Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:45 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

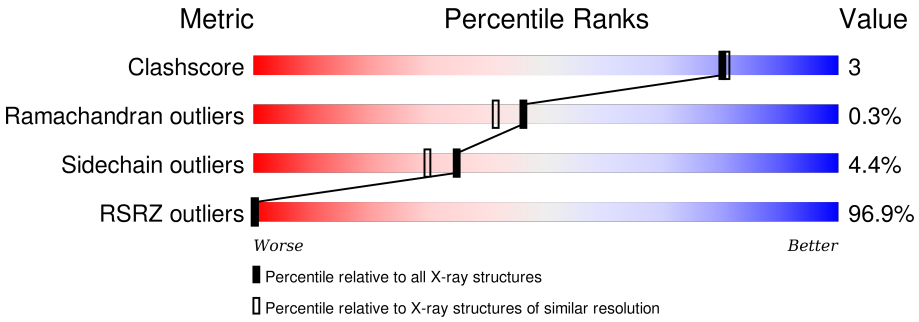
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	97%, 84%, 13%

2 Entry composition

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

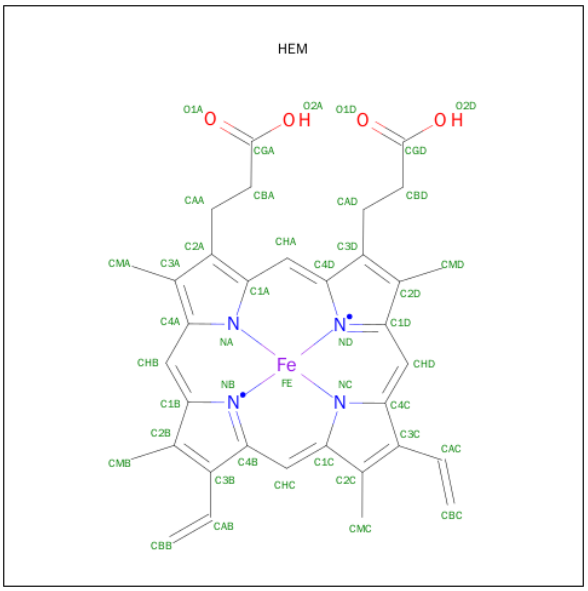
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

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

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

- Molecule 3 is water.

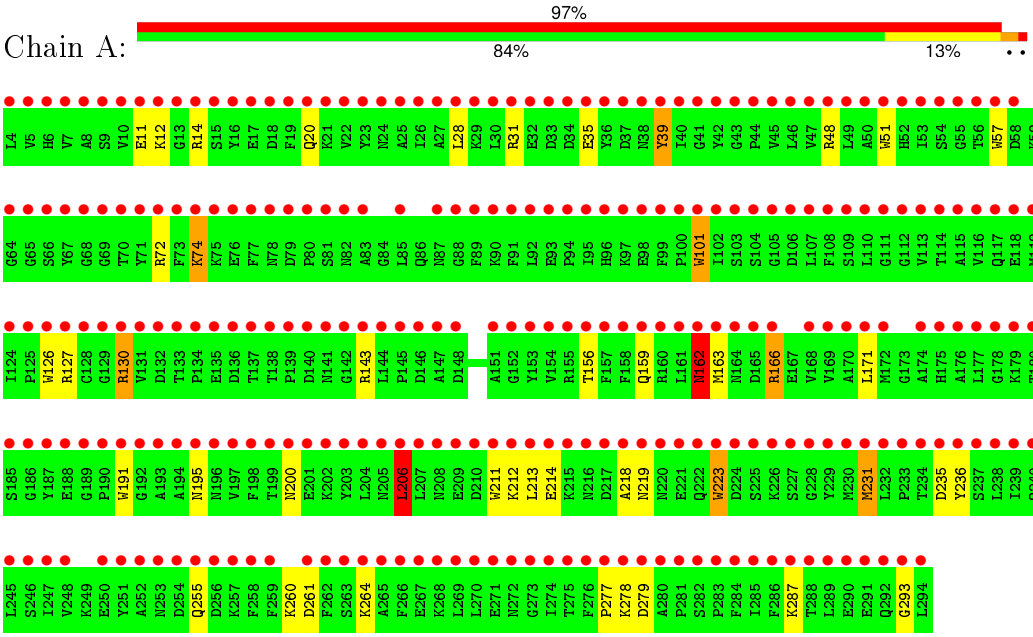
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0

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: CYTOCHROME C PEROXIDASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.01 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.79	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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	2348	515	2232	16	45
2	A	43	0	30	0	0
3	A	107	0	0	2	12
All	All	2498	515	2262	16	45

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 3.

All (16) 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:20:GLN:HE22	1:A:287:LYS:H	1.40	0.69
1:A:231:MET:HE1	1:A:236:TYR:HD1	1.67	0.59
1:A:74:LYS:H	1:A:74:LYS:HD2	1.67	0.58
1:A:200:ASN:H	1:A:255:GLN:HE21	1.51	0.56
1:A:20:GLN:HE22	1:A:287:LYS:N	2.04	0.54
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:20:GLN:NE2	1:A:287:LYS:H	2.10	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:231:MET:HG2	1:A:235:ASP:CB	2.50	0.41
1:A:74:LYS:H	1:A:74:LYS:CD	2.33	0.41
1:A:218:ALA:O	1:A:219:ASN:HB2	2.21	0.41

All (45) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:NH2	1:A:213:LEU:C[4_5610]	0.42	1.78
1:A:14:ARG:CZ	1:A:213:LEU:O[4_5610]	0.83	1.37
1:A:12:LYS:CA	1:A:214:GLU:OE2[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:264:LYS:HZ3	3:A:389:HOH:O[3_559]	0.73	0.87
1:A:12:LYS:C	1:A:214:GLU:OE2[4_5610]	1.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:14:ARG:HH22	1:A:213:LEU:CA[4_5610]	0.77	0.83
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
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:214:GLU:CG	3:A:373:HOH:O[4_4610]	1.53	0.67
1:A:212:LYS:CE	3:A:374: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:14:ARG:HH21	1:A:213:LEU:C[4_5610]	1.17	0.43
1:A:12:LYS:CB	1:A:214:GLU:OE2[4_5610]	1.80	0.40
1:A:11:GLU:CA	1:A:212:LYS:HZ1[4_5610]	1.22	0.38
1:A:101:TRP:CB	1:A:213:LEU:H[4_5610]	1.23	0.37
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:14:ARG:HE	1:A:213:LEU:O[4_5610]	1.26	0.34
1:A:212:LYS:HZ3	3:A:374:HOH:O[4_4610]	1.26	0.34
1:A:14:ARG:HH22	1:A:213:LEU:C[4_5610]	1.27	0.33
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:HH21	1:A:213:LEU:CA[4_5610]	1.47	0.13
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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	289/291 (99%)	279 (96%)	9 (3%)	1 (0%)	46 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	249/249 (100%)	238 (96%)	11 (4%)	35 30

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

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Mol	Chain	Res	Type
1	A	279	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	87	ASN
1	A	208	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 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

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	30,50,50	3.94	12 (40%)	24,82,82	2.42	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
2	HEM	A	1	1,3	-	0/10/54/54	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	C3B-C4B	-13.20	1.40	1.51
2	A	1	HEM	C3D-C4D	-9.60	1.39	1.51
2	A	1	HEM	C2C-C1C	-6.54	1.40	1.52
2	A	1	HEM	C3B-CAB	-5.60	1.40	1.51
2	A	1	HEM	C3C-CAC	-5.35	1.41	1.51
2	A	1	HEM	C2D-C3D	-5.24	1.38	1.54
2	A	1	HEM	C2D-C1D	-3.75	1.39	1.51
2	A	1	HEM	C2B-C1B	-3.39	1.40	1.51
2	A	1	HEM	FE-NB	2.09	2.08	1.97
2	A	1	HEM	FE-NC	2.58	2.06	1.95
2	A	1	HEM	CBB-CAB	2.62	1.44	1.29
2	A	1	HEM	CBC-CAC	2.80	1.45	1.29

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	HEM	C1D-CHD-C4C	2.14	129.39	125.82
2	A	1	HEM	C4B-CHC-C1C	2.20	129.51	125.82
2	A	1	HEM	CMD-C2D-C3D	2.64	126.01	114.35
2	A	1	HEM	C3C-CAC-CBC	2.65	128.53	124.46
2	A	1	HEM	C2D-C3D-C4D	2.86	106.34	101.50
2	A	1	HEM	CAD-C3D-C4D	4.33	127.74	112.47
2	A	1	HEM	CAD-C3D-C2D	4.41	125.91	113.22
2	A	1	HEM	CMC-C2C-C3C	5.08	129.20	116.53
2	A	1	HEM	CMB-C2B-C3B	5.58	130.45	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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^2)	Q<0.9
1	A	291/291 (100%)	5.00	282 (96%)	0 0	11, 21, 35, 47	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	TRP	13.3
1	A	4	LEU	13.1
1	A	36	TYR	12.5
1	A	83	ALA	12.0
1	A	10	VAL	11.7
1	A	191	TRP	10.3
1	A	231	MET	10.2
1	A	276	PHE	10.1
1	A	7	VAL	9.9
1	A	251	TYR	9.9
1	A	63	THR	9.6
1	A	286	PHE	9.3
1	A	27	ALA	9.2
1	A	279	ASP	9.2
1	A	131	VAL	9.1
1	A	206	LEU	9.1
1	A	22	VAL	9.0
1	A	80	PRO	9.0
1	A	57	TRP	8.9
1	A	23	TYR	8.9
1	A	277	PRO	8.9
1	A	85	LEU	8.9
1	A	213	LEU	8.9
1	A	278	LYS	8.8
1	A	107	LEU	8.8
1	A	161	LEU	8.7
1	A	40	ILE	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	53	ILE	8.4
1	A	282	SER	8.4
1	A	153	TYR	8.3
1	A	5	VAL	8.3
1	A	78	ASN	8.3
1	A	97	LYS	8.1
1	A	177	LEU	8.0
1	A	110	LEU	7.8
1	A	74	LYS	7.8
1	A	258	PHE	7.7
1	A	44	PRO	7.6
1	A	62	ASN	7.5
1	A	157	PHE	7.5
1	A	39	TYR	7.3
1	A	125	PRO	7.3
1	A	203	TYR	7.3
1	A	142	GLY	7.2
1	A	16	TYR	7.2
1	A	66	SER	7.2
1	A	254	ASP	7.1
1	A	259	PHE	7.1
1	A	77	PHE	7.0
1	A	229	TYR	7.0
1	A	128	CYS	7.0
1	A	45	VAL	7.0
1	A	171	LEU	6.9
1	A	126	TRP	6.9
1	A	75	LYS	6.9
1	A	19	PHE	6.9
1	A	109	SER	6.9
1	A	101	TRP	6.8
1	A	288	THR	6.6
1	A	42	TYR	6.6
1	A	168	VAL	6.6
1	A	15	SER	6.6
1	A	8	ALA	6.5
1	A	275	THR	6.5
1	A	26	ILE	6.4
1	A	51	TRP	6.4
1	A	95	ILE	6.4
1	A	236	TYR	6.4
1	A	73	PHE	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	248	VAL	6.4
1	A	211	TRP	6.3
1	A	266	PHE	6.3
1	A	198	PHE	6.3
1	A	187	TYR	6.2
1	A	89	PHE	6.2
1	A	270	LEU	6.1
1	A	241	ASP	6.1
1	A	294	LEU	6.0
1	A	158	PHE	6.0
1	A	156	THR	6.0
1	A	197	VAL	5.9
1	A	240	GLN	5.9
1	A	226	LYS	5.9
1	A	199	THR	5.8
1	A	116	VAL	5.8
1	A	242	PRO	5.8
1	A	178	GLY	5.8
1	A	30	LEU	5.8
1	A	225	SER	5.8
1	A	169	VAL	5.7
1	A	143	ARG	5.7
1	A	105	GLY	5.7
1	A	145	PRO	5.6
1	A	138	THR	5.6
1	A	25	ALA	5.6
1	A	61	ASP	5.6
1	A	216	ASN	5.6
1	A	219	ASN	5.6
1	A	154	VAL	5.6
1	A	155	ARG	5.6
1	A	33	ASP	5.6
1	A	67	TYR	5.6
1	A	49	LEU	5.6
1	A	230	MET	5.6
1	A	227	SER	5.5
1	A	71	TYR	5.5
1	A	108	PHE	5.5
1	A	34	ASP	5.5
1	A	274	ILE	5.5
1	A	32	GLU	5.5
1	A	87	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	136	ASP	5.4
1	A	239	ILE	5.4
1	A	124	ILE	5.3
1	A	28	LEU	5.3
1	A	79	ASP	5.2
1	A	46	LEU	5.2
1	A	237	SER	5.2
1	A	179	LYS	5.2
1	A	133	THR	5.2
1	A	11	GLU	5.1
1	A	283	PRO	5.1
1	A	115	ALA	5.0
1	A	194	ALA	5.0
1	A	220	ASN	4.9
1	A	100	PRO	4.9
1	A	265	ALA	4.8
1	A	208	ASN	4.8
1	A	262	PHE	4.8
1	A	159	GLN	4.8
1	A	91	PHE	4.8
1	A	6	HIS	4.8
1	A	9	SER	4.8
1	A	193	ALA	4.7
1	A	261	ASP	4.7
1	A	96	HIS	4.7
1	A	280	ALA	4.7
1	A	113	VAL	4.6
1	A	228	GLY	4.6
1	A	247	ILE	4.6
1	A	111	GLY	4.5
1	A	47	VAL	4.5
1	A	218	ALA	4.5
1	A	202	LYS	4.5
1	A	56	THR	4.5
1	A	182	LEU	4.5
1	A	129	GLY	4.4
1	A	253	ASN	4.4
1	A	146	ASP	4.4
1	A	52	HIS	4.4
1	A	99	PHE	4.3
1	A	12	LYS	4.3
1	A	114	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	4.3
1	A	284	PHE	4.3
1	A	170	ALA	4.3
1	A	192	GLY	4.2
1	A	60	HIS	4.2
1	A	207	LEU	4.2
1	A	221	GLU	4.2
1	A	141	ASN	4.2
1	A	264	LYS	4.2
1	A	269	LEU	4.2
1	A	244	TYR	4.2
1	A	64	GLY	4.2
1	A	210	ASP	4.2
1	A	190	PRO	4.2
1	A	31	ARG	4.1
1	A	163	MET	4.1
1	A	48	ARG	4.1
1	A	92	LEU	4.1
1	A	55	GLY	4.0
1	A	119	MET	4.0
1	A	121	GLY	4.0
1	A	174	ALA	4.0
1	A	82	ASN	4.0
1	A	102	ILE	4.0
1	A	54	SER	3.9
1	A	263	SER	3.9
1	A	38	ASN	3.9
1	A	139	PRO	3.9
1	A	41	GLY	3.9
1	A	243	LYS	3.9
1	A	70	THR	3.9
1	A	166	ARG	3.8
1	A	147	ALA	3.8
1	A	144	LEU	3.8
1	A	24	ASN	3.8
1	A	18	ASP	3.8
1	A	17	GLU	3.8
1	A	164	ASN	3.8
1	A	204	LEU	3.8
1	A	188	GLU	3.8
1	A	118	GLU	3.8
1	A	72	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	104	SER	3.7
1	A	233	PRO	3.7
1	A	65	GLY	3.7
1	A	122	PRO	3.7
1	A	212	LYS	3.6
1	A	245	LEU	3.6
1	A	160	ARG	3.5
1	A	180	THR	3.5
1	A	252	ALA	3.5
1	A	272	ASN	3.5
1	A	50	ALA	3.5
1	A	200	ASN	3.5
1	A	35	GLU	3.4
1	A	94	PRO	3.4
1	A	76	GLU	3.4
1	A	189	GLY	3.4
1	A	222	GLN	3.4
1	A	14	ARG	3.4
1	A	181	HIS	3.4
1	A	217	ASP	3.4
1	A	235	ASP	3.3
1	A	69	GLY	3.3
1	A	293	GLY	3.3
1	A	183	LYS	3.3
1	A	135	GLU	3.3
1	A	209	GLU	3.3
1	A	232	LEU	3.3
1	A	81	SER	3.3
1	A	257	LYS	3.2
1	A	20	GLN	3.2
1	A	103	SER	3.2
1	A	268	LYS	3.2
1	A	196	ASN	3.2
1	A	292	GLN	3.2
1	A	184	ASN	3.1
1	A	130	ARG	3.1
1	A	205	ASN	3.1
1	A	151	ALA	3.1
1	A	224	ASP	3.1
1	A	234	THR	3.1
1	A	37	ASP	3.1
1	A	120	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLU	3.0
1	A	290	GLU	3.0
1	A	112	GLY	3.0
1	A	195	ASN	3.0
1	A	127	ARG	3.0
1	A	175	HIS	3.0
1	A	172	MET	3.0
1	A	152	GLY	3.0
1	A	134	PRO	3.0
1	A	162	ASN	3.0
1	A	98	GLU	2.9
1	A	165	ASP	2.9
1	A	93	GLU	2.9
1	A	13	GLY	2.9
1	A	117	GLN	2.9
1	A	186	GLY	2.8
1	A	285	ILE	2.8
1	A	289	LEU	2.8
1	A	132	ASP	2.8
1	A	267	GLU	2.8
1	A	246	SER	2.8
1	A	273	GLY	2.8
1	A	281	PRO	2.7
1	A	123	LYS	2.7
1	A	214	GLU	2.7
1	A	58	ASP	2.6
1	A	148	ASP	2.6
1	A	185	SER	2.6
1	A	255	GLN	2.6
1	A	21	LYS	2.6
1	A	250	GLU	2.6
1	A	256	ASP	2.6
1	A	215	LYS	2.5
1	A	176	ALA	2.5
1	A	201	GLU	2.5
1	A	90	LYS	2.5
1	A	291	GLU	2.5
1	A	140	ASP	2.5
1	A	29	LYS	2.5
1	A	43	GLY	2.4
1	A	106	ASP	2.4
1	A	68	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	GLY	2.1
1	A	287	LYS	2.1
1	A	137	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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^{th} 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^2)	Q<0.9
2	HEM	A	1	43/43	0.75	0.33	-0.57	12,15,18,25	0

6.5 Other polymers (i)

There are no such residues in this entry.