Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:06 PM GMT

PDB ID	:	1IT3
Title	:	Hagfish CO ligand hemoglobin
Authors	:	Mito, M.; Chong, K.T.; Park, S.-Y.; Tame, J.R.
Deposited on	:	2002-01-05
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

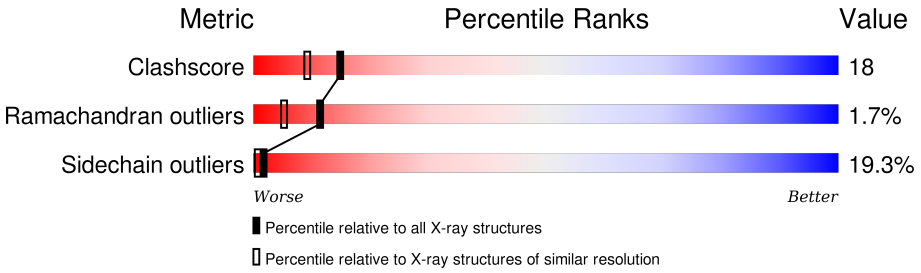
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	146	49% 42% 9%
1	B	146	54% 33% 11%
1	C	146	55% 36% 8%
1	D	146	59% 36% 5%

2 Entry composition

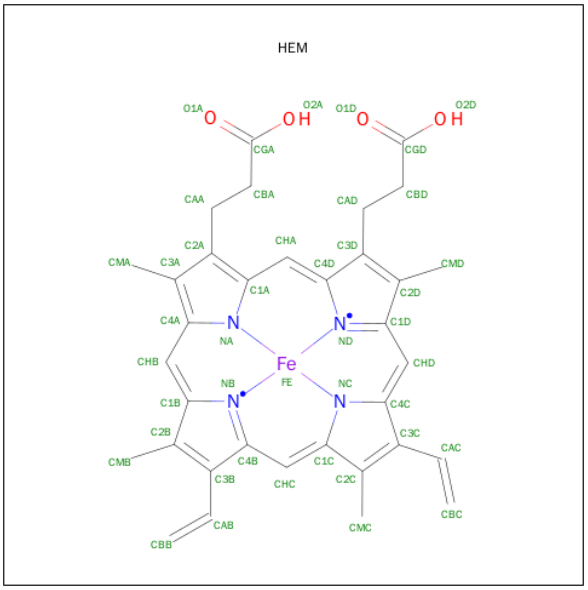
There are 4 unique types of molecules in this entry. The entry contains 5210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	146	Total	C	N	O	S	0	0	0
			1190	776	191	220	3			
1	B	146	Total	C	N	O	S	0	0	0
			1190	776	191	220	3			
1	C	146	Total	C	N	O	S	0	0	0
			1190	776	191	220	3			
1	D	146	Total	C	N	O	S	0	0	0
			1190	776	191	220	3			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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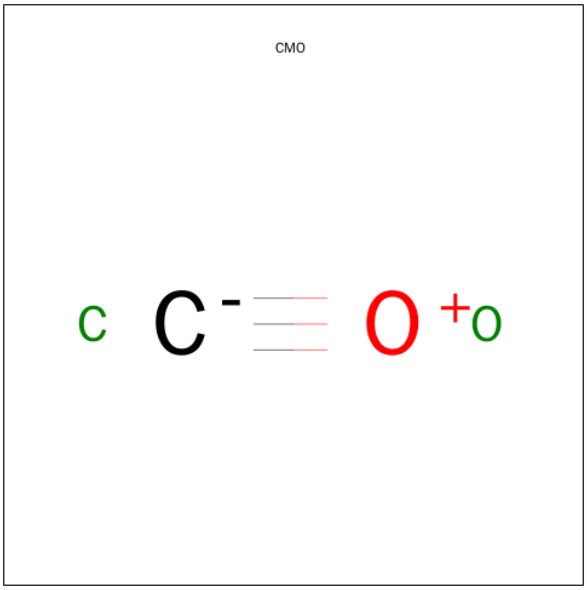
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	58	Total	O	0	0
			58	58		
4	C	60	Total	O	0	0
			60	60		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	85	Total	O	0	0
			85	85		

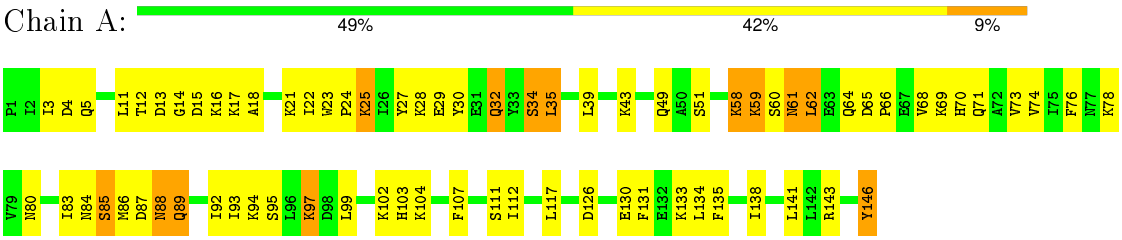
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

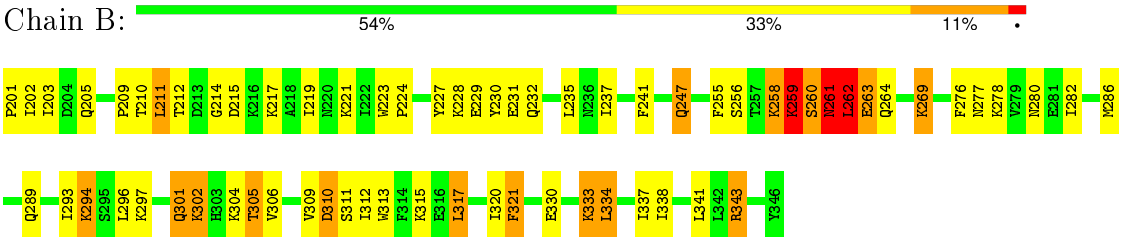
- Molecule 1: hemoglobin

Chain A:



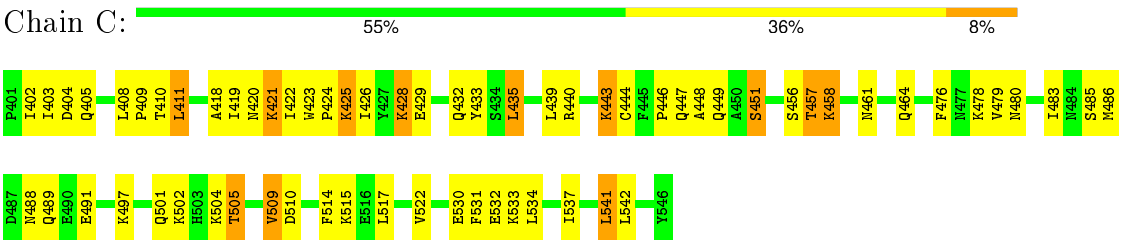
- Molecule 1: hemoglobin

Chain B:



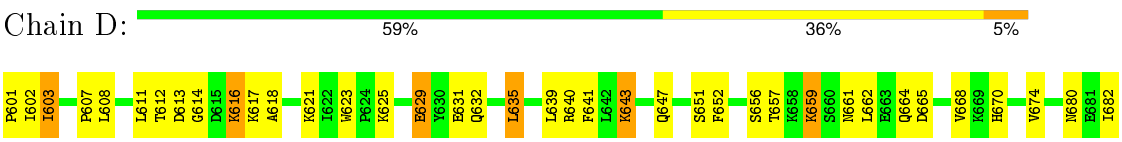
- Molecule 1: hemoglobin

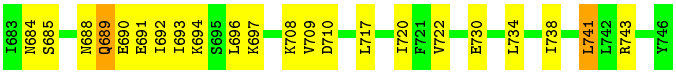
Chain C:



- Molecule 1: hemoglobin

Chain D:




I683
N684
S685
N688
Q689
E690
E691
I692
I693
K694
S695
L696
K697
K708
V709
D710
L717
I720
F721
V722
E730
L734
I738
L741
L742
R743
Y746

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.97Å 150.64Å 51.94Å 90.00° 106.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	84.1 (20.00-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.196 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5210	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: CMO, 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	0.37	0/1216	0.55	0/1637
1	B	0.38	0/1216	0.54	0/1637
1	C	0.40	0/1216	0.58	0/1637
1	D	0.39	0/1216	0.59	0/1637
All	All	0.39	0/4864	0.57	0/6548

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1190	0	1223	62	0
1	B	1190	0	1221	47	0
1	C	1190	0	1221	38	0
1	D	1190	0	1221	38	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	67	0	0	3	0
4	B	58	0	0	3	0
4	C	60	0	0	2	0
4	D	85	0	0	5	0
All	All	5210	0	5006	175	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 18.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HA	1:A:69:LYS:HD2	1.34	1.05
1:B:223:TRP:HE1	1:B:280:ASN:HD22	1.03	0.95
1:A:12:THR:HG22	1:A:14:GLY:H	1.29	0.95
1:D:612:THR:HG22	1:D:614:GLY:H	1.30	0.95
1:C:440:ARG:HA	1:C:443:LYS:HD3	1.48	0.95
1:A:23:TRP:HE1	1:A:80:ASN:HD22	1.11	0.91
1:B:201:PRO:HA	1:D:647:GLN:NE2	1.86	0.89
1:A:12:THR:HG22	1:A:14:GLY:N	1.88	0.88
1:B:223:TRP:HE1	1:B:280:ASN:ND2	1.71	0.87
1:A:65:ASP:HB3	1:A:68:VAL:HB	1.61	0.82
1:C:423:TRP:HE1	1:C:480:ASN:HD22	1.29	0.81
1:D:623:TRP:HE1	1:D:680:ASN:HD22	1.28	0.79
1:B:259:LYS:HA	1:B:262:LEU:HD21	1.66	0.78
1:A:12:THR:O	1:A:16:LYS:HG3	1.83	0.78
1:C:429:GLU:HB3	1:C:432:GLN:HE21	1.49	0.78
1:A:23:TRP:HE1	1:A:80:ASN:ND2	1.81	0.77
1:A:12:THR:CG2	1:A:14:GLY:H	1.98	0.75
1:D:612:THR:HG22	1:D:614:GLY:N	2.01	0.75
1:A:30:TYR:O	1:A:34:SER:HB3	1.88	0.73
1:A:18:ALA:HB3	1:A:130:GLU:HG2	1.72	0.70
1:A:12:THR:HG23	4:B:349:HOH:O	1.93	0.67
1:C:428:LYS:HD2	1:C:429:GLU:HG3	1.76	0.67
1:A:5:GLN:NE2	1:A:143:ARG:HH21	1.92	0.67
1:A:59:LYS:HA	1:A:62:LEU:HD22	1.75	0.67
1:B:201:PRO:HA	1:D:647:GLN:HE21	1.60	0.66
1:A:58:LYS:HG2	1:A:58:LYS:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:GLN:HB3	4:D:218:HOH:O	1.96	0.65
1:C:479:VAL:O	1:C:483:ILE:HG13	1.97	0.65
1:B:223:TRP:HB3	1:B:224:PRO:HD3	1.80	0.63
1:B:309:VAL:CG1	2:B:347:HEM:HAC	2.29	0.62
1:B:209:PRO:HG2	1:B:337:ILE:HG13	1.83	0.61
1:B:294:LYS:HB3	1:B:294:LYS:HZ2	1.66	0.60
1:D:629:GLU:HG3	4:D:90:HOH:O	2.01	0.60
1:B:215:ASP:O	1:B:219:ILE:HD12	2.02	0.60
1:D:651:SER:HB3	1:D:709:VAL:HG22	1.83	0.60
1:B:212:THR:HG22	1:B:214:GLY:H	1.67	0.59
1:A:27:TYR:HB2	1:D:607:PRO:HD3	1.85	0.59
1:B:263:GLU:HB3	4:B:359:HOH:O	2.02	0.59
1:A:102:LYS:HB3	1:A:107:PHE:CE1	2.36	0.58
1:C:432:GLN:HG2	4:C:10:HOH:O	2.03	0.58
1:C:440:ARG:HA	1:C:443:LYS:CD	2.29	0.58
1:A:66:PRO:HB2	1:C:501:GLN:HG2	1.85	0.57
1:C:422:ILE:O	1:C:425:LYS:HG2	2.05	0.57
1:A:65:ASP:O	1:A:69:LYS:HG3	2.04	0.56
1:A:66:PRO:CB	1:C:501:GLN:HG2	2.36	0.56
1:A:89:GLN:HG3	1:B:310:ASP:OD1	2.05	0.56
1:D:682:ILE:HG23	1:D:692:ILE:HD12	1.87	0.56
1:D:689:GLN:O	1:D:693:ILE:HG13	2.05	0.56
1:B:293:ILE:O	1:B:297:LYS:HB2	2.05	0.56
1:C:440:ARG:HG3	1:C:443:LYS:HE2	1.88	0.56
1:A:117:LEU:O	1:A:117:LEU:HD23	2.06	0.55
1:B:317:LEU:HD12	2:B:347:HEM:HMC1	1.88	0.55
1:D:682:ILE:HD11	1:D:696:LEU:HD21	1.88	0.55
1:A:35:LEU:HD22	1:A:39:LEU:HG	1.88	0.55
1:C:458:LYS:HG2	1:C:461:ASN:HB2	1.89	0.54
1:C:410:THR:O	1:C:533:LYS:HE2	2.07	0.54
1:A:84:ASN:ND2	1:D:603:ILE:HG13	2.23	0.54
1:B:294:LYS:HB3	1:B:294:LYS:NZ	2.23	0.53
1:A:70:HIS:O	1:A:74:VAL:HG23	2.07	0.53
1:D:709:VAL:HG21	2:D:747:HEM:HHD	1.91	0.53
1:D:631:GLU:HB2	4:D:17:HOH:O	2.08	0.52
1:B:282:ILE:HD11	1:B:296:LEU:HD21	1.91	0.52
1:A:5:GLN:NE2	1:A:143:ARG:NH2	2.56	0.52
1:B:309:VAL:HG11	2:B:347:HEM:HAC	1.91	0.52
1:C:402:ILE:HG13	1:C:532:GLU:HG2	1.90	0.52
1:B:227:TYR:OH	1:B:277:ASN:ND2	2.43	0.52
1:B:211:LEU:HD23	1:B:286:MET:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:HIS:HA	1:A:107:PHE:HD1	1.75	0.52
1:D:670:HIS:O	1:D:674:VAL:HG23	2.09	0.52
4:A:204:HOH:O	1:D:601:PRO:HB3	2.10	0.52
1:B:309:VAL:HG13	2:B:347:HEM:HAC	1.93	0.51
1:A:71:GLN:HE22	2:A:147:HEM:HBD1	1.75	0.51
1:C:488:ASN:OD1	1:C:491:GLU:HB2	2.10	0.51
1:C:429:GLU:CB	1:C:432:GLN:HE21	2.22	0.51
1:C:418:ALA:HB3	1:C:530:GLU:HG2	1.92	0.51
1:C:435:LEU:HD22	1:C:439:LEU:HG	1.91	0.50
1:B:259:LYS:HA	1:B:262:LEU:CD2	2.38	0.50
1:B:311:SER:HB2	1:B:343:ARG:CG	2.42	0.50
1:D:730:GLU:CD	1:D:730:GLU:H	2.14	0.49
1:C:537:ILE:O	1:C:541:LEU:HB2	2.12	0.49
1:C:423:TRP:N	1:C:424:PRO:CD	2.75	0.49
1:A:88:ASN:C	1:A:88:ASN:HD22	2.15	0.49
1:B:334:LEU:O	1:B:338:ILE:HG13	2.12	0.49
1:C:448:ALA:O	1:C:451:SER:HB2	2.12	0.49
1:B:247:GLN:HG3	1:B:313:TRP:CH2	2.48	0.49
1:A:49:GLN:NE2	1:A:59:LYS:NZ	2.61	0.48
1:A:111:SER:HB3	1:A:146:TYR:CD2	2.47	0.48
1:A:103:HIS:HA	1:A:107:PHE:CD1	2.48	0.48
1:B:202:ILE:O	1:B:315:LYS:HE2	2.13	0.48
1:A:83:ILE:HA	1:A:86:MET:HG3	1.95	0.48
1:B:210:THR:C	1:B:333:LYS:HZ1	2.15	0.48
1:A:4:ASP:HB2	1:A:143:ARG:HD3	1.96	0.48
1:B:269:LYS:HE2	4:B:401:HOH:O	2.13	0.48
1:B:258:LYS:HG3	1:B:260:SER:HB2	1.94	0.47
1:C:422:ILE:O	1:C:426:ILE:HG12	2.14	0.47
1:D:691:GLU:HA	1:D:694:LYS:HE2	1.95	0.47
1:B:241:PHE:HA	1:B:320:ILE:HD13	1.97	0.47
1:B:255:PHE:HD1	1:B:255:PHE:O	1.96	0.47
1:D:612:THR:O	1:D:616:LYS:HG2	2.15	0.47
1:A:93:ILE:O	1:A:97:LYS:HB2	2.14	0.47
1:D:618:ALA:HB3	1:D:730:GLU:HG2	1.96	0.47
1:A:58:LYS:HG2	1:A:60:SER:H	1.80	0.47
1:D:643:LYS:HA	1:D:659:LYS:HZ3	1.79	0.46
1:D:602:ILE:HD11	1:D:722:VAL:HG21	1.97	0.46
1:A:64:GLN:O	1:A:69:LYS:HE3	2.14	0.46
1:C:432:GLN:HG3	1:C:433:TYR:H	1.80	0.46
1:B:312:ILE:HD13	1:B:312:ILE:N	2.30	0.46
1:A:32:GLN:NE2	4:A:188:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:HB2	1:A:76:PHE:CE2	2.52	0.45
1:D:689:GLN:HG2	1:D:689:GLN:H	1.62	0.45
1:B:311:SER:HB2	1:B:343:ARG:HG2	1.99	0.45
1:B:203:ILE:HG23	1:B:205:GLN:H	1.80	0.45
1:B:255:PHE:O	1:B:255:PHE:CD1	2.70	0.45
1:B:258:LYS:HB2	1:B:258:LYS:HE2	1.69	0.45
1:B:293:ILE:HG23	1:B:297:LYS:HE3	1.99	0.44
1:D:682:ILE:HD13	1:D:738:ILE:HG12	1.99	0.44
1:C:403:ILE:CG2	1:C:404:ASP:N	2.80	0.44
1:A:112:ILE:O	1:A:112:ILE:HG22	2.17	0.44
1:B:302:LYS:HE3	1:B:306:VAL:HG21	2.00	0.44
1:B:263:GLU:O	1:B:263:GLU:HG2	2.17	0.44
1:B:237:ILE:HG12	1:B:321:PHE:HA	2.00	0.44
1:A:69:LYS:H	1:A:69:LYS:HG3	1.63	0.44
1:D:618:ALA:HA	4:D:256:HOH:O	2.18	0.44
1:C:409:PRO:HD2	1:C:537:ILE:HG13	1.98	0.44
1:A:95:SER:HB2	4:A:172:HOH:O	2.18	0.43
1:A:49:GLN:NE2	1:A:59:LYS:HZ2	2.16	0.43
1:A:111:SER:HB2	1:A:143:ARG:HG2	1.99	0.43
1:B:201:PRO:HA	1:D:647:GLN:HE22	1.78	0.43
1:D:641:PHE:HA	1:D:720:ILE:HD12	2.01	0.43
1:A:12:THR:CG2	1:A:13:ASP:N	2.81	0.43
1:A:24:PRO:HA	1:A:27:TYR:CE2	2.53	0.43
1:A:87:ASP:HB3	1:B:312:ILE:HG13	2.01	0.43
1:C:419:ILE:C	1:C:421:LYS:H	2.22	0.43
1:C:443:LYS:HG2	1:C:444:CYS:N	2.33	0.43
1:D:693:ILE:CG2	1:D:697:LYS:HE3	2.49	0.43
1:C:514:PHE:CD2	1:C:542:LEU:HD13	2.54	0.42
1:C:411:LEU:HA	1:C:411:LEU:HD12	1.93	0.42
1:B:261:ASN:OD1	1:B:261:ASN:N	2.48	0.42
1:B:212:THR:HG22	1:B:214:GLY:N	2.33	0.42
1:D:689:GLN:HE21	1:D:689:GLN:HB3	1.65	0.42
1:D:690:GLU:HG3	4:D:260:HOH:O	2.19	0.42
1:A:61:ASN:O	1:A:61:ASN:CG	2.56	0.42
1:A:111:SER:HB3	1:A:146:TYR:CE2	2.55	0.42
1:B:301:GLN:OE1	1:B:305:THR:HG21	2.19	0.42
1:D:665:ASP:HB3	1:D:668:VAL:HG23	2.02	0.42
1:A:22:ILE:O	1:A:25:LYS:HG2	2.19	0.42
1:C:504:LYS:HE3	1:C:505:THR:HG22	2.00	0.42
1:A:22:ILE:HD12	1:A:131:PHE:HE1	1.83	0.42
1:D:608:LEU:HD11	1:D:741:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:VAL:HG22	1:C:531:PHE:HB3	2.00	0.42
1:A:117:LEU:C	1:A:117:LEU:HD23	2.39	0.42
1:B:227:TYR:O	1:B:230:TYR:HB3	2.20	0.42
1:D:635:LEU:HD22	1:D:639:LEU:HG	2.02	0.42
1:A:135:PHE:HA	1:A:138:ILE:HB	2.03	0.41
1:D:709:VAL:CG1	1:D:710:ASP:N	2.83	0.41
1:C:446:PRO:O	1:C:449:GLN:HB2	2.19	0.41
1:C:483:ILE:O	1:C:486:MET:HG3	2.20	0.41
1:A:58:LYS:O	1:A:60:SER:N	2.52	0.41
1:A:32:GLN:O	1:A:32:GLN:HG2	2.21	0.41
1:C:403:ILE:HG23	1:C:405:GLN:H	1.85	0.41
1:C:509:VAL:HG21	2:C:547:HEM:CAC	2.51	0.41
1:D:652:PHE:CE1	2:D:747:HEM:HAC	2.56	0.41
1:C:514:PHE:HB2	4:C:6:HOH:O	2.21	0.41
1:D:612:THR:CG2	1:D:613:ASP:N	2.84	0.40
1:B:228:LYS:HB3	1:B:229:GLU:OE1	2.21	0.40
1:A:84:ASN:ND2	1:D:603:ILE:HA	2.36	0.40
1:A:25:LYS:HG2	1:A:25:LYS:H	1.48	0.40
1:A:89:GLN:HE21	1:A:89:GLN:HB3	1.61	0.40
1:C:403:ILE:CG2	1:C:405:GLN:O	2.70	0.40
1:A:85:SER:O	1:A:92:ILE:HD11	2.20	0.40
1:C:432:GLN:HG3	1:C:433:TYR:N	2.36	0.40
1:A:78:LYS:HE3	2:A:147:HEM:HMA3	2.02	0.40
1:A:15:ASP:OD2	1:A:133:LYS:HE2	2.21	0.40
1:A:62:LEU:O	1:A:68:VAL:HG11	2.21	0.40
1:A:99:LEU:HA	1:A:102:LYS:HZ2	1.85	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	144/146 (99%)	136 (94%)	7 (5%)	1 (1%)	26 21
1	B	144/146 (99%)	136 (94%)	5 (4%)	3 (2%)	9 3
1	C	144/146 (99%)	138 (96%)	3 (2%)	3 (2%)	9 3
1	D	144/146 (99%)	137 (95%)	4 (3%)	3 (2%)	9 3
All	All	576/584 (99%)	547 (95%)	19 (3%)	10 (2%)	11 5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	LEU
1	D	662	LEU
1	A	59	LYS
1	B	261	ASN
1	C	456	SER
1	C	457	THR
1	D	659	LYS
1	B	259	LYS
1	C	420	ASN
1	D	656	SER

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	136/136 (100%)	110 (81%)	26 (19%)	2 1
1	B	136/136 (100%)	104 (76%)	32 (24%)	1 0
1	C	136/136 (100%)	111 (82%)	25 (18%)	2 1
1	D	136/136 (100%)	114 (84%)	22 (16%)	3 1
All	All	544/544 (100%)	439 (81%)	105 (19%)	2 1

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	17	LYS
1	A	21	LYS
1	A	25	LYS
1	A	28	LYS
1	A	29	GLU
1	A	32	GLN
1	A	34	SER
1	A	35	LEU
1	A	43	LYS
1	A	51	SER
1	A	58	LYS
1	A	61	ASN
1	A	62	LEU
1	A	73	VAL
1	A	85	SER
1	A	88	ASN
1	A	89	GLN
1	A	94	LYS
1	A	97	LYS
1	A	104	LYS
1	A	126	ASP
1	A	134	LEU
1	A	141	LEU
1	A	146	TYR
1	B	211	LEU
1	B	217	LYS
1	B	221	LYS
1	B	231	GLU
1	B	232	GLN
1	B	235	LEU
1	B	247	GLN
1	B	256	SER
1	B	258	LYS
1	B	259	LYS
1	B	260	SER
1	B	261	ASN
1	B	262	LEU
1	B	263	GLU
1	B	264	GLN
1	B	269	LYS
1	B	276	PHE

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Mol	Chain	Res	Type
1	B	278	LYS
1	B	289	GLN
1	B	294	LYS
1	B	301	GLN
1	B	302	LYS
1	B	304	LYS
1	B	305	THR
1	B	310	ASP
1	B	317	LEU
1	B	321	PHE
1	B	330	GLU
1	B	333	LYS
1	B	334	LEU
1	B	341	LEU
1	B	343	ARG
1	C	408	LEU
1	C	411	LEU
1	C	421	LYS
1	C	425	LYS
1	C	428	LYS
1	C	435	LEU
1	C	443	LYS
1	C	447	GLN
1	C	451	SER
1	C	457	THR
1	C	458	LYS
1	C	464	GLN
1	C	476	PHE
1	C	478	LYS
1	C	485	SER
1	C	489	GLN
1	C	497	LYS
1	C	502	LYS
1	C	505	THR
1	C	509	VAL
1	C	510	ASP
1	C	515	LYS
1	C	517	LEU
1	C	534	LEU
1	C	541	LEU
1	D	603	ILE
1	D	611	LEU

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Mol	Chain	Res	Type
1	D	616	LYS
1	D	617	LYS
1	D	621	LYS
1	D	625	LYS
1	D	629	GLU
1	D	632	GLN
1	D	635	LEU
1	D	640	ARG
1	D	643	LYS
1	D	657	THR
1	D	661	ASN
1	D	684	ASN
1	D	685	SER
1	D	688	ASN
1	D	689	GLN
1	D	708	LYS
1	D	717	LEU
1	D	734	LEU
1	D	741	LEU
1	D	743	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	32	GLN
1	A	49	GLN
1	A	71	GLN
1	A	80	ASN
1	A	84	ASN
1	A	88	ASN
1	A	89	GLN
1	B	247	GLN
1	B	277	ASN
1	B	280	ASN
1	C	432	GLN
1	C	436	ASN
1	C	464	GLN
1	C	480	ASN
1	C	501	GLN
1	D	632	GLN
1	D	647	GLN

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Mol	Chain	Res	Type
1	D	680	ASN
1	D	688	ASN
1	D	689	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	147	1,3	30,50,50	2.86	10 (33%)	24,82,82	2.01	6 (25%)
3	CMO	A	148	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	B	347	1,3	30,50,50	3.03	8 (26%)	24,82,82	2.14	6 (25%)
3	CMO	B	348	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	C	547	1,3	30,50,50	2.82	10 (33%)	24,82,82	2.04	7 (29%)
3	CMO	C	548	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	D	747	1,3	30,50,50	3.02	10 (33%)	24,82,82	2.05	8 (33%)
3	CMO	D	748	2	0,1,1	0.00	-	0,0,0	0.00	-

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
2	HEM	A	147	1,3	-	0/10/54/54	0/0/8/8
3	CMO	A	148	2	-	0/0/0/0	0/0/0/0
2	HEM	B	347	1,3	-	0/10/54/54	0/0/8/8
3	CMO	B	348	2	-	0/0/0/0	0/0/0/0
2	HEM	C	547	1,3	-	0/10/54/54	0/0/8/8
3	CMO	C	548	2	-	0/0/0/0	0/0/0/0
2	HEM	D	747	1,3	-	0/10/54/54	0/0/8/8
3	CMO	D	748	2	-	0/0/0/0	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	347	HEM	C3B-C4B	-7.68	1.45	1.51
2	A	147	HEM	C3B-C4B	-7.42	1.45	1.51
2	D	747	HEM	C3B-C4B	-7.17	1.45	1.51
2	D	747	HEM	C3C-CAC	-6.98	1.38	1.51
2	D	747	HEM	C2D-C3D	-6.93	1.33	1.54
2	C	547	HEM	C3C-CAC	-6.57	1.39	1.51
2	C	547	HEM	C2D-C3D	-6.45	1.35	1.54
2	B	347	HEM	C2D-C3D	-6.38	1.35	1.54
2	B	347	HEM	C3B-CAB	-6.33	1.39	1.51
2	D	747	HEM	C3B-CAB	-6.06	1.40	1.51
2	A	147	HEM	C3B-CAB	-6.02	1.40	1.51
2	C	547	HEM	C3D-C4D	-5.85	1.44	1.51
2	C	547	HEM	C3B-CAB	-5.82	1.40	1.51
2	A	147	HEM	C3C-CAC	-5.81	1.40	1.51
2	A	147	HEM	C2D-C3D	-5.71	1.37	1.54
2	B	347	HEM	C3C-CAC	-5.48	1.41	1.51
2	C	547	HEM	C3B-C4B	-5.10	1.47	1.51
2	B	347	HEM	C3D-C4D	-4.59	1.45	1.51
2	D	747	HEM	C2C-C1C	-4.51	1.44	1.52
2	B	347	HEM	C2C-C1C	-4.28	1.44	1.52
2	A	147	HEM	C3D-C4D	-3.98	1.46	1.51
2	D	747	HEM	C3D-C4D	-3.72	1.46	1.51
2	A	147	HEM	C2C-C1C	-3.25	1.46	1.52
2	C	547	HEM	C2C-C1C	-2.84	1.47	1.52
2	C	547	HEM	C2D-C1D	-2.83	1.42	1.51
2	D	747	HEM	C2D-C1D	-2.23	1.44	1.51
2	C	547	HEM	CBB-CAB	2.13	1.41	1.29
2	A	147	HEM	CHC-C1C	2.14	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	147	HEM	CHD-C4C	2.20	1.41	1.36
2	D	747	HEM	CBB-CAB	2.21	1.42	1.29
2	A	147	HEM	C1C-NC	3.41	1.40	1.36
2	C	547	HEM	C4C-NC	3.47	1.40	1.36
2	D	747	HEM	C4C-NC	3.47	1.40	1.36
2	C	547	HEM	C1C-NC	3.77	1.40	1.36
2	B	347	HEM	C4C-NC	4.27	1.41	1.36
2	A	147	HEM	C4C-NC	4.34	1.41	1.36
2	D	747	HEM	C1C-NC	4.35	1.41	1.36
2	B	347	HEM	C1C-NC	5.04	1.42	1.36

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	747	HEM	C1D-CHD-C4C	-2.39	121.82	125.82
2	D	747	HEM	CAA-C2A-C1A	-2.15	124.67	127.01
2	D	747	HEM	CMD-C2D-C3D	2.33	124.66	114.35
2	C	547	HEM	CMD-C2D-C3D	2.38	124.87	114.35
2	B	347	HEM	CMD-C2D-C3D	2.75	126.52	114.35
2	A	147	HEM	CMD-C2D-C3D	2.75	126.52	114.35
2	C	547	HEM	CBA-CAA-C2A	2.81	117.56	112.53
2	A	147	HEM	CMB-C2B-C3B	3.19	124.50	116.53
2	C	547	HEM	CMC-C2C-C3C	3.41	125.03	116.53
2	D	747	HEM	CAD-C3D-C2D	3.48	123.23	113.22
2	C	547	HEM	CMB-C2B-C3B	3.51	125.30	116.53
2	A	147	HEM	C2D-C3D-C4D	3.57	107.55	101.50
2	D	747	HEM	C2D-C3D-C4D	3.58	107.57	101.50
2	B	347	HEM	CAD-C3D-C4D	3.61	125.19	112.47
2	A	147	HEM	CAD-C3D-C4D	3.75	125.70	112.47
2	D	747	HEM	CMB-C2B-C3B	3.77	125.94	116.53
2	B	347	HEM	C2D-C3D-C4D	3.80	107.94	101.50
2	C	547	HEM	CAD-C3D-C4D	4.00	126.59	112.47
2	C	547	HEM	C2D-C3D-C4D	4.03	108.33	101.50
2	C	547	HEM	CAD-C3D-C2D	4.13	125.08	113.22
2	D	747	HEM	CMC-C2C-C3C	4.22	127.06	116.53
2	B	347	HEM	CMC-C2C-C3C	4.38	127.45	116.53
2	B	347	HEM	CMB-C2B-C3B	4.49	127.73	116.53
2	D	747	HEM	CAD-C3D-C4D	4.54	128.48	112.47
2	A	147	HEM	CAD-C3D-C2D	4.60	126.43	113.22
2	B	347	HEM	CAD-C3D-C2D	4.70	126.74	113.22
2	A	147	HEM	CMC-C2C-C3C	4.73	128.34	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	147	HEM	2	0
2	B	347	HEM	4	0
2	C	547	HEM	1	0
2	D	747	HEM	2	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.