



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:28 am GMT

PDB ID : 1BCF  
Title : THE STRUCTURE OF A UNIQUE, TWO-FOLD SYMMETRIC, HAEM-BINDING SITE  
Authors : Frolow, F.; Kalb(Gilboa), A.J.; Yariv, J.  
Deposited on : 1993-12-06  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

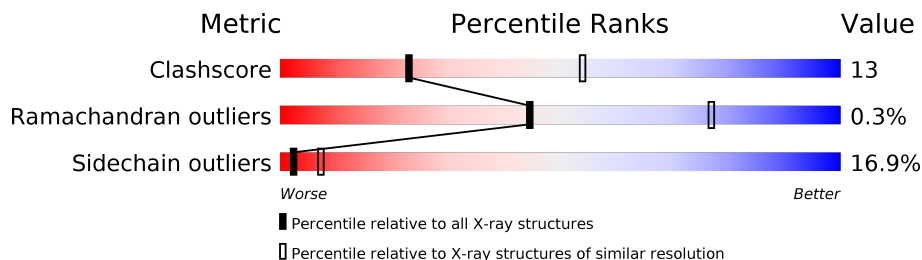
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)




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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	158	
1	B	158	
1	C	158	
1	D	158	
1	E	158	
1	F	158	
1	G	158	

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Mol	Chain	Length	Quality of chain
1	H	158	 60% 34% 6%
1	I	158	 61% 33% 6%
1	J	158	 59% 35% 6%
1	K	158	 61% 33% 6%
1	L	158	 58% 36% 6%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15846 atoms, of which 0 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 BACTERIOFERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	B	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	C	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	D	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	E	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	F	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	G	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	H	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	I	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	J	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	K	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	L	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

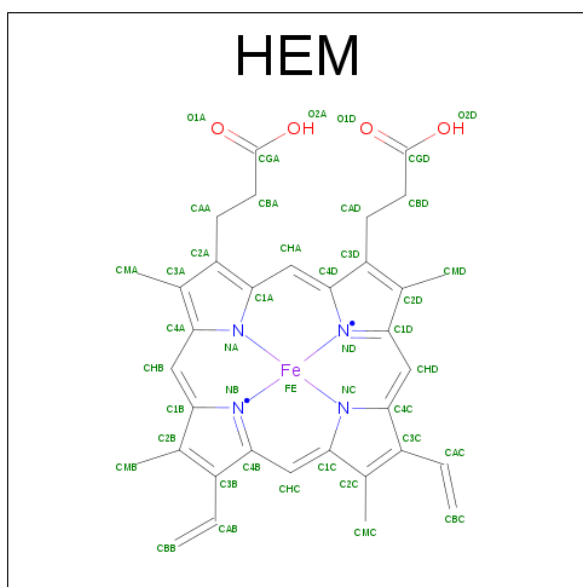
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	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	
			43	34	1	4	4	
							0	0

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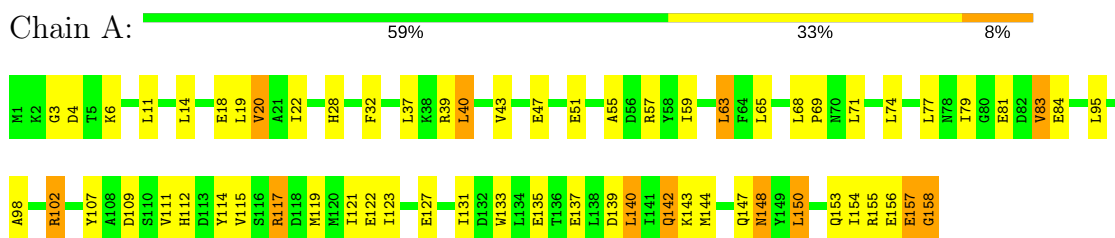
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

### 3 Residue-property plots [i](#)

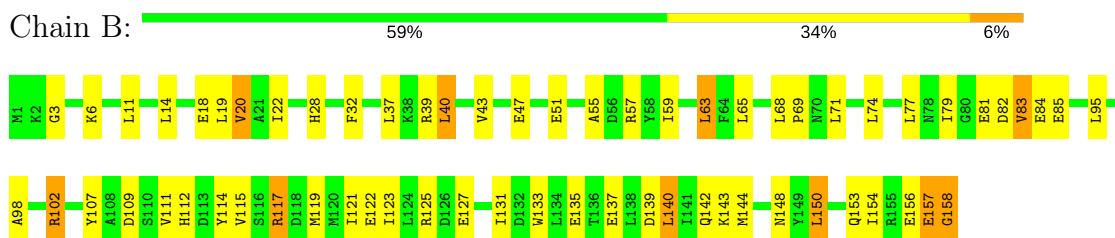
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

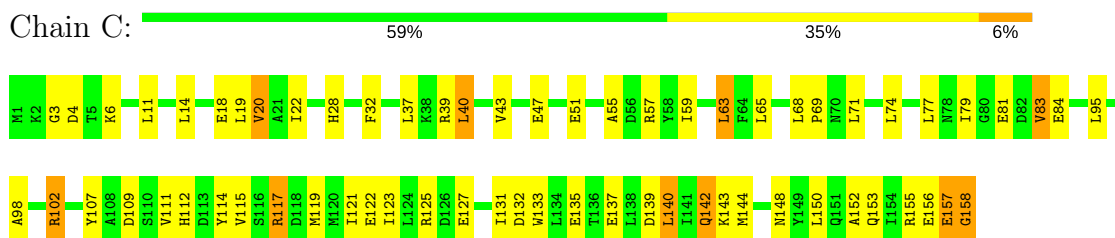
#### • Molecule 1: BACTERIOFERRITIN



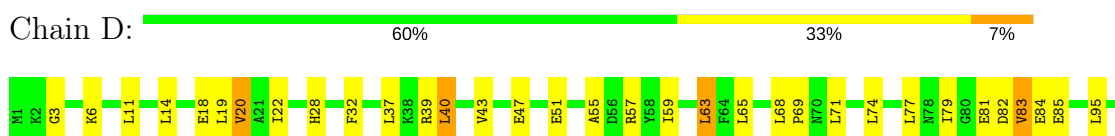
#### • Molecule 1: BACTERIOFERRITIN



#### • Molecule 1: BACTERIOFERRITIN



#### • Molecule 1: BACTERIOFERRITIN





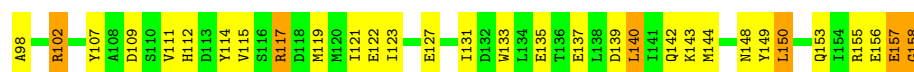
• Molecule 1: BACTERIOFERRITIN

Chain E: 61% 32% 6%



• Molecule 1: BACTERIOFERRITIN

Chain F: 59% 34% 6%



• Molecule 1: BACTERIOFERRITIN

Chain G: 61% 32% 6%



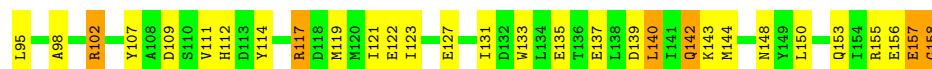
• Molecule 1: BACTERIOFERRITIN

Chain H: 60% 34% 6%

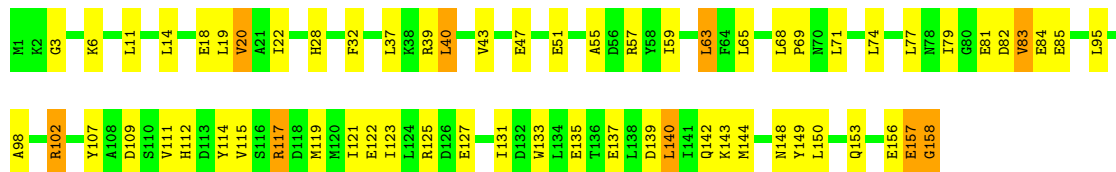


• Molecule 1: BACTERIOFERRITIN

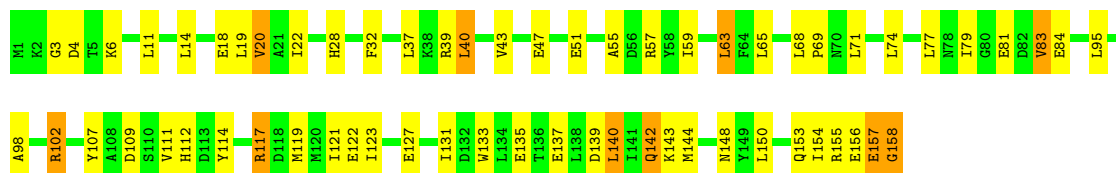
Chain I: 61% 33% 6%



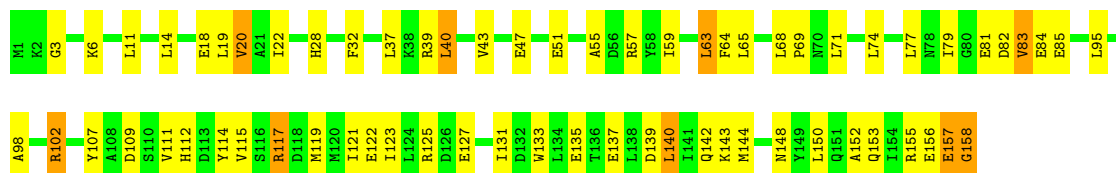
## ● Molecule 1: BACTERIOFERRITIN

Chain J:  59% 35% 6%

## ● Molecule 1: BACTERIOFERRITIN

Chain K:  61% 33% 6%

## ● Molecule 1: BACTERIOFERRITIN

Chain L:  58% 36% 6%

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.10Å 211.10Å 145.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, MN

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	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	B	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	C	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	D	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	E	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	F	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	G	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	H	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	I	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	J	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	K	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	L	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
All	All	0.77	12/15792 (0.1%)	0.83	24/21228 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	GLU	CG-CD	6.28	1.61	1.51
1	A	81	GLU	CG-CD	6.27	1.61	1.51
1	E	81	GLU	CG-CD	6.26	1.61	1.51
1	I	81	GLU	CG-CD	6.24	1.61	1.51
1	G	81	GLU	CG-CD	6.23	1.61	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3	GLY	N-CA-C	6.68	129.80	113.10
1	K	3	GLY	N-CA-C	6.67	129.78	113.10
1	C	3	GLY	N-CA-C	6.67	129.78	113.10
1	A	3	GLY	N-CA-C	6.66	129.76	113.10
1	I	3	GLY	N-CA-C	6.66	129.76	113.10

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	1297	0	1280	44	0
1	B	1297	0	1280	43	0
1	C	1297	0	1280	39	0
1	D	1297	0	1280	43	0
1	E	1297	0	1280	28	0
1	F	1297	0	1280	33	0
1	G	1297	0	1280	35	0
1	H	1297	0	1280	31	0
1	I	1297	0	1280	33	0
1	J	1297	0	1280	34	0
1	K	1297	0	1280	30	0
1	L	1297	0	1280	46	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	43	0	30	3	0
3	C	43	0	30	3	0
3	E	43	0	30	3	0
3	G	43	0	30	3	0
3	I	43	0	30	3	0
3	K	43	0	30	3	0
All	All	15846	0	15540	405	0

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 13.

The worst 5 of 405 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:B:157:GLU:HA	1:D:155:ARG:NH1	1.75	1.02
1:G:157:GLU:HA	1:I:155:ARG:NH1	1.91	0.85
1:J:20:VAL:HG23	1:J:77:LEU:HD23	1.60	0.84
1:K:20:VAL:HG23	1:K:77:LEU:HD23	1.61	0.83
1:F:20:VAL:HG23	1:F:77:LEU:HD23	1.60	0.83

There are no symmetry-related clashes.

## 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	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	28	64
1	B	156/158 (99%)	151 (97%)	5 (3%)	0	100	100
1	C	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	28	64
1	D	156/158 (99%)	151 (97%)	5 (3%)	0	100	100
1	E	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	28	64
1	F	156/158 (99%)	151 (97%)	5 (3%)	0	100	100
1	G	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	28	64
1	H	156/158 (99%)	151 (97%)	5 (3%)	0	100	100
1	I	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	28	64
1	J	156/158 (99%)	151 (97%)	5 (3%)	0	100	100
1	K	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	28	64
1	L	156/158 (99%)	151 (97%)	5 (3%)	0	100	100
All	All	1872/1896 (99%)	1812 (97%)	54 (3%)	6 (0%)	44	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	C	4	ASP
1	E	4	ASP
1	G	4	ASP
1	I	4	ASP

### 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	139/139 (100%)	115 (83%)	24 (17%)	2	7
1	B	139/139 (100%)	116 (84%)	23 (16%)	2	8
1	C	139/139 (100%)	115 (83%)	24 (17%)	2	7
1	D	139/139 (100%)	116 (84%)	23 (16%)	2	8
1	E	139/139 (100%)	115 (83%)	24 (17%)	2	7
1	F	139/139 (100%)	116 (84%)	23 (16%)	2	8
1	G	139/139 (100%)	115 (83%)	24 (17%)	2	7
1	H	139/139 (100%)	116 (84%)	23 (16%)	2	8
1	I	139/139 (100%)	115 (83%)	24 (17%)	2	7
1	J	139/139 (100%)	116 (84%)	23 (16%)	2	8
1	K	139/139 (100%)	115 (83%)	24 (17%)	2	7
1	L	139/139 (100%)	116 (84%)	23 (16%)	2	8
All	All	1668/1668 (100%)	1386 (83%)	282 (17%)	2	7

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	68	LEU
1	G	117	ARG
1	L	14	LEU
1	F	95	LEU

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Mol	Chain	Res	Type
1	G	20	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	28	HIS
1	G	112	HIS
1	K	148	ASN
1	F	78	ASN
1	G	24	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](#)

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z  > 2$
3	HEM	A	200	1	28,50,50	2.96	11 (39%)	17,82,82	2.17	6 (35%)
3	HEM	C	201	1	28,50,50	2.96	12 (42%)	17,82,82	2.18	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	E	202	1	28,50,50	2.96	11 (39%)	17,82,82	2.16	6 (35%)
3	HEM	G	203	1	28,50,50	2.96	11 (39%)	17,82,82	2.16	6 (35%)
3	HEM	I	204	1	28,50,50	2.96	11 (39%)	17,82,82	2.17	6 (35%)
3	HEM	K	205	1	28,50,50	2.96	12 (42%)	17,82,82	2.16	6 (35%)

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
3	HEM	A	200	1	-	0/6/54/54	0/0/8/8
3	HEM	C	201	1	-	0/6/54/54	0/0/8/8
3	HEM	E	202	1	-	0/6/54/54	0/0/8/8
3	HEM	G	203	1	-	0/6/54/54	0/0/8/8
3	HEM	I	204	1	-	0/6/54/54	0/0/8/8
3	HEM	K	205	1	-	0/6/54/54	0/0/8/8

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	205	HEM	C3C-CAC	-4.96	1.37	1.47
3	G	203	HEM	C3C-CAC	-4.94	1.37	1.47
3	I	204	HEM	C3C-CAC	-4.93	1.37	1.47
3	A	200	HEM	C3C-CAC	-4.92	1.37	1.47
3	C	201	HEM	C3C-CAC	-4.92	1.37	1.47

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	204	HEM	C4A-C3A-C2A	-3.55	104.52	107.00
3	C	201	HEM	C4A-C3A-C2A	-3.54	104.53	107.00
3	G	203	HEM	C4A-C3A-C2A	-3.53	104.54	107.00
3	A	200	HEM	C4A-C3A-C2A	-3.53	104.54	107.00
3	K	205	HEM	C4A-C3A-C2A	-3.52	104.55	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	200	HEM	3	0
3	C	201	HEM	3	0
3	E	202	HEM	3	0
3	G	203	HEM	3	0
3	I	204	HEM	3	0
3	K	205	HEM	3	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.