



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:29 PM GMT

PDB ID : 1A3O  
Title : ARTIFICIAL MUTANT (ALPHA Y42H) OF DEOXY HEMOGLOBIN  
Authors : Tame, J.; Vallone, B.  
Deposited on : 1998-01-22  
Resolution : 1.80 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>

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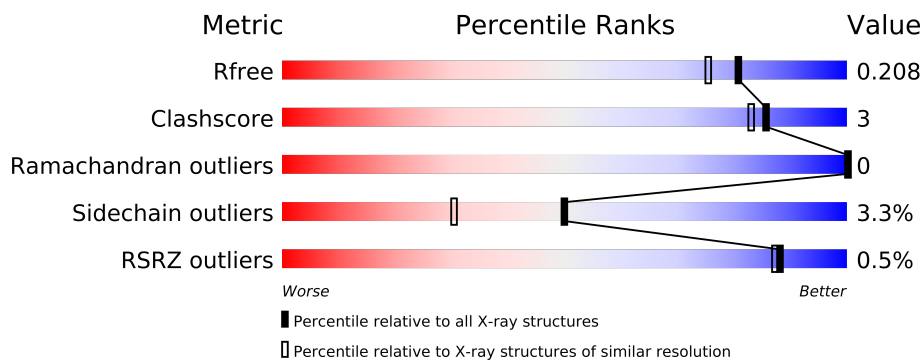
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 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))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
2	B	146	
2	D	146	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4956 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	141	Total	C	N	O	S	12	0	0
			1067	682	189	193	3			
1	C	141	Total	C	N	O	S	15	1	0
			1069	683	189	194	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	HIS	TYR	ENGINEERED	UNP P69905
C	42	HIS	TYR	ENGINEERED	UNP P69905

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	16	1	0
			1120	721	195	201	3			
2	D	145	Total	C	N	O	S	20	0	0
			1116	719	194	200	3			

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	106	Total	O	0	0
			106	106		
4	C	92	Total	O	0	0
			92	92		
4	D	101	Total	O	0	0
			101	101		

### 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.

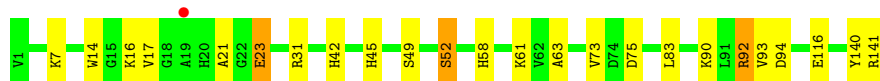
- Molecule 1: HEMOGLOBIN (ALPHA CHAIN)

Chain A: 



- Molecule 1: HEMOGLOBIN (ALPHA CHAIN)

Chain C: 



- Molecule 2: HEMOGLOBIN (BETA CHAIN)

Chain B: 



- Molecule 2: HEMOGLOBIN (BETA CHAIN)

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.44Å 81.16Å 53.32Å 90.00° 99.65° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 14.88 – 1.78	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-1.80) 95.0 (14.88-1.78)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.78Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.227 0.168 , 0.208	Depositor DCC
$R_{free}$ test set	2378 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 47408 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.96	2/1095 (0.2%)	1.50	15/1488 (1.0%)
1	C	1.02	3/1101 (0.3%)	1.55	16/1496 (1.1%)
2	B	0.78	2/1154 (0.2%)	1.51	11/1567 (0.7%)
2	D	0.87	3/1146 (0.3%)	1.33	7/1556 (0.4%)
All	All	0.91	10/4496 (0.2%)	1.47	49/6107 (0.8%)

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
2	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	GLU	CG-CD	-23.74	1.16	1.51
1	A	60	LYS	CG-CD	20.65	2.22	1.52
2	D	2	HIS	CA-CB	14.03	1.84	1.53
2	D	43	GLU	CB-CG	-10.66	1.31	1.52
2	B	82	LYS	CD-CE	-8.06	1.31	1.51
1	C	16	LYS	CG-CD	-7.45	1.27	1.52
2	B	66	LYS	CB-CG	-7.40	1.32	1.52
2	D	104	ARG	CD-NE	-7.02	1.34	1.46
1	C	75	ASP	CB-CG	-5.94	1.39	1.51
1	A	61	LYS	CG-CD	-5.08	1.35	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	LYS	CG-CD-CE	17.81	165.33	111.90
1	A	99	LYS	CB-CG-CD	15.52	151.96	111.60
2	B	66	LYS	CA-CB-CG	14.93	146.24	113.40
2	B	104	ARG	NE-CZ-NH2	-14.12	113.24	120.30
2	B	104	ARG	CD-NE-CZ	13.79	142.91	123.60
1	C	16	LYS	CB-CG-CD	13.00	145.40	111.60
2	B	2	HIS	CA-CB-CG	11.99	133.98	113.60
1	A	60	LYS	CB-CG-CD	-11.76	81.02	111.60
1	C	75	ASP	CB-CG-OD2	-11.63	107.83	118.30
1	C	75	ASP	CB-CG-OD1	11.05	128.25	118.30
2	D	6	GLU	CA-CB-CG	11.03	137.66	113.40
1	A	92	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	47	ASP	CB-CG-OD1	9.26	126.63	118.30
2	B	30	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	A	90	LYS	CB-CG-CD	8.53	133.77	111.60
1	A	141	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	C	23	GLU	CB-CG-CD	8.22	136.39	114.20
1	C	94	ASP	CB-CG-OD2	7.95	125.46	118.30
1	C	31	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	31	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	60	LYS	CG-CD-CE	7.20	133.51	111.90
1	C	31	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	C	141	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	D	104	ARG	NE-CZ-NH2	6.70	123.65	120.30
2	D	2	HIS	N-CA-CB	-6.67	98.60	110.60
1	A	74	ASP	CB-CG-OD1	6.64	124.27	118.30
1	C	23	GLU	CG-CD-OE1	-6.54	105.21	118.30
1	A	116	GLU	OE1-CD-OE2	6.52	131.13	123.30
2	D	2	HIS	CA-CB-CG	6.50	124.65	113.60
2	B	94	ASP	CB-CG-OD2	6.42	124.08	118.30
2	B	130	TYR	CB-CG-CD2	-6.41	117.16	121.00
2	B	103	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	A	24	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	C	23	GLU	CG-CD-OE2	5.90	130.09	118.30
2	B	104	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	C	141	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	D	103	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	C	116	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	C	140	TYR	CB-CG-CD2	-5.77	117.54	121.00
2	D	104	ARG	CG-CD-NE	5.77	123.91	111.80
1	A	92	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	B	43	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	C	92	ARG	NE-CZ-NH1	5.23	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	LYS	CB-CG-CD	5.20	125.12	111.60
1	A	66	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	126	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	75	ASP	CA-CB-CG	5.17	124.77	113.40
2	D	142	ALA	CB-CA-C	-5.11	102.44	110.10
1	A	94	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2	HIS	Sidechain

## 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	1067	0	1071	2	0
1	C	1069	0	1072	10	0
2	B	1120	0	1108	12	0
2	D	1116	0	1106	1	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	1	0
3	D	43	0	30	1	0
4	A	113	0	0	2	0
4	B	106	0	0	0	0
4	C	92	0	0	1	0
4	D	101	0	0	1	0
All	All	4956	0	4477	24	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 3.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:4:THR:HB	2:B:5:PRO:HD2	1.49	0.94
2:B:3:LEU:HD22	2:B:7:GLU:HB3	1.64	0.78
2:B:40:ARG:HH11	2:B:40:ARG:HA	1.47	0.78
2:B:3:LEU:HD23	2:B:132:LYS:HD2	1.72	0.72
1:A:116:GLU:HB2	4:A:191:HOH:O	1.91	0.71
2:B:40:ARG:HG3	1:C:92:ARG:HB3	1.80	0.62
2:B:4:THR:HB	2:B:5:PRO:CD	2.27	0.61
2:B:40:ARG:HA	2:B:40:ARG:NH1	2.14	0.60
1:C:21:ALA:HB1	1:C:63:ALA:HB1	1.88	0.56
1:A:30:GLU:OE1	4:A:208:HOH:O	2.18	0.56
3:D:147:HEM:HMC2	3:D:147:HEM:HBC2	1.89	0.54
1:C:49:SER:O	1:C:52:SER:HB3	2.11	0.51
2:B:40:ARG:HD2	1:C:90:LYS:O	2.14	0.47
2:B:21:ASP:OD1	2:B:65:LYS:HG3	2.15	0.47
2:D:51:PRO:HD2	4:D:176:HOH:O	2.16	0.46
1:C:23:GLU:HG2	4:C:180:HOH:O	2.18	0.44
1:C:7:LYS:HD3	1:C:73:VAL:HG13	2.00	0.44
2:B:57:ASN:HA	2:B:58:PRO:HD2	1.90	0.43
1:C:83:LEU:HD11	3:C:142:HEM:C3A	2.55	0.42
1:C:14:TRP:O	1:C:17:VAL:HB	2.20	0.41
1:C:58:HIS:HA	1:C:61:LYS:HD3	2.02	0.41
2:B:51:PRO:O	2:B:55:MET:HG2	2.21	0.41
2:B:4:THR:CB	2:B:5:PRO:HD2	2.35	0.41
1:C:42:HIS:CE1	1:C:93:VAL:HA	2.55	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	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	C	140/141 (99%)	138 (99%)	2 (1%)	0	100	100
2	B	144/146 (99%)	144 (100%)	0	0	100	100
2	D	143/146 (98%)	141 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	566/574 (99%)	559 (99%)	7 (1%)	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	113/113 (100%)	108 (96%)	5 (4%)	39	18
1	C	114/113 (101%)	112 (98%)	2 (2%)	71	58
2	B	118/118 (100%)	115 (98%)	3 (2%)	60	42
2	D	117/118 (99%)	112 (96%)	5 (4%)	40	19
All	All	462/462 (100%)	447 (97%)	15 (3%)	50	32

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	16	LYS
1	A	60	LYS
1	A	66	LEU
1	A	90	LYS
2	B	14	LEU
2	B	40	ARG
2	B	65	LYS
1	C	45	HIS
1	C	52	SER
2	D	2	HIS
2	D	6	GLU
2	D	22	GLU
2	D	65	LYS
2	D	79	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	ASN

### 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 ⓘ

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	49,50,50	2.53	12 (24%)	46,82,82	2.02	11 (23%)
3	HEM	B	147	2	49,50,50	2.29	11 (22%)	46,82,82	1.82	10 (21%)
3	HEM	C	142	1	49,50,50	2.31	14 (28%)	46,82,82	1.90	11 (23%)
3	HEM	D	147	2	49,50,50	2.09	10 (20%)	46,82,82	1.57	5 (10%)

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	-	0/14/114/114	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	147	2	-	0/14/114/114	0/0/8/8
3	HEM	C	142	1	-	0/14/114/114	0/0/8/8
3	HEM	D	147	2	-	0/14/114/114	0/0/8/8

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	C3D-C4D	-9.14	1.42	1.44
3	D	147	HEM	C3D-C2D	-7.01	1.31	1.43
3	A	142	HEM	C3B-C2B	-6.72	1.32	1.43
3	B	147	HEM	C3D-C2D	-6.36	1.32	1.43
3	A	142	HEM	C3C-C2C	-6.34	1.32	1.43
3	C	142	HEM	C3C-C2C	-6.22	1.32	1.43
3	B	147	HEM	C3C-C2C	-6.16	1.33	1.43
3	D	147	HEM	C3B-C2B	-6.10	1.33	1.43
3	C	142	HEM	C3B-C2B	-5.87	1.33	1.43
3	C	142	HEM	C3D-C2D	-5.76	1.33	1.43
3	B	147	HEM	C3B-C2B	-5.53	1.34	1.43
3	B	147	HEM	C2B-C1B	-5.44	1.43	1.44
3	D	147	HEM	C3C-C2C	-5.44	1.34	1.43
3	C	142	HEM	C4A-C3A	5.18	1.46	1.40
3	A	142	HEM	C3D-C2D	-4.91	1.35	1.43
3	B	147	HEM	C3B-CAB	4.65	1.55	1.40
3	A	142	HEM	C3B-CAB	4.55	1.54	1.40
3	B	147	HEM	C4A-C3A	4.50	1.45	1.40
3	D	147	HEM	C3B-CAB	4.36	1.54	1.40
3	A	142	HEM	C3C-CAC	4.31	1.53	1.40
3	C	142	HEM	C3B-CAB	4.30	1.53	1.40
3	A	142	HEM	C4A-C3A	4.09	1.45	1.40
3	C	142	HEM	C3C-CAC	3.88	1.52	1.40
3	D	147	HEM	C3C-CAC	3.82	1.52	1.40
3	C	142	HEM	C2B-C1B	3.67	1.45	1.44
3	B	147	HEM	C3C-CAC	3.64	1.51	1.40
3	C	142	HEM	C2D-C1D	-3.34	1.43	1.44
3	D	147	HEM	C4A-C3A	3.17	1.44	1.40
3	C	142	HEM	C3D-C4D	3.01	1.45	1.44
3	D	147	HEM	CMC-C2C	2.46	1.55	1.47
3	A	142	HEM	C2B-C1B	-2.42	1.44	1.44
3	C	142	HEM	FE-NB	2.40	2.06	1.97
3	B	147	HEM	CMC-C2C	2.39	1.54	1.47
3	A	142	HEM	CMB-C2B	2.32	1.54	1.47
3	C	142	HEM	CMB-C2B	2.27	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	CHB-C1B	2.22	1.39	1.35
3	A	142	HEM	FE-NA	2.21	2.01	1.92
3	D	147	HEM	FE-NA	2.18	2.01	1.92
3	D	147	HEM	C2B-C1B	2.15	1.45	1.44
3	B	147	HEM	CMD-C2D	2.14	1.54	1.47
3	C	142	HEM	CMD-C2D	2.14	1.54	1.47
3	A	142	HEM	CMD-C2D	2.12	1.54	1.47
3	B	147	HEM	FE-NA	2.12	2.01	1.92
3	D	147	HEM	CMD-C2D	2.11	1.53	1.47
3	C	142	HEM	CMC-C2C	2.09	1.53	1.47
3	C	142	HEM	FE-NA	2.05	2.01	1.92
3	A	142	HEM	C2A-C3A	-2.04	1.31	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	C3B-C4B-NB	-6.20	109.56	114.00
3	D	147	HEM	C3B-C4B-NB	-5.79	109.86	114.00
3	A	142	HEM	C3B-C4B-NB	-5.50	110.06	114.00
3	A	142	HEM	CMA-C3A-C4A	-5.27	120.51	128.62
3	B	147	HEM	C3B-C4B-NB	-5.00	110.42	114.00
3	C	142	HEM	CHD-C4C-NC	4.49	128.63	124.73
3	C	142	HEM	CMA-C3A-C4A	-4.37	121.89	128.62
3	A	142	HEM	C1A-CHA-C4D	-4.13	122.03	127.47
3	A	142	HEM	CMA-C3A-C2A	4.10	132.68	124.94
3	A	142	HEM	CHD-C1D-ND	4.03	127.93	124.58
3	B	147	HEM	CHC-C1C-NC	4.00	128.21	124.73
3	B	147	HEM	CMA-C3A-C4A	-3.99	122.48	128.62
3	B	147	HEM	CBD-CAD-C3D	-3.96	105.74	114.37
3	A	142	HEM	CHD-C4C-NC	3.76	128.00	124.73
3	D	147	HEM	C1A-CHA-C4D	-3.55	122.80	127.47
3	A	142	HEM	CHC-C1C-NC	3.47	127.74	124.73
3	B	147	HEM	CHD-C4C-NC	3.46	127.74	124.73
3	C	142	HEM	CBA-CAA-C2A	3.38	118.65	112.69
3	C	142	HEM	CMA-C3A-C2A	3.19	130.96	124.94
3	B	147	HEM	C1A-CHA-C4D	-2.79	123.80	127.47
3	B	147	HEM	C4A-CHB-C1B	-2.75	123.86	127.47
3	C	142	HEM	C4A-CHB-C1B	-2.74	123.87	127.47
3	C	142	HEM	CHC-C1C-NC	2.67	127.05	124.73
3	B	147	HEM	CMA-C3A-C2A	2.65	129.93	124.94
3	D	147	HEM	CMA-C3A-C4A	-2.64	124.55	128.62
3	B	147	HEM	C2D-C1D-ND	-2.63	109.82	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	C4C-NC-C1C	2.56	108.20	105.53
3	C	142	HEM	CHC-C4B-NB	2.54	126.70	124.58
3	D	147	HEM	C2D-C1D-ND	-2.47	110.01	112.93
3	A	142	HEM	C1D-CHD-C4C	-2.40	120.24	126.57
3	A	142	HEM	C4A-CHB-C1B	-2.26	124.50	127.47
3	C	142	HEM	O1A-CGA-CBA	-2.26	115.26	123.03
3	D	147	HEM	CBD-CAD-C3D	-2.24	109.49	114.37
3	A	142	HEM	CBD-CAD-C3D	-2.23	109.51	114.37
3	A	142	HEM	C2D-C1D-ND	-2.18	110.35	112.93
3	C	142	HEM	CAD-CBD-CGD	2.13	120.14	113.48
3	C	142	HEM	O1D-CGD-CBD	-2.10	115.80	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 ⓘ

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%)	-0.50	0 100 100	12, 18, 26, 42	4 (2%)
1	C	141/141 (100%)	-0.38	1 (0%) 84 83	14, 20, 32, 38	5 (3%)
2	B	145/146 (99%)	-0.44	2 (1%) 72 68	13, 18, 30, 52	4 (2%)
2	D	145/146 (99%)	-0.44	0 100 100	14, 19, 29, 40	5 (3%)
All	All	572/574 (99%)	-0.44	3 (0%) 88 87	12, 19, 30, 52	18 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	5	PRO	4.0
2	B	2	HIS	3.2
1	C	19	ALA	2.8

### 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEM	A	142	43/43	0.09	1.14	11,17,27,37	0
3	HEM	C	142	43/43	0.09	0.03	15,18,33,42	0
3	HEM	B	147	43/43	0.07	-0.12	12,16,29,35	4
3	HEM	D	147	43/43	0.07	-0.51	12,16,28,39	0

## 6.5 Other polymers

There are no such residues in this entry.