



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:20 PM GMT

PDB ID : 1V4U  
Title : Crystal structure of bluefin tuna carbonmonoxy-hemoglobin  
Authors : Yokoyama, T.; Chong, K.T.; Miyazaki, Y.; Nakatsukasa, T.; Unzai, S.;  
Miyazaki, G.; Morimoto, H.; Jeremy, R.H.T.; Park, S.Y.  
Deposited on : 2003-11-19  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

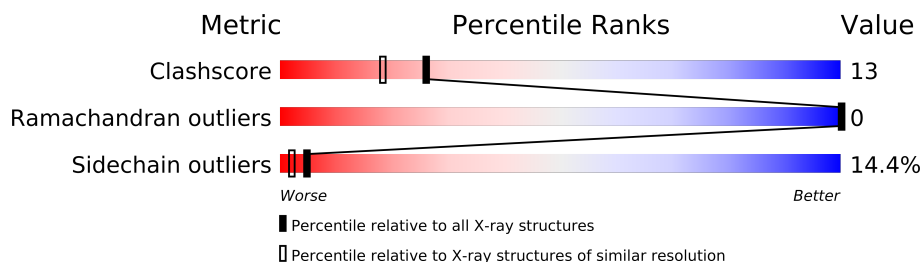
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	144	
1	C	144	
2	B	146	
2	D	146	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4694 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called hemoglobin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1088	699	184	199	6			
1	C	144	Total	C	N	O	S	0	0	0
			1088	699	184	199	6			

- Molecule 2 is a protein called hemoglobin beta chain.

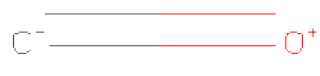
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1100	706	187	203	4			
2	D	142	Total	C	N	O	S	0	0	0
			1100	706	187	203	4			

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total	O	0	0
			42	42		
5	B	42	Total	O	0	0
			42	42		

*Continued on next page...*

*Continued from previous page...*

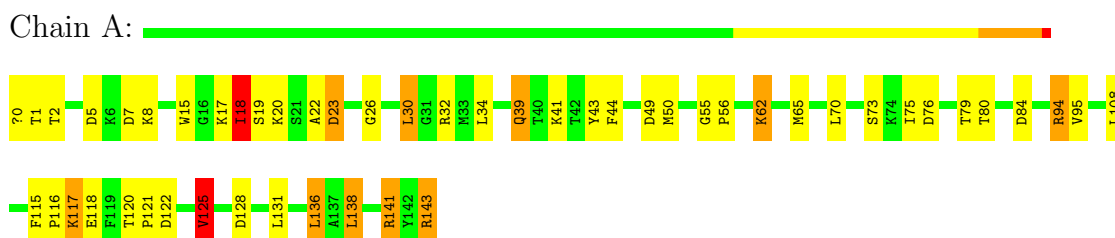
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	35	Total 35	O 35	0	0
5	D	19	Total 19	O 19	0	0

### 3 Residue-property plots

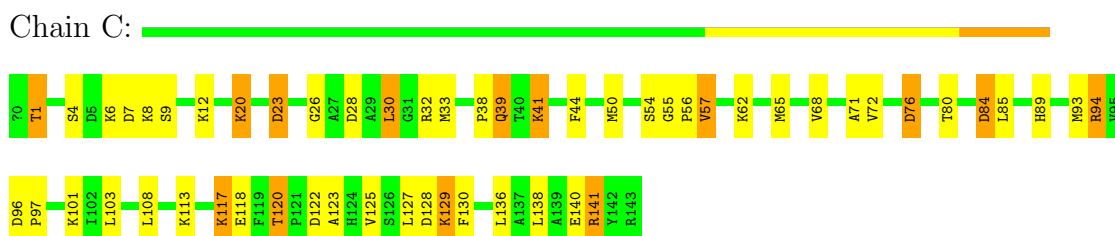
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

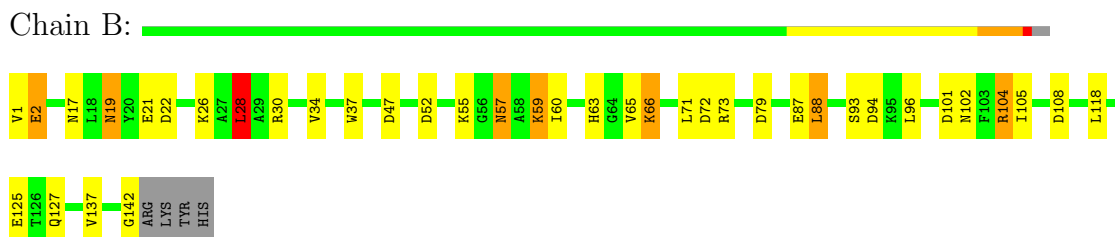
- Molecule 1: hemoglobin alpha chain



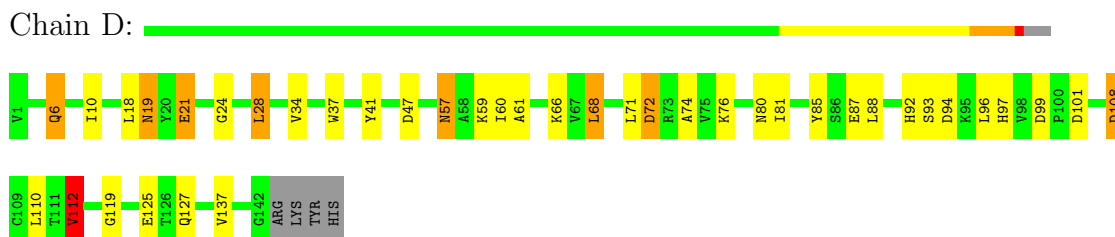
- Molecule 1: hemoglobin alpha chain



- Molecule 2: hemoglobin beta chain



- Molecule 2: hemoglobin beta chain



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.02Å 102.54Å 108.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.00)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.22	Depositor
R, $R_{free}$	0.204 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4694	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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: CMO, HEM, ACE

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	1.28	2/1110 (0.2%)	1.32	18/1499 (1.2%)
1	C	1.25	0/1110	1.29	10/1499 (0.7%)
2	B	1.25	1/1123 (0.1%)	1.17	9/1527 (0.6%)
2	D	1.18	1/1123 (0.1%)	1.12	7/1527 (0.5%)
All	All	1.24	4/4466 (0.1%)	1.23	44/6052 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	125	GLU	CD-OE2	5.27	1.31	1.25
1	A	22	ALA	CA-CB	5.16	1.63	1.52
2	D	61	ALA	CA-CB	5.14	1.63	1.52
1	A	44	PHE	CE1-CZ	5.06	1.47	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	A	128	ASP	CB-CG-OD2	8.95	126.36	118.30
1	C	76	ASP	CB-CG-OD2	8.84	126.26	118.30
1	C	28	ASP	CB-CG-OD1	8.82	126.24	118.30
1	C	23	ASP	CB-CG-OD2	8.28	125.75	118.30
2	D	72	ASP	CB-CG-OD2	8.18	125.67	118.30
2	B	52	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	125	VAL	CB-CA-C	-7.49	97.17	111.40
2	D	99	ASP	CB-CG-OD2	7.47	125.03	118.30
2	B	72	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	30	LEU	CB-CG-CD2	7.13	123.12	111.00
1	A	143	ARG	NE-CZ-NH1	-6.86	116.87	120.30
2	D	112	VAL	CG1-CB-CG2	6.72	121.65	110.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	A	1	THR	CA-CB-CG2	6.58	121.62	112.40
2	B	30	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	141	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	C	128	ASP	CB-CG-OD2	6.34	124.00	118.30
2	B	108	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	1	THR	N-CA-CB	6.22	122.11	110.30
1	A	49	ASP	CB-CG-OD2	6.18	123.87	118.30
1	C	76	ASP	CB-CG-OD1	-6.14	112.78	118.30
1	A	23	ASP	CB-CG-OD2	6.12	123.81	118.30
2	B	47	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	129	LYS	CD-CE-NZ	-5.90	98.13	111.70
1	C	7	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	18	ILE	CG1-CB-CG2	5.81	124.18	111.40
2	D	47	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	94	ASP	CB-CG-OD2	5.63	123.36	118.30
2	D	108	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	84	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	138	LEU	CB-CG-CD1	5.56	120.46	111.00
1	C	85	LEU	CB-CG-CD1	-5.44	101.75	111.00
2	B	79	ASP	CB-CG-OD2	5.38	123.14	118.30
2	D	110	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	A	136	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	A	5	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	84	ASP	CB-CG-OD2	5.16	122.94	118.30
2	D	94	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	7	ASP	CB-CG-OD2	5.11	122.90	118.30
2	B	28	LEU	CB-CG-CD2	5.11	119.69	111.00
2	B	104	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	76	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	0	ACE	C-N-CA	-5.06	109.05	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1088	0	1120	39	0
1	C	1088	0	1120	39	0
2	B	1100	0	1093	22	0
2	D	1100	0	1093	22	0
3	A	43	0	30	4	0
3	B	43	0	30	5	0
3	C	43	0	30	2	0
3	D	43	0	30	6	0
4	A	2	0	0	4	0
4	B	2	0	0	4	0
4	C	2	0	0	0	0
4	D	2	0	0	4	0
5	A	42	0	0	0	0
5	B	42	0	0	0	0
5	C	35	0	0	0	0
5	D	19	0	0	0	0
All	All	4694	0	4546	119	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:117:LYS:HD2	1:C:117:LYS:H	1.31	0.93
3:A:144:HEM:ND	4:A:145:CMO:C	2.32	0.92
1:C:32:ARG:HH11	2:D:127:GLN:HE21	1.11	0.92
1:A:117:LYS:HD2	1:A:117:LYS:H	1.37	0.90
3:B:147:HEM:ND	4:B:148:CMO:C	2.34	0.90
1:A:41:LYS:HD3	1:A:50:MET:HE2	1.51	0.90
1:A:41:LYS:CG	1:A:50:MET:HE1	2.05	0.87
2:B:57:ASN:HD21	2:B:59:LYS:HD2	1.41	0.86
1:A:41:LYS:HD3	1:A:50:MET:CE	2.05	0.85
1:C:32:ARG:HH11	2:D:127:GLN:NE2	1.76	0.84
1:A:117:LYS:CD	1:A:117:LYS:H	1.87	0.83
3:A:144:HEM:NC	4:A:145:CMO:C	2.43	0.81
3:B:147:HEM:NC	4:B:148:CMO:C	2.43	0.81
1:A:32:ARG:HH11	2:B:127:GLN:HE21	1.28	0.80
1:A:39:GLN:HE21	1:A:39:GLN:H	1.29	0.80
1:A:117:LYS:HD3	1:A:118:GLU:OE1	1.84	0.77
1:C:117:LYS:HD3	1:C:118:GLU:OE1	1.85	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:147:HEM:ND	4:D:148:CMO:C	2.49	0.76
1:C:120:THR:CG2	1:C:123:ALA:H	1.99	0.76
1:A:32:ARG:HH11	2:B:127:GLN:NE2	1.83	0.76
1:A:136:LEU:HD11	1:C:1:THR:HB	1.69	0.74
1:C:120:THR:HG22	1:C:123:ALA:H	1.54	0.73
1:C:39:GLN:H	1:C:39:GLN:HE21	1.36	0.73
1:C:117:LYS:CD	1:C:117:LYS:H	2.04	0.71
1:A:41:LYS:HG2	1:A:50:MET:HE1	1.74	0.68
3:A:144:HEM:NB	4:A:145:CMO:C	2.57	0.68
2:B:57:ASN:ND2	2:B:59:LYS:HD2	2.07	0.68
1:A:41:LYS:CD	1:A:50:MET:CE	2.72	0.68
3:B:147:HEM:NA	4:B:148:CMO:C	2.57	0.67
1:A:41:LYS:CD	1:A:50:MET:HE1	2.25	0.67
2:B:1:VAL:CG1	2:B:2:GLU:H	2.07	0.67
3:D:147:HEM:NA	4:D:148:CMO:C	2.57	0.66
3:A:144:HEM:NA	4:A:145:CMO:C	2.60	0.65
1:A:18:ILE:HG13	1:A:115:PHE:CE2	2.34	0.63
1:C:32:ARG:NH1	2:D:127:GLN:HE21	1.92	0.62
1:A:8:LYS:HD3	1:A:75:ILE:HG23	1.81	0.62
2:B:1:VAL:HG12	2:B:2:GLU:H	1.64	0.62
1:C:108:LEU:HD23	1:C:127:LEU:HD23	1.81	0.61
2:D:57:ASN:HD22	2:D:60:ILE:H	1.48	0.61
1:A:41:LYS:CB	1:A:50:MET:HE1	2.31	0.60
1:C:44:PHE:HB2	1:C:50:MET:CE	2.30	0.60
1:C:125:VAL:HG22	2:D:34:VAL:HA	1.82	0.59
3:D:147:HEM:NC	4:D:148:CMO:C	2.66	0.59
3:D:147:HEM:NB	4:D:148:CMO:C	2.66	0.58
2:D:108:ASP:O	2:D:112:VAL:HG13	2.04	0.57
2:B:37:TRP:HA	1:C:94:ARG:HG3	1.86	0.57
2:B:19:ASN:HD22	2:B:19:ASN:C	2.07	0.57
1:C:23:ASP:OD1	1:C:62:LYS:HE2	2.05	0.56
1:A:23:ASP:OD1	1:A:62:LYS:HE3	2.05	0.56
2:B:28:LEU:HD13	2:B:60:ILE:HG23	1.86	0.56
1:C:120:THR:HG23	1:C:122:ASP:N	2.21	0.55
1:A:15:TRP:O	1:A:19:SER:HB3	2.06	0.54
1:A:32:ARG:HD3	2:B:127:GLN:HE22	1.71	0.54
1:A:116:PRO:HD2	1:A:117:LYS:HE3	1.89	0.54
1:A:39:GLN:NE2	1:A:39:GLN:H	2.02	0.54
1:C:1:THR:HG21	1:C:136:LEU:HD22	1.89	0.54
3:C:144:HEM:CMB	3:C:144:HEM:HBB2	2.37	0.53
1:A:32:ARG:NH1	2:B:127:GLN:HE21	2.03	0.53
3:B:147:HEM:NB	4:B:148:CMO:C	2.71	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:92:HIS:HE1	3:D:147:HEM:NA	2.05	0.53
1:A:117:LYS:HD2	1:A:117:LYS:N	2.17	0.52
1:C:120:THR:HG23	1:C:122:ASP:H	1.75	0.52
1:C:108:LEU:CD2	1:C:127:LEU:HD23	2.40	0.52
2:D:74:ALA:HB2	2:D:85:TYR:CE2	2.45	0.51
2:B:17:ASN:ND2	2:B:118:LEU:HD21	2.26	0.50
2:D:68:LEU:HD13	2:D:71:LEU:HD12	1.94	0.50
1:A:108:LEU:HD21	1:A:131:LEU:HD12	1.94	0.50
2:B:22:ASP:OD1	2:B:26:LYS:HE2	2.12	0.49
1:A:116:PRO:N	1:A:117:LYS:HD2	2.27	0.49
2:D:72:ASP:OD2	2:D:76:LYS:NZ	2.43	0.49
2:D:6:GLN:O	2:D:10:ILE:HG13	2.12	0.49
1:A:120:THR:HB	1:A:121:PRO:HD2	1.95	0.48
1:A:2:THR:HB	1:C:140:GLU:OE1	2.14	0.48
2:D:19:ASN:HD21	2:D:21:GLU:HG3	1.77	0.48
1:A:17:LYS:HD3	1:A:118:GLU:HG2	1.95	0.47
2:B:1:VAL:CG1	2:B:2:GLU:N	2.74	0.47
3:C:144:HEM:HMB1	3:C:144:HEM:HBB2	1.96	0.47
1:A:55:GLY:N	1:A:56:PRO:CD	2.78	0.47
1:C:55:GLY:N	1:C:56:PRO:CD	2.78	0.47
1:C:26:GLY:CA	1:C:65:MET:HG2	2.44	0.47
2:D:24:GLY:CA	2:D:68:LEU:HD23	2.45	0.46
1:C:113:LYS:HE2	2:D:119:GLY:O	2.16	0.46
2:B:88:LEU:HD11	3:B:147:HEM:HBA1	1.98	0.46
1:A:26:GLY:CA	1:A:65:MET:HG2	2.45	0.46
1:A:117:LYS:CD	1:A:117:LYS:N	2.66	0.46
1:C:54:SER:OG	1:C:57:VAL:HG13	2.14	0.46
1:A:34:LEU:O	1:A:41:LYS:HE2	2.16	0.46
1:C:4:SER:O	1:C:8:LYS:HG3	2.16	0.46
2:B:102:ASN:ND2	1:C:96:ASP:OD2	2.26	0.46
1:A:70:LEU:O	1:A:73:SER:HB2	2.17	0.45
2:D:81:ILE:O	2:D:85:TYR:HB2	2.16	0.45
2:B:93:SER:OG	2:B:142:GLY:HA2	2.17	0.45
1:C:89:HIS:HA	1:C:93:MET:HE2	1.99	0.44
1:C:118:GLU:N	1:C:118:GLU:OE1	2.50	0.44
1:C:32:ARG:HD3	2:D:127:GLN:HE22	1.83	0.44
1:C:26:GLY:HA3	1:C:65:MET:HG2	1.99	0.44
1:C:33:MET:SD	1:C:103:LEU:HB2	2.58	0.44
1:C:38:PRO:O	1:C:41:LYS:HG3	2.17	0.44
1:A:23:ASP:OD1	1:A:62:LYS:CE	2.65	0.44
1:A:94:ARG:HG3	2:D:37:TRP:HA	2.00	0.44
1:A:125:VAL:HG13	2:B:34:VAL:HA	2.00	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:20:LYS:HG2	1:C:20:LYS:O	2.18	0.43
2:B:71:LEU:HD23	2:B:71:LEU:HA	1.90	0.43
2:D:6:GLN:HE21	2:D:6:GLN:HA	1.85	0.42
1:A:143:ARG:HG3	1:C:129:LYS:HD2	2.02	0.42
1:C:68:VAL:O	1:C:72:VAL:HG23	2.20	0.42
2:D:28:LEU:HD13	2:D:60:ILE:HG23	2.01	0.42
2:D:68:LEU:HD13	2:D:68:LEU:HA	1.85	0.42
2:D:57:ASN:HB3	2:D:60:ILE:HB	2.01	0.41
1:C:96:ASP:HA	1:C:97:PRO:HD3	1.85	0.41
2:B:63:HIS:HA	2:B:66:LYS:HG3	2.03	0.41
2:B:57:ASN:C	2:B:57:ASN:HD22	2.24	0.41
1:C:120:THR:HG22	1:C:123:ALA:CB	2.50	0.41
1:A:41:LYS:CG	1:A:50:MET:CE	2.89	0.41
2:D:41:TYR:CD1	3:D:147:HEM:HBC1	2.56	0.40
1:A:43:TYR:CE2	1:A:95:VAL:HA	2.56	0.40
2:B:60:ILE:HD13	2:B:60:ILE:HA	1.95	0.40
1:C:26:GLY:O	1:C:30:LEU:HB2	2.21	0.40
1:C:71:ALA:HB3	1:C:130:PHE:HZ	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	C	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
2	B	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
2	D	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
All	All	564/580 (97%)	548 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	117/117 (100%)	104 (89%)	13 (11%)	9	5
1	C	117/117 (100%)	99 (85%)	18 (15%)	4	1
2	B	115/119 (97%)	98 (85%)	17 (15%)	4	2
2	D	115/119 (97%)	96 (84%)	19 (16%)	3	1
All	All	464/472 (98%)	397 (86%)	67 (14%)	5	2

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	20	LYS
1	A	30	LEU
1	A	39	GLN
1	A	62	LYS
1	A	79	THR
1	A	80	THR
1	A	94	ARG
1	A	117	LYS
1	A	122	ASP
1	A	125	VAL
1	A	138	LEU
1	A	141	ARG
2	B	2	GLU
2	B	19	ASN
2	B	21	GLU
2	B	28	LEU
2	B	55	LYS
2	B	57	ASN
2	B	59	LYS
2	B	65	VAL
2	B	66	LYS
2	B	73	ARG
2	B	87	GLU
2	B	88	LEU
2	B	96	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	101	ASP
2	B	104	ARG
2	B	105	ILE
2	B	137	VAL
1	C	1	THR
1	C	6	LYS
1	C	9	SER
1	C	12	LYS
1	C	20	LYS
1	C	30	LEU
1	C	39	GLN
1	C	41	LYS
1	C	57	VAL
1	C	76	ASP
1	C	80	THR
1	C	84	ASP
1	C	94	ARG
1	C	101	LYS
1	C	117	LYS
1	C	120	THR
1	C	138	LEU
1	C	141	ARG
2	D	6	GLN
2	D	18	LEU
2	D	19	ASN
2	D	21	GLU
2	D	28	LEU
2	D	57	ASN
2	D	59	LYS
2	D	66	LYS
2	D	68	LEU
2	D	80	ASN
2	D	87	GLU
2	D	88	LEU
2	D	93	SER
2	D	96	LEU
2	D	97	HIS
2	D	101	ASP
2	D	112	VAL
2	D	125	GLU
2	D	137	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
2	B	17	ASN
2	B	19	ASN
2	B	39	GLN
2	B	57	ASN
2	B	127	GLN
2	B	131	GLN
1	C	39	GLN
2	D	6	GLN
2	D	17	ASN
2	D	19	ASN
2	D	39	GLN
2	D	57	ASN
2	D	69	HIS
2	D	77	ASN
2	D	82	ASN
2	D	127	GLN
2	D	131	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
3	HEM	A	144	1,4	49,50,50	2.36	16 (32%)	46,82,82	1.97	10 (21%)
4	CMO	A	145	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	B	147	2,4	49,50,50	3.96	17 (34%)	46,82,82	1.90	11 (23%)
4	CMO	B	148	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	C	144	1,4	49,50,50	2.50	16 (32%)	46,82,82	2.23	13 (28%)
4	CMO	C	145	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	D	147	2,4	49,50,50	2.24	15 (30%)	46,82,82	1.92	10 (21%)
4	CMO	D	148	3	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
3	HEM	A	144	1,4	-	0/14/114/114	0/0/8/8
4	CMO	A	145	3	-	0/0/0/0	0/0/0/0
3	HEM	B	147	2,4	-	0/14/114/114	0/0/8/8
4	CMO	B	148	3	-	0/0/0/0	0/0/0/0
3	HEM	C	144	1,4	-	0/14/114/114	0/0/8/8
4	CMO	C	145	3	-	0/0/0/0	0/0/0/0
3	HEM	D	147	2,4	-	0/14/114/114	0/0/8/8
4	CMO	D	148	3	-	0/0/0/0	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C2D-C1D	18.61	1.49	1.44
3	B	147	HEM	C3D-C4D	12.96	1.47	1.44
3	C	144	HEM	C4A-C3A	6.82	1.48	1.40
3	C	144	HEM	FE-NA	6.15	2.18	1.92
3	B	147	HEM	C3C-C2C	-5.99	1.33	1.43
3	A	144	HEM	C4A-C3A	5.77	1.47	1.40
3	C	144	HEM	C3C-C2C	-5.56	1.34	1.43
3	B	147	HEM	C3D-C2D	5.47	1.53	1.43
3	D	147	HEM	C3B-C2B	-5.44	1.34	1.43
3	C	144	HEM	C3B-C2B	-5.38	1.34	1.43
3	A	144	HEM	C3B-C2B	-5.17	1.34	1.43
3	D	147	HEM	C3B-CAB	5.08	1.56	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	147	HEM	C3C-C2C	-5.06	1.34	1.43
3	A	144	HEM	C3C-C2C	-4.98	1.35	1.43
3	B	147	HEM	C4A-C3A	4.97	1.46	1.40
3	A	144	HEM	C3B-CAB	4.94	1.56	1.40
3	B	147	HEM	C3B-C2B	-4.94	1.35	1.43
3	C	144	HEM	C3B-CAB	4.78	1.55	1.40
3	C	144	HEM	C3C-CAC	4.73	1.55	1.40
3	B	147	HEM	C3C-CAC	4.57	1.54	1.40
3	D	147	HEM	C3D-C2D	4.56	1.51	1.43
3	B	147	HEM	C3B-CAB	4.46	1.54	1.40
3	D	147	HEM	C4A-C3A	4.42	1.45	1.40
3	D	147	HEM	C3C-CAC	4.42	1.54	1.40
3	A	144	HEM	CAA-C2A	4.24	1.59	1.52
3	A	144	HEM	C3C-CAC	4.18	1.53	1.40
3	A	144	HEM	FE-ND	-4.08	1.83	1.97
3	D	147	HEM	FE-NB	3.75	2.11	1.97
3	C	144	HEM	CMB-C2B	3.74	1.59	1.47
3	A	144	HEM	FE-NA	3.41	2.07	1.92
3	C	144	HEM	FE-NB	-3.37	1.85	1.97
3	A	144	HEM	C3D-C4D	-3.34	1.43	1.44
3	A	144	HEM	C3D-C2D	3.31	1.49	1.43
3	C	144	HEM	C3D-C2D	3.29	1.49	1.43
3	A	144	HEM	CMB-C2B	3.22	1.57	1.47
3	C	144	HEM	CHA-C4D	3.17	1.40	1.35
3	C	144	HEM	CMC-C2C	3.16	1.57	1.47
3	B	147	HEM	CMB-C2B	3.14	1.57	1.47
3	D	147	HEM	FE-NC	3.03	2.09	1.97
3	B	147	HEM	CAA-C2A	3.00	1.57	1.52
3	D	147	HEM	CAA-C2A	2.91	1.57	1.52
3	C	144	HEM	FE-NC	2.80	2.08	1.97
3	D	147	HEM	CMB-C2B	2.75	1.56	1.47
3	B	147	HEM	C2B-C1B	-2.74	1.43	1.44
3	B	147	HEM	FE-NC	2.71	2.08	1.97
3	B	147	HEM	FE-NB	2.71	2.07	1.97
3	D	147	HEM	C3D-C4D	2.53	1.45	1.44
3	A	144	HEM	C2D-C1D	-2.47	1.43	1.44
3	D	147	HEM	CMD-C2D	2.43	1.55	1.47
3	A	144	HEM	CMD-C2D	2.41	1.54	1.47
3	B	147	HEM	CMA-C3A	2.39	1.56	1.51
3	B	147	HEM	CMD-C2D	2.38	1.54	1.47
3	B	147	HEM	O1D-CGD	2.36	1.30	1.22
3	A	144	HEM	C3B-C4B	2.33	1.47	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	147	HEM	C2D-C1D	2.31	1.45	1.44
3	D	147	HEM	CMC-C2C	2.30	1.54	1.47
3	C	144	HEM	CMD-C2D	2.27	1.54	1.47
3	B	147	HEM	C1B-NB	-2.22	1.35	1.39
3	A	144	HEM	C1A-CHA	-2.22	1.33	1.39
3	A	144	HEM	C4C-NC	-2.19	1.34	1.38
3	D	147	HEM	CMA-C3A	2.14	1.56	1.51
3	C	144	HEM	CMA-C3A	2.07	1.56	1.51
3	C	144	HEM	C1D-ND	2.04	1.42	1.37
3	C	144	HEM	C2C-C1C	2.00	1.49	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	C3B-C4B-NB	-7.54	108.61	114.00
3	C	144	HEM	C3B-C4B-NB	-6.85	109.10	114.00
3	D	147	HEM	C3B-C4B-NB	-6.49	109.36	114.00
3	A	144	HEM	CHD-C4C-NC	5.35	129.38	124.73
3	C	144	HEM	CMA-C3A-C4A	-5.29	120.48	128.62
3	A	144	HEM	C3B-C4B-NB	-5.17	110.30	114.00
3	D	147	HEM	C4D-ND-C1D	4.70	109.97	105.16
3	B	147	HEM	C4D-ND-C1D	4.62	109.89	105.16
3	D	147	HEM	CHD-C4C-NC	4.47	128.61	124.73
3	A	144	HEM	CMA-C3A-C4A	-4.44	121.79	128.62
3	A	144	HEM	C4C-NC-C1C	4.35	110.06	105.53
3	C	144	HEM	CHA-C4D-ND	4.28	130.19	124.31
3	C	144	HEM	CHD-C1D-ND	4.23	128.10	124.58
3	B	147	HEM	CHC-C4B-NB	4.11	128.00	124.58
3	C	144	HEM	C4A-CHB-C1B	-4.08	122.10	127.47
3	C	144	HEM	CHC-C4B-NB	4.02	127.92	124.58
3	C	144	HEM	CMA-C3A-C2A	3.98	132.44	124.94
3	A	144	HEM	C4A-C3A-C2A	3.62	109.51	107.00
3	B	147	HEM	C2D-C1D-ND	-3.40	108.92	112.93
3	D	147	HEM	C4C-NC-C1C	3.32	108.99	105.53
3	D	147	HEM	C1A-CHA-C4D	-3.21	123.24	127.47
3	A	144	HEM	CAD-C3D-C4D	3.16	130.21	124.53
3	A	144	HEM	C1A-C2A-C3A	-3.14	103.67	106.92
3	C	144	HEM	C1D-CHD-C4C	-2.83	119.11	126.57
3	B	147	HEM	CHC-C1C-NC	2.75	127.12	124.73
3	D	147	HEM	C2D-C1D-ND	-2.58	109.88	112.93
3	C	144	HEM	O1A-CGA-CBA	-2.55	114.26	123.03
3	B	147	HEM	C4C-NC-C1C	2.46	108.09	105.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	CBD-CAD-C3D	2.39	119.60	114.37
3	C	144	HEM	C3A-C4A-NA	-2.38	107.61	109.41
3	A	144	HEM	C3A-C4A-NA	-2.20	107.75	109.41
3	C	144	HEM	O2A-CGA-O1A	2.20	128.88	123.30
3	A	144	HEM	CHB-C1B-NB	2.18	127.31	124.31
3	D	147	HEM	CMB-C2B-C3B	2.18	131.29	126.16
3	B	147	HEM	CBA-CAA-C2A	-2.18	108.86	112.69
3	B	147	HEM	CAD-C3D-C2D	2.15	132.04	127.25
3	C	144	HEM	C4C-NC-C1C	2.08	107.70	105.53
3	A	144	HEM	C4A-CHB-C1B	-2.07	124.74	127.47
3	D	147	HEM	C3A-C4A-NA	-2.07	107.85	109.41
3	D	147	HEM	CHA-C4D-ND	2.06	127.14	124.31
3	C	144	HEM	C4A-NA-C1A	2.06	109.48	106.76
3	B	147	HEM	CMB-C2B-C3B	2.06	131.01	126.16
3	D	147	HEM	CAA-CBA-CGA	2.05	120.05	113.47
3	B	147	HEM	O1A-CGA-CBA	-2.02	116.07	123.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 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.