Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2023 – 12:30 AM EST

PDB ID	:	1HGC
Title	:	HIGH RESOLUTION CRYSTAL STRUCTURES AND COMPARISONS OF T STATE DEOXYHAEMOGLOBIN AND TWO LIGANDED T-STATE HAEMOGLOBINS: T(ALPHA-OXY)HAEMOGLOBIN AND T(MET)HAEMOGLOBIN
Authors	:	Liddington, R.; Derewenda, Z.; Dodson, E.; Hubbard, R.; Dodson, G.
Deposited on	:	1991-10-31
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 (1)) were used in the production of this report:

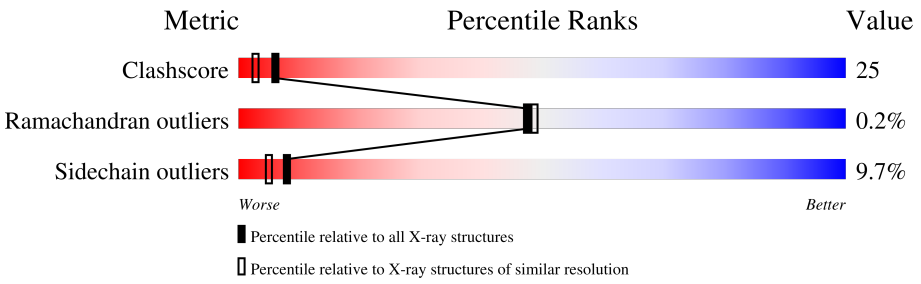
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	60% 32% 6% •
1	C	141	64% 28% 7% •
2	B	146	55% 34% 10% •
2	D	146	51% 38% 10% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4649 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.

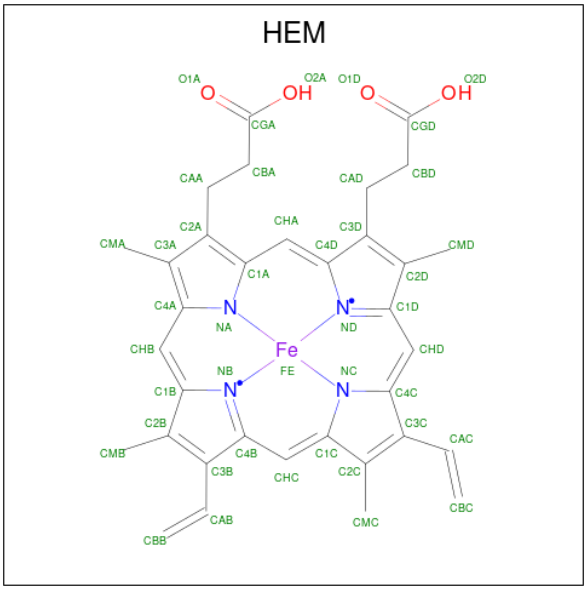
- Molecule 1 is a protein called HEMOGLOBIN (OXY) (ALPHA CHAIN).

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 (DEOXY) (BETA CHAIN).

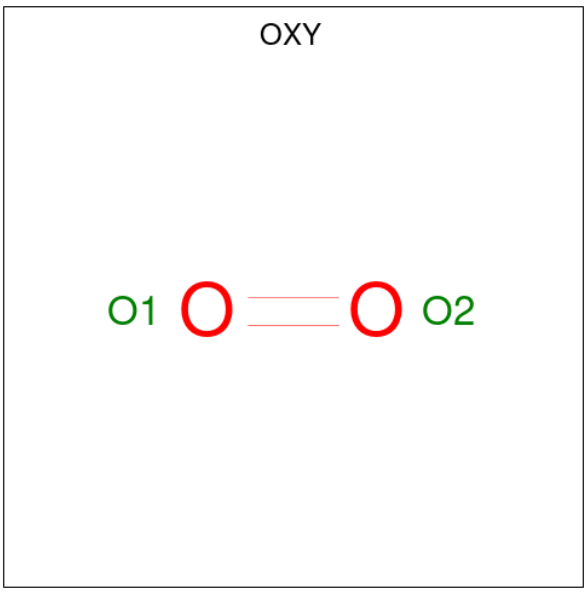
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1123	724	195	201	3	0	0	0
2	D	146	1123	724	195	201	3	0	0	0

- 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
3	B	1	43	34	1	4	4	0	0
3	C	1	43	34	1	4	4	0	0
3	D	1	43	34	1	4	4	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	2	2	0	0
4	C	1	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	16	16	16	0	0
5	B	33	33	33	0	0
5	C	21	21	21	0	0
5	D	19	19	19	0	0

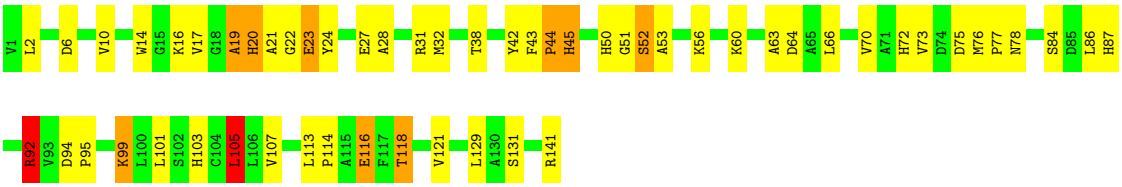
3 Residue-property plots (i)

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.

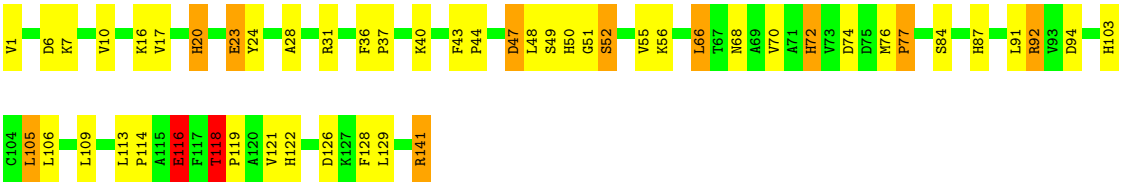
• Molecule 1: HEMOGLOBIN (OXY) (ALPHA CHAIN)

Chain A:



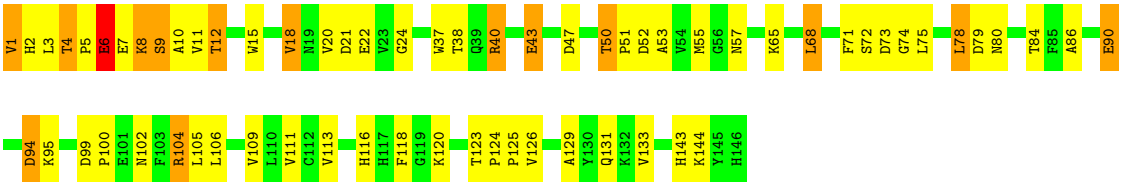
• Molecule 1: HEMOGLOBIN (OXY) (ALPHA CHAIN)

Chain C:



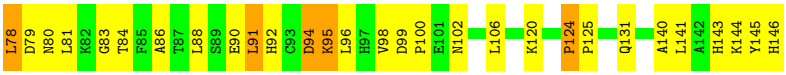
• Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)

Chain B:



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

Chain D:


L78
D79
N80
L81
K82
G83
T84
F85
A86
T87
L88
S89
E90
L91
H92
C93
D94
K95
L96
H97
V98
D99
P100
E101
N102
L106
K120
P124
P125
Q131
A140
L141
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 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.78Å 97.78Å 65.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4649	wwPDB-VP
Average B, all atoms ($Å^2$)	22.0	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: OXY, 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	0.77	0/1097	1.81	17/1491 (1.1%)
1	C	0.79	0/1097	1.65	18/1491 (1.2%)
2	B	0.77	0/1153	1.60	14/1566 (0.9%)
2	D	0.81	0/1153	1.66	12/1566 (0.8%)
All	All	0.79	0/4500	1.68	61/6114 (1.0%)

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	2
2	B	0	1
All	All	0	4

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	CD-NE-CZ	19.35	150.69	123.60
1	A	92	ARG	NE-CZ-NH2	19.31	129.96	120.30
1	C	23	GLU	CA-CB-CG	14.11	144.44	113.40
1	A	31	ARG	NE-CZ-NH1	11.75	126.17	120.30
1	C	31	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	23	GLU	CA-CB-CG	10.37	136.21	113.40
2	B	40	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	C	31	ARG	NE-CZ-NH2	-9.65	115.48	120.30
2	B	40	ARG	CD-NE-CZ	9.31	136.64	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	79	ASP	CB-CG-OD1	8.80	126.22	118.30
2	B	90	GLU	OE1-CD-OE2	8.64	133.66	123.30
1	C	141	ARG	NE-CZ-NH2	-8.42	116.09	120.30
2	B	79	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	C	47	ASP	CB-CG-OD2	-7.81	111.27	118.30
2	D	40	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	B	47	ASP	CB-CG-OD1	-7.80	111.28	118.30
1	A	92	ARG	NH1-CZ-NH2	-7.67	110.97	119.40
2	B	104	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	B	43	GLU	OE1-CD-OE2	7.49	132.29	123.30
1	A	20	HIS	O-C-N	7.25	134.30	122.70
1	A	31	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	D	52	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	118	THR	N-CA-CB	-7.06	96.89	110.30
1	C	118	THR	N-CA-CB	-6.78	97.42	110.30
1	A	64	ASP	CB-CG-OD1	6.76	124.38	118.30
2	D	10	ALA	N-CA-CB	-6.65	100.79	110.10
1	A	19	ALA	N-CA-CB	-6.54	100.95	110.10
2	B	6	GLU	OE1-CD-OE2	-6.38	115.65	123.30
1	C	126	ASP	CB-CG-OD1	6.35	124.02	118.30
2	D	47	ASP	CB-CG-OD1	-6.32	112.61	118.30
2	D	52	ASP	CA-CB-CG	6.24	127.12	113.40
1	A	23	GLU	CB-CA-C	-6.16	98.08	110.40
1	A	105	LEU	CA-CB-CG	6.13	129.39	115.30
1	C	94	ASP	CB-CG-OD1	-6.05	112.86	118.30
2	B	6	GLU	CG-CD-OE1	6.00	130.29	118.30
1	C	72	HIS	CA-CB-CG	-5.98	103.43	113.60
1	C	20	HIS	O-C-N	5.94	132.21	122.70
2	D	8	LYS	CA-CB-CG	5.92	126.42	113.40
1	C	47	ASP	N-CA-C	-5.85	95.20	111.00
1	C	116	GLU	CG-CD-OE1	-5.85	106.60	118.30
1	A	116	GLU	CG-CD-OE1	-5.74	106.83	118.30
2	D	21	ASP	CB-CG-OD1	5.72	123.45	118.30
2	D	2	HIS	O-C-N	5.71	131.84	122.70
2	D	19	ASN	N-CA-C	-5.71	95.58	111.00
1	A	72	HIS	CA-CB-CG	-5.57	104.13	113.60
2	B	94	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	C	92	ARG	CD-NE-CZ	-5.55	115.82	123.60
1	A	27	GLU	CG-CD-OE2	5.54	129.38	118.30
1	A	116	GLU	OE1-CD-OE2	5.54	129.94	123.30
2	B	1	VAL	O-C-N	5.50	131.50	122.70
1	A	141	ARG	NE-CZ-NH2	-5.43	117.58	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	94	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	36	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	C	105	LEU	CB-CG-CD2	-5.28	102.03	111.00
2	B	4	THR	N-CA-C	-5.25	96.81	111.00
2	D	6	GLU	CG-CD-OE1	5.24	128.78	118.30
1	C	77	PRO	O-C-N	5.22	131.05	122.70
1	C	116	GLU	OE1-CD-OE2	5.19	129.52	123.30
2	D	14	LEU	CB-CA-C	5.17	120.03	110.20
2	D	94	ASP	CB-CG-OD2	5.05	122.84	118.30
2	B	2	HIS	N-CA-CB	5.03	119.65	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	ARG	Sidechain
2	B	104	ARG	Sidechain
1	C	141	ARG	Sidechain
1	C	92	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	1
1	C	1069	0	1073	35	0
2	B	1123	0	1118	62	0
2	D	1123	0	1118	81	0
3	A	43	0	30	0	0
3	B	43	0	30	5	0
3	C	43	0	30	0	0
3	D	43	0	30	14	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	16	0	0	1	0
5	B	33	0	0	5	1
5	C	21	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	19	0	0	0	0
All	All	4649	0	4502	224	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (224) 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)
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.24	1.10
2:B:4:THR:CG2	2:B:5:PRO:HD2	1.88	1.03
3:B:147:HEM:HHC	3:B:147:HEM:HBB2	1.41	1.02
3:D:147:HEM:HHC	3:D:147:HEM:HBB2	1.36	1.02
2:D:21:ASP:HA	2:D:65:LYS:HG3	1.45	0.97
2:D:5:PRO:HA	2:D:8:LYS:HG3	1.46	0.96
2:B:50:THR:HG22	2:B:51:PRO:HD2	1.47	0.95
1:C:113:LEU:HB3	1:C:116:GLU:HG3	1.57	0.87
2:D:4:THR:O	2:D:8:LYS:HG2	1.75	0.86
1:A:42:TYR:C	1:A:44:PRO:HD3	1.98	0.84
2:B:4:THR:HG22	2:B:6:GLU:H	1.42	0.83
2:B:4:THR:HG23	2:B:5:PRO:CD	2.08	0.82
2:D:124:PRO:HB2	2:D:125:PRO:HD3	1.62	0.81
2:B:74:GLY:HA3	5:B:160:HOH:O	1.81	0.80
2:B:143:HIS:ND1	2:B:144:LYS:HE2	1.97	0.79
2:D:4:THR:HG22	2:D:6:GLU:H	1.47	0.78
1:C:113:LEU:HB3	1:C:116:GLU:CG	2.14	0.78
1:A:6:ASP:O	1:A:10:VAL:HG13	1.84	0.77
2:D:73:ASP:O	2:D:77:HIS:HD2	1.67	0.76
2:D:73:ASP:O	2:D:77:HIS:CD2	2.38	0.76
1:A:113:LEU:HB3	1:A:116:GLU:HG2	1.68	0.76
1:C:66:LEU:O	1:C:70:VAL:HG23	1.86	0.76
2:D:66:LYS:HE2	3:D:147:HEM:CAA	2.16	0.76
1:C:7:LYS:NZ	1:C:74:ASP:OD1	2.16	0.75
2:B:21:ASP:HA	2:B:65:LYS:HG2	1.70	0.74
2:D:38:THR:HG22	2:D:102:ASN:ND2	2.02	0.73
2:B:4:THR:CG2	2:B:5:PRO:CD	2.66	0.72
2:D:5:PRO:O	2:D:9:SER:HB3	1.90	0.72
1:A:99:LYS:HD2	1:A:99:LYS:N	2.03	0.72
1:C:52:SER:O	1:C:56:LYS:HG3	1.90	0.71
2:B:3:LEU:HD23	2:B:8:LYS:HA	1.74	0.70
2:D:66:LYS:HE2	3:D:147:HEM:HAA1	1.70	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:ASN:ND2	2:D:83:GLY:H	1.90	0.70
2:D:6:GLU:OE1	2:D:6:GLU:HA	1.92	0.69
2:B:50:THR:HG22	2:B:51:PRO:CD	2.23	0.68
2:D:38:THR:HG22	2:D:102:ASN:HD22	1.59	0.67
1:A:44:PRO:HD2	1:A:45:HIS:ND1	2.09	0.67
1:A:43:PHE:N	1:A:44:PRO:HD3	2.09	0.67
2:D:90:GLU:O	2:D:94:ASP:HB2	1.94	0.67
1:A:19:ALA:HB3	1:A:20:HIS:CD2	2.30	0.67
2:D:4:THR:CG2	2:D:5:PRO:CD	2.74	0.66
1:A:20:HIS:O	1:A:23:GLU:HB2	1.95	0.66
2:D:15:TRP:HH2	2:D:68:LEU:HD11	1.59	0.65
2:B:24:GLY:HA2	2:B:68:LEU:HD23	1.79	0.65
2:D:124:PRO:CB	2:D:125:PRO:HD3	2.27	0.65
2:B:4:THR:O	2:B:8:LYS:HG2	1.98	0.64
2:D:4:THR:HG22	2:D:5:PRO:HD2	1.80	0.63
2:D:50:THR:OG1	2:D:53:ALA:HB2	1.98	0.62
1:A:53:ALA:HA	1:A:56:LYS:HB2	1.80	0.62
2:B:129:ALA:O	2:B:133:VAL:HG23	1.99	0.62
2:D:91:LEU:O	2:D:95:LYS:HB2	2.00	0.62
2:D:66:LYS:CE	3:D:147:HEM:HAA1	2.29	0.61
1:A:92:ARG:HH11	2:D:40:ARG:HB2	1.64	0.61
2:D:96:LEU:HD13	3:D:147:HEM:C3D	2.34	0.61
1:C:103:HIS:HE1	2:D:131:GLN:OE1	1.84	0.61
2:D:51:PRO:O	2:D:55:MET:HG2	2.00	0.61
2:D:66:LYS:HE2	3:D:147:HEM:HAA2	1.83	0.61
2:B:124:PRO:HB2	2:B:125:PRO:HD3	1.82	0.61
2:B:4:THR:O	2:B:8:LYS:HE3	2.01	0.60
2:B:90:GLU:O	2:B:94:ASP:HB2	2.01	0.60
2:B:3:LEU:HD23	2:B:8:LYS:CA	2.30	0.60
1:A:76:MET:N	1:A:77:PRO:CD	2.65	0.60
2:D:4:THR:HG22	2:D:5:PRO:CD	2.32	0.59
3:D:147:HEM:HHC	3:D:147:HEM:CBB	2.22	0.59
1:C:66:LEU:HD21	1:C:105:LEU:HD21	1.84	0.59
2:B:86:ALA:O	2:B:90:GLU:HG3	2.02	0.59
2:B:74:GLY:HA2	2:B:84:THR:HG21	1.84	0.59
2:B:7:GLU:HG2	2:B:129:ALA:HB2	1.84	0.58
2:B:74:GLY:CA	5:B:160:HOH:O	2.45	0.58
2:D:4:THR:CG2	2:D:5:PRO:HD2	2.34	0.58
1:C:43:PHE:N	1:C:44:PRO:CD	2.66	0.58
2:D:124:PRO:N	2:D:125:PRO:CD	2.66	0.58
2:B:4:THR:C	2:B:8:LYS:HE3	2.23	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ALA:O	2:D:90:GLU:HG3	2.04	0.58
2:D:80:ASN:HD21	2:D:83:GLY:H	1.50	0.58
2:B:111:VAL:HG11	2:B:131:GLN:OE1	2.03	0.57
2:B:38:THR:HG22	2:B:102:ASN:ND2	2.20	0.57
2:B:123:THR:O	2:B:126:VAL:N	2.38	0.57
3:D:147:HEM:HBB2	3:D:147:HEM:CHC	2.18	0.56
2:D:50:THR:H	2:D:53:ALA:HB3	1.71	0.55
1:C:50:HIS:ND1	1:C:51:GLY:N	2.55	0.55
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.89	0.55
3:B:147:HEM:HHC	3:B:147:HEM:CBB	2.23	0.55
2:D:74:GLY:HA2	2:D:84:THR:HG21	1.87	0.55
2:D:4:THR:HB	2:D:7:GLU:HG3	1.89	0.54
1:C:17:VAL:HG13	1:C:24:TYR:CD2	2.43	0.54
1:A:43:PHE:HA	1:A:45:HIS:CE1	2.42	0.53
1:C:76:MET:N	1:C:77:PRO:CD	2.71	0.53
2:D:45:PHE:O	2:D:59:LYS:HG3	2.09	0.53
1:C:76:MET:HB2	1:C:77:PRO:HD3	1.90	0.53
2:D:106:LEU:HD23	3:D:147:HEM:CBB	2.39	0.53
2:B:15:TRP:HH2	2:B:68:LEU:HD11	1.73	0.52
2:D:50:THR:OG1	2:D:53:ALA:CB	2.58	0.52
2:B:109:VAL:O	2:B:113:VAL:HG23	2.10	0.52
2:B:3:LEU:HD21	2:B:11:VAL:HG21	1.92	0.52
1:A:66:LEU:O	1:A:70:VAL:HG23	2.11	0.51
1:C:43:PHE:N	1:C:44:PRO:HD3	2.25	0.51
1:A:42:TYR:O	1:A:44:PRO:HD3	2.10	0.51
2:B:38:THR:HG22	2:B:102:ASN:HD21	1.74	0.51
2:B:72:SER:O	2:B:75:LEU:HB2	2.11	0.51
1:C:68:ASN:O	1:C:72:HIS:HD2	1.93	0.51
1:C:76:MET:N	1:C:77:PRO:HD2	2.24	0.51
2:D:50:THR:O	2:D:54:VAL:HG23	2.11	0.51
2:D:94:ASP:OD1	2:D:146:HIS:NE2	2.38	0.51
2:D:45:PHE:HA	2:D:59:LYS:HE3	1.92	0.51
1:A:114:PRO:O	2:B:116:HIS:NE2	2.33	0.50
2:D:15:TRP:CH2	2:D:68:LEU:HD11	2.44	0.50
2:B:5:PRO:HA	2:B:8:LYS:CG	2.41	0.50
2:B:20:VAL:HG13	2:B:68:LEU:HB3	1.92	0.50
2:B:5:PRO:HA	2:B:8:LYS:HG2	1.94	0.50
2:B:15:TRP:CH2	2:B:68:LEU:HD11	2.47	0.50
2:B:8:LYS:O	2:B:12:THR:HB	2.12	0.49
2:D:140:ALA:O	2:D:143:HIS:CB	2.60	0.49
1:C:118:THR:HG22	1:C:121:VAL:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:PRO:O	2:B:55:MET:HG2	2.12	0.49
2:B:53:ALA:O	2:B:57:ASN:HB2	2.11	0.49
2:D:5:PRO:HA	2:D:8:LYS:CG	2.30	0.49
2:D:30:ARG:O	2:D:34:VAL:HG23	2.12	0.49
3:B:147:HEM:HBB2	3:B:147:HEM:CHC	2.21	0.49
1:A:2:LEU:HD22	1:A:6:ASP:HB3	1.94	0.48
3:B:147:HEM:HAA1	5:B:168:HOH:O	2.13	0.48
1:A:92:ARG:HB3	2:D:37:TRP:HB2	1.95	0.48
2:D:1:VAL:HG23	2:D:3:LEU:HD13	1.95	0.48
1:A:21:ALA:HB1	1:A:63:ALA:HB1	1.96	0.48
2:D:38:THR:O	2:D:41:PHE:HD1	1.96	0.48
1:A:118:THR:HG22	1:A:121:VAL:H	1.79	0.48
2:B:143:HIS:HB3	5:B:158:HOH:O	2.13	0.48
2:B:5:PRO:O	2:B:9:SER:HB3	2.13	0.48
1:A:16:LYS:HG3	1:A:116:GLU:OE1	2.14	0.47
2:B:10:ALA:HA	5:B:164:HOH:O	2.14	0.47
1:A:103:HIS:O	1:A:107:VAL:HG23	2.14	0.47
1:C:20:HIS:O	1:C:23:GLU:HB2	2.14	0.47
2:D:57:ASN:HA	2:D:58:PRO:HD2	1.60	0.47
1:A:38:THR:CG2	2:D:100:PRO:HG2	2.44	0.47
1:A:103:HIS:HD2	5:A:163:HOH:O	1.97	0.47
2:D:140:ALA:O	2:D:143:HIS:HB3	2.14	0.47
2:B:3:LEU:HG	2:B:7:GLU:HB3	1.97	0.47
1:C:105:LEU:O	1:C:109:LEU:HG	2.14	0.47
1:C:28:ALA:CB	1:C:105:LEU:HD13	2.44	0.47
2:B:37:TRP:O	2:B:40:ARG:HG2	2.15	0.47
2:B:75:LEU:O	2:B:78:LEU:HD22	2.15	0.47
2:D:78:LEU:HD12	2:D:78:LEU:HA	1.73	0.46
2:D:80:ASN:O	2:D:84:THR:OG1	2.18	0.46
2:B:106:LEU:HD23	3:B:147:HEM:CBB	2.45	0.46
2:D:15:TRP:CE3	2:D:18:VAL:HG21	2.51	0.46
2:D:66:LYS:HD3	3:D:147:HEM:C2A	2.49	0.46
2:D:96:LEU:HB2	2:D:98:VAL:HG23	1.96	0.46
1:A:75:ASP:OD1	1:A:78:ASN:OD1	2.32	0.46
2:D:1:VAL:CG2	2:D:3:LEU:HD13	2.45	0.46
1:A:51:GLY:O	1:A:52:SER:C	2.54	0.46
2:B:21:ASP:HA	2:B:65:LYS:CG	2.44	0.46
2:D:40:ARG:HG2	2:D:41:PHE:CD1	2.50	0.46
1:C:106:LEU:HD13	1:C:129:LEU:HD12	1.98	0.45
1:C:118:THR:HG22	1:C:121:VAL:H	1.81	0.45
2:D:88:LEU:HD11	3:D:147:HEM:HMA1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:HIS:N	2:D:146:HIS:CD2	2.84	0.45
2:B:68:LEU:O	2:B:72:SER:HB2	2.16	0.45
1:A:60:LYS:HB2	1:A:60:LYS:HE2	1.57	0.45
2:B:18:VAL:HG12	2:B:118:PHE:CZ	2.52	0.45
1:C:116:GLU:H	1:C:116:GLU:HG2	1.44	0.45
1:C:6:ASP:O	1:C:10:VAL:HG13	2.17	0.45
2:D:4:THR:HG23	2:D:5:PRO:CD	2.45	0.45
1:C:49:SER:O	1:C:52:SER:HB3	2.16	0.44
2:B:124:PRO:N	2:B:125:PRO:CD	2.81	0.44
2:B:1:VAL:HG23	2:B:3:LEU:HD13	2.00	0.44
2:B:3:LEU:HD23	2:B:8:LYS:N	2.31	0.44
1:A:94:ASP:HA	1:A:95:PRO:HD3	1.84	0.44
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.72	0.44
2:D:21:ASP:HA	2:D:65:LYS:CG	2.34	0.44
2:D:99:ASP:OD1	2:D:100:PRO:HD2	2.17	0.44
2:D:63:HIS:ND1	2:D:66:LYS:HD2	2.32	0.43
1:C:106:LEU:HA	1:C:106:LEU:HD12	1.75	0.43
1:A:20:HIS:CD2	1:A:20:HIS:N	2.84	0.43
2:D:63:HIS:HE1	3:D:147:HEM:CHA	2.31	0.43
2:B:3:LEU:HB3	2:B:8:LYS:HD3	2.01	0.43
1:A:28:ALA:HB1	1:A:105:LEU:HD13	2.00	0.43
2:D:1:VAL:HG13	2:D:81:LEU:HD12	2.00	0.43
2:B:124:PRO:CB	2:B:125:PRO:HD3	2.45	0.43
1:A:28:ALA:CB	1:A:105:LEU:HD13	2.49	0.43
1:A:43:PHE:N	1:A:44:PRO:CD	2.81	0.43
1:A:86:LEU:HD23	1:A:87:HIS:CE1	2.54	0.42
2:B:3:LEU:C	2:B:4:THR:O	2.56	0.42
2:B:80:ASN:HD22	2:B:80:ASN:HA	1.60	0.42
1:C:66:LEU:HD12	1:C:66:LEU:HA	1.76	0.42
1:A:70:VAL:O	1:A:73:VAL:HB	2.19	0.42
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.90	0.42
1:A:22:GLY:HA2	1:A:60:LYS:HA	2.02	0.42
1:A:99:LYS:HD2	1:A:99:LYS:H	1.83	0.42
1:A:14:TRP:O	1:A:17:VAL:HB	2.20	0.42
1:C:1:VAL:HG13	1:C:1:VAL:O	2.19	0.42
2:B:105:LEU:HA	2:B:105:LEU:HD23	1.81	0.42
2:D:77:HIS:C	2:D:79:ASP:H	2.23	0.42
1:A:38:THR:HG21	2:D:100:PRO:HG2	2.01	0.42
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.87	0.42
1:A:32:MET:SD	1:A:101:LEU:HB2	2.60	0.41
1:C:122:HIS:HD2	1:C:122:HIS:O	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:HA	1:C:119:PRO:HD3	1.85	0.41
2:B:99:ASP:HA	2:B:100:PRO:HD3	1.91	0.41
1:C:10:VAL:HG11	1:C:128:PHE:HB2	2.02	0.41
2:D:57:ASN:OD1	2:D:59:LYS:N	2.53	0.41
1:A:86:LEU:HD23	1:A:87:HIS:ND1	2.35	0.41
1:C:87:HIS:HA	1:C:91:LEU:HB2	2.03	0.41
2:D:92:HIS:HB3	2:D:145:TYR:OH	2.20	0.41
2:D:143:HIS:CE1	2:D:144:LYS:HE2	2.56	0.41
1:A:51:GLY:HA2	1:A:56:LYS:HE3	2.02	0.41
1:C:37:PRO:HA	1:C:40:LYS:HD3	2.03	0.41
2:D:5:PRO:O	2:D:9:SER:N	2.47	0.41
2:D:72:SER:O	2:D:75:LEU:HB2	2.20	0.41
2:D:77:HIS:CD2	2:D:77:HIS:N	2.89	0.41
1:A:20:HIS:HB2	1:A:24:TYR:CZ	2.56	0.41
3:D:147:HEM:HBD2	3:D:147:HEM:HHA	2.03	0.41
1:A:113:LEU:N	1:A:114:PRO:CD	2.84	0.40
2:B:3:LEU:CD2	2:B:8:LYS:HA	2.47	0.40
2:D:51:PRO:O	2:D:55:MET:N	2.45	0.40
2:D:144:LYS:O	2:D:146:HIS:HD2	2.04	0.40
2:B:68:LEU:HD13	2:B:71:PHE:HB3	2.03	0.40
1:A:16:LYS:HB3	1:A:16:LYS:HE3	1.20	0.40
2:D:6:GLU:OE1	2:D:6:GLU:CA	2.63	0.40
2:D:43:GLU:H	2:D:43:GLU:HG3	1.64	0.40
2:D:63:HIS:CE1	2:D:66:LYS:HD2	2.56	0.40
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.90	0.40
1:C:48:LEU:HD23	1:C:55:VAL:CG2	2.52	0.40
2:D:57:ASN:OD1	2:D:59:LYS:HB2	2.21	0.40
2:D:141:LEU:CD1	3:D:147:HEM:CAB	3.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:OE1	5:B:148:HOH:O[3_555]	1.80	0.40

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%)	135 (97%)	4 (3%)	0	100	100
1	C	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	18
2	B	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
2	D	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
All	All	566/574 (99%)	542 (96%)	23 (4%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	114	PRO

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	11
1	C	113/113 (100%)	106 (94%)	7 (6%)	18	15
2	B	118/118 (100%)	104 (88%)	14 (12%)	5	2
2	D	118/118 (100%)	102 (86%)	16 (14%)	3	2
All	All	462/462 (100%)	417 (90%)	45 (10%)	8	5

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	A	45	HIS
1	A	50	HIS
1	A	52	SER
1	A	84	SER
1	A	99	LYS
1	A	105	LEU
1	A	131	SER
2	B	6	GLU
2	B	8	LYS
2	B	9	SER
2	B	12	THR
2	B	18	VAL
2	B	22	GLU
2	B	43	GLU
2	B	50	THR
2	B	52	ASP
2	B	68	LEU
2	B	73	ASP
2	B	78	LEU
2	B	95	LYS
2	B	120	LYS
1	C	16	LYS
1	C	47	ASP
1	C	52	SER
1	C	66	LEU
1	C	84	SER
1	C	116	GLU
1	C	118	THR
2	D	6	GLU
2	D	8	LYS
2	D	14	LEU
2	D	17	LYS
2	D	43	GLU
2	D	50	THR
2	D	52	ASP
2	D	65	LYS
2	D	68	LEU
2	D	73	ASP
2	D	77	HIS
2	D	78	LEU
2	D	91	LEU
2	D	95	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	120	LYS
2	D	124	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	78	ASN
1	A	97	ASN
1	A	103	HIS
2	B	63	HIS
2	B	77	HIS
2	B	80	ASN
2	B	102	ASN
1	C	20	HIS
1	C	72	HIS
1	C	78	ASN
1	C	97	ASN
1	C	103	HIS
2	D	63	HIS
2	D	77	HIS
2	D	80	ASN
2	D	102	ASN

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	$\#\|Z\| > 2$
4	OXY	C	150	3	1,1,1	0.15	0	-		
3	HEM	B	147	2	41,50,50	1.55	5 (12%)	45,82,82	1.32	5 (11%)
3	HEM	C	142	4,1	41,50,50	1.52	4 (9%)	45,82,82	1.45	5 (11%)
3	HEM	A	142	4,1	41,50,50	1.47	4 (9%)	45,82,82	1.41	9 (20%)
3	HEM	D	147	2	41,50,50	1.50	4 (9%)	45,82,82	2.11	12 (26%)
4	OXY	A	150	3	1,1,1	0.00	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	147	2	-	4/12/54/54	-
3	HEM	A	142	4,1	-	3/12/54/54	-
3	HEM	C	142	4,1	-	3/12/54/54	-
3	HEM	D	147	2	-	5/12/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C3C-C2C	-4.92	1.33	1.40
3	B	147	HEM	C3C-C2C	-4.69	1.33	1.40
3	D	147	HEM	C3C-C2C	-4.04	1.34	1.40
3	A	142	HEM	C3C-C2C	-3.93	1.34	1.40
3	A	142	HEM	C3C-CAC	3.57	1.55	1.47
3	C	142	HEM	C3C-CAC	3.49	1.55	1.47
3	D	147	HEM	FE-NB	3.33	2.13	1.96
3	B	147	HEM	C3C-CAC	3.09	1.54	1.47
3	C	142	HEM	CAB-C3B	2.93	1.55	1.47
3	D	147	HEM	C3C-CAC	2.90	1.53	1.47
3	B	147	HEM	CAB-C3B	2.86	1.55	1.47
3	A	142	HEM	CAB-C3B	2.78	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	147	HEM	CAB-C3B	2.59	1.54	1.47
3	C	142	HEM	CAA-C2A	2.28	1.55	1.52
3	B	147	HEM	CMB-C2B	2.14	1.55	1.50
3	B	147	HEM	CBD-CAD	2.07	1.58	1.52
3	A	142	HEM	CMB-C2B	2.05	1.55	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	147	HEM	CBA-CAA-C2A	8.04	126.34	112.62
3	D	147	HEM	CMA-C3A-C4A	-4.26	121.91	128.46
3	D	147	HEM	O1D-CGD-CBD	-3.94	110.44	123.08
3	D	147	HEM	O2D-CGD-O1D	3.87	132.95	123.30
3	B	147	HEM	CMA-C3A-C4A	-3.52	123.06	128.46
3	D	147	HEM	CMA-C3A-C2A	3.36	131.27	124.94
3	C	142	HEM	CBA-CAA-C2A	3.27	118.21	112.62
3	B	147	HEM	CMC-C2C-C3C	3.18	130.62	124.68
3	A	142	HEM	O1D-CGD-CBD	-3.16	112.94	123.08
3	A	142	HEM	CAD-CBD-CGD	3.12	120.32	113.60
3	D	147	HEM	O2A-CGA-O1A	3.00	130.79	123.30
3	C	142	HEM	CMA-C3A-C4A	-2.92	123.97	128.46
3	C	142	HEM	O1D-CGD-CBD	-2.90	113.76	123.08
3	D	147	HEM	CHB-C1B-NB	2.84	127.89	124.38
3	C	142	HEM	CMB-C2B-C1B	-2.77	120.82	125.04
3	A	142	HEM	O2A-CGA-O1A	2.75	130.15	123.30
3	A	142	HEM	CMB-C2B-C1B	-2.53	121.19	125.04
3	C	142	HEM	CMC-C2C-C3C	2.50	129.36	124.68
3	D	147	HEM	CAA-CBA-CGA	2.50	120.75	113.76
3	B	147	HEM	CMA-C3A-C2A	2.44	129.55	124.94
3	D	147	HEM	C4C-CHD-C1D	2.42	125.75	122.56
3	A	142	HEM	O1A-CGA-CBA	-2.36	115.49	123.08
3	A	142	HEM	O2D-CGD-O1D	2.34	129.12	123.30
3	D	147	HEM	C4B-CHC-C1C	2.23	125.50	122.56
3	B	147	HEM	C4B-CHC-C1C	2.21	125.47	122.56
3	A	142	HEM	C3B-C2B-C1B	2.20	108.12	106.49
3	B	147	HEM	CAD-C3D-C4D	-2.20	120.82	124.66
3	A	142	HEM	CAD-C3D-C4D	-2.14	120.92	124.66
3	D	147	HEM	CBD-CAD-C3D	-2.10	106.79	112.63
3	D	147	HEM	CMC-C2C-C3C	2.02	128.46	124.68
3	A	142	HEM	C4C-CHD-C1D	2.02	125.22	122.56

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

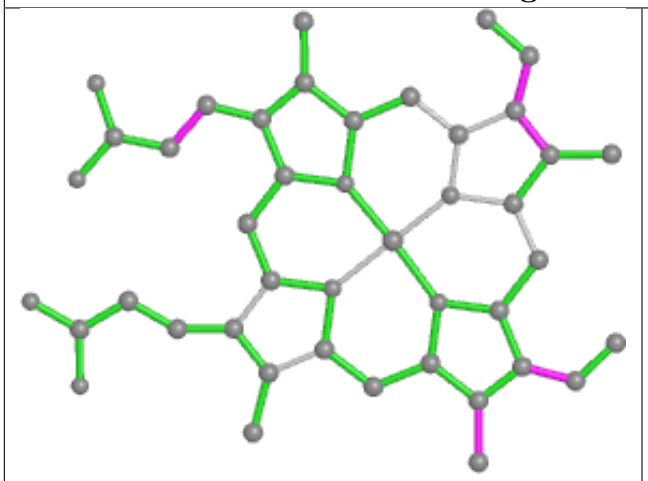
There are no ring outliers.

2 monomers are involved in 19 short contacts:

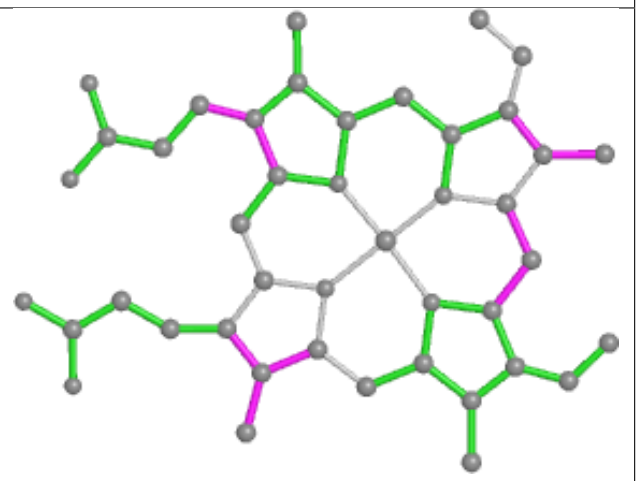
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	147	HEM	5	0
3	D	147	HEM	14	0

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

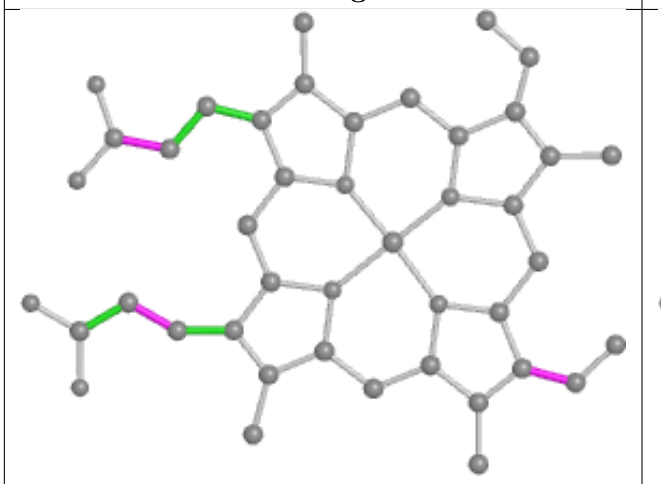
Ligand HEM B 147



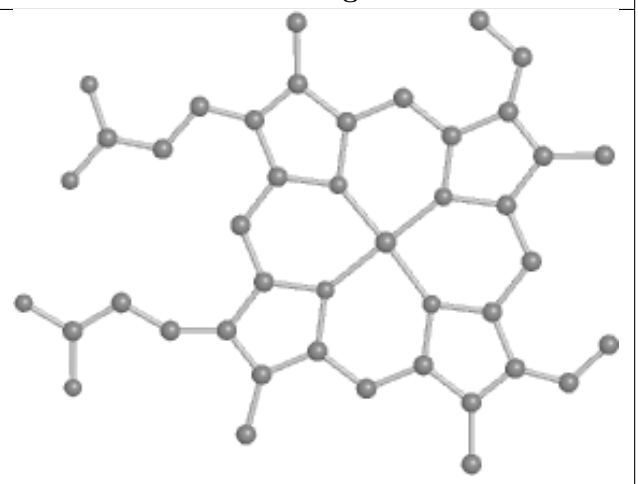
Bond lengths



Bond angles

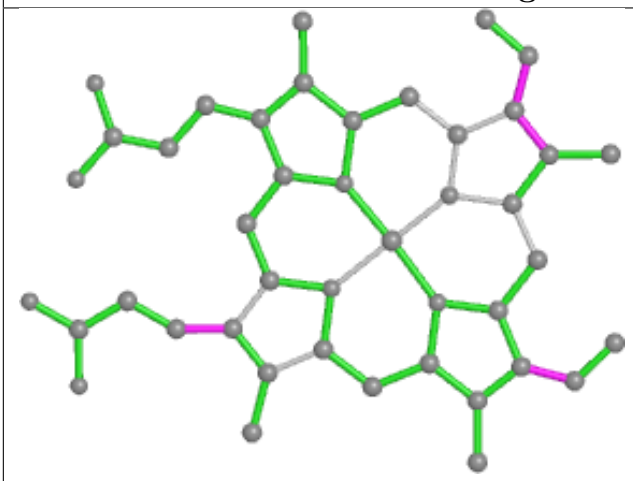


Torsions

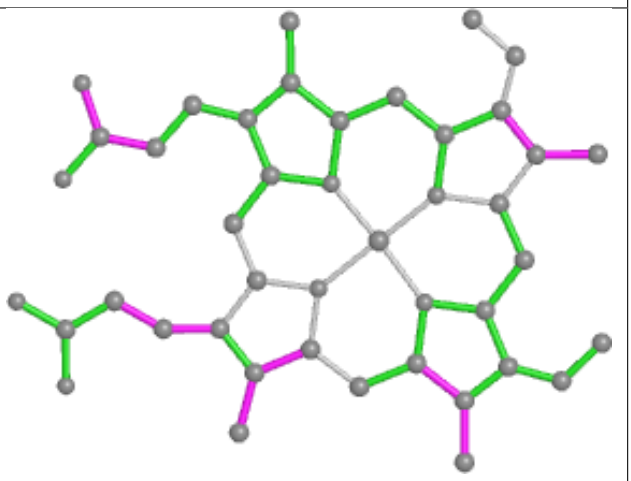


Rings

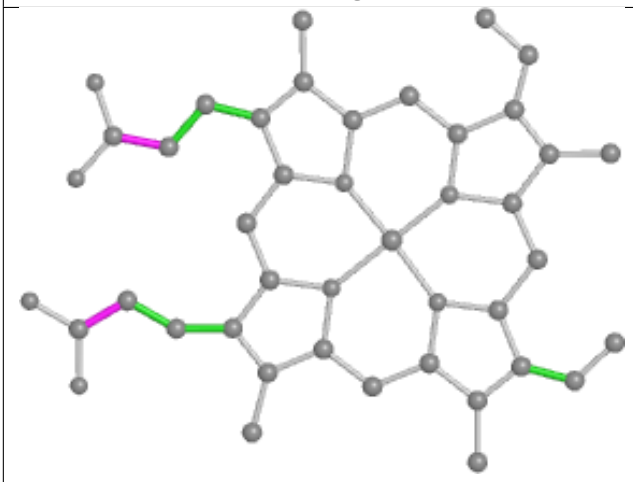
Ligand HEM C 142



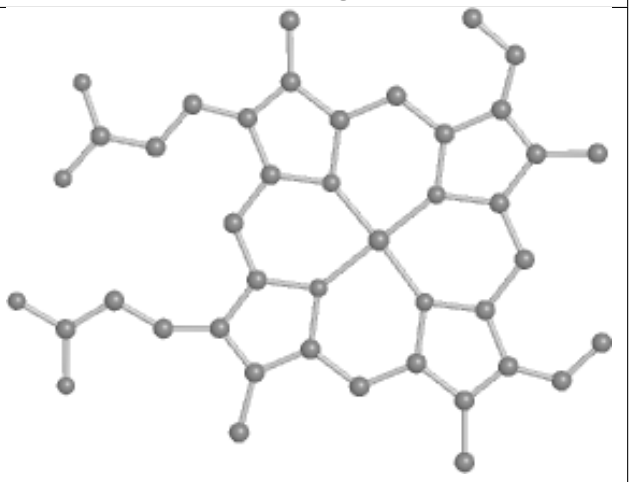
Bond lengths



Bond angles

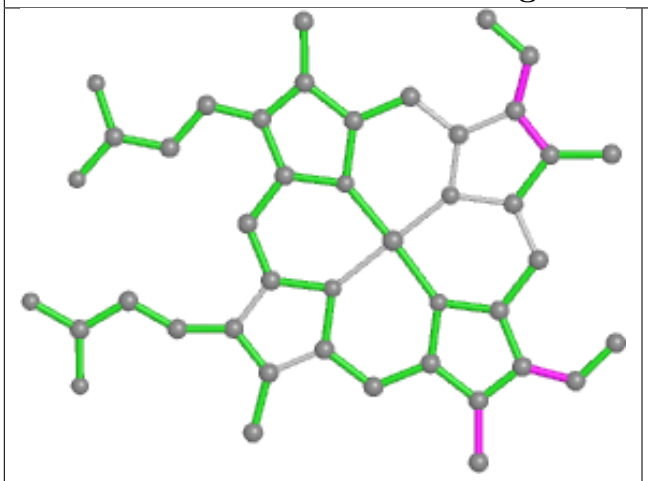


Torsions

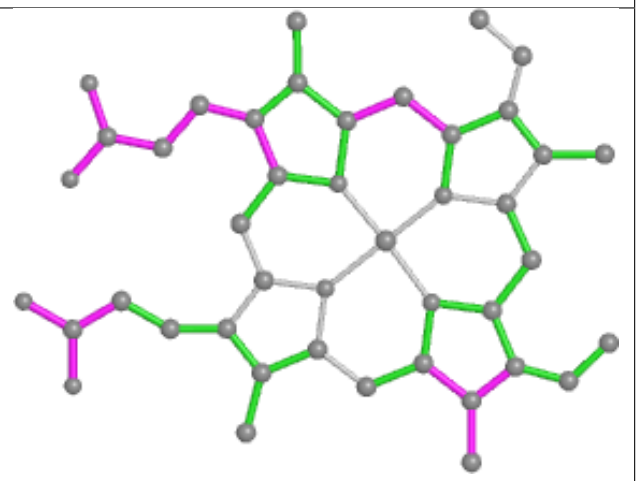


Rings

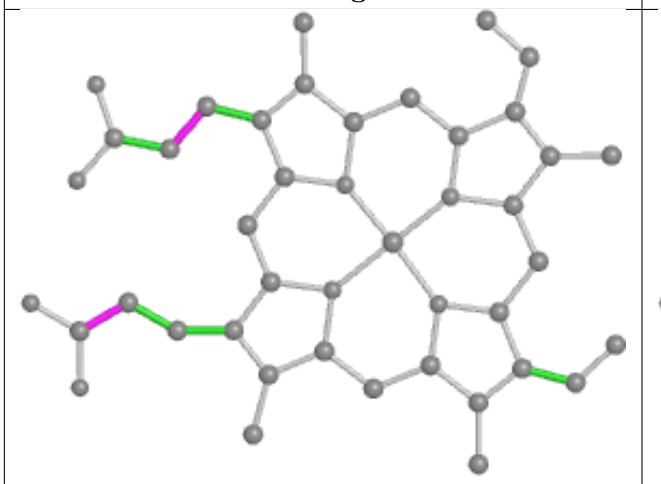
Ligand HEM A 142



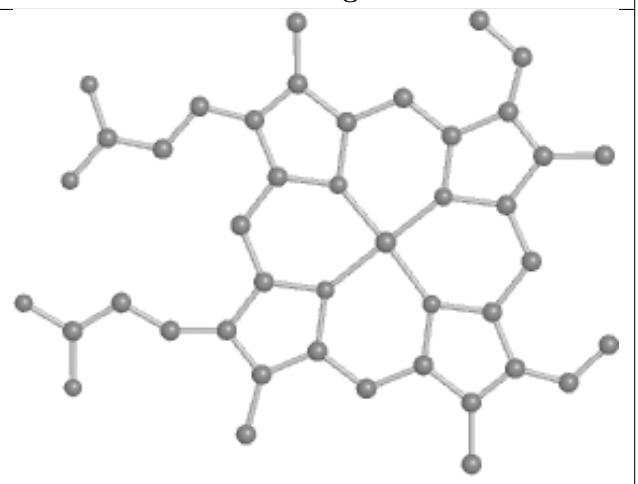
Bond lengths



Bond angles

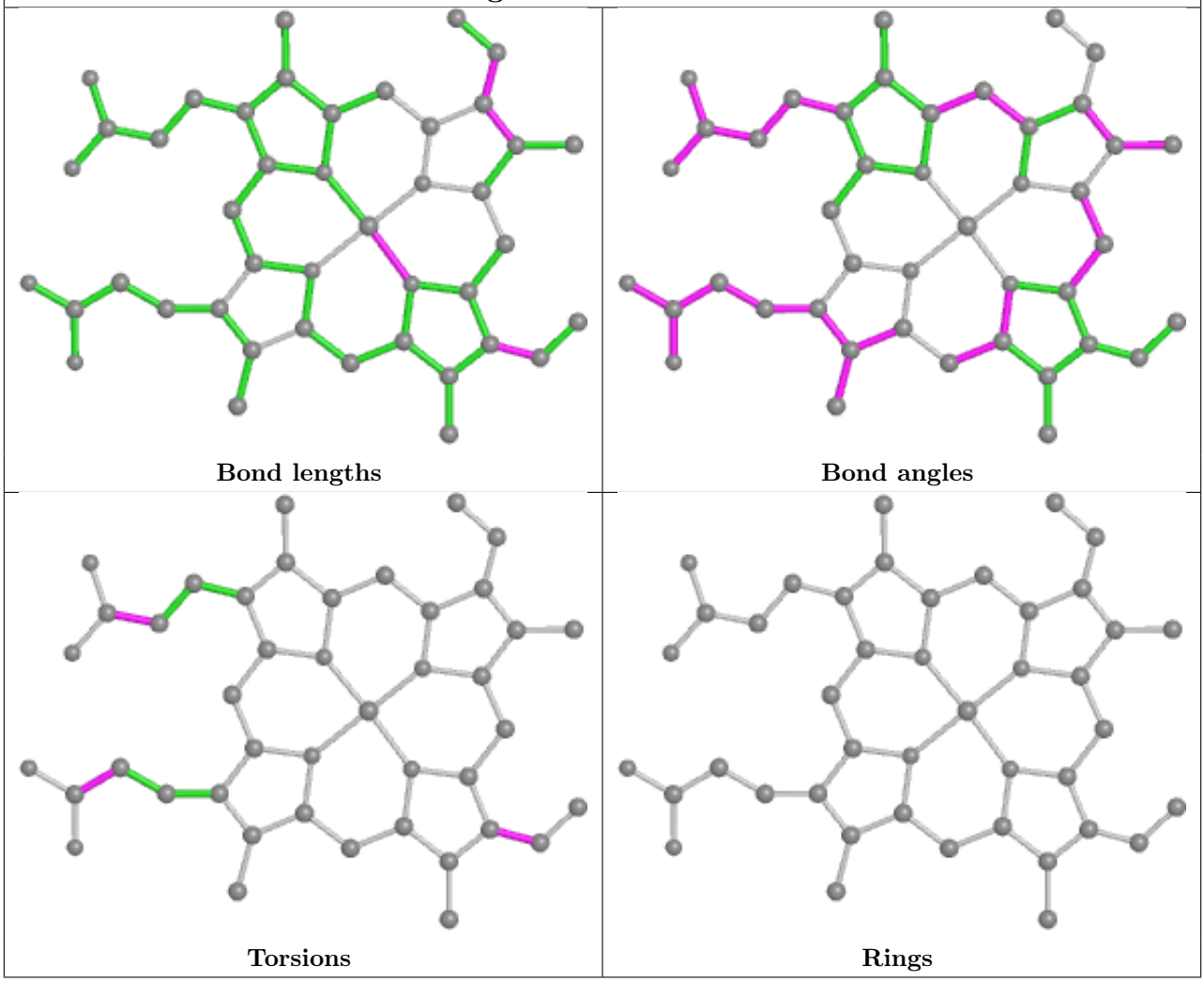


Torsions



Rings

Ligand HEM D 147



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.