W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:16 pm GMT

PDB ID	:	1CCK
Title	:	ALTERING SUBSTRATE SPECIFICITY OF CYTOCHROME C PEROX-IDASE TOWARDS A SMALL MOLECULAR SUBSTRATE PEROXIDASE BY SUBSTITUTING TYROSINE FOR PHE 202
Authors	:	Cao, Y.; Musah, R.A.; Wilcox, S.K.; Goodin, D.B.; Mcree, D.E.
Deposited on	:	1998-01-02
Resolution	:	2.10 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 ⓘ symbol.

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

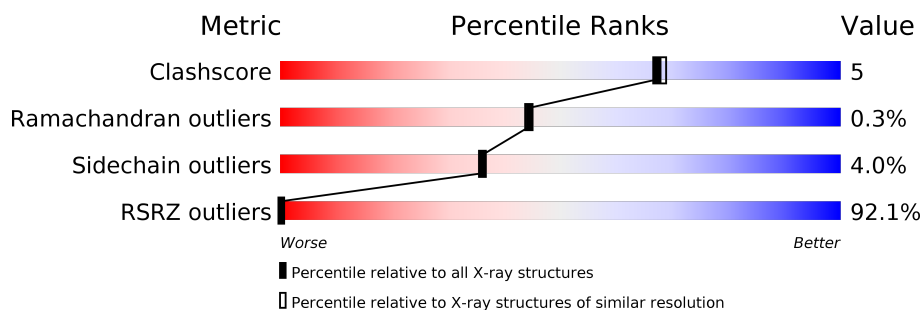|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.10 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		4.0%
RSRZ outliers		92.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	92% / 80% / 18% / •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3014 atoms, of which 513 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 2864	C 1501	H 513	N 392	O 452	S 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	TYR	PHE	SUBSTITUTION	UNP P00431

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
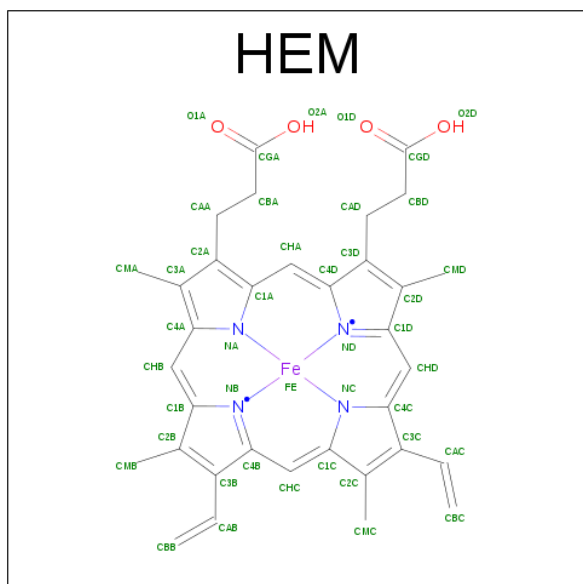
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

• 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 the various outlier classes 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
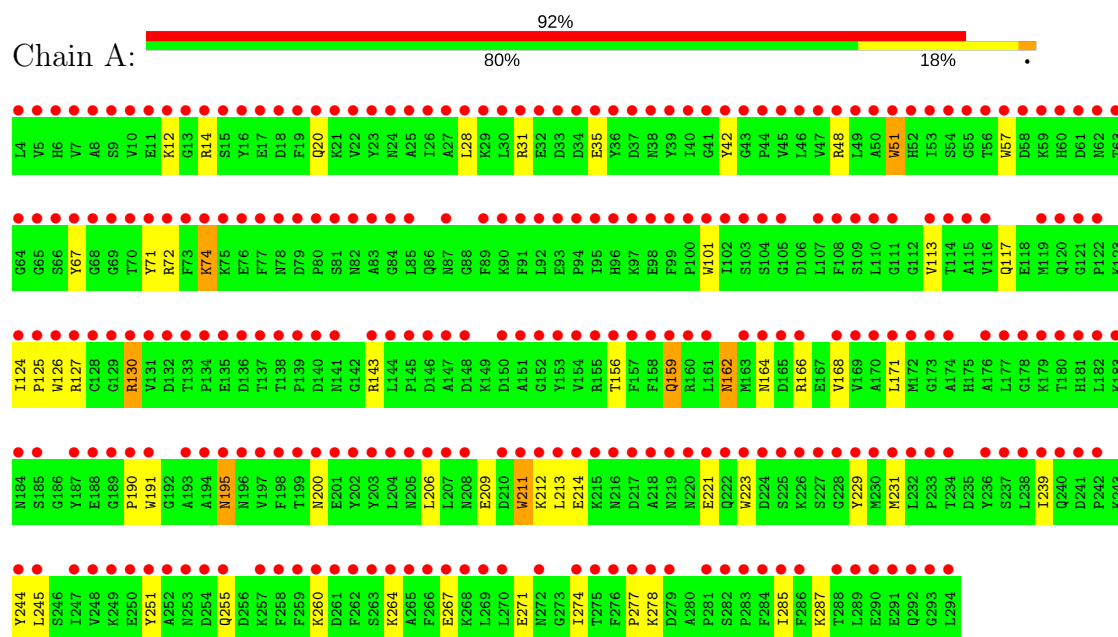
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.50Å 73.40Å 44.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.10 18.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.10) 75.5 (18.77-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 1.90Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , (Not available) 0.469 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.59	EDS
Total number of atoms	3014	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 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.84	0/2417	1.56	39/3272 (1.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	127	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	31	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	143	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	51	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	A	127	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	229	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	A	51	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	101	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	211	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	223	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	191	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	A	211	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	126	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	A	223	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	A	48	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	101	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	191	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	A	57	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	A	72	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	51	TRP	CB-CG-CD1	-6.39	118.70	127.00
1	A	251	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	A	57	TRP	CD1-CG-CD2	6.19	111.25	106.30
1	A	162	ASN	CA-C-N	-6.17	103.62	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	LYS	CA-CB-CG	-6.17	99.83	113.40
1	A	126	TRP	CE2-CD2-CG	-6.07	102.44	107.30
1	A	51	TRP	CG-CD1-NE1	-6.02	104.08	110.10
1	A	244	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	191	TRP	CG-CD2-CE3	5.85	139.16	133.90
1	A	72	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	101	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	42	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	31	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	191	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	A	277	PRO	CA-C-N	5.36	129.00	117.20
1	A	51	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	A	71	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	130	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	244	TYR	CB-CG-CD1	5.09	124.06	121.00

There are no chirality outliers.

There are no planarity outliers.

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	2351	513	2228	21	32
2	A	43	0	30	0	0
3	A	107	0	0	3	11
All	All	2501	513	2258	21	32

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 5.

All (21) 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:195:ASN:H	1:A:195:ASN:HD22	1.48	0.62
1:A:206:LEU:HD13	1:A:231:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:H	1:A:74:LYS:HD2	1.71	0.55
1:A:200:ASN:H	1:A:255:GLN:HE21	1.57	0.53
1:A:113:VAL:HG13	1:A:124:ILE:HB	1.90	0.52
1:A:130:ARG:NE	3:A:326:HOH:O	2.44	0.51
1:A:20:GLN:HE22	1:A:287:LYS:N	2.09	0.50
1:A:20:GLN:HE22	1:A:287:LYS:H	1.59	0.49
1:A:164:ASN:O	1:A:168:VAL:HG23	2.13	0.47
1:A:20:GLN:NE2	1:A:287:LYS:H	2.13	0.47
1:A:67:TYR:O	1:A:130:ARG:HB3	2.15	0.46
1:A:156:THR:O	1:A:159:GLN:HB3	2.16	0.46
1:A:209:GLU:HB2	1:A:211:TRP:CE2	2.51	0.46
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.98	0.45
1:A:113:VAL:O	1:A:117:GLN:HG3	2.18	0.43
1:A:130:ARG:CZ	3:A:326:HOH:O	2.67	0.42
1:A:271:GLU:HA	1:A:274:ILE:HD12	2.01	0.42
1:A:239:ILE:HG22	1:A:245:LEU:HD13	2.01	0.41
1:A:213:LEU:HD11	1:A:221:GLU:HB3	2.03	0.41
1:A:195:ASN:H	1:A:195:ASN:ND2	2.17	0.40
1:A:267:GLU:HG3	3:A:323:HOH:O	2.22	0.40

All (32) 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:HH21	1:A:213:LEU:C[4_5610]	0.13	1.47
1:A:14:ARG:NH2	1:A:213:LEU:C[4_5610]	0.92	1.28
1:A:212:LYS:CG	3:A:372:HOH:O[4_4610]	1.11	1.09
1:A:212:LYS:CE	3:A:374:HOH:O[4_4610]	1.34	0.86
1:A:212:LYS:CD	3:A:372:HOH:O[4_4610]	1.35	0.85
1:A:212:LYS:NZ	3:A:374:HOH:O[4_4610]	1.37	0.83
1:A:12:LYS:N	1:A:214:GLU:OE2[4_5610]	1.41	0.79
1:A:214:GLU:CG	3:A:373:HOH:O[4_4610]	1.48	0.72
1:A:12:LYS:O	1:A:214:GLU:CB[4_5610]	1.49	0.71
1:A:12:LYS:CB	1:A:214:GLU:OE2[4_5610]	1.50	0.70
1:A:14:ARG:NH2	1:A:214:GLU:N[4_5610]	1.52	0.68
1:A:14:ARG:NH2	1:A:213:LEU:O[4_5610]	1.53	0.67
1:A:264:LYS:NZ	3:A:389:HOH:O[3_559]	1.54	0.66
1:A:12:LYS:CA	1:A:214:GLU:OE2[4_5610]	1.55	0.65
1:A:212:LYS:CE	3:A:372:HOH:O[4_4610]	1.62	0.58
1:A:14:ARG:NE	1:A:213:LEU:O[4_5610]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HH21	1:A:213:LEU:O[4_5610]	1.13	0.47
1:A:212:LYS:HZ3	3:A:374:HOH:O[4_4610]	1.13	0.47
1:A:12:LYS:CB	1:A:214:GLU:CD[4_5610]	1.77	0.43
1:A:14:ARG:CZ	1:A:213:LEU:O[4_5610]	1.78	0.42
1:A:12:LYS:CB	1:A:214:GLU:OE1[4_5610]	1.86	0.34
1:A:14:ARG:NH2	1:A:213:LEU:CA[4_5610]	1.87	0.33
1:A:264:LYS:HZ1	3:A:389:HOH:O[3_559]	1.30	0.30
1:A:14:ARG:HE	1:A:213:LEU:O[4_5610]	1.30	0.30
1:A:12:LYS:H	1:A:214:GLU:OE2[4_5610]	1.33	0.27
1:A:14:ARG:CZ	1:A:213:LEU:C[4_5610]	2.01	0.19
1:A:14:ARG:HH21	1:A:214:GLU:N[4_5610]	1.43	0.17
1:A:14:ARG:HH21	1:A:213:LEU:CA[4_5610]	1.52	0.08
1:A:212:LYS:CB	3:A:372:HOH:O[4_4610]	2.12	0.08
1:A:264:LYS:HZ3	3:A:389:HOH:O[3_559]	1.56	0.04
1:A:14:ARG:HH22	1:A:213:LEU:CG[4_5610]	1.58	0.02
1:A:12:LYS:O	1:A:214:GLU:CG[4_5610]	2.19	0.01

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%)	44	44

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%)	239 (96%)	10 (4%)	36	36

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	GLU
1	A	51	TRP
1	A	74	LYS
1	A	159	GLN
1	A	166	ARG
1	A	171	LEU
1	A	190	PRO
1	A	195	ASN
1	A	260	LYS

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	195	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	28,50,50	1.67	7 (25%)	17,82,82	1.74	4 (23%)

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	-	0/6/54/54	0/0/8/8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	C3B-CAB	-3.84	1.40	1.47
2	A	1	HEM	C3C-CAC	-3.34	1.41	1.47
2	A	1	HEM	C4C-NC	-3.33	1.32	1.36
2	A	1	HEM	C4D-ND	-3.06	1.33	1.36
2	A	1	HEM	C1B-NB	-2.97	1.33	1.36
2	A	1	HEM	CBC-CAC	2.05	1.43	1.28
2	A	1	HEM	CBB-CAB	2.29	1.45	1.28

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	HEM	C1D-C2D-C3D	-3.12	104.83	107.00
2	A	1	HEM	C4A-C3A-C2A	-2.19	105.47	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	HEM	CMC-C2C-C3C	2.43	129.39	124.89
2	A	1	HEM	CMB-C2B-C3B	4.02	132.36	124.89

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95th 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(Å²)	Q<0.9
1	A	291/291 (100%)	4.45	268 (92%)	0	0	10, 21, 36, 46	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	TRP	13.4
1	A	218	ALA	12.6
1	A	4	LEU	11.8
1	A	171	LEU	11.6
1	A	10	VAL	11.2
1	A	16	TYR	10.5
1	A	294	LEU	10.0
1	A	53	ILE	9.0
1	A	211	TRP	8.8
1	A	206	LEU	8.5
1	A	145	PRO	8.3
1	A	36	TYR	8.3
1	A	286	PHE	8.1
1	A	71	TYR	8.1
1	A	169	VAL	8.1
1	A	277	PRO	7.9
1	A	156	THR	7.9
1	A	187	TYR	7.8
1	A	203	TYR	7.7
1	A	22	VAL	7.6
1	A	251	TYR	7.5
1	A	85	LEU	7.4
1	A	89	PHE	7.3
1	A	5	VAL	7.3
1	A	276	PHE	7.2
1	A	124	ILE	7.1
1	A	46	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	231	MET	7.1
1	A	270	LEU	6.8
1	A	38	ASN	6.8
1	A	213	LEU	6.8
1	A	138	THR	6.7
1	A	230	MET	6.7
1	A	282	SER	6.6
1	A	265	ALA	6.6
1	A	275	THR	6.6
1	A	33	ASP	6.5
1	A	247	ILE	6.5
1	A	67	TYR	6.5
1	A	259	PHE	6.4
1	A	128	CYS	6.4
1	A	153	TYR	6.4
1	A	202	TYR	6.3
1	A	30	LEU	6.2
1	A	12	LYS	6.2
1	A	28	LEU	6.2
1	A	61	ASP	6.2
1	A	240	GLN	6.2
1	A	109	SER	6.2
1	A	168	VAL	6.2
1	A	23	TYR	6.1
1	A	49	LEU	6.1
1	A	65	GLY	6.0
1	A	288	THR	6.0
1	A	108	PHE	6.0
1	A	236	TYR	6.0
1	A	177	LEU	6.0
1	A	269	LEU	5.9
1	A	79	ASP	5.9
1	A	83	ALA	5.9
1	A	219	ASN	5.8
1	A	77	PHE	5.8
1	A	25	ALA	5.8
1	A	64	GLY	5.8
1	A	229	TYR	5.8
1	A	41	GLY	5.8
1	A	39	TYR	5.7
1	A	252	ALA	5.7
1	A	34	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	105	GLY	5.6
1	A	245	LEU	5.6
1	A	40	ILE	5.6
1	A	144	LEU	5.5
1	A	262	PHE	5.4
1	A	42	TYR	5.4
1	A	159	GLN	5.4
1	A	126	TRP	5.3
1	A	57	TRP	5.3
1	A	6	HIS	5.3
1	A	193	ALA	5.3
1	A	97	LYS	5.3
1	A	37	ASP	5.3
1	A	131	VAL	5.2
1	A	9	SER	5.2
1	A	45	VAL	5.2
1	A	62	ASN	5.2
1	A	228	GLY	5.2
1	A	35	GLU	5.2
1	A	191	TRP	5.2
1	A	161	LEU	5.2
1	A	52	HIS	5.2
1	A	255	GLN	5.1
1	A	266	PHE	5.1
1	A	75	LYS	5.1
1	A	73	PHE	5.1
1	A	207	LEU	5.1
1	A	283	PRO	5.0
1	A	248	VAL	5.0
1	A	19	PHE	5.0
1	A	291	GLU	5.0
1	A	254	ASP	5.0
1	A	141	ASN	5.0
1	A	198	PHE	5.0
1	A	63	THR	4.9
1	A	279	ASP	4.9
1	A	101	TRP	4.9
1	A	244	TYR	4.9
1	A	107	LEU	4.8
1	A	44	PRO	4.8
1	A	278	LYS	4.8
1	A	284	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	237	SER	4.7
1	A	7	VAL	4.7
1	A	292	GLN	4.7
1	A	14	ARG	4.7
1	A	158	PHE	4.7
1	A	70	THR	4.6
1	A	8	ALA	4.6
1	A	214	GLU	4.6
1	A	127	ARG	4.6
1	A	217	ASP	4.6
1	A	13	GLY	4.6
1	A	233	PRO	4.6
1	A	60	HIS	4.6
1	A	104	SER	4.5
1	A	15	SER	4.5
1	A	234	THR	4.5
1	A	154	VAL	4.4
1	A	258	PHE	4.4
1	A	55	GLY	4.4
1	A	157	PHE	4.4
1	A	51	TRP	4.4
1	A	147	ALA	4.4
1	A	196	ASN	4.4
1	A	293	GLY	4.4
1	A	133	THR	4.4
1	A	11	GLU	4.3
1	A	115	ALA	4.3
1	A	274	ILE	4.2
1	A	190	PRO	4.2
1	A	72	ARG	4.2
1	A	74	LYS	4.2
1	A	263	SER	4.2
1	A	102	ILE	4.2
1	A	205	ASN	4.1
1	A	225	SER	4.1
1	A	78	ASN	4.1
1	A	215	LYS	4.1
1	A	170	ALA	4.0
1	A	253	ASN	4.0
1	A	87	ASN	4.0
1	A	137	THR	4.0
1	A	197	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	26	ILE	4.0
1	A	80	PRO	4.0
1	A	136	ASP	4.0
1	A	140	ASP	4.0
1	A	216	ASN	4.0
1	A	182	LEU	3.9
1	A	125	PRO	3.9
1	A	114	THR	3.9
1	A	241	ASP	3.9
1	A	268	LYS	3.9
1	A	249	LYS	3.9
1	A	81	SER	3.9
1	A	93	GLU	3.8
1	A	116	VAL	3.8
1	A	242	PRO	3.8
1	A	110	LEU	3.8
1	A	264	LYS	3.8
1	A	121	GLY	3.8
1	A	155	ARG	3.8
1	A	27	ALA	3.8
1	A	166	ARG	3.7
1	A	92	LEU	3.7
1	A	139	PRO	3.7
1	A	95	ILE	3.7
1	A	238	LEU	3.7
1	A	250	GLU	3.7
1	A	289	LEU	3.6
1	A	189	GLY	3.6
1	A	48	ARG	3.6
1	A	21	LYS	3.6
1	A	32	GLU	3.6
1	A	76	GLU	3.6
1	A	201	GLU	3.6
1	A	54	SER	3.6
1	A	91	PHE	3.5
1	A	132	ASP	3.5
1	A	66	SER	3.5
1	A	290	GLU	3.4
1	A	165	ASP	3.4
1	A	220	ASN	3.4
1	A	143	ARG	3.4
1	A	47	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	68	GLY	3.4
1	A	20	GLN	3.4
1	A	152	GLY	3.3
1	A	119	MET	3.3
1	A	163	MET	3.3
1	A	31	ARG	3.3
1	A	113	VAL	3.3
1	A	56	THR	3.3
1	A	99	PHE	3.3
1	A	285	ILE	3.3
1	A	226	LYS	3.3
1	A	239	ILE	3.3
1	A	50	ALA	3.3
1	A	212	LYS	3.3
1	A	222	GLN	3.3
1	A	17	GLU	3.2
1	A	122	PRO	3.2
1	A	281	PRO	3.2
1	A	188	GLU	3.2
1	A	183	LYS	3.1
1	A	199	THR	3.1
1	A	204	LEU	3.1
1	A	59	LYS	3.0
1	A	180	THR	3.0
1	A	69	GLY	3.0
1	A	164	ASN	3.0
1	A	221	GLU	3.0
1	A	129	GLY	3.0
1	A	90	LYS	3.0
1	A	103	SER	2.9
1	A	43	GLY	2.8
1	A	184	ASN	2.8
1	A	100	PRO	2.8
1	A	135	GLU	2.8
1	A	179	LYS	2.8
1	A	160	ARG	2.8
1	A	146	ASP	2.8
1	A	181	HIS	2.7
1	A	130	ARG	2.7
1	A	195	ASN	2.7
1	A	261	ASP	2.7
1	A	174	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	94	PRO	2.7
1	A	58	ASP	2.7
1	A	257	LYS	2.6
1	A	172	MET	2.6
1	A	267	GLU	2.6
1	A	24	ASN	2.6
1	A	194	ALA	2.5
1	A	232	LEU	2.5
1	A	120	GLN	2.5
1	A	84	GLY	2.5
1	A	260	LYS	2.5
1	A	18	ASP	2.4
1	A	227	SER	2.4
1	A	272	ASN	2.4
1	A	134	PRO	2.4
1	A	210	ASP	2.4
1	A	82	ASN	2.3
1	A	208	ASN	2.3
1	A	98	GLU	2.3
1	A	178	GLY	2.3
1	A	200	ASN	2.2
1	A	96	HIS	2.2
1	A	173	GLY	2.2
1	A	185	SER	2.2
1	A	224	ASP	2.1
1	A	29	LYS	2.1
1	A	151	ALA	2.1
1	A	148	ASP	2.1
1	A	176	ALA	2.1
1	A	111	GLY	2.0
1	A	150	ASP	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, 95th 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	0.76	0.33	-0.41	9,14,18,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.