



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:25 pm GMT

PDB ID : 1CCI  
Title : HOW FLEXIBLE ARE PROTEINS? TRAPPING OF A FLEXIBLE LOOP  
Authors : Cao, Y.; Musah, R.A.; Wilcox, S.K.; Goodin, D.B.; Mcree, D.E.  
Deposited on : 1996-12-18  
Resolution : 2.40 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.

---

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

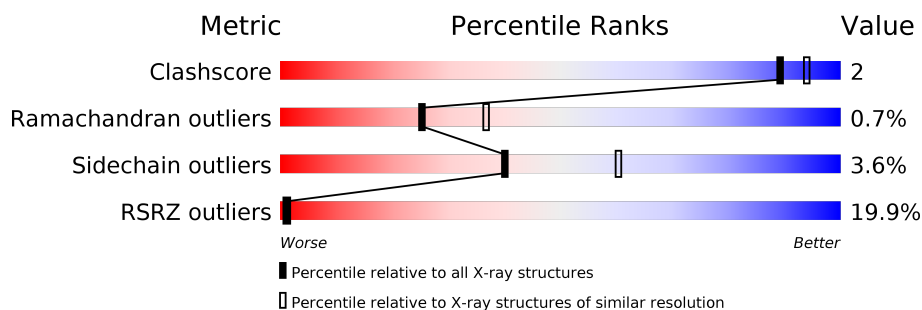
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	294	<div> <div>20%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3003 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.

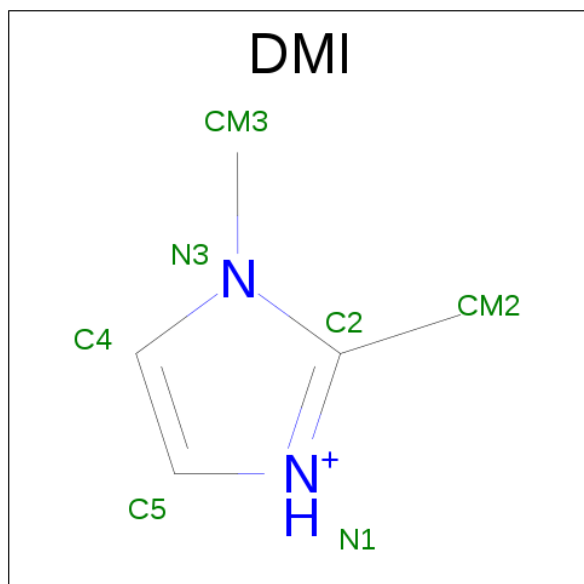
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	0	0
			2855	1494	512	392	451	6			

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 2,3-DIMETHYLIMIDAZOLIUM ION (three-letter code: DMI) (formula: C<sub>5</sub>H<sub>9</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	N	0	0
			8	5	1	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

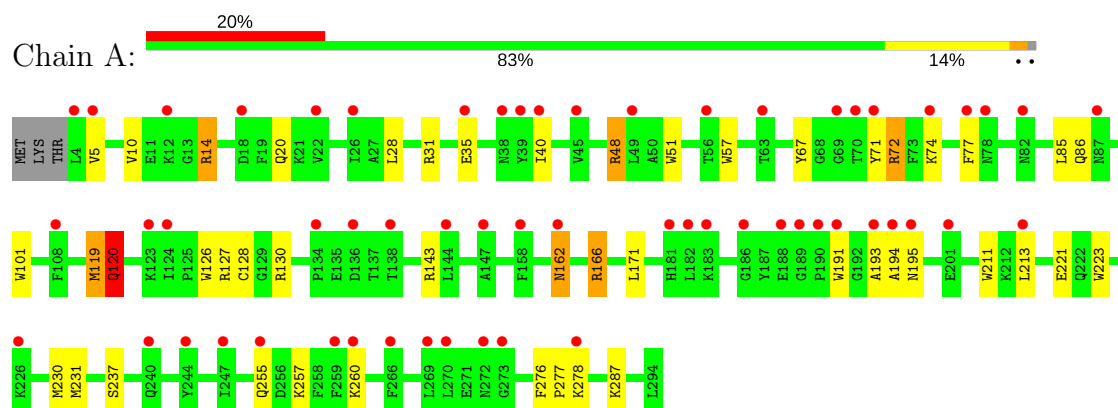
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		

### 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, $\alpha$ , $\beta$ , $\gamma$	107.72Å 76.63Å 51.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.40 46.60 – 2.01	Depositor EDS
% Data completeness (in resolution range)	67.1 (5.00-2.40) 73.2 (46.60-2.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.370 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.0	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	0.76	EDS
Total number of atoms	3003	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: DMI, 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	0/2408	1.64	46/3259 (1.4%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH2	-15.03	112.78	120.30
1	A	48	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	A	166	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	A	31	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	162	ASN	CA-C-N	-8.23	99.09	117.20
1	A	223	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	A	127	ARG	CB-CG-CD	-8.16	90.38	111.60
1	A	101	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	A	143	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	48	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	191	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	72	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	51	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	101	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	A	211	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	A	51	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	166	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	191	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	A	126	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	A	71	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	A	223	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	A	211	TRP	CE2-CD2-CG	-7.02	101.69	107.30
1	A	127	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	126	TRP	CE2-CD2-CG	-6.91	101.77	107.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	14	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	57	TRP	CD1-CG-CD2	6.51	111.51	106.30
1	A	57	TRP	CE2-CD2-CG	-6.37	102.20	107.30
1	A	67	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	A	162	ASN	N-CA-C	6.28	127.96	111.00
1	A	195	ASN	N-CA-CB	-5.84	100.08	110.60
1	A	126	TRP	CB-CG-CD1	-5.79	119.48	127.00
1	A	126	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	A	231	MET	CA-CB-CG	5.56	122.75	113.30
1	A	51	TRP	CB-CG-CD1	-5.52	119.82	127.00
1	A	166	ARG	CG-CD-NE	-5.35	100.57	111.80
1	A	223	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	A	143	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	5	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	A	126	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	A	120	GLN	N-CA-C	5.18	125.00	111.00
1	A	162	ASN	CA-C-O	5.18	130.99	120.10
1	A	230	MET	CA-CB-CG	5.07	121.92	113.30
1	A	119	MET	CG-SD-CE	5.05	108.28	100.20
1	A	101	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	237	SER	CB-CA-C	-5.00	100.60	110.10

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	2343	512	2222	10	3
2	A	7	1	9	0	0
3	A	43	0	30	0	0
4	A	97	0	0	2	0
All	All	2490	513	2261	10	3

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 2.

All (10) 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:128:CYS:HA	4:A:326:HOH:O	1.81	0.81
1:A:130:ARG:NH1	4:A:326:HOH:O	2.37	0.56
1:A:20:GLN:HE22	1:A:287:LYS:H	1.64	0.45
1:A:276:PHE:HA	1:A:277:PRO:HD3	1.92	0.43
1:A:48:ARG:HG2	1:A:85:LEU:HD21	2.00	0.43
1:A:119:MET:O	1:A:120:GLN:HG2	2.19	0.42
1:A:166:ARG:HH21	1:A:257:LYS:NZ	2.19	0.40
1:A:10:VAL:HG13	1:A:128:CYS:SG	2.61	0.40
1:A:40:ILE:HD11	1:A:194:ALA:HB3	2.03	0.40
1:A:77:PHE:CE1	1:A:86:GLN:HG3	2.57	0.40

All (3) 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_477]	1.16	0.44
1:A:14:ARG:HH12	1:A:221:GLU:OE2[4_477]	1.31	0.29
1:A:14:ARG:NH2	1:A:213:LEU:O[4_477]	2.00	0.20

## 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	289/294 (98%)	278 (96%)	9 (3%)	2 (1%)	25	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	193	ALA

### 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	248/251 (99%)	239 (96%)	9 (4%)	40 60

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	72	ARG
1	A	74	LYS
1	A	120	GLN
1	A	171	LEU
1	A	255	GLN
1	A	260	LYS
1	A	278	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	78	ASN
1	A	220	ASN
1	A	240	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 [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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	DMI	A	499	-	6,7,7	1.92	1 (16%)	5,9,9	2.13	1 (20%)
3	HEM	A	500	1,4	28,50,50	1.58	6 (21%)	17,82,82	1.93	5 (29%)

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	DMI	A	499	-	-	0/0/0/0	0/1/1/1
3	HEM	A	500	1,4	-	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)
3	A	500	HEM	C3B-CAB	-3.96	1.40	1.47
2	A	499	DMI	C4-N3	-3.91	1.30	1.37
3	A	500	HEM	C3C-CAC	-3.38	1.41	1.47
3	A	500	HEM	C4D-ND	-2.54	1.33	1.36
3	A	500	HEM	C1B-NB	-2.31	1.34	1.36
3	A	500	HEM	CBB-CAB	2.50	1.46	1.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	CBC-CAC	2.56	1.46	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	HEM	C4A-C3A-C2A	-2.63	105.16	107.00
3	A	500	HEM	C1D-C2D-C3D	-2.56	105.21	107.00
3	A	500	HEM	CMD-C2D-C3D	2.12	128.95	124.94
3	A	500	HEM	CMB-C2B-C3B	3.27	130.97	124.89
3	A	500	HEM	CMC-C2C-C3C	4.15	132.60	124.89
2	A	499	DMI	CM2-C2-N3	4.34	128.72	124.88

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	291/294 (98%)	1.27	58 (19%) 1 1	9, 24, 44, 58	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	LYS	5.1
1	A	38	ASN	4.7
1	A	188	GLU	3.9
1	A	269	LEU	3.9
1	A	63	THR	3.3
1	A	45	VAL	3.3
1	A	77	PHE	3.2
1	A	70	THR	3.1
1	A	144	LEU	3.1
1	A	270	LEU	3.1
1	A	138	THR	3.0
1	A	189	GLY	2.9
1	A	158	PHE	2.9
1	A	226	LYS	2.8
1	A	49	LEU	2.8
1	A	35	GLU	2.8
1	A	195	ASN	2.7
1	A	240	GLN	2.7
1	A	186	GLY	2.5
1	A	201	GLU	2.5
1	A	273	GLY	2.5
1	A	193	ALA	2.5
1	A	191	TRP	2.4
1	A	213	LEU	2.4
1	A	136	ASP	2.4
1	A	26	ILE	2.4
1	A	124	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	278	LYS	2.4
1	A	40	ILE	2.3
1	A	147	ALA	2.3
1	A	78	ASN	2.3
1	A	134	PRO	2.3
1	A	39	TYR	2.3
1	A	71	TYR	2.3
1	A	266	PHE	2.3
1	A	272	ASN	2.2
1	A	194	ALA	2.2
1	A	190	PRO	2.2
1	A	255	GLN	2.2
1	A	244	TYR	2.2
1	A	82	ASN	2.2
1	A	4	LEU	2.2
1	A	5	VAL	2.2
1	A	22	VAL	2.2
1	A	260	LYS	2.2
1	A	247	ILE	2.2
1	A	87	ASN	2.1
1	A	162	ASN	2.1
1	A	56	THR	2.1
1	A	259	PHE	2.1
1	A	69	GLY	2.1
1	A	181	HIS	2.1
1	A	182	LEU	2.1
1	A	12	LYS	2.1
1	A	108	PHE	2.0
1	A	123	LYS	2.0
1	A	74	LYS	2.0
1	A	18	ASP	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
3	HEM	A	500	43/43	0.79	0.26	0.14	10,20,24,25	0
2	DMI	A	499	7/7	0.77	0.26	-0.04	20,35,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.