN	CA-CB-CG	5.77	118.37	112.60
1	C	31	ARG	CA-C-N	5.77	127.94	120.44
1	C	31	ARG	C-N-CA	5.77	127.94	120.44
1	A	104	CYS	CA-C-O	-5.73	112.55	119.49
1	C	47	ASP	N-CA-C	-5.72	100.49	109.25
1	C	106	LEU	CA-C-N	5.72	127.98	120.60
1	C	106	LEU	C-N-CA	5.72	127.98	120.60
1	C	38	THR	N-CA-C	-5.71	105.06	111.28
2	B	13	ALA	N-CA-CB	5.70	118.48	109.82
2	B	20	VAL	CB-CA-C	5.69	119.49	112.04
1	C	53	ALA	CA-C-N	5.67	127.81	120.44
1	C	53	ALA	C-N-CA	5.67	127.81	120.44
2	B	6	GLU	CB-CG-CD	5.66	122.23	112.60
1	A	10	VAL	O-C-N	5.64	127.77	121.90
2	B	113	VAL	CB-CA-C	5.64	119.11	111.88
2	D	113	VAL	CB-CA-C	5.64	119.19	111.97
2	B	110	LEU	CA-C-O	-5.64	114.87	120.90
2	B	79	ASP	CA-CB-CG	-5.63	106.97	112.60
1	A	44	PRO	CB-CA-C	5.62	120.36	111.31
1	A	89	HIS	N-CA-C	5.62	120.29	113.38
2	D	116	HIS	N-CA-C	-5.61	105.09	111.14
2	D	119	GLY	CA-C-N	5.61	132.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	119	GLY	C-N-CA	5.61	132.25	121.54
1	A	134	THR	O-C-N	5.60	128.06	122.12
2	B	5	PRO	CA-C-N	5.60	128.06	120.38
2	B	5	PRO	C-N-CA	5.60	128.06	120.38
2	B	104	ARG	CA-C-N	5.60	128.04	120.65
2	B	104	ARG	C-N-CA	5.60	128.04	120.65
1	C	96	VAL	CA-C-O	-5.58	114.44	120.47
1	C	94	ASP	CA-C-N	5.58	125.94	119.47
1	C	94	ASP	C-N-CA	5.58	125.94	119.47
2	B	67	VAL	CB-CA-C	5.57	118.77	111.81
2	D	112	CYS	O-C-N	5.57	128.11	122.09
1	A	87	HIS	CA-CB-CG	-5.56	108.24	113.80
1	C	104	CYS	CA-C-N	5.54	127.97	120.44
1	C	104	CYS	C-N-CA	5.54	127.97	120.44
1	C	56	LYS	O-C-N	5.53	127.78	122.03
1	A	132	VAL	O-C-N	5.52	127.64	121.90
1	A	56	LYS	CA-C-O	-5.50	115.04	120.70
1	A	105	LEU	O-C-N	5.46	129.33	122.23
1	A	75	ASP	O-C-N	5.45	129.41	121.78
1	C	94	ASP	CA-C-O	-5.45	114.74	120.02
1	A	83	LEU	N-CA-CB	-5.45	101.91	110.30
2	B	68	LEU	CB-CA-C	5.44	120.69	110.63
2	D	143	HIS	CA-CB-CG	-5.44	108.36	113.80
1	C	126	ASP	CB-CA-C	5.44	119.38	110.95
2	D	12	THR	O-C-N	5.43	127.66	122.07
2	D	137	VAL	CB-CA-C	5.43	119.15	112.04
2	D	108	ASN	O-C-N	5.43	127.95	122.09
1	A	103	HIS	N-CA-CB	5.40	119.62	110.49
1	C	22	GLY	CA-C-O	5.39	126.30	120.75
1	C	6	ASP	O-C-N	5.38	127.82	122.12
2	B	121	GLU	N-CA-C	-5.36	106.70	113.18
1	C	116	GLU	N-CA-C	5.35	118.03	111.82
2	D	83	GLY	CA-C-N	5.35	127.71	120.65
2	D	83	GLY	C-N-CA	5.35	127.71	120.65
2	B	127	GLN	CA-C-N	5.35	127.76	120.54
2	B	127	GLN	C-N-CA	5.35	127.76	120.54
2	B	71	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	99	LYS	N-CA-C	-5.33	105.92	112.90
1	A	85	ASP	N-CA-CB	5.30	117.64	109.91
1	C	58	HIS	N-CA-C	-5.29	105.69	111.82
1	A	107	VAL	N-CA-CB	5.28	116.37	110.51
1	C	107	VAL	N-CA-CB	5.28	116.37	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	53	ALA	CA-C-O	5.28	126.55	120.90
2	D	131	GLN	N-CA-C	-5.28	105.61	111.36
2	B	105	LEU	N-CA-C	-5.28	105.22	110.97
1	A	137	THR	CA-CB-CG2	5.27	119.46	110.50
2	D	38	THR	CA-CB-OG1	-5.26	101.70	109.60
1	C	72	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	2	LEU	O-C-N	5.24	129.33	122.68
1	C	130	ALA	O-C-N	5.24	128.12	122.15
2	B	8	LYS	CA-C-N	5.23	128.67	120.82
2	B	8	LYS	C-N-CA	5.23	128.67	120.82
2	B	53	ALA	CA-C-N	5.22	127.22	120.70
2	B	53	ALA	C-N-CA	5.22	127.22	120.70
2	D	48	LEU	CB-CA-C	5.21	119.20	110.44
1	C	70	VAL	N-CA-CB	5.21	116.64	110.55
1	A	46	PHE	CA-C-O	5.19	126.21	120.71
1	A	132	VAL	CA-C-N	5.19	127.55	120.54
1	A	132	VAL	C-N-CA	5.19	127.55	120.54
1	C	96	VAL	O-C-N	5.19	127.66	121.80
2	B	129	ALA	N-CA-CB	5.18	117.66	109.94
2	B	55	MET	CA-C-N	5.16	126.85	120.34
2	B	55	MET	C-N-CA	5.16	126.85	120.34
2	B	34	VAL	CA-C-O	-5.16	114.90	120.47
2	B	116	HIS	N-CA-C	-5.16	105.57	111.14
2	D	113	VAL	N-CA-CB	-5.16	104.51	110.55
1	C	93	VAL	N-CA-CB	-5.16	105.12	111.00
2	B	31	LEU	N-CA-C	-5.13	105.58	111.07
2	B	52	ASP	CB-CA-C	5.13	119.00	110.90
1	A	91	LEU	O-C-N	5.12	128.89	122.23
2	B	30	ARG	CD-NE-CZ	5.11	131.56	124.40
2	B	37	TRP	CB-CA-C	5.11	120.48	110.67
1	C	58	HIS	CB-CA-C	5.11	120.47	110.67
2	B	108	ASN	CB-CG-ND2	-5.10	108.75	116.40
1	A	40	LYS	O-C-N	5.10	129.26	122.43
2	B	43	GLU	CB-CA-C	5.09	119.78	110.11
1	C	56	LYS	CG-CD-CE	5.09	123.01	111.30
2	D	31	LEU	CA-C-O	5.09	126.67	121.07
1	C	31	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	C	65	ALA	O-C-N	5.08	127.30	122.07
2	D	139	ASN	O-C-N	5.07	127.50	122.12
1	C	33	PHE	CB-CA-C	5.07	119.21	110.79
1	C	94	ASP	O-C-N	5.07	126.18	121.27
2	D	69	GLY	O-C-N	5.05	127.03	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	GLN	CA-C-O	-5.05	115.70	121.00
1	C	109	LEU	CB-CA-C	5.04	119.92	110.70
2	D	108	ASN	CB-CG-ND2	-5.04	108.84	116.40
2	D	12	THR	CA-CB-OG1	-5.04	102.05	109.60
2	D	19	ASN	N-CA-CB	5.03	117.84	110.35
2	D	105	LEU	CB-CA-C	5.02	118.77	110.88
2	B	88	LEU	CB-CA-C	5.01	120.30	110.67
1	C	130	ALA	CA-C-O	-5.01	115.11	120.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	ARG	Sidechain
2	B	131	GLN	Mainchain
1	C	31	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	45	0
1	C	1069	0	1073	56	0
2	B	1114	0	1111	38	0
2	D	1114	0	1111	56	0
3	A	43	0	30	2	0
3	B	43	0	30	4	0
3	C	43	0	30	7	0
3	D	43	0	30	5	0
4	A	92	0	0	3	0
4	B	107	0	0	2	0
4	C	117	0	0	4	0
4	D	118	0	0	8	0
All	All	4972	0	4488	189	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 21.

All (189) 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:113:LEU:HB3	1:C:116:GLU:HG2	1.53	0.91
3:B:147:HEM:HHA	3:B:147:HEM:HBA1	1.55	0.86
2:D:104:ARG:NH2	2:D:139:ASN:OD1	2.13	0.80
2:B:63:HIS:ND1	2:B:66:LYS:HE3	2.01	0.76
1:A:42:TYR:CE2	1:A:93:VAL:HA	2.23	0.73
2:B:82:LYS:HZ3	2:B:140:ALA:HA	1.52	0.73
1:A:9:ASN:HB3	1:A:121:VAL:HG22	1.73	0.70
1:A:7:LYS:HE3	1:A:74:ASP:OD1	1.93	0.69
1:C:121:VAL:O	1:C:125:LEU:HG	1.91	0.69
2:D:124:PRO:HB2	2:D:125:PRO:HD3	1.75	0.69
2:D:28:LEU:O	2:D:32:LEU:HD22	1.94	0.68
2:B:146:HIS:OXT	1:C:40:LYS:NZ	2.28	0.66
1:A:103:HIS:NE2	2:B:131:GLN:OE1	2.29	0.66
1:A:89:HIS:HB2	1:A:90:LYS:HE2	1.78	0.66
2:B:8:LYS:HG2	2:B:78:LEU:HD23	1.78	0.65
3:B:147:HEM:HBA1	3:B:147:HEM:CHA	2.22	0.65
2:D:44:SER:O	2:D:46:GLY:N	2.30	0.65
2:D:1:MET:SD	2:D:3:LEU:HG	2.39	0.63
2:B:86:ALA:O	2:B:90:GLU:HG3	1.99	0.63
2:D:3:LEU:HD21	2:D:132:LYS:HB2	1.80	0.62
1:C:40:LYS:HG2	1:C:48:LEU:CD1	2.30	0.62
2:B:1:MET:HB2	2:B:78:LEU:O	1.99	0.62
3:C:142:HEM:CMC	3:C:142:HEM:HBC2	2.30	0.61
1:A:110:ALA:O	2:B:116:HIS:HA	2.01	0.61
2:D:143:HIS:HB3	4:D:217:HOH:O	2.00	0.60
2:B:40:ARG:HA	1:C:92:ARG:HH11	1.66	0.60
2:B:40:ARG:HA	1:C:92:ARG:NH1	2.18	0.59
2:D:1:MET:N	4:D:206:HOH:O	2.36	0.58
3:D:147:HEM:HBC2	3:D:147:HEM:HMC2	1.85	0.58
2:B:50:THR:O	2:B:54:VAL:HG23	2.03	0.58
1:C:58:HIS:O	1:C:62:VAL:HG23	2.04	0.58
1:A:96:VAL:HB	4:D:220:HOH:O	2.03	0.58
2:B:29:GLY:O	2:B:33:VAL:HG23	2.04	0.58
2:B:28:LEU:CD2	2:B:63:HIS:HB3	2.35	0.57
2:D:24:GLY:HA2	2:D:68:LEU:HG	1.87	0.57
2:B:91:LEU:HD12	2:B:95:LYS:HB2	1.86	0.57
2:D:142:ALA:HA	2:D:145:TYR:CD1	2.38	0.57
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.40	0.56
2:D:5:PRO:HG2	2:D:6:GLU:OE2	2.04	0.56
1:A:92:ARG:HG2	2:D:37:TRP:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:SER:HB2	1:C:4:PRO:HD2	1.87	0.55
2:D:4:THR:OG1	2:D:6:GLU:HG2	2.06	0.55
2:D:41:PHE:HA	4:D:243:HOH:O	2.05	0.55
2:B:41:PHE:CD2	3:B:147:HEM:HBC1	2.41	0.55
2:D:104:ARG:HD2	4:D:226:HOH:O	2.06	0.55
1:C:52:SER:HB3	1:C:55:VAL:HG23	1.87	0.55
1:A:17:VAL:O	1:A:20:HIS:HB2	2.07	0.54
1:C:17:VAL:HG13	1:C:24:TYR:CD2	2.43	0.54
1:C:85:ASP:OD1	1:C:139:LYS:NZ	2.38	0.54
1:C:80:LEU:HD13	1:C:136:LEU:HD21	1.90	0.54
1:A:57:GLY:O	1:A:61:LYS:HG3	2.07	0.54
1:A:42:TYR:OH	2:D:99:ASP:OD2	2.15	0.53
2:D:15:TRP:NE1	2:D:72:SER:OG	2.37	0.53
2:D:75:LEU:HA	2:D:78:LEU:HD13	1.89	0.53
1:C:83:LEU:HD11	3:C:142:HEM:HMA1	1.91	0.52
2:D:38:THR:HG22	2:D:102:ASN:OD1	2.07	0.52
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.09	0.52
2:B:142:ALA:O	2:B:145:TYR:HB2	2.10	0.52
1:C:96:VAL:O	1:C:99:LYS:NZ	2.43	0.52
1:C:132:VAL:O	1:C:136:LEU:HG	2.08	0.52
1:A:16:LYS:HE3	1:A:16:LYS:HA	1.91	0.52
1:C:45:HIS:HB2	4:C:258:HOH:O	2.10	0.52
1:A:7:LYS:C	1:A:11:LYS:HE3	2.35	0.52
1:A:7:LYS:HD2	1:A:73:VAL:HG13	1.92	0.52
2:B:43:GLU:HA	4:B:247:HOH:O	2.09	0.52
3:C:142:HEM:CMB	3:C:142:HEM:HBB2	2.39	0.52
2:B:98:VAL:HG13	2:B:102:ASN:HD22	1.75	0.52
2:D:4:THR:HB	2:D:5:PRO:HD2	1.92	0.51
2:D:71:PHE:O	2:D:75:LEU:HD12	2.10	0.51
1:C:40:LYS:HG2	1:C:48:LEU:HD13	1.91	0.51
1:A:42:TYR:HE2	1:A:93:VAL:HA	1.72	0.51
1:C:25:GLY:O	1:C:28:ALA:HB3	2.10	0.51
2:B:32:LEU:HD23	2:B:39:GLN:HG2	1.93	0.50
1:A:14:TRP:O	1:A:17:VAL:HB	2.11	0.50
2:B:82:LYS:HE2	4:B:171:HOH:O	2.11	0.50
2:D:28:LEU:CD2	2:D:63:HIS:HD2	2.24	0.50
1:C:26:ALA:HB2	1:C:56:LYS:HA	1.93	0.50
1:A:7:LYS:HD2	1:A:73:VAL:CG1	2.41	0.50
1:A:78:ASN:N	1:A:78:ASN:OD1	2.45	0.50
2:B:8:LYS:O	2:B:12:THR:HG23	2.12	0.50
1:C:6:ASP:O	1:C:10:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:HIS:O	1:C:92:ARG:N	2.40	0.49
2:D:133:VAL:O	2:D:137:VAL:HG23	2.12	0.49
1:C:30:GLU:OE2	1:C:50:HIS:ND1	2.45	0.49
1:C:92:ARG:NH2	4:C:180:HOH:O	2.45	0.49
2:B:3:LEU:H	2:B:3:LEU:HD12	1.76	0.49
2:D:3:LEU:CD2	2:D:132:LYS:HD2	2.43	0.49
1:C:88:ALA:O	1:C:92:ARG:HG2	2.13	0.48
1:C:94:ASP:OD1	1:C:95:PRO:HD2	2.13	0.48
1:A:86:LEU:HA	1:A:90:LYS:HE3	1.95	0.48
1:C:43:PHE:HA	1:C:45:HIS:CE1	2.48	0.48
1:C:88:ALA:HB1	1:C:139:LYS:O	2.14	0.48
1:C:17:VAL:O	1:C:20:HIS:HB2	2.13	0.48
1:C:137:THR:HA	1:C:140:TYR:CD1	2.49	0.48
2:D:3:LEU:HD23	2:D:132:LYS:HD2	1.95	0.48
3:D:147:HEM:HBB2	3:D:147:HEM:HMB1	1.95	0.48
1:A:58:HIS:HE1	3:A:142:HEM:C1A	2.31	0.48
1:A:98:PHE:HB3	1:A:133:SER:OG	2.13	0.48
3:C:142:HEM:HBB2	3:C:142:HEM:HMB2	1.96	0.48
1:A:7:LYS:O	1:A:11:LYS:HE3	2.14	0.48
1:C:83:LEU:HD23	1:C:86:LEU:HD23	1.95	0.48
1:A:92:ARG:HB3	2:D:37:TRP:HB2	1.97	0.47
2:B:99:ASP:O	2:B:101:GLU:N	2.47	0.47
2:D:81:LEU:HB2	4:D:178:HOH:O	2.14	0.47
2:D:96:LEU:HD13	3:D:147:HEM:C3D	2.49	0.47
1:C:92:ARG:NE	4:C:188:HOH:O	2.45	0.47
1:C:109:LEU:HD12	1:C:125:LEU:HD13	1.96	0.47
1:A:76:MET:N	1:A:77:PRO:CD	2.77	0.47
1:C:7:LYS:O	1:C:11:LYS:HE3	2.14	0.47
1:C:37:PRO:O	1:C:40:LYS:HB2	2.15	0.47
1:A:7:LYS:O	1:A:11:LYS:HG3	2.15	0.46
1:C:84:SER:HB2	4:C:148:HOH:O	2.16	0.46
2:D:50:THR:O	2:D:54:VAL:HG23	2.16	0.46
2:D:14:LEU:O	2:D:14:LEU:HD13	2.15	0.46
4:A:219:HOH:O	1:C:99:LYS:HD3	2.16	0.46
2:D:67:VAL:HG13	3:D:147:HEM:C3B	2.51	0.46
2:D:109:VAL:O	2:D:112:CYS:HB2	2.16	0.46
2:D:123:THR:OG1	2:D:126:VAL:HG23	2.16	0.46
1:C:80:LEU:O	1:C:83:LEU:N	2.47	0.45
1:A:45:HIS:HE2	3:A:142:HEM:HBD1	1.81	0.45
1:C:13:ALA:O	1:C:17:VAL:HG23	2.17	0.45
1:A:40:LYS:NZ	2:D:146:HIS:OXT	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:SER:HA	2:D:75:LEU:HD13	1.98	0.45
1:A:38:THR:HB	2:D:100:PRO:HD2	1.99	0.45
2:D:92:HIS:HA	2:D:96:LEU:HB2	1.98	0.44
2:D:113:VAL:O	2:D:114:LEU:C	2.59	0.44
1:C:116:GLU:CD	1:C:116:GLU:H	2.24	0.44
1:A:45:HIS:ND1	1:A:45:HIS:N	2.64	0.44
1:C:112:HIS:O	1:C:113:LEU:HD23	2.18	0.44
1:A:7:LYS:HE3	1:A:74:ASP:CG	2.43	0.44
1:A:21:ALA:O	1:A:24:TYR:N	2.51	0.44
1:A:52:SER:O	1:A:56:LYS:HG3	2.18	0.44
1:A:88:ALA:O	1:A:92:ARG:HG3	2.17	0.44
2:B:23:VAL:O	2:B:24:GLY:C	2.61	0.44
1:C:20:HIS:HB3	1:C:24:TYR:CE1	2.53	0.44
2:B:62:ALA:O	2:B:65:LYS:HG3	2.18	0.44
1:A:126:ASP:OD2	1:C:141:ARG:NH1	2.42	0.44
2:B:5:PRO:HG2	2:B:6:GLU:OE1	2.17	0.43
1:C:20:HIS:HB3	1:C:24:TYR:CZ	2.53	0.43
1:C:61:LYS:HD3	3:C:142:HEM:HAA2	1.98	0.43
2:D:7:GLU:HB3	2:D:129:ALA:CB	2.48	0.43
2:D:47:ASP:OD1	2:D:49:SER:HB3	2.19	0.43
2:D:28:LEU:HD21	2:D:63:HIS:HD2	1.83	0.43
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.85	0.43
1:C:93:VAL:O	1:C:94:ASP:C	2.62	0.43
2:D:111:VAL:HG13	2:D:122:PHE:HE2	1.84	0.43
2:D:3:LEU:HD11	2:D:133:VAL:CG2	2.48	0.43
2:B:63:HIS:CE1	2:B:66:LYS:HE3	2.51	0.43
2:B:1:MET:N	2:B:79:ASP:OD1	2.40	0.42
2:B:81:LEU:HD22	2:B:85:PHE:HE2	1.84	0.42
1:C:136:LEU:HD11	3:C:142:HEM:HMB3	2.00	0.42
2:B:124:PRO:HB2	2:B:125:PRO:HD3	2.02	0.42
1:A:102:SER:OG	1:A:129:LEU:HB3	2.19	0.42
2:D:57:ASN:HA	2:D:58:PRO:HD2	1.79	0.42
1:A:102:SER:HA	1:A:129:LEU:HD13	2.01	0.42
1:C:21:ALA:HB1	1:C:63:ALA:HB1	2.02	0.42
1:C:53:ALA:HA	1:C:56:LYS:HB2	2.00	0.42
1:A:35:SER:C	1:A:37:PRO:HD3	2.44	0.42
2:B:67:VAL:HG13	3:B:147:HEM:C3B	2.55	0.42
2:D:130:TYR:O	2:D:134:VAL:HG22	2.20	0.42
1:A:32:MET:HE2	1:A:32:MET:HB3	1.92	0.41
2:D:16:GLY:HA3	4:D:237:HOH:O	2.19	0.41
1:C:94:ASP:HA	1:C:95:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:THR:CB	2:D:5:PRO:HD2	2.50	0.41
2:D:68:LEU:HA	2:D:71:PHE:HB3	2.02	0.41
1:C:32:MET:HE3	1:C:33:PHE:CE1	2.55	0.41
1:C:114:PRO:HD3	4:D:173:HOH:O	2.21	0.41
2:D:85:PHE:CD2	2:D:88:LEU:HD12	2.55	0.41
2:B:30:ARG:O	2:B:34:VAL:HG23	2.20	0.41
2:D:85:PHE:HD2	2:D:88:LEU:HD12	1.86	0.41
1:A:115:ALA:HA	4:A:213:HOH:O	2.21	0.41
1:A:137:THR:HG22	4:A:165:HOH:O	2.19	0.41
2:B:45:PHE:CZ	2:B:63:HIS:HB2	2.55	0.41
2:D:67:VAL:HG13	3:D:147:HEM:C2B	2.56	0.41
2:B:53:ALA:O	2:B:57:ASN:N	2.53	0.41
1:C:45:HIS:ND1	1:C:45:HIS:N	2.63	0.41
1:A:21:ALA:O	1:A:24:TYR:HB2	2.20	0.41
1:C:107:VAL:O	1:C:110:ALA:HB3	2.21	0.41
1:C:52:SER:OG	1:C:54:GLN:HB2	2.20	0.41
2:B:30:ARG:O	2:B:34:VAL:N	2.38	0.40
2:D:86:ALA:O	2:D:90:GLU:HG3	2.21	0.40
2:D:100:PRO:HB3	2:D:142:ALA:HB2	2.03	0.40
1:A:3:SER:HB2	1:A:4:PRO:HD2	2.03	0.40
2:D:99:ASP:O	2:D:101:GLU:N	2.54	0.40
2:B:120:LYS:HB3	2:B:120:LYS:HE2	1.99	0.40
3:C:142:HEM:CMC	3:C:142:HEM:CBC	2.98	0.40
1:A:119:PRO:HG2	2:B:55:MET:HG3	2.04	0.40
2:B:37:TRP:HB2	1:C:92:ARG:HB3	2.03	0.40
2:D:48:LEU:HD23	2:D:54:VAL:HA	2.04	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%)	125 (90%)	14 (10%)	0	100 100
1	C	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
2	B	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	9 7
2	D	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	9 7
All	All	564/572 (99%)	514 (91%)	46 (8%)	4 (1%)	18 19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	45	PHE
2	B	143	HIS
2	D	120	LYS
2	B	86	ALA

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%)	100 (88%)	13 (12%)	5 5
1	C	113/113 (100%)	107 (95%)	6 (5%)	20 26
2	B	117/117 (100%)	105 (90%)	12 (10%)	7 7
2	D	117/117 (100%)	105 (90%)	12 (10%)	7 7
All	All	460/460 (100%)	417 (91%)	43 (9%)	8 9

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

Mol	Chain	Res	Type
1	A	1	VAL
1	A	8	THR
1	A	16	LYS
1	A	42	TYR
1	A	52	SER
1	A	56	LYS
1	A	75	ASP

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	90	LYS
1	A	105	LEU
1	A	106	LEU
1	A	121	VAL
1	A	137	THR
2	B	1	MET
2	B	3	LEU
2	B	6	GLU
2	B	18	VAL
2	B	61	LYS
2	B	65	LYS
2	B	67	VAL
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	94	ASP
2	B	100	PRO
1	C	1	VAL
1	C	16	LYS
1	C	95	PRO
1	C	102	SER
1	C	105	LEU
1	C	116	GLU
2	D	1	MET
2	D	4	THR
2	D	6	GLU
2	D	14	LEU
2	D	26	GLU
2	D	32	LEU
2	D	50	THR
2	D	68	LEU
2	D	75	LEU
2	D	78	LEU
2	D	91	LEU
2	D	124	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	97	HIS
2	B	102	ASN

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Mol	Chain	Res	Type
2	D	63	HIS
2	D	116	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	50,50,50	1.48	9 (18%)	67,82,82	1.32	9 (13%)
3	HEM	C	142	1	50,50,50	1.49	8 (16%)	67,82,82	1.47	15 (22%)
3	HEM	D	147	2	50,50,50	1.35	7 (14%)	67,82,82	1.18	7 (10%)
3	HEM	B	147	2	50,50,50	1.28	8 (16%)	67,82,82	1.67	10 (14%)

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	A	142	1	-	5/14/54/54	-
3	HEM	C	142	1	-	3/14/54/54	-
3	HEM	D	147	2	-	5/14/54/54	-
3	HEM	B	147	2	-	3/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	CAB-C3B	3.66	1.57	1.47
3	C	142	HEM	FE-NB	3.56	2.05	1.94
3	A	142	HEM	FE-NB	3.32	2.05	1.94
3	D	147	HEM	FE-NC	3.10	2.05	1.95
3	C	142	HEM	CAB-C3B	3.06	1.55	1.47
3	D	147	HEM	FE-NA	2.90	2.04	1.95
3	C	142	HEM	CMA-C3A	2.82	1.56	1.50
3	C	142	HEM	CAC-C3C	2.75	1.54	1.47
3	C	142	HEM	C2A-C3A	-2.68	1.31	1.38
3	C	142	HEM	CMB-C2B	2.66	1.56	1.50
3	A	142	HEM	C2A-C3A	-2.56	1.32	1.38
3	A	142	HEM	CMD-C2D	2.53	1.56	1.50
3	A	142	HEM	CAC-C3C	2.45	1.53	1.47
3	D	147	HEM	CAC-C3C	2.43	1.53	1.47
3	D	147	HEM	C2A-C3A	-2.37	1.32	1.38
3	D	147	HEM	CAB-C3B	2.34	1.53	1.47
3	B	147	HEM	CAB-C3B	2.34	1.53	1.47
3	B	147	HEM	O1A-CGA	2.30	1.29	1.22
3	B	147	HEM	CMC-C2C	2.28	1.55	1.50
3	B	147	HEM	FE-NA	2.26	2.02	1.95
3	C	142	HEM	CBA-CAA	2.24	1.59	1.51
3	C	142	HEM	CAA-C2A	2.23	1.57	1.51
3	A	142	HEM	CMB-C2B	2.23	1.55	1.50
3	B	147	HEM	FE-NC	2.16	2.02	1.95
3	A	142	HEM	FE-ND	2.14	2.01	1.94
3	D	147	HEM	CBD-CAD	2.12	1.59	1.51
3	B	147	HEM	CMA-C3A	2.12	1.55	1.50
3	A	142	HEM	C3C-C2C	-2.09	1.32	1.37
3	B	147	HEM	O1D-CGD	2.09	1.28	1.22
3	A	142	HEM	FE-NA	2.03	2.01	1.95
3	B	147	HEM	C3B-C2B	-2.02	1.33	1.37
3	D	147	HEM	O1A-CGA	2.00	1.28	1.22

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	147	HEM	CBC-CAC-C3C	7.85	166.75	127.53
3	C	142	HEM	CHD-C1D-ND	3.54	128.23	124.42
3	D	147	HEM	CHC-C4B-NB	3.54	128.23	124.42
3	B	147	HEM	O1A-CGA-CBA	-3.52	111.94	123.09
3	A	142	HEM	CBD-CAD-C3D	3.41	121.95	112.53
3	D	147	HEM	O2A-CGA-O1A	3.06	131.21	123.33
3	A	142	HEM	CHA-C1A-NA	3.06	129.41	123.86
3	B	147	HEM	CAA-CBA-CGA	3.04	121.74	113.67
3	A	142	HEM	O2A-CGA-O1A	2.93	130.86	123.33
3	C	142	HEM	CBA-CAA-C2A	-2.92	104.45	112.53
3	C	142	HEM	CHB-C1B-NB	2.81	127.84	124.37
3	C	142	HEM	CHC-C1C-NC	2.79	127.50	124.45
3	C	142	HEM	CMA-C3A-C4A	-2.78	121.19	125.42
3	B	147	HEM	O2A-CGA-O1A	2.74	130.37	123.33
3	C	142	HEM	CBD-CAD-C3D	2.67	119.90	112.53
3	A	142	HEM	CAA-C2A-C1A	-2.64	119.78	124.94
3	C	142	HEM	O2A-CGA-O1A	2.63	130.09	123.33
3	C	142	HEM	CAD-CBD-CGD	2.59	120.53	113.67
3	A	142	HEM	C1A-CHA-C4D	-2.57	120.20	126.25
3	C	142	HEM	CMA-C3A-C2A	2.56	131.05	125.62
3	C	142	HEM	C4A-CHB-C1B	-2.56	120.23	126.25
3	A	142	HEM	O2D-CGD-CBD	2.52	121.96	114.00
3	C	142	HEM	CHB-C4A-NA	2.50	128.40	123.86
3	C	142	HEM	CBC-CAC-C3C	-2.43	115.38	127.53
3	D	147	HEM	C1C-CHC-C4B	-2.40	120.93	126.02
3	B	147	HEM	CHC-C1C-NC	2.36	127.02	124.45
3	C	142	HEM	CBB-CAB-C3B	-2.36	115.76	127.53
3	A	142	HEM	CBB-CAB-C3B	-2.35	115.80	127.53
3	D	147	HEM	C3B-C2B-C1B	2.34	108.17	106.41
3	A	142	HEM	CHA-C4D-ND	2.34	127.26	124.37
3	B	147	HEM	C4C-CHD-C1D	-2.31	121.10	126.02
3	B	147	HEM	CHB-C4A-NA	2.30	128.02	123.86
3	D	147	HEM	CHD-C4C-NC	2.18	126.83	124.45
3	D	147	HEM	CHC-C1C-NC	2.18	126.82	124.45
3	C	142	HEM	C4C-CHD-C1D	-2.16	121.43	126.02
3	A	142	HEM	O2D-CGD-O1D	-2.15	117.81	123.33
3	B	147	HEM	CHD-C1D-ND	2.15	126.73	124.42
3	D	147	HEM	O1D-CGD-CBD	-2.10	116.44	123.09
3	B	147	HEM	CMA-C3A-C2A	2.08	130.04	125.62
3	C	142	HEM	O1A-CGA-CBA	-2.05	116.59	123.09
3	B	147	HEM	C4A-CHB-C1B	-2.02	121.49	126.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C1A-C2A-CAA-CBA
3	B	147	HEM	C3A-C2A-CAA-CBA
3	D	147	HEM	C2A-CAA-CBA-CGA
3	A	142	HEM	C3D-CAD-CBD-CGD
3	A	142	HEM	C2B-C3B-CAB-CBB
3	A	142	HEM	C4D-C3D-CAD-CBD
3	A	142	HEM	C2D-C3D-CAD-CBD
3	A	142	HEM	C4B-C3B-CAB-CBB
3	D	147	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	C2A-CAA-CBA-CGA
3	C	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAA-CBA-CGA-O2A
3	D	147	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	C3D-CAD-CBD-CGD

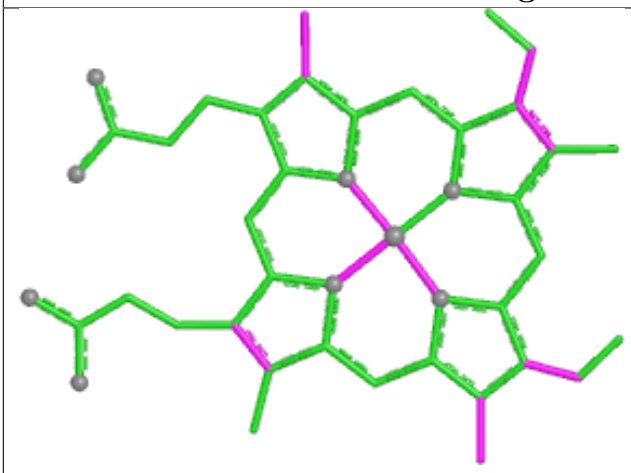
There are no ring outliers.

4 monomers are involved in 18 short contacts:

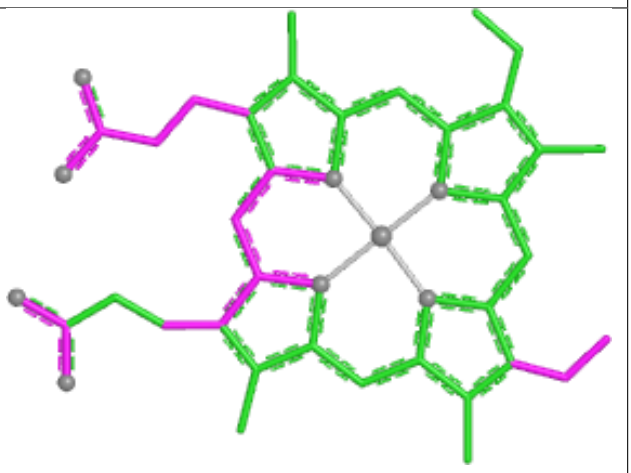
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	HEM	2	0
3	C	142	HEM	7	0
3	D	147	HEM	5	0
3	B	147	HEM	4	0

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.

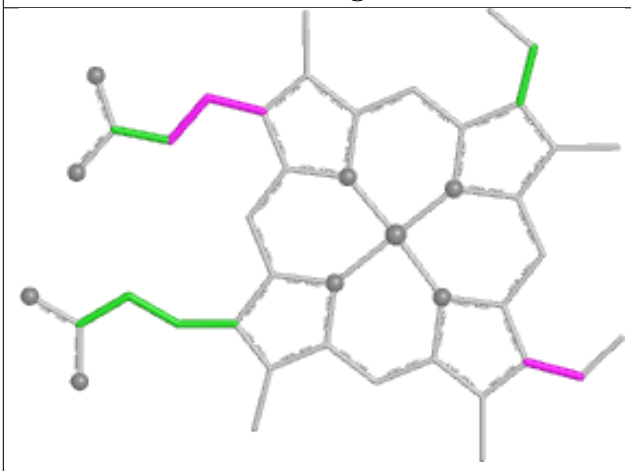
Ligand HEM A 142



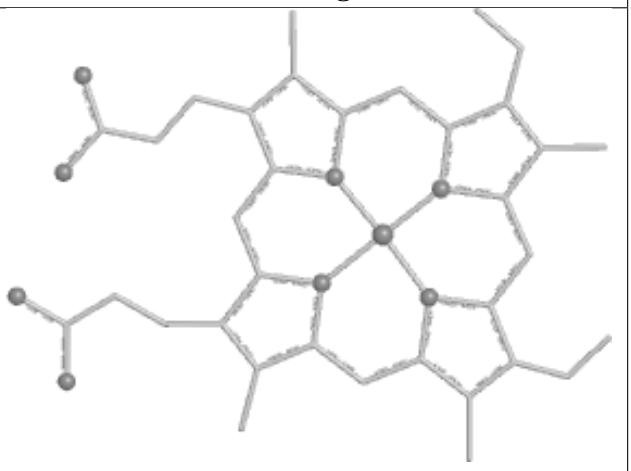
Bond lengths



Bond angles

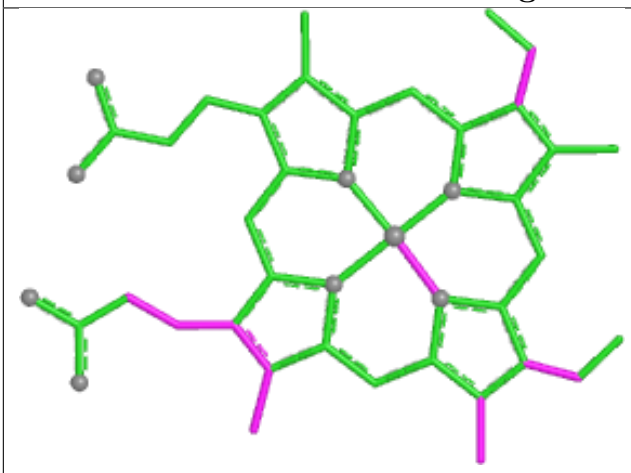


Torsions



Rings

Ligand HEM C 142



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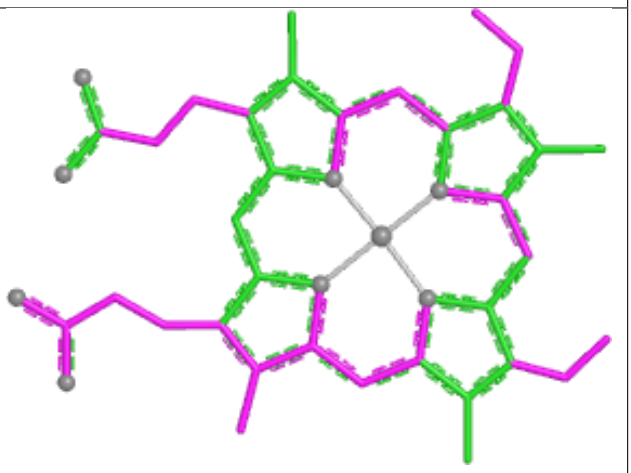
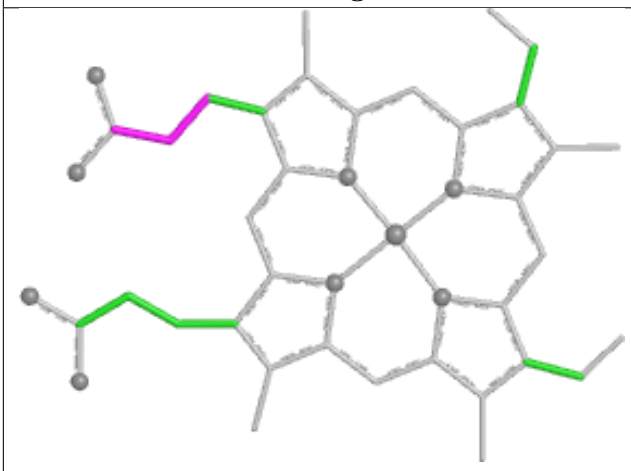


Bond angles



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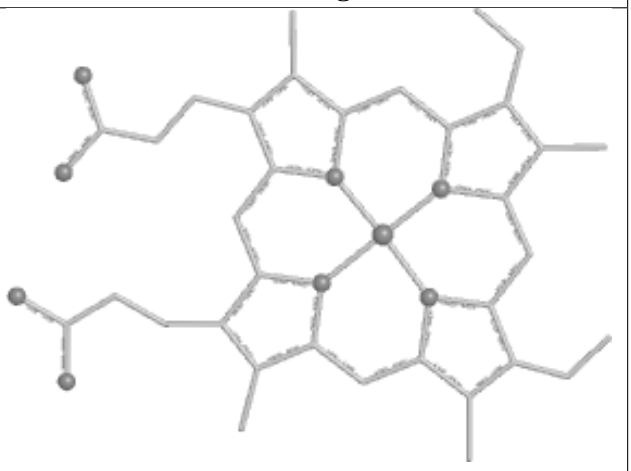
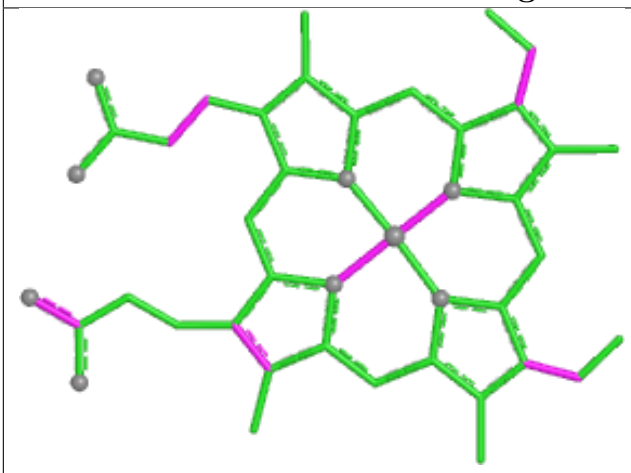
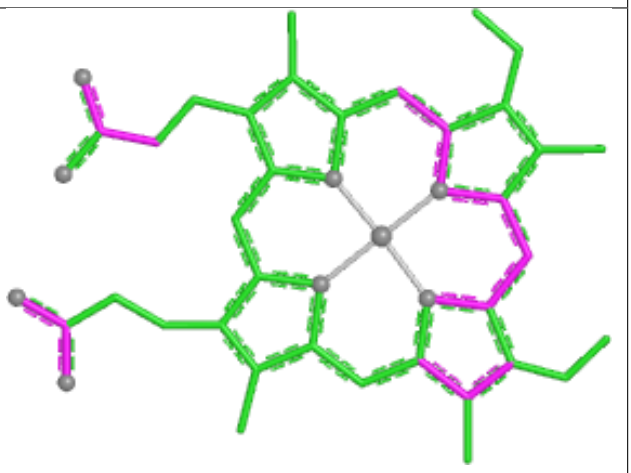


Rings

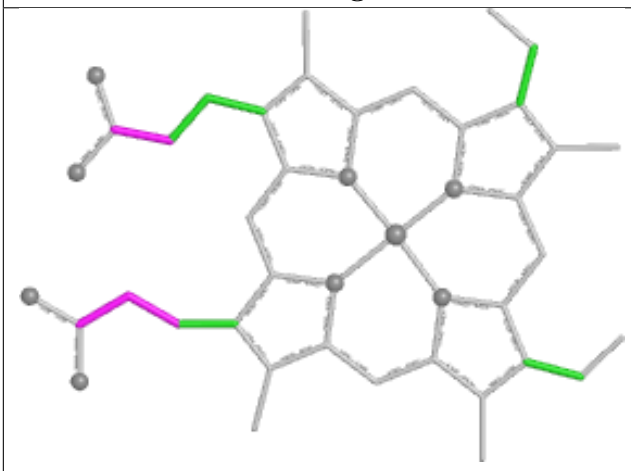
Ligand HEM D 147



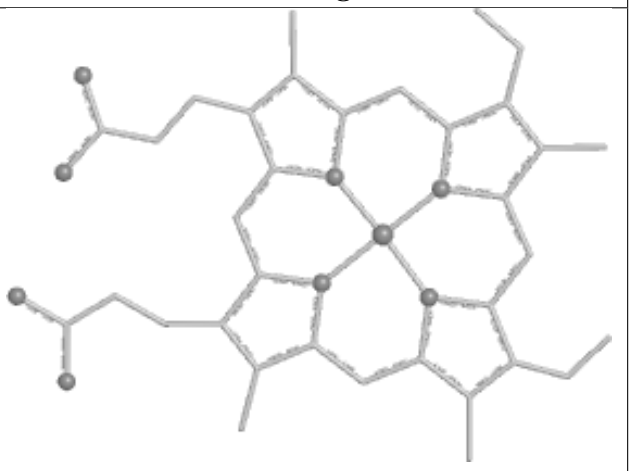
Bond lengths



Bond angles

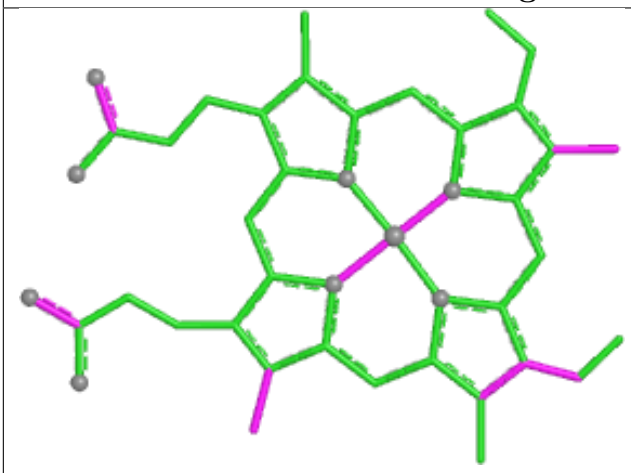


Torsions

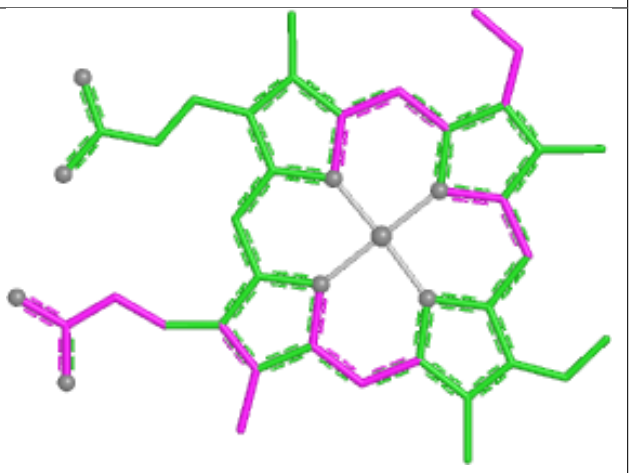


Rings

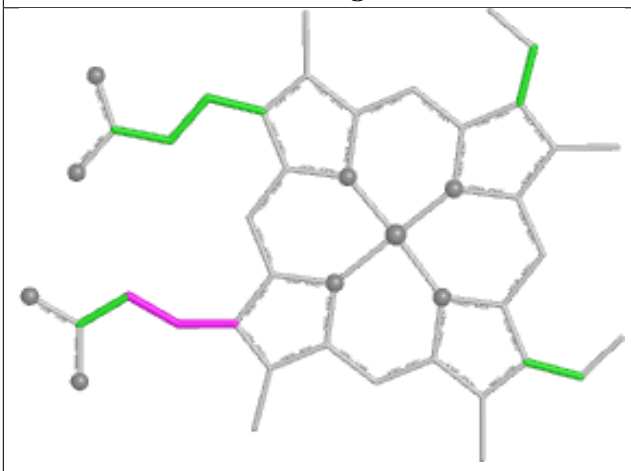
Ligand HEM B 147



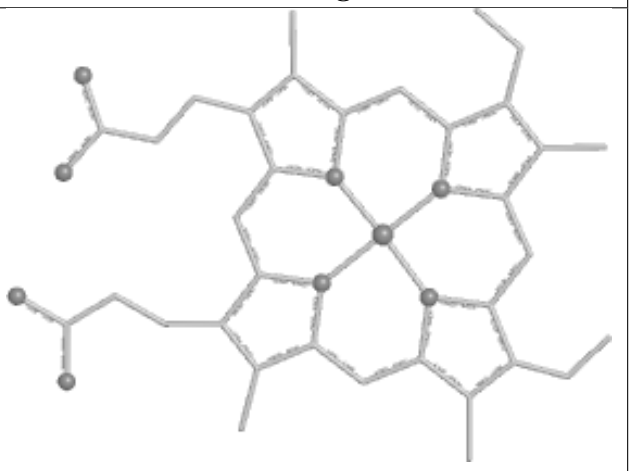
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.