



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FHJ  
Title : CRYSTAL STRUCTURE OF AQUOMET HEMOGLOBIN-I OF THE  
MANED WOLF (CHRYSOCYON BRACHYURUS) AT 2.0 RESOLUTION.  
Authors : Fadel, V.; de Azevedo, W.F.  
Deposited on : 2000-08-01  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

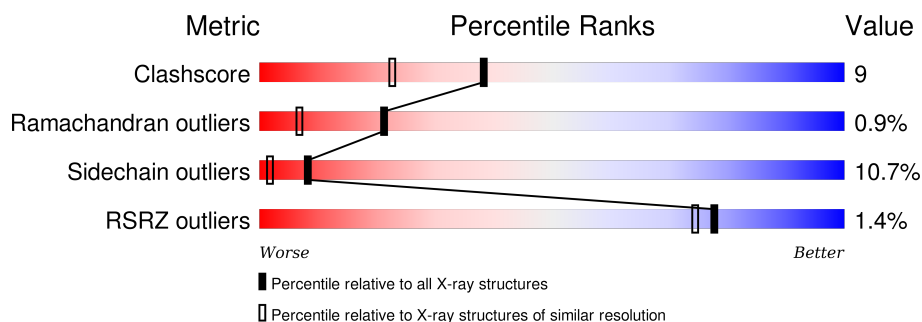
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	141	<div> <div>2%</div> <div>76%</div> <div>17%</div> <div>6%</div> <div>•</div> </div>
1	C	141	<div> <div>77%</div> <div>20%</div> <div>•</div> </div>
2	B	146	<div> <div>2%</div> <div>68%</div> <div>27%</div> <div>5%</div> <div>•</div> </div>
2	D	146	<div> <div>2%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4900 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 (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1079	692	184	201	2			
1	C	141	Total	C	N	O	S	0	0	0
			1079	692	184	201	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	THR	ALA	SEE REMARK 999	UNP P01952
C	130	THR	ALA	SEE REMARK 999	UNP P01952

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1131	727	196	205	3			
2	D	146	Total	C	N	O	S	0	0	0
			1131	727	196	205	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

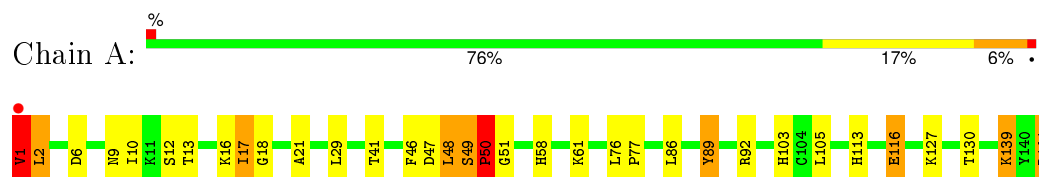
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	69	Total	O	0	0
			69	69		
4	C	75	Total	O	0	0
			75	75		
4	D	74	Total	O	0	0
			74	74		

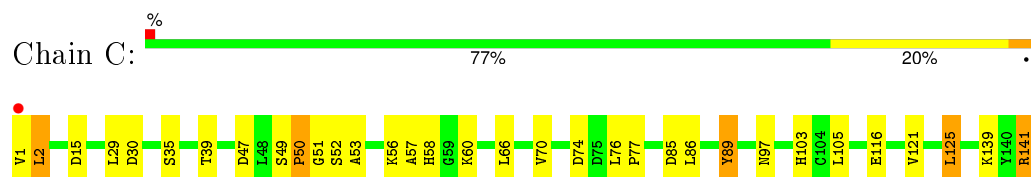
### 3 Residue-property plots [i](#)

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.

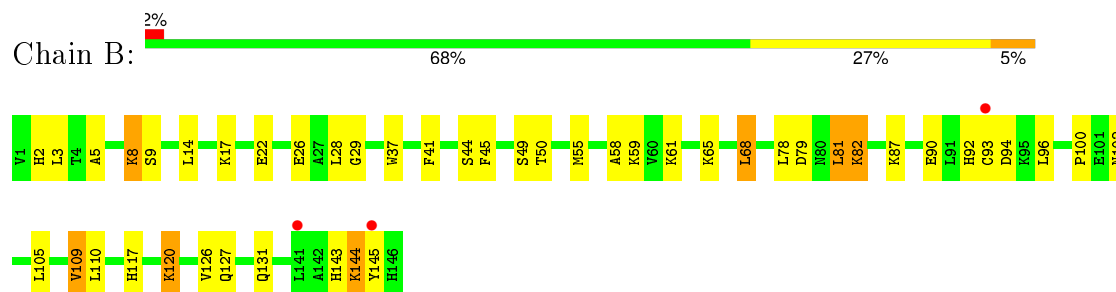
- Molecule 1: HEMOGLOBIN (ALPHA CHAIN)



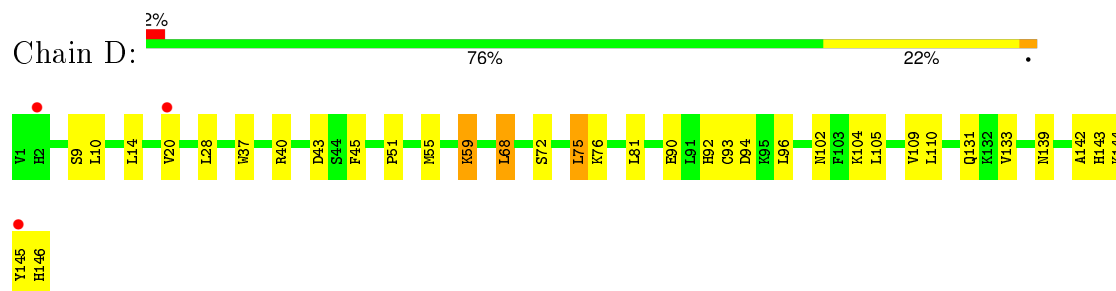
- Molecule 1: HEMOGLOBIN (ALPHA CHAIN)



- Molecule 2: HEMOGLOBIN (BETA CHAIN)



- Molecule 2: HEMOGLOBIN (BETA CHAIN)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.18Å 87.72Å 133.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 73.30 – 1.86	Depositor EDS
% Data completeness (in resolution range)	93.5 (10.00-1.80) 93.1 (73.30-1.86)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.60 (at 1.87Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.194 , 0.246 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 68.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50259 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	0.62	0/1109	0.90	6/1510 (0.4%)
1	C	0.58	0/1109	0.77	3/1510 (0.2%)
2	B	0.57	0/1157	0.73	0/1564
2	D	0.53	0/1157	0.75	0/1564
All	All	0.58	0/4532	0.79	9/6148 (0.1%)

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	50	PRO	CA-C-N	7.95	132.10	116.20
1	A	47	ASP	N-CA-C	-5.84	95.22	111.00
1	A	50	PRO	N-CA-CB	5.74	110.19	103.30
1	A	49	SER	N-CA-CB	5.64	118.97	110.50
1	C	50	PRO	CA-C-N	5.57	127.34	116.20
1	C	47	ASP	N-CA-C	-5.48	96.21	111.00
1	A	2	LEU	CA-C-N	-5.45	105.22	117.20
1	C	51	GLY	O-C-N	-5.17	114.43	122.70
1	A	51	GLY	CA-C-N	5.02	128.24	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain

## 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	1079	0	1071	26	0
1	C	1079	0	1071	18	0
2	B	1131	0	1135	25	0
2	D	1131	0	1135	21	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0
3	D	43	0	30	1	0
4	A	90	0	0	0	0
4	B	69	0	0	0	0
4	C	75	0	0	0	0
4	D	74	0	0	0	0
All	All	4900	0	4532	83	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (83) 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:1:VAL:HG22	1:A:2:LEU:N	1.66	1.11
1:A:1:VAL:CG1	1:C:141:ARG:O	2.21	0.89
2:B:120:LYS:HA	2:B:120:LYS:HE3	1.52	0.89
1:A:1:VAL:HG12	1:C:141:ARG:O	1.74	0.87
2:B:3:LEU:HD23	2:B:8:LYS:HD2	1.62	0.81
1:A:89:TYR:CD1	1:A:139:LYS:HD3	2.16	0.80
1:A:58:HIS:HA	1:A:61:LYS:HE3	1.64	0.79
1:A:17:ILE:HD11	1:A:21:ALA:HB2	1.65	0.78
1:A:9:ASN:O	1:A:13:THR:HG23	1.88	0.73
2:B:90:GLU:O	2:B:94:ASP:HB2	1.88	0.72
1:C:39:THR:HG22	1:C:97:ASN:ND2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD11	1:A:58:HIS:HD2	1.55	0.70
1:A:127:LYS:O	1:A:130:THR:HG22	1.94	0.68
1:A:92:ARG:HD3	2:D:37:TRP:HA	1.76	0.68
1:C:29:LEU:HD11	1:C:58:HIS:HD2	1.60	0.66
1:A:139:LYS:HG3	1:A:139:LYS:O	1.96	0.65
2:D:20:VAL:HG23	2:D:68:LEU:HD12	1.79	0.64
2:D:90:GLU:HG3	2:D:144:LYS:HE2	1.80	0.64
2:B:58:ALA:HA	2:B:61:LYS:HE2	1.78	0.63
2:D:93:CYS:SG	2:D:145:TYR:CE2	2.85	0.62
1:A:46:PHE:HB3	1:A:48:LEU:HD13	1.82	0.60
2:B:29:GLY:HA3	2:B:55:MET:HE1	1.84	0.58
1:A:12:SER:O	1:A:16:LYS:HG2	2.04	0.57
1:A:17:ILE:HD13	1:A:18:GLY:N	2.19	0.57
2:D:20:VAL:HG23	2:D:68:LEU:HB3	1.86	0.57
1:A:89:TYR:CE1	1:A:139:LYS:HD3	2.40	0.56
1:A:141:ARG:O	1:C:1:VAL:HG23	2.06	0.55
2:D:105:LEU:O	2:D:109:VAL:HG13	2.07	0.55
1:C:53:ALA:HA	1:C:56:LYS:HE2	1.88	0.55
1:A:141:ARG:HB3	1:A:141:ARG:NH1	2.22	0.55
2:B:45:PHE:CD1	2:B:59:LYS:HB3	2.42	0.55
2:D:37:TRP:HE1	2:D:102:ASN:HD21	1.56	0.54
1:C:66:LEU:O	1:C:70:VAL:HG23	2.09	0.53
2:B:105:LEU:O	2:B:109:VAL:HG13	2.09	0.53
2:B:26:GLU:OE2	2:B:117:HIS:HE1	1.91	0.52
2:B:82:LYS:H	2:B:82:LYS:CD	2.22	0.52
1:C:1:VAL:O	1:C:2:LEU:HB2	2.10	0.52
2:D:45:PHE:CD1	2:D:59:LYS:HB3	2.44	0.52
1:C:52:SER:O	1:C:56:LYS:HG3	2.09	0.52
2:D:143:HIS:HA	2:D:146:HIS:CD2	2.45	0.51
1:A:141:ARG:HB3	1:A:141:ARG:HH11	1.76	0.50
3:D:147:HEM:HHA	3:D:147:HEM:HBA1	1.93	0.50
1:A:6:ASP:O	1:A:10:ILE:HG12	2.11	0.49
2:D:90:GLU:O	2:D:94:ASP:HB2	2.12	0.49
2:D:142:ALA:O	2:D:145:TYR:HB2	2.12	0.49
2:D:72:SER:O	2:D:76:LYS:HG2	2.13	0.48
2:B:143:HIS:HD2	2:B:144:LYS:HD2	1.79	0.48
2:B:120:LYS:HE3	2:B:120:LYS:CA	2.35	0.48
2:B:78:LEU:HD23	2:B:81:LEU:HD21	1.94	0.48
1:A:1:VAL:HG22	1:A:2:LEU:H	1.71	0.47
2:B:82:LYS:H	2:B:82:LYS:HD2	1.79	0.47
1:C:35:SER:HB3	2:D:131:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:LEU:HD12	2:B:126:VAL:HG11	1.97	0.47
2:B:92:HIS:HA	2:B:96:LEU:HB2	1.96	0.46
1:C:89:TYR:CE1	1:C:139:LYS:HE2	2.50	0.46
1:C:29:LEU:HD11	1:C:58:HIS:CD2	2.45	0.46
1:C:57:ALA:HA	1:C:60:LYS:HD2	1.97	0.46
2:D:51:PRO:O	2:D:55:MET:HG2	2.16	0.45
1:A:1:VAL:HG13	1:C:141:ARG:O	2.11	0.45
1:A:49:SER:HB2	1:A:50:PRO:HD2	1.98	0.44
1:A:113:HIS:HB3	1:A:116:GLU:HG2	1.98	0.44
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.99	0.44
1:C:76:LEU:N	1:C:77:PRO:CD	2.80	0.44
2:B:68:LEU:HD22	2:B:68:LEU:HA	1.85	0.44
2:B:127:GLN:O	2:B:131:GLN:HG2	2.18	0.43
2:B:93:CYS:SG	2:B:145:TYR:CE2	3.03	0.43
2:D:92:HIS:HA	2:D:96:LEU:HD12	2.00	0.43
2:D:68:LEU:HA	2:D:68:LEU:HD22	1.72	0.42
1:A:49:SER:CB	1:A:50:PRO:HD2	2.50	0.42
1:A:76:LEU:N	1:A:77:PRO:CD	2.82	0.42
2:D:143:HIS:C	2:D:145:TYR:H	2.23	0.42
2:B:37:TRP:HE1	2:B:102:ASN:HD21	1.67	0.42
2:D:75:LEU:HD11	2:D:133:VAL:HG11	2.01	0.42
2:B:78:LEU:O	2:B:81:LEU:HD22	2.19	0.41
2:B:8:LYS:HE2	2:B:78:LEU:HD12	2.02	0.41
2:B:45:PHE:HA	2:B:59:LYS:HD2	2.01	0.41
1:C:103:HIS:HE1	2:D:131:GLN:OE1	2.03	0.41
2:B:41:PHE:CD1	3:B:147:HEM:HBC1	2.56	0.41
2:D:144:LYS:HB3	2:D:144:LYS:HE3	1.73	0.41
1:C:49:SER:O	1:C:52:SER:CB	2.69	0.41
2:B:100:PRO:HG3	2:B:145:TYR:CD2	2.56	0.41
2:D:93:CYS:SG	2:D:145:TYR:CD2	3.11	0.41
1:C:121:VAL:HG12	1:C:125:LEU:HD22	2.03	0.41

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	139/141 (99%)	135 (97%)	3 (2%)	1 (1%)	26	11
1	C	139/141 (99%)	135 (97%)	2 (1%)	2 (1%)	14	3
2	B	144/146 (99%)	136 (94%)	6 (4%)	2 (1%)	14	3
2	D	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
All	All	566/574 (99%)	543 (96%)	18 (3%)	5 (1%)	21	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	49	SER
2	B	5	ALA
1	C	2	LEU
1	C	50	PRO
1	A	50	PRO

### 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%)	107 (92%)	10 (8%)	13	3
1	C	117/117 (100%)	107 (92%)	10 (8%)	13	3
2	B	121/121 (100%)	103 (85%)	18 (15%)	4	0
2	D	121/121 (100%)	108 (89%)	13 (11%)	8	2
All	All	476/476 (100%)	425 (89%)	51 (11%)	8	2

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	17	ILE
1	A	41	THR

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Mol	Chain	Res	Type
1	A	48	LEU
1	A	86	LEU
1	A	89	TYR
1	A	105	LEU
1	A	116	GLU
1	A	139	LYS
1	A	141	ARG
2	B	2	HIS
2	B	8	LYS
2	B	9	SER
2	B	17	LYS
2	B	22	GLU
2	B	28	LEU
2	B	44	SER
2	B	50	THR
2	B	65	LYS
2	B	68	LEU
2	B	79	ASP
2	B	81	LEU
2	B	82	LYS
2	B	87	LYS
2	B	109	VAL
2	B	110	LEU
2	B	120	LYS
2	B	144	LYS
1	C	15	ASP
1	C	30	ASP
1	C	74	ASP
1	C	85	ASP
1	C	86	LEU
1	C	89	TYR
1	C	105	LEU
1	C	116	GLU
1	C	125	LEU
1	C	141	ARG
2	D	9	SER
2	D	10	LEU
2	D	14	LEU
2	D	28	LEU
2	D	40	ARG
2	D	43	ASP
2	D	59	LYS

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Mol	Chain	Res	Type
2	D	68	LEU
2	D	75	LEU
2	D	81	LEU
2	D	104	LYS
2	D	110	LEU
2	D	139	ASN

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

Mol	Chain	Res	Type
1	A	9	ASN
1	A	34	GLN
1	A	103	HIS
2	B	102	ASN
2	B	108	ASN
2	B	117	HIS
2	B	139	ASN
2	B	143	HIS
1	C	9	ASN
1	C	34	GLN
1	C	58	HIS
1	C	97	ASN
1	C	103	HIS
1	C	113	HIS
2	D	102	ASN
2	D	108	ASN
2	D	146	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 carbohydrates 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	1,4	30,50,50	2.57	8 (26%)	24,82,82	2.35	9 (37%)
3	HEM	B	147	2	30,50,50	2.52	9 (30%)	24,82,82	2.51	10 (41%)
3	HEM	C	142	1,4	30,50,50	2.58	8 (26%)	24,82,82	2.31	9 (37%)
3	HEM	D	147	2,4	30,50,50	2.50	7 (23%)	24,82,82	2.45	9 (37%)

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	1,4	-	0/10/54/54	0/0/8/8
3	HEM	B	147	2	-	0/10/54/54	0/0/8/8
3	HEM	C	142	1,4	-	0/10/54/54	0/0/8/8
3	HEM	D	147	2,4	-	0/10/54/54	0/0/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C3B-CAB	-6.83	1.38	1.51
3	D	147	HEM	C3C-CAC	-6.80	1.38	1.51
3	B	147	HEM	C3C-CAC	-6.43	1.39	1.51
3	B	147	HEM	C2D-C3D	-6.42	1.35	1.54
3	D	147	HEM	C2D-C3D	-6.01	1.36	1.54
3	C	142	HEM	C2C-C1C	-5.71	1.41	1.52
3	C	142	HEM	C2D-C3D	-5.65	1.37	1.54
3	D	147	HEM	C3B-CAB	-5.64	1.40	1.51
3	A	142	HEM	C3C-CAC	-5.64	1.40	1.51
3	A	142	HEM	C3B-CAB	-5.58	1.40	1.51
3	A	142	HEM	C2D-C3D	-5.50	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	C3D-C4D	-5.35	1.44	1.51
3	A	142	HEM	C3B-C4B	-5.26	1.47	1.51
3	B	147	HEM	C3D-C4D	-5.23	1.44	1.51
3	C	142	HEM	C3C-CAC	-4.64	1.42	1.51
3	C	142	HEM	C3B-C4B	-4.61	1.47	1.51
3	B	147	HEM	C3B-CAB	-4.55	1.42	1.51
3	A	142	HEM	C2C-C1C	-4.38	1.44	1.52
3	B	147	HEM	C3B-C4B	-3.39	1.48	1.51
3	D	147	HEM	C2C-C1C	-3.35	1.46	1.52
3	C	142	HEM	C3D-C4D	-2.77	1.48	1.51
3	B	147	HEM	C2C-C1C	-2.74	1.47	1.52
3	A	142	HEM	C2B-C1B	-2.19	1.44	1.51
3	A	142	HEM	C2D-C1D	-2.08	1.45	1.51
3	B	147	HEM	CBB-CAB	2.03	1.41	1.29
3	D	147	HEM	FE-NC	2.06	2.03	1.95
3	C	142	HEM	CHD-C4C	2.06	1.41	1.36
3	B	147	HEM	C1C-NC	2.27	1.38	1.36
3	D	147	HEM	C4C-NC	2.39	1.38	1.36
3	B	147	HEM	C4C-NC	3.47	1.40	1.36
3	C	142	HEM	C1C-NC	3.63	1.40	1.36
3	D	147	HEM	C1C-NC	4.94	1.42	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CAA-C2A-C1A	-3.13	123.61	127.01
3	C	142	HEM	CAA-C2A-C3A	-3.08	120.21	129.00
3	A	142	HEM	CBD-CAD-C3D	-2.40	106.56	113.55
3	B	147	HEM	CBD-CAD-C3D	2.12	119.72	113.55
3	C	142	HEM	CMD-C2D-C3D	2.20	124.08	114.35
3	B	147	HEM	C3C-CAC-CBC	2.37	128.09	124.46
3	B	147	HEM	CAD-C3D-C4D	2.38	120.86	112.47
3	A	142	HEM	C4B-CHC-C1C	2.39	129.82	125.82
3	D	147	HEM	C3B-C4B-CHC	2.44	126.60	123.16
3	C	142	HEM	CAA-C2A-C1A	2.55	129.78	127.01
3	D	147	HEM	CMD-C2D-C3D	2.60	125.87	114.35
3	B	147	HEM	C2D-C3D-C4D	2.73	106.13	101.50
3	D	147	HEM	C2D-C3D-C4D	2.79	106.23	101.50
3	C	142	HEM	CBA-CAA-C2A	3.00	117.90	112.53
3	B	147	HEM	CBA-CAA-C2A	3.02	117.94	112.53
3	D	147	HEM	C3C-CAC-CBC	3.18	129.34	124.46
3	B	147	HEM	CMD-C2D-C3D	3.21	128.56	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CMD-C2D-C3D	3.28	128.86	114.35
3	B	147	HEM	C3B-CAB-CBB	3.52	129.85	124.46
3	C	142	HEM	C2D-C3D-C4D	3.54	107.50	101.50
3	C	142	HEM	CAD-C3D-C4D	3.82	125.95	112.47
3	A	142	HEM	CAD-C3D-C2D	3.90	124.44	113.22
3	A	142	HEM	CAD-C3D-C4D	3.93	126.32	112.47
3	A	142	HEM	C2D-C3D-C4D	4.08	108.42	101.50
3	C	142	HEM	CAD-C3D-C2D	4.17	125.20	113.22
3	D	147	HEM	CAD-C3D-C2D	4.18	125.25	113.22
3	A	142	HEM	CMC-C2C-C3C	4.38	127.47	116.53
3	D	147	HEM	CMB-C2B-C3B	4.40	127.52	116.53
3	D	147	HEM	CAD-C3D-C4D	4.41	128.03	112.47
3	D	147	HEM	CMC-C2C-C3C	4.44	127.60	116.53
3	B	147	HEM	CMB-C2B-C3B	4.45	127.63	116.53
3	C	142	HEM	CMB-C2B-C3B	4.50	127.76	116.53
3	B	147	HEM	CMC-C2C-C3C	4.50	127.77	116.53
3	A	142	HEM	CMB-C2B-C3B	4.51	127.80	116.53
3	C	142	HEM	CMC-C2C-C3C	4.69	128.25	116.53
3	D	147	HEM	C3B-CAB-CBB	4.91	131.98	124.46
3	B	147	HEM	CAD-C3D-C2D	6.82	132.84	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	147	HEM	1	0
3	D	147	HEM	1	0

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	141/141 (100%)	-0.18	1 (0%) 89 87	13, 21, 39, 50	0
1	C	141/141 (100%)	-0.16	1 (0%) 89 87	10, 22, 41, 55	0
2	B	146/146 (100%)	0.15	3 (2%) 67 62	12, 32, 54, 58	0
2	D	146/146 (100%)	0.05	3 (2%) 67 62	10, 25, 48, 59	0
All	All	574/574 (100%)	-0.03	8 (1%) 78 74	10, 25, 48, 59	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	20	VAL	4.2
1	A	1	VAL	3.7
1	C	1	VAL	3.6
2	D	2	HIS	2.6
2	B	145	TYR	2.3
2	D	145	TYR	2.3
2	B	93	CYS	2.2
2	B	141	LEU	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	HEM	C	142	43/43	0.97	0.12	1.65	13,19,33,40	0
3	HEM	A	142	43/43	0.97	0.10	0.41	15,18,33,39	0
3	HEM	B	147	43/43	0.96	0.11	-0.22	26,30,42,46	0
3	HEM	D	147	43/43	0.97	0.10	-0.59	24,31,49,56	0

## 6.5 Other polymers

There are no such residues in this entry.