



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:16 pm GMT

PDB ID : 1A2F  
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 : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (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

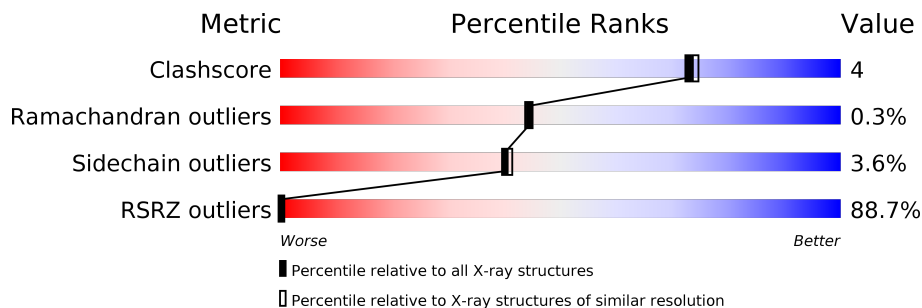
# 1 Overall quality at a glance

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	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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	<div> <div>89%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3016 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.

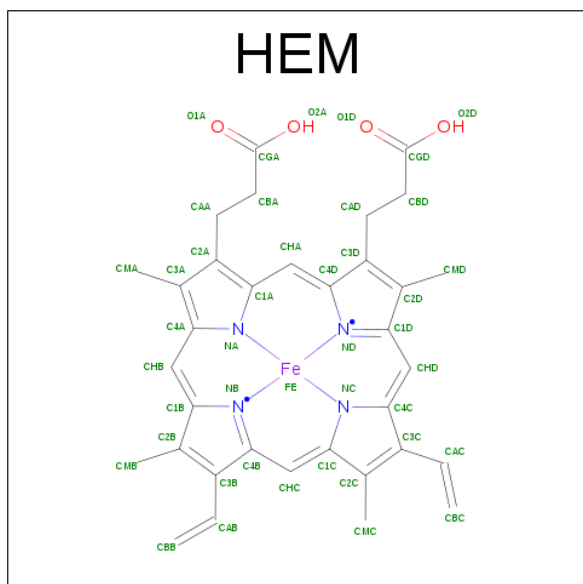
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	291	Total	C	H	N	O	S	0	0	0
			2866	1502	515	393	451	5			

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	172	LYS	MET	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		

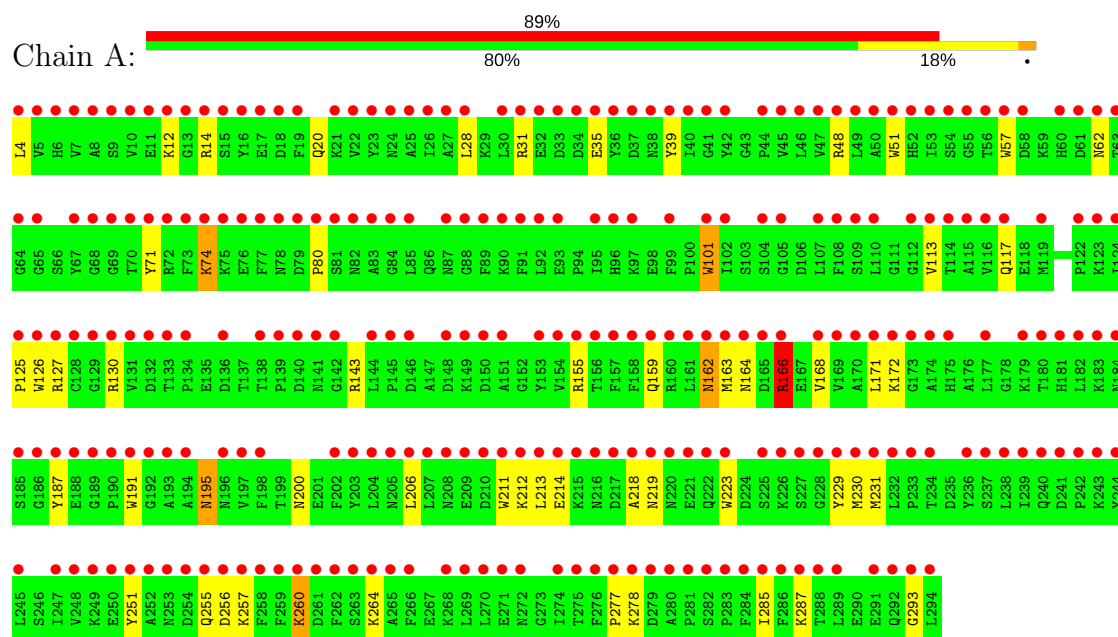
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	103.80Å 73.50Å 44.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.10 14.92 – 1.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.10) 78.9 (14.92-1.91)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.91Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.184 , (Not available) 0.473 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.62	EDS
Total number of atoms	3016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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	0.86	0/2417	1.58	40/3271 (1.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	A	51	TRP	CD1-CG-CD2	9.44	113.85	106.30
1	A	31	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	51	TRP	CE2-CD2-CG	-8.24	100.71	107.30
1	A	191	TRP	CE2-CD2-CG	-8.17	100.77	107.30
1	A	101	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	143	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	191	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	211	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	223	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	126	TRP	CD1-CG-CD2	7.27	112.11	106.30
1	A	51	TRP	CB-CG-CD1	-7.24	117.59	127.00
1	A	101	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	A	127	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	57	TRP	CD1-CG-CD2	6.83	111.76	106.30
1	A	223	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	48	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	51	TRP	CG-CD2-CE3	6.62	139.86	133.90
1	A	211	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	51	TRP	CG-CD1-NE1	-6.52	103.58	110.10
1	A	229	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	A	57	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	A	127	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	126	TRP	CE2-CD2-CG	-6.24	102.31	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	LYS	CA-CB-CG	-6.16	99.84	113.40
1	A	162	ASN	CA-C-N	-5.99	104.03	117.20
1	A	251	TYR	CB-CG-CD2	-5.84	117.49	121.00
1	A	101	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	A	187	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	A	155	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	230	MET	CA-CB-CG	5.70	122.99	113.30
1	A	163	MET	CG-SD-CE	-5.55	91.31	100.20
1	A	71	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	A	277	PRO	CA-C-N	5.42	129.12	117.20
1	A	166	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	191	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	A	39	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	101	TRP	CG-CD2-CE3	5.16	138.55	133.90
1	A	230	MET	CG-SD-CE	-5.09	92.06	100.20
1	A	101	TRP	CB-CG-CD1	-5.08	120.39	127.00

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	515	2232	18	23
2	A	43	0	30	0	0
3	A	107	0	0	2	13
All	All	2501	515	2262	18	23

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 4.

All (18) 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:168:VAL:O	1:A:172:LYS:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:HD22	1:A:195:ASN:H	1.47	0.63
1:A:206:LEU:HD13	1:A:231:MET:SD	2.38	0.62
1:A:20:GLN:HE22	1:A:287:LYS:H	1.51	0.58
1:A:74:LYS:H	1:A:74:LYS:HD2	1.70	0.57
1:A:200:ASN:H	1:A:255:GLN:HE21	1.56	0.53
1:A:130:ARG:NE	3:A:326:HOH:O	2.43	0.51
1:A:256:ASP:O	1:A:260:LYS:HD2	2.17	0.44
1:A:164:ASN:O	1:A:168:VAL:HG23	2.17	0.44
1:A:20:GLN:HE22	1:A:287:LYS:N	2.13	0.44
1:A:218:ALA:O	1:A:219:ASN:HB2	2.18	0.44
1:A:195:ASN:ND2	1:A:195:ASN:H	2.14	0.43
1:A:125:PRO:HG3	1:A:285:ILE:HD11	2.01	0.42
1:A:113:VAL:O	1:A:117:GLN:HG3	2.20	0.41
1:A:195:ASN:HD22	1:A:195:ASN:N	2.18	0.41
1:A:4:LEU:HB2	1:A:62:ASN:HB3	2.02	0.41
1:A:130:ARG:CZ	3:A:326:HOH:O	2.69	0.40
1:A:166:ARG:HH21	1:A:257:LYS:HZ2	1.68	0.40

All (23) 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:O[4_5610]	1.01	0.59
1:A:14:ARG:HH21	1:A:213:LEU:C[4_5610]	1.01	0.59
1:A:212:LYS:NZ	3:A:374:HOH:O[4_4610]	1.70	0.50
1:A:212:LYS:CG	3:A:372:HOH:O[4_4610]	1.70	0.50
1:A:212:LYS:CD	3:A:372:HOH:O[4_4610]	1.74	0.46
1:A:14:ARG:NH2	1:A:213:LEU:C[4_5610]	1.81	0.39
1:A:264:LYS:HZ1	3:A:389:HOH:O[3_559]	1.22	0.38
1:A:264:LYS:NZ	3:A:389:HOH:O[3_559]	1.83	0.37
1:A:212:LYS:CE	3:A:374:HOH:O[4_4610]	1.86	0.34
1:A:14:ARG:NH2	1:A:213:LEU:O[4_5610]	1.86	0.34
1:A:12:LYS:CB	1:A:214:GLU:OE2[4_5610]	1.87	0.33
1:A:214:GLU:OE2	3:A:374:HOH:O[4_4610]	1.89	0.31
1:A:212:LYS:HZ3	3:A:374:HOH:O[4_4610]	1.35	0.25
1:A:212:LYS:CE	3:A:372:HOH:O[4_4610]	1.97	0.23
1:A:14:ARG:NH2	1:A:214:GLU:N[4_5610]	2.02	0.18
1:A:214:GLU:CG	3:A:373:HOH:O[4_4610]	2.05	0.15
1:A:101:TRP:CB	1:A:213:LEU:O[4_5610]	2.07	0.13
1:A:14:ARG:HH21	1:A:214:GLU:N[4_5610]	1.54	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:N	1:A:214:GLU:OE2[4_5610]	2.15	0.05
1:A:12:LYS:H	1:A:214:GLU:OE2[4_5610]	1.56	0.04
1:A:214:GLU:CB	3:A:373:HOH:O[4_4610]	2.17	0.03
1:A:213:LEU:O	3:A:373:HOH:O[4_4610]	2.18	0.02
1:A:293:GLY:O	3:A:330:HOH:O[3_549]	2.18	0.02

## 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%)	282 (98%)	6 (2%)	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%)	240 (96%)	9 (4%)	40 41

All (9) 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	80	PRO
1	A	159	GLN
1	A	166	ARG
1	A	171	LEU
1	A	195	ASN
1	A	260	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	208	ASN
1	A	220	ASN
1	A	240	GLN
1	A	255	GLN
1	A	292	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	1.64	6 (21%)	17,82,82	1.70	3 (17%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	C3B-CAB	-4.33	1.39	1.47
2	A	1	HEM	C3C-CAC	-3.23	1.41	1.47
2	A	1	HEM	C4D-ND	-3.08	1.33	1.36
2	A	1	HEM	C4C-NC	-2.98	1.33	1.36
2	A	1	HEM	CBB-CAB	2.03	1.43	1.28
2	A	1	HEM	CBC-CAC	2.52	1.46	1.28

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HEM	C1D-C2D-C3D	-2.98	104.92	107.00
2	A	1	HEM	CMC-C2C-C3C	2.82	130.12	124.89
2	A	1	HEM	CMB-C2B-C3B	3.49	131.37	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, 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%)	3.85	258 (88%) <b>0</b> <b>0</b>	10, 20, 35, 45	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	THR	12.3
1	A	171	LEU	11.3
1	A	73	PHE	8.5
1	A	79	ASP	8.4
1	A	4	LEU	8.0
1	A	211	TRP	7.9
1	A	38	ASN	7.9
1	A	53	ILE	7.8
1	A	251	TYR	7.5
1	A	57	TRP	7.3
1	A	25	ALA	7.2
1	A	276	PHE	6.9
1	A	223	TRP	6.9
1	A	206	LEU	6.9
1	A	22	VAL	6.9
1	A	64	GLY	6.7
1	A	77	PHE	6.7
1	A	5	VAL	6.7
1	A	187	TYR	6.6
1	A	10	VAL	6.6
1	A	294	LEU	6.4
1	A	277	PRO	6.4
1	A	213	LEU	6.4
1	A	71	TYR	6.4
1	A	124	ILE	6.3
1	A	89	PHE	6.3
1	A	16	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	36	TYR	6.2
1	A	255	GLN	6.1
1	A	30	LEU	6.1
1	A	131	VAL	6.0
1	A	39	TYR	6.0
1	A	90	LYS	6.0
1	A	169	VAL	6.0
1	A	67	TYR	6.0
1	A	46	LEU	5.8
1	A	254	ASP	5.8
1	A	230	MET	5.6
1	A	231	MET	5.6
1	A	203	TYR	5.6
1	A	286	PHE	5.6
1	A	8	ALA	5.6
1	A	266	PHE	5.6
1	A	85	LEU	5.5
1	A	92	LEU	5.5
1	A	202	PHE	5.5
1	A	282	SER	5.4
1	A	49	LEU	5.4
1	A	134	PRO	5.4
1	A	245	LEU	5.4
1	A	218	ALA	5.4
1	A	233	PRO	5.3
1	A	272	ASN	5.3
1	A	229	TYR	5.3
1	A	156	THR	5.3
1	A	269	LEU	5.3
1	A	75	LYS	5.2
1	A	174	ALA	5.2
1	A	262	PHE	5.2
1	A	275	THR	5.2
1	A	244	TYR	5.2
1	A	160	ARG	5.2
1	A	60	HIS	5.2
1	A	42	TYR	5.1
1	A	63	THR	5.1
1	A	78	ASN	5.0
1	A	52	HIS	5.0
1	A	68	GLY	5.0
1	A	207	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	153	TYR	4.9
1	A	182	LEU	4.9
1	A	109	SER	4.9
1	A	127	ARG	4.9
1	A	12	LYS	4.9
1	A	128	CYS	4.8
1	A	219	ASN	4.8
1	A	9	SER	4.7
1	A	145	PRO	4.7
1	A	228	GLY	4.7
1	A	283	PRO	4.7
1	A	144	LEU	4.6
1	A	258	PHE	4.6
1	A	191	TRP	4.6
1	A	26	ILE	4.6
1	A	65	GLY	4.6
1	A	93	GLU	4.6
1	A	80	PRO	4.5
1	A	104	SER	4.5
1	A	125	PRO	4.5
1	A	265	ALA	4.5
1	A	270	LEU	4.5
1	A	154	VAL	4.5
1	A	81	SER	4.4
1	A	236	TYR	4.4
1	A	239	ILE	4.4
1	A	241	ASP	4.4
1	A	97	LYS	4.4
1	A	72	ARG	4.4
1	A	238	LEU	4.4
1	A	14	ARG	4.3
1	A	161	LEU	4.3
1	A	163	MET	4.3
1	A	74	LYS	4.3
1	A	51	TRP	4.3
1	A	288	THR	4.3
1	A	45	VAL	4.3
1	A	139	PRO	4.2
1	A	136	ASP	4.2
1	A	7	VAL	4.2
1	A	102	ILE	4.2
1	A	198	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	204	LEU	4.2
1	A	44	PRO	4.1
1	A	101	TRP	4.1
1	A	242	PRO	4.1
1	A	105	GLY	4.1
1	A	116	VAL	4.1
1	A	48	ARG	4.0
1	A	226	LYS	4.0
1	A	133	THR	4.0
1	A	248	VAL	4.0
1	A	28	LEU	3.9
1	A	168	VAL	3.9
1	A	96	HIS	3.9
1	A	279	ASP	3.9
1	A	34	ASP	3.9
1	A	35	GLU	3.9
1	A	62	ASN	3.9
1	A	99	PHE	3.9
1	A	249	LYS	3.9
1	A	205	ASN	3.9
1	A	225	SER	3.8
1	A	240	GLN	3.8
1	A	155	ARG	3.7
1	A	61	ASP	3.7
1	A	33	ASP	3.7
1	A	54	SER	3.7
1	A	189	GLY	3.7
1	A	119	MET	3.7
1	A	23	TYR	3.6
1	A	108	PHE	3.6
1	A	150	ASP	3.6
1	A	289	LEU	3.6
1	A	41	GLY	3.6
1	A	141	ASN	3.6
1	A	165	ASP	3.6
1	A	126	TRP	3.5
1	A	196	ASN	3.5
1	A	149	LYS	3.5
1	A	278	LYS	3.5
1	A	193	ALA	3.5
1	A	183	LYS	3.5
1	A	234	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	173	GLY	3.5
1	A	95	ILE	3.5
1	A	6	HIS	3.4
1	A	13	GLY	3.4
1	A	214	GLU	3.4
1	A	56	THR	3.4
1	A	55	GLY	3.4
1	A	21	LYS	3.3
1	A	257	LYS	3.3
1	A	292	GLN	3.3
1	A	113	VAL	3.3
1	A	19	PHE	3.3
1	A	180	THR	3.3
1	A	212	LYS	3.3
1	A	31	ARG	3.3
1	A	252	ALA	3.2
1	A	58	ASP	3.2
1	A	210	ASP	3.2
1	A	263	SER	3.2
1	A	11	GLU	3.1
1	A	157	PHE	3.1
1	A	87	ASN	3.1
1	A	264	LYS	3.1
1	A	37	ASP	3.1
1	A	259	PHE	3.0
1	A	190	PRO	3.0
1	A	132	ASP	3.0
1	A	220	ASN	3.0
1	A	32	GLU	3.0
1	A	274	ILE	2.9
1	A	285	ILE	2.9
1	A	175	HIS	2.9
1	A	221	GLU	2.9
1	A	215	LYS	2.9
1	A	237	SER	2.9
1	A	130	ARG	2.9
1	A	188	GLU	2.9
1	A	17	GLU	2.9
1	A	217	ASP	2.9
1	A	159	GLN	2.9
1	A	146	ASP	2.9
1	A	186	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	2.9
1	A	177	LEU	2.9
1	A	115	ALA	2.8
1	A	140	ASP	2.8
1	A	76	GLU	2.8
1	A	222	GLN	2.8
1	A	69	GLY	2.8
1	A	117	GLN	2.8
1	A	166	ARG	2.8
1	A	123	LYS	2.8
1	A	243	LYS	2.8
1	A	197	VAL	2.7
1	A	216	ASN	2.7
1	A	27	ALA	2.7
1	A	91	PHE	2.7
1	A	253	ASN	2.7
1	A	122	PRO	2.7
1	A	110	LEU	2.7
1	A	268	LYS	2.7
1	A	162	ASN	2.7
1	A	184	ASN	2.7
1	A	291	GLU	2.7
1	A	151	ALA	2.7
1	A	181	HIS	2.6
1	A	84	GLY	2.6
1	A	129	GLY	2.6
1	A	158	PHE	2.6
1	A	170	ALA	2.6
1	A	247	ILE	2.6
1	A	142	GLY	2.6
1	A	24	ASN	2.6
1	A	179	LYS	2.6
1	A	284	PHE	2.5
1	A	232	LEU	2.5
1	A	83	ALA	2.5
1	A	250	GLU	2.5
1	A	70	THR	2.5
1	A	281	PRO	2.4
1	A	208	ASN	2.4
1	A	293	GLY	2.4
1	A	280	ALA	2.4
1	A	18	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	15	SER	2.3
1	A	50	ALA	2.3
1	A	185	SER	2.3
1	A	88	GLY	2.3
1	A	172	LYS	2.3
1	A	82	ASN	2.3
1	A	227	SER	2.3
1	A	287	LYS	2.2
1	A	261	ASP	2.2
1	A	209	GLU	2.2
1	A	256	ASP	2.2
1	A	271	GLU	2.2
1	A	148	ASP	2.1
1	A	260	LYS	2.1
1	A	192	GLY	2.1
1	A	47	VAL	2.1
1	A	114	THR	2.1
1	A	112	GLY	2.1
1	A	164	ASN	2.0
1	A	40	ILE	2.0
1	A	194	ALA	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	A	1	43/43	0.78	0.31	-0.23	10,14,18,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.