



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:39 PM GMT

PDB ID : 1CCL  
Title : PROBING THE STRENGTH AND CHARACTER OF AN ASP-HIS-X HYDROGEN BOND BY INTRODUCING BURIED CHARGES  
Authors : Cao, Y.; Goodin, D.B.; Mcree, D.E.  
Deposited on : 1998-01-02  
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>

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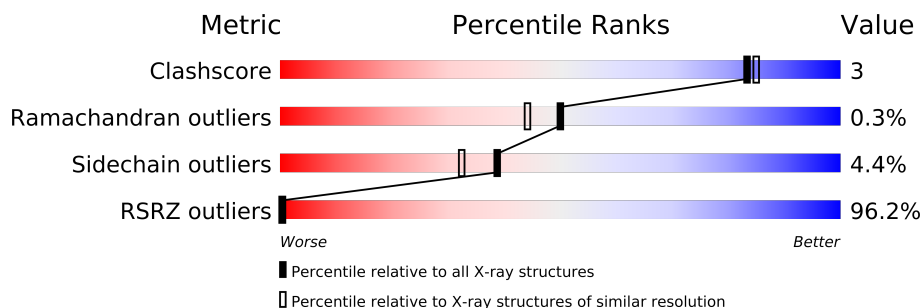
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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)
RSRZ outliers	66119	4890 (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.

Mol	Chain	Length	Quality of chain
1	A	291	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3013 atoms, of which 515 are hydrogens 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 CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	291	2863	1498	515	393	451	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	SUBSTITUTION	UNP P00431
A	152	GLY	ASP	SUBSTITUTION	UNP P00431
A	202	LYS	PHE	SUBSTITUTION	UNP P00431

- 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

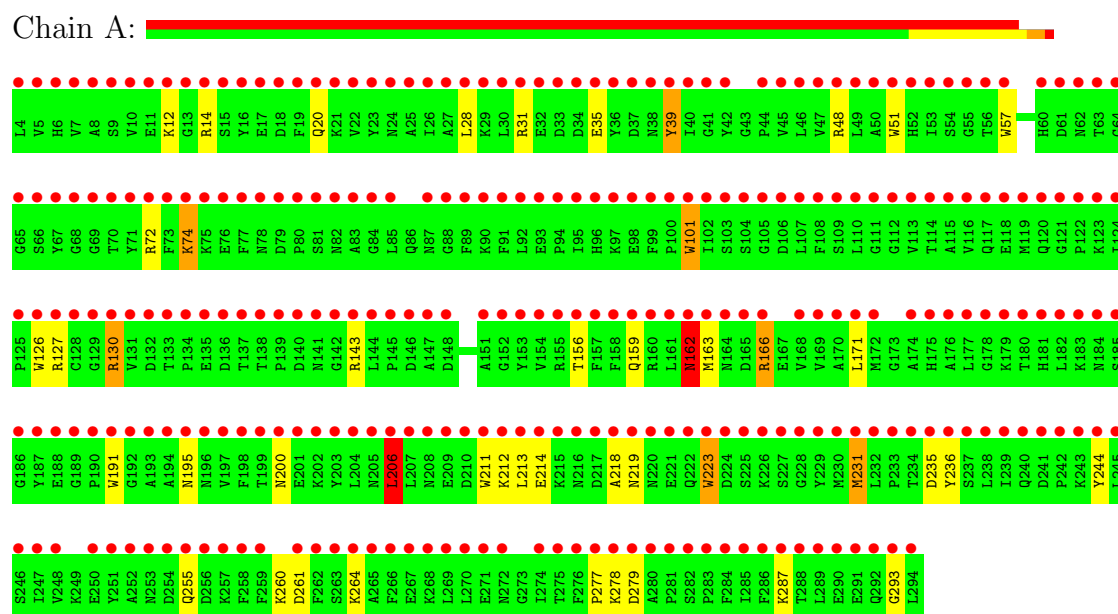
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total 107	O 107	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.

#### • Molecule 1: CYTOCHROME C PEROXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.40Å 73.20Å 44.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00 27.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.00) 81.6 (27.25-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.184 , (Not available) 0.502 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 30.8	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 19325 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.55	EDS
Total number of atoms	3013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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	0.79	0/2413	1.52	42/3265 (1.3%)

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 (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	A	127	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	A	48	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	143	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	101	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	A	51	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	A	223	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	A	191	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	A	191	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	51	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	211	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	A	101	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	143	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	223	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	A	57	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	A	31	ARG	NE-CZ-NH2	-6.92	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	A	162	ASN	CA-C-N	-6.64	102.58	117.20
1	A	191	TRP	CB-CG-CD1	-6.59	118.43	127.00
1	A	126	TRP	CD1-CG-CD2	6.58	111.57	106.30
1	A	211	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	A	244	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	48	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	51	TRP	CB-CG-CD1	-6.33	118.77	127.00
1	A	163	MET	CG-SD-CE	-6.31	90.11	100.20
1	A	31	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	130	ARG	CG-CD-NE	-6.18	98.83	111.80
1	A	101	TRP	CG-CD1-NE1	-6.06	104.04	110.10
1	A	101	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	A	166	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	278	LYS	CA-CB-CG	-5.86	100.51	113.40
1	A	72	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	101	TRP	CB-CG-CD1	-5.76	119.51	127.00
1	A	51	TRP	CG-CD2-CE3	5.66	138.99	133.90
1	A	191	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	A	126	TRP	CE2-CD2-CG	-5.48	102.92	107.30
1	A	277	PRO	CA-C-N	5.39	129.07	117.20
1	A	51	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	A	231	MET	CA-CB-CG	5.35	122.39	113.30
1	A	156	THR	CA-CB-CG2	5.34	119.88	112.40
1	A	206	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	39	TYR	CB-CG-CD2	-5.10	117.94	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	TYR	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	2348	515	1718	14	36
2	A	43	0	30	0	0
3	A	107	0	0	2	10
All	All	2498	515	1748	14	36

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:MET:HE1	1:A:236:TYR:HD1	1.67	0.59
1:A:74:LYS:H	1:A:74:LYS:HD2	1.70	0.55
1:A:231:MET:HE1	1:A:236:TYR:CD1	2.43	0.54
1:A:231:MET:HG2	1:A:235:ASP:HB2	1.91	0.51
1:A:130:ARG:NE	3:A:326:HOH:O	2.47	0.48
1:A:200:ASN:H	1:A:255:GLN:HE22	1.63	0.47
1:A:20:GLN:HE21	1:A:287:LYS:N	2.13	0.47
1:A:231:MET:HE1	1:A:236:TYR:HB2	1.98	0.46
1:A:206:LEU:HD12	1:A:231:MET:SD	2.56	0.45
1:A:223:TRP:HB2	1:A:231:MET:HE2	1.99	0.45
1:A:130:ARG:CZ	3:A:326:HOH:O	2.65	0.43
1:A:20:GLN:HE21	1:A:287:LYS:H	1.67	0.43
1:A:231:MET:HG2	1:A:235:ASP:CB	2.50	0.41
1:A:218:ALA:O	1:A:219:ASN:HB2	2.21	0.41

All (36) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:ARG:NH2	1:A:213:LEU:C[4.5610]	0.42	1.78
1:A:12:LYS:CA	1:A:214:GLU:OE2[4.5610]	0.83	1.37
1:A:14:ARG:CZ	1:A:213:LEU:O[4.5610]	0.83	1.37
1:A:14:ARG:NE	1:A:213:LEU:O[4.5610]	0.94	1.26
1:A:14:ARG:CZ	1:A:213:LEU:C[4.5610]	1.07	1.13
1:A:14:ARG:NH2	1:A:213:LEU:CA[4.5610]	1.11	1.09
1:A:212:LYS:CG	3:A:372:HOH:O[4.4610]	1.15	1.05
1:A:12:LYS:C	1:A:214:GLU:OE2[4.5610]	1.33	0.87
1:A:212:LYS:CD	3:A:372:HOH:O[4.4610]	1.33	0.87
1:A:212:LYS:CB	3:A:372:HOH:O[4.4610]	1.34	0.86
1:A:212:LYS:NZ	3:A:374:HOH:O[4.4610]	1.37	0.83
1:A:12:LYS:O	1:A:214:GLU:CG[4.5610]	1.38	0.82
1:A:12:LYS:N	1:A:214:GLU:OE2[4.5610]	1.40	0.80
1:A:14:ARG:NH2	1:A:213:LEU:O[4.5610]	1.41	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:LYS:O	1:A:214:GLU:CB[4.5610]	1.43	0.77
1:A:264:LYS:NZ	3:A:389:HOH:O[3.559]	1.46	0.74
1:A:12:LYS:O	1:A:214:GLU:CD[4.5610]	1.49	0.71
1:A:212:LYS:CE	3:A:374:HOH:O[4.4610]	1.53	0.67
1:A:214:GLU:CG	3:A:373:HOH:O[4.4610]	1.53	0.67
1:A:14:ARG:NH2	1:A:214:GLU:N[4.5610]	1.62	0.58
1:A:261:ASP:OD1	3:A:389:HOH:O[3.559]	1.68	0.52
1:A:12:LYS:CB	1:A:214:GLU:OE1[4.5610]	1.72	0.48
1:A:12:LYS:C	1:A:214:GLU:CD[4.5610]	1.75	0.45
1:A:12:LYS:CB	1:A:214:GLU:OE2[4.5610]	1.80	0.40
1:A:14:ARG:CZ	1:A:214:GLU:N[4.5610]	1.83	0.37
1:A:12:LYS:O	1:A:214:GLU:OE2[4.5610]	1.84	0.36
1:A:212:LYS:CE	3:A:372:HOH:O[4.4610]	1.84	0.36
1:A:12:LYS:CA	1:A:214:GLU:CD[4.5610]	1.89	0.31
1:A:101:TRP:CB	1:A:213:LEU:N[4.5610]	1.97	0.23
1:A:12:LYS:CB	1:A:214:GLU:CD[4.5610]	2.00	0.20
1:A:14:ARG:NE	1:A:213:LEU:C[4.5610]	2.01	0.19
1:A:293:GLY:O	3:A:331:HOH:O[3.549]	2.03	0.17
1:A:14:ARG:NH2	1:A:213:LEU:N[4.5610]	2.08	0.12
1:A:14:ARG:NH1	1:A:213:LEU:O[4.5610]	2.10	0.10
1:A:14:ARG:NH1	1:A:213:LEU:C[4.5610]	2.13	0.07
1:A:14:ARG:NH2	1:A:213:LEU:CB[4.5610]	2.15	0.05

## 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	289/291 (99%)	279 (96%)	9 (3%)	1 (0%)	50 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

### 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	249/249 (100%)	238 (96%)	11 (4%)	39 32

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	GLU
1	A	74	LYS
1	A	159	GLN
1	A	162	ASN
1	A	166	ARG
1	A	171	LEU
1	A	195	ASN
1	A	206	LEU
1	A	260	LYS
1	A	279	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	87	ASN
1	A	220	ASN
1	A	240	GLN
1	A	255	GLN
1	A	292	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 ⓘ

1 ligand is 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	1	1,3	49,50,50	5.09	21 (42%)	46,82,82	1.37	4 (8%)

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	1	1,3	-	0/14/114/114	0/0/8/8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	C3D-C4D	-21.31	1.39	1.44
2	A	1	HEM	C2D-C1D	-19.98	1.39	1.44
2	A	1	HEM	C2B-C1B	-15.32	1.40	1.44
2	A	1	HEM	CHB-C1B	3.73	1.41	1.35
2	A	1	HEM	C3B-C4B	-3.67	1.40	1.44
2	A	1	HEM	CHA-C4D	3.60	1.41	1.35
2	A	1	HEM	FE-NA	3.32	2.06	1.92
2	A	1	HEM	C4C-NC	-3.04	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	FE-NB	2.94	2.08	1.97
2	A	1	HEM	C1A-C2A	-2.87	1.38	1.43
2	A	1	HEM	CBC-CAC	2.86	1.45	1.28
2	A	1	HEM	C1B-NB	-2.86	1.33	1.39
2	A	1	HEM	C3D-C2D	-2.83	1.38	1.43
2	A	1	HEM	C4D-ND	-2.73	1.34	1.39
2	A	1	HEM	FE-ND	2.69	2.07	1.97
2	A	1	HEM	CBB-CAB	2.68	1.44	1.28
2	A	1	HEM	CHD-C4C	2.63	1.41	1.36
2	A	1	HEM	CHC-C1C	2.59	1.41	1.36
2	A	1	HEM	FE-NC	2.17	2.06	1.97
2	A	1	HEM	CMC-C2C	2.07	1.53	1.47
2	A	1	HEM	O2A-CGA	-2.02	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HEM	C3B-C4B-NB	-4.66	110.66	114.00
2	A	1	HEM	C3A-C4A-NA	2.46	111.27	109.41
2	A	1	HEM	C4A-C3A-C2A	-2.41	105.32	107.00
2	A	1	HEM	C4D-ND-C1D	2.03	107.24	105.16

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	291/291 (100%)	4.74	280 (96%) 0 0	11, 21, 35, 47	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	VAL	13.4
1	A	223	TRP	12.6
1	A	63	THR	12.2
1	A	36	TYR	12.0
1	A	4	LEU	11.5
1	A	83	ALA	11.2
1	A	153	TYR	10.0
1	A	231	MET	9.4
1	A	278	LYS	9.3
1	A	22	VAL	9.2
1	A	282	SER	9.1
1	A	85	LEU	9.1
1	A	27	ALA	9.0
1	A	276	PHE	8.8
1	A	213	LEU	8.8
1	A	191	TRP	8.7
1	A	286	PHE	8.7
1	A	251	TYR	8.4
1	A	66	SER	8.3
1	A	277	PRO	8.3
1	A	42	TYR	8.1
1	A	78	ASN	8.0
1	A	279	ASP	7.9
1	A	161	LEU	7.8
1	A	5	VAL	7.7
1	A	128	CYS	7.7
1	A	75	LYS	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	131	VAL	7.6
1	A	258	PHE	7.4
1	A	57	TRP	7.4
1	A	23	TYR	7.3
1	A	275	THR	7.3
1	A	7	VAL	7.3
1	A	206	LEU	7.3
1	A	145	PRO	7.2
1	A	53	ILE	7.2
1	A	219	ASN	7.2
1	A	171	LEU	7.2
1	A	203	TYR	7.1
1	A	157	PHE	7.1
1	A	177	LEU	7.0
1	A	178	GLY	7.0
1	A	110	LEU	6.9
1	A	62	ASN	6.8
1	A	16	TYR	6.8
1	A	19	PHE	6.7
1	A	125	PRO	6.6
1	A	116	VAL	6.6
1	A	216	ASN	6.6
1	A	220	ASN	6.6
1	A	248	VAL	6.5
1	A	45	VAL	6.5
1	A	187	TYR	6.5
1	A	44	PRO	6.5
1	A	294	LEU	6.4
1	A	95	ILE	6.4
1	A	274	ILE	6.4
1	A	288	THR	6.3
1	A	80	PRO	6.3
1	A	107	LEU	6.2
1	A	259	PHE	6.2
1	A	254	ASP	6.2
1	A	40	ILE	6.2
1	A	51	TRP	6.2
1	A	97	LYS	6.2
1	A	198	PHE	6.1
1	A	74	LYS	6.1
1	A	199	THR	6.1
1	A	30	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	79	ASP	6.1
1	A	236	TYR	6.1
1	A	156	THR	6.0
1	A	126	TRP	6.0
1	A	197	VAL	6.0
1	A	39	TYR	6.0
1	A	67	TYR	6.0
1	A	71	TYR	6.0
1	A	229	TYR	6.0
1	A	77	PHE	5.9
1	A	124	ILE	5.8
1	A	138	THR	5.8
1	A	241	ASP	5.8
1	A	133	THR	5.8
1	A	109	SER	5.8
1	A	266	PHE	5.8
1	A	8	ALA	5.6
1	A	89	PHE	5.6
1	A	143	ARG	5.6
1	A	101	TRP	5.5
1	A	211	TRP	5.5
1	A	28	LEU	5.4
1	A	11	GLU	5.4
1	A	270	LEU	5.4
1	A	218	ALA	5.4
1	A	154	VAL	5.4
1	A	46	LEU	5.4
1	A	221	GLU	5.3
1	A	26	ILE	5.3
1	A	226	LYS	5.3
1	A	32	GLU	5.3
1	A	15	SER	5.3
1	A	225	SER	5.3
1	A	194	ALA	5.3
1	A	142	GLY	5.2
1	A	9	SER	5.1
1	A	179	LYS	5.1
1	A	113	VAL	5.0
1	A	108	PHE	5.0
1	A	158	PHE	5.0
1	A	49	LEU	4.9
1	A	159	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	136	ASP	4.9
1	A	227	SER	4.9
1	A	155	ARG	4.8
1	A	56	THR	4.8
1	A	180	THR	4.8
1	A	244	TYR	4.8
1	A	64	GLY	4.8
1	A	192	GLY	4.8
1	A	217	ASP	4.7
1	A	12	LYS	4.7
1	A	210	ASP	4.7
1	A	283	PRO	4.6
1	A	169	VAL	4.6
1	A	230	MET	4.6
1	A	87	ASN	4.6
1	A	262	PHE	4.6
1	A	115	ALA	4.5
1	A	284	PHE	4.5
1	A	228	GLY	4.5
1	A	33	ASP	4.5
1	A	240	GLN	4.5
1	A	261	ASP	4.5
1	A	73	PHE	4.5
1	A	34	ASP	4.5
1	A	65	GLY	4.5
1	A	91	PHE	4.4
1	A	257	LYS	4.4
1	A	129	GLY	4.4
1	A	61	ASP	4.4
1	A	52	HIS	4.3
1	A	252	ALA	4.3
1	A	102	ILE	4.3
1	A	114	THR	4.3
1	A	204	LEU	4.3
1	A	168	VAL	4.3
1	A	6	HIS	4.3
1	A	96	HIS	4.3
1	A	200	ASN	4.2
1	A	208	ASN	4.2
1	A	105	GLY	4.2
1	A	239	ILE	4.2
1	A	269	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	47	VAL	4.2
1	A	92	LEU	4.1
1	A	265	ALA	4.1
1	A	25	ALA	4.1
1	A	238	LEU	4.1
1	A	99	PHE	4.0
1	A	242	PRO	4.0
1	A	100	PRO	4.0
1	A	247	ILE	4.0
1	A	122	PRO	4.0
1	A	264	LYS	3.9
1	A	31	ARG	3.9
1	A	41	GLY	3.9
1	A	82	ASN	3.9
1	A	233	PRO	3.9
1	A	55	GLY	3.9
1	A	118	GLU	3.9
1	A	182	LEU	3.9
1	A	146	ASP	3.9
1	A	160	ARG	3.9
1	A	139	PRO	3.8
1	A	170	ALA	3.8
1	A	190	PRO	3.8
1	A	130	ARG	3.8
1	A	141	ASN	3.8
1	A	193	ALA	3.8
1	A	263	SER	3.8
1	A	280	ALA	3.8
1	A	185	SER	3.7
1	A	164	ASN	3.7
1	A	215	LYS	3.7
1	A	243	LYS	3.7
1	A	24	ASN	3.7
1	A	163	MET	3.7
1	A	72	ARG	3.7
1	A	111	GLY	3.7
1	A	268	LYS	3.6
1	A	60	HIS	3.6
1	A	144	LEU	3.6
1	A	172	MET	3.6
1	A	17	GLU	3.6
1	A	188	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	205	ASN	3.6
1	A	48	ARG	3.6
1	A	202	LYS	3.6
1	A	134	PRO	3.6
1	A	119	MET	3.5
1	A	234	THR	3.5
1	A	38	ASN	3.5
1	A	285	ILE	3.4
1	A	76	GLU	3.4
1	A	165	ASP	3.4
1	A	253	ASN	3.4
1	A	222	GLN	3.4
1	A	151	ALA	3.4
1	A	196	ASN	3.4
1	A	209	GLU	3.4
1	A	135	GLU	3.3
1	A	174	ALA	3.3
1	A	18	ASP	3.3
1	A	207	LEU	3.3
1	A	103	SER	3.3
1	A	104	SER	3.3
1	A	186	GLY	3.3
1	A	290	GLU	3.2
1	A	70	THR	3.2
1	A	237	SER	3.2
1	A	121	GLY	3.2
1	A	189	GLY	3.2
1	A	123	LYS	3.2
1	A	54	SER	3.2
1	A	147	ALA	3.2
1	A	245	LEU	3.2
1	A	14	ARG	3.1
1	A	183	LYS	3.1
1	A	293	GLY	3.1
1	A	181	HIS	3.1
1	A	20	GLN	3.1
1	A	166	ARG	3.1
1	A	224	ASP	3.0
1	A	37	ASP	3.0
1	A	292	GLN	3.0
1	A	232	LEU	2.9
1	A	235	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLU	2.9
1	A	127	ARG	2.8
1	A	94	PRO	2.8
1	A	289	LEU	2.8
1	A	50	ALA	2.8
1	A	255	GLN	2.8
1	A	35	GLU	2.8
1	A	272	ASN	2.7
1	A	267	GLU	2.7
1	A	175	HIS	2.7
1	A	148	ASP	2.7
1	A	84	GLY	2.7
1	A	176	ALA	2.7
1	A	120	GLN	2.7
1	A	29	LYS	2.6
1	A	93	GLU	2.6
1	A	88	GLY	2.6
1	A	256	ASP	2.6
1	A	212	LYS	2.6
1	A	250	GLU	2.6
1	A	112	GLY	2.6
1	A	281	PRO	2.5
1	A	13	GLY	2.5
1	A	291	GLU	2.5
1	A	69	GLY	2.5
1	A	184	ASN	2.5
1	A	21	LYS	2.4
1	A	195	ASN	2.4
1	A	140	ASP	2.4
1	A	162	ASN	2.4
1	A	106	ASP	2.3
1	A	98	GLU	2.3
1	A	132	ASP	2.3
1	A	117	GLN	2.3
1	A	68	GLY	2.3
1	A	152	GLY	2.3
1	A	201	GLU	2.3
1	A	246	SER	2.2
1	A	90	LYS	2.2
1	A	287	LYS	2.2
1	A	137	THR	2.1
1	A	214	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	SER	2.0

## 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
2	HEM	A	1	43/43	0.36	-0.50	12,15,18,25	0

## 6.5 Other polymers

There are no such residues in this entry.