



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2017 – 10:01 am GMT

PDB ID : 5GYR  
Title : Tetrameric Allochromatium vinosum cytochrome c'  
Authors : Yamanaka, M.; Hoshizumi, M.; Nagao, S.; Nakayama, R.; Shibata, N.; Higuchi, Y.; Hirota, S.  
Deposited on : 2016-09-23  
Resolution : 1.60 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 : recalc29047  
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) : recalc29047

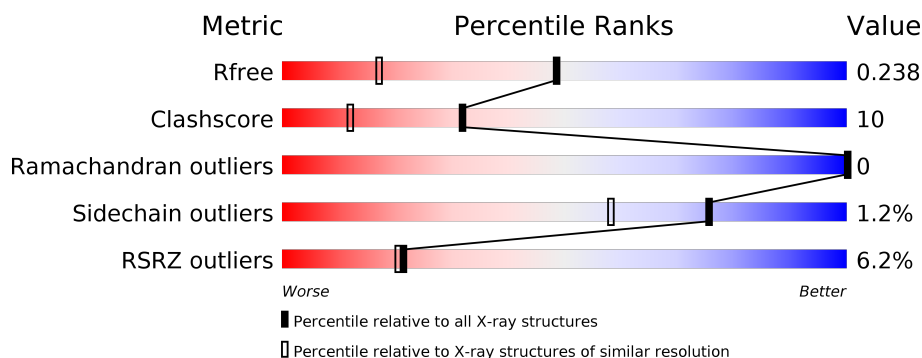
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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.




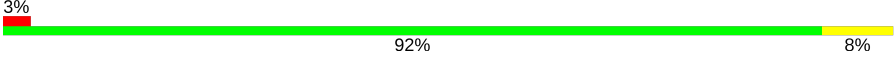
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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	131	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	131	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	E	131	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	F	131	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	I	131	<div> <div>11%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	J	131	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	131	
1	N	131	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8888 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 Cytochrome c'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			
1	B	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			
1	E	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			
1	F	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			
1	I	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			
1	J	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			
1	M	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			
1	N	131	Total	C	N	O	S	0	0	0
			967	600	168	193	6			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	I	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	J	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	N	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O		
			113	113	0	0
3	B	138	Total	O		
			138	138	0	0
3	E	125	Total	O		
			125	125	0	0
3	F	140	Total	O		
			140	140	0	0

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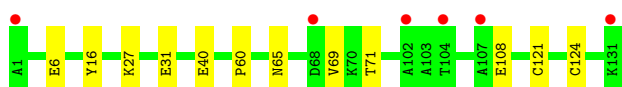
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	52	Total 52	O 52	0	0
3	J	97	Total 97	O 97	0	0
3	M	48	Total 48	O 48	0	0
3	N	95	Total 95	O 95	0	0

### 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.

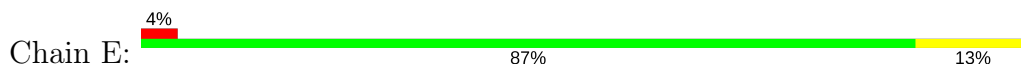
- Molecule 1: Cytochrome c'



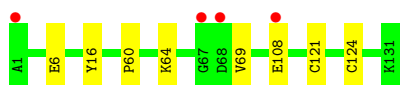
- Molecule 1: Cytochrome c'



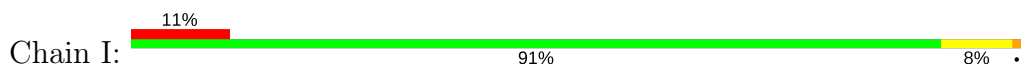
- Molecule 1: Cytochrome c'



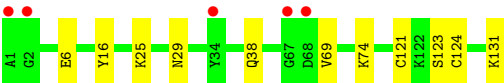
- Molecule 1: Cytochrome c'



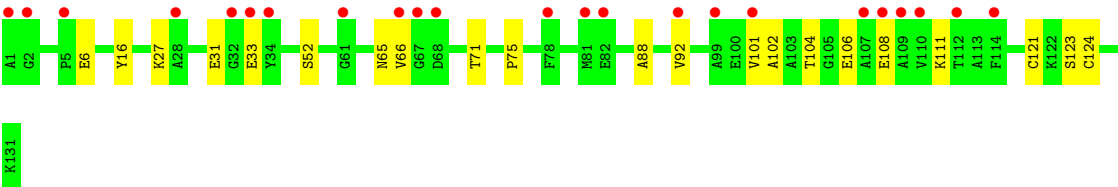
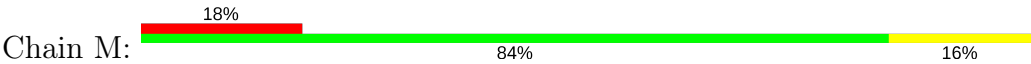
- Molecule 1: Cytochrome c'



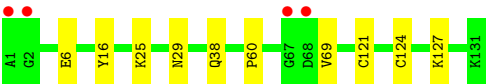
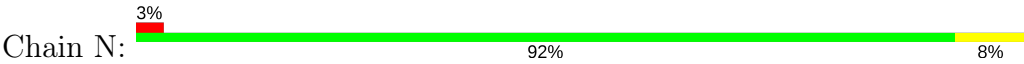
- Molecule 1: Cytochrome c'



● Molecule 1: Cytochrome c'



● Molecule 1: Cytochrome c'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.95Å 48.62Å 130.55Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	41.40 – 1.60 40.16 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (41.40-1.60) 98.6 (40.16-1.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.204 , 0.232 0.213 , 0.238	Depositor DCC
$R_{free}$ test set	6704 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 91.11 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7269e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.45	0/981	0.57	0/1319
1	B	0.50	0/981	0.64	0/1319
1	E	0.50	1/981 (0.1%)	0.57	0/1319
1	F	0.48	0/981	0.62	0/1319
1	I	0.47	0/981	0.65	0/1319
1	J	0.47	0/981	0.60	0/1319
1	M	0.49	0/981	0.66	0/1319
1	N	0.47	0/981	0.61	0/1319
All	All	0.48	1/7848 (0.0%)	0.62	0/10552

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	I	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	123	SER	CB-OG	-6.17	1.34	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	2	GLY	Peptide

## 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	967	0	940	15	0
1	B	967	0	940	13	0
1	E	967	0	940	21	0
1	F	967	0	940	14	1
1	I	967	0	937	17	0
1	J	967	0	940	18	0
1	M	967	0	939	23	0
1	N	967	0	940	18	0
2	A	43	0	30	10	0
2	B	43	0	30	11	0
2	E	43	0	30	11	0
2	F	43	0	30	13	0
2	I	43	0	30	11	0
2	J	43	0	30	11	0
2	M	43	0	30	11	0
2	N	43	0	30	12	0
3	A	113	0	0	0	0
3	B	138	0	0	1	0
3	E	125	0	0	0	0
3	F	140	0	0	0	0
3	I	52	0	0	0	0
3	J	97	0	0	1	1
3	M	48	0	0	1	0
3	N	95	0	0	1	0
All	All	8888	0	7756	144	1

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 10.

All (144) 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:124:CYS:HG	2:B:201:HEM:CAC	1.43	1.31
1:M:124:CYS:HG	2:M:201:HEM:CAC	1.40	1.28
1:E:124:CYS:HG	2:E:201:HEM:CAC	1.43	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:124:CYS:SG	2:N:201:HEM:HAC	1.80	1.16
1:F:124:CYS:SG	2:F:201:HEM:HAC	1.82	1.11
1:B:124:CYS:HG	2:B:201:HEM:HAC	1.13	1.07
1:I:124:CYS:SG	2:I:201:HEM:HAC	1.93	1.07
1:J:124:CYS:SG	2:J:201:HEM:HAC	1.84	1.07
1:M:124:CYS:HG	2:M:201:HEM:HAC	1.10	1.06
1:A:124:CYS:SG	2:A:201:HEM:HAC	1.90	1.04
1:M:124:CYS:SG	2:M:201:HEM:HAC	1.85	1.04
1:J:124:CYS:HG	2:J:201:HEM:CAC	1.60	1.03
1:B:124:CYS:SG	2:B:201:HEM:HAC	1.84	1.03
1:N:121:CYS:SG	2:N:201:HEM:HAB	1.94	1.02
1:J:121:CYS:SG	2:J:201:HEM:HAB	2.00	1.01
1:I:124:CYS:HG	2:I:201:HEM:CAC	1.61	1.00
1:E:124:CYS:SG	2:E:201:HEM:HAC	1.87	1.00
1:E:124:CYS:HG	2:E:201:HEM:HAC	1.14	0.97
1:I:31:GLU:HB3	1:M:31:GLU:HG2	1.46	0.96
1:F:124:CYS:HG	2:F:201:HEM:CAC	1.67	0.96
1:N:124:CYS:HG	2:N:201:HEM:CAC	1.69	0.93
1:E:121:CYS:SG	2:E:201:HEM:HAB	2.07	0.92
1:I:121:CYS:SG	2:I:201:HEM:HAB	2.06	0.92
1:M:121:CYS:SG	2:M:201:HEM:HAB	2.09	0.92
1:F:121:CYS:SG	2:F:201:HEM:HAB	2.09	0.91
1:E:72:ARG:HG2	1:J:131:LYS:HE3	1.54	0.90
1:B:121:CYS:SG	2:B:201:HEM:HAB	2.10	0.90
1:I:124:CYS:HG	2:I:201:HEM:HAC	1.29	0.90
1:A:121:CYS:SG	2:A:201:HEM:HAB	2.12	0.89
1:B:121:CYS:SG	2:B:201:HEM:CBB	2.61	0.88
1:M:121:CYS:SG	2:M:201:HEM:CBB	2.60	0.88
1:E:121:CYS:SG	2:E:201:HEM:CBB	2.61	0.87
1:J:121:CYS:SG	2:J:201:HEM:CBB	2.64	0.85
1:F:121:CYS:SG	2:F:201:HEM:CBB	2.65	0.84
1:N:121:CYS:SG	2:N:201:HEM:CBB	2.67	0.82
1:A:6:GLU:HG3	1:A:69:VAL:HG21	1.62	0.81
1:J:6:GLU:HG3	1:J:69:VAL:HG21	1.63	0.81
1:A:121:CYS:SG	2:A:201:HEM:CBB	2.70	0.80
1:B:124:CYS:SG	2:B:201:HEM:CBC	2.69	0.80
1:F:6:GLU:HG3	1:F:69:VAL:HG21	1.63	0.80
1:E:6:GLU:HG3	1:E:69:VAL:HG21	1.64	0.80
2:A:201:HEM:HBC2	2:A:201:HEM:HMC2	1.63	0.79
1:B:6:GLU:HG3	1:B:69:VAL:HG21	1.63	0.79
1:N:6:GLU:HG3	1:N:69:VAL:HG21	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:31:GLU:CB	1:M:31:GLU:HG2	2.14	0.78
1:M:104:THR:OG1	1:M:106:GLU:HG3	1.83	0.78
1:F:124:CYS:HG	2:F:201:HEM:HAC	1.29	0.78
1:M:121:CYS:SG	2:M:201:HEM:C3B	2.77	0.78
1:N:121:CYS:SG	2:N:201:HEM:C3B	2.78	0.77
1:I:121:CYS:SG	2:I:201:HEM:CBB	2.73	0.77
1:J:124:CYS:SG	2:J:201:HEM:CBC	2.73	0.77
1:J:124:CYS:HG	2:J:201:HEM:HAC	1.27	0.76
1:N:124:CYS:HG	2:N:201:HEM:HAC	1.31	0.76
1:N:124:CYS:SG	2:N:201:HEM:C3C	2.79	0.76
1:E:27:LYS:HE2	1:E:31:GLU:OE2	1.86	0.76
1:M:124:CYS:SG	2:M:201:HEM:CBC	2.75	0.75
1:M:124:CYS:SG	2:M:201:HEM:C3C	2.77	0.75
1:E:124:CYS:SG	2:E:201:HEM:CBC	2.75	0.75
1:F:124:CYS:SG	2:F:201:HEM:CBC	2.75	0.75
1:M:33:GLU:OE1	1:N:127:LYS:NZ	2.21	0.74
1:J:131:LYS:HG2	1:N:6:GLU:OE2	1.88	0.74
1:I:124:CYS:SG	2:I:201:HEM:CBC	2.74	0.74
1:J:124:CYS:SG	2:J:201:HEM:C3C	2.80	0.74
1:E:124:CYS:SG	2:E:201:HEM:C3C	2.79	0.73
1:J:121:CYS:SG	2:J:201:HEM:C3B	2.81	0.73
1:F:124:CYS:SG	2:F:201:HEM:C3C	2.82	0.73
1:I:124:CYS:SG	2:I:201:HEM:C3C	2.83	0.72
1:B:124:CYS:SG	2:B:201:HEM:C3C	2.81	0.72
1:E:121:CYS:SG	2:E:201:HEM:C3B	2.82	0.71
1:B:108:GLU:HG2	3:B:396:HOH:O	1.89	0.71
2:E:201:HEM:HMC2	2:E:201:HEM:HBC2	1.72	0.70
1:E:72:ARG:HG2	1:J:131:LYS:CE	2.21	0.70
1:F:121:CYS:SG	2:F:201:HEM:C3B	2.86	0.69
1:A:121:CYS:SG	2:A:201:HEM:C3B	2.86	0.69
1:A:124:CYS:SG	2:A:201:HEM:C3C	2.86	0.68
1:N:124:CYS:SG	2:N:201:HEM:CBC	2.79	0.68
1:M:27:LYS:HG2	1:M:31:GLU:OE2	1.94	0.68
1:B:121:CYS:SG	2:B:201:HEM:C3B	2.85	0.68
1:A:124:CYS:SG	2:A:201:HEM:CBC	2.83	0.66
1:E:6:GLU:CG	1:E:69:VAL:HG21	2.26	0.65
1:F:6:GLU:CG	1:F:69:VAL:HG21	2.27	0.65
1:N:6:GLU:CG	1:N:69:VAL:HG21	2.26	0.65
1:J:6:GLU:CG	1:J:69:VAL:HG21	2.26	0.65
2:M:201:HEM:HMC2	2:M:201:HEM:HBC2	1.78	0.65
1:A:6:GLU:CG	1:A:69:VAL:HG21	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLU:CG	1:B:69:VAL:HG21	2.26	0.64
1:I:26:ILE:O	1:I:30:LEU:HD13	1.98	0.64
2:J:201:HEM:HMC2	2:J:201:HEM:HBC2	1.80	0.64
2:B:201:HEM:HBC2	2:B:201:HEM:HMC2	1.80	0.63
1:I:121:CYS:SG	2:I:201:HEM:C3B	2.92	0.62
2:F:201:HEM:HBC2	2:F:201:HEM:HMC2	1.82	0.62
1:F:6:GLU:HG3	1:F:69:VAL:CG2	2.30	0.61
1:E:6:GLU:HG3	1:E:69:VAL:CG2	2.31	0.60
1:A:6:GLU:HG3	1:A:69:VAL:CG2	2.30	0.60
2:A:201:HEM:HBC2	2:A:201:HEM:CMC	2.32	0.60
1:J:6:GLU:HG3	1:J:69:VAL:CG2	2.32	0.60
1:A:27:LYS:HE3	1:A:31:GLU:OE2	2.01	0.59
1:B:6:GLU:HG3	1:B:69:VAL:CG2	2.32	0.59
1:E:27:LYS:CE	1:E:31:GLU:OE2	2.49	0.59
2:I:201:HEM:HMC2	2:I:201:HEM:HBC2	1.84	0.59
1:N:6:GLU:HG3	1:N:69:VAL:CG2	2.32	0.59
1:A:40:GLU:HG3	3:N:332:HOH:O	2.05	0.56
1:I:16:TYR:HB3	2:I:201:HEM:C4A	2.41	0.55
2:N:201:HEM:HMC2	2:N:201:HEM:HBC2	1.90	0.54
1:M:101:VAL:HG23	1:M:102:ALA:N	2.24	0.53
1:I:31:GLU:HG3	1:M:31:GLU:HA	1.91	0.53
2:E:201:HEM:CMC	2:E:201:HEM:HBC2	2.38	0.53
1:M:88:ALA:O	1:M:92:VAL:HG13	2.11	0.51
1:E:16:TYR:HB3	2:J:201:HEM:C4A	2.46	0.50
2:M:201:HEM:CMC	2:M:201:HEM:HBC2	2.41	0.50
1:I:31:GLU:HB3	1:M:31:GLU:CG	2.30	0.50
2:J:201:HEM:CMC	2:J:201:HEM:HBC2	2.41	0.50
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.12	0.50
1:M:16:TYR:HB3	2:M:201:HEM:C4A	2.47	0.49
1:I:52:SER:O	1:J:25:LYS:NZ	2.46	0.49
2:F:201:HEM:HBC2	2:F:201:HEM:CMC	2.42	0.48
2:B:201:HEM:CMC	2:B:201:HEM:HBC2	2.42	0.48
1:M:6:GLU:OE1	1:M:66:VAL:HG12	2.13	0.48
1:E:108:GLU:HA	1:E:108:GLU:OE1	2.14	0.48
1:A:16:TYR:HB3	2:N:201:HEM:C4A	2.48	0.48
2:A:201:HEM:CMC	2:A:201:HEM:HMC2	2.40	0.47
2:A:201:HEM:C4A	1:N:16:TYR:HB3	2.49	0.47
2:E:201:HEM:C4A	1:J:16:TYR:HB3	2.50	0.47
1:B:16:TYR:HB3	2:B:201:HEM:C4A	2.50	0.47
1:I:122:LYS:O	1:I:126:GLU:HG3	2.15	0.46
2:N:201:HEM:CMC	2:N:201:HEM:HBC2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:SER:O	1:N:25:LYS:NZ	2.49	0.46
2:I:201:HEM:CMC	2:I:201:HEM:HBC2	2.45	0.46
1:F:124:CYS:HG	2:F:201:HEM:CHD	2.31	0.44
1:F:16:TYR:HB3	2:F:201:HEM:C4A	2.52	0.44
1:E:65:ASN:ND2	1:E:71:THR:H	2.15	0.44
1:N:124:CYS:HG	2:N:201:HEM:CHD	2.31	0.44
1:E:40:GLU:HG3	3:J:307:HOH:O	2.16	0.43
1:E:128:TYR:HA	1:J:74:LYS:HD3	2.01	0.43
1:A:65:ASN:ND2	1:A:71:THR:H	2.17	0.43
1:I:65:ASN:ND2	1:I:71:THR:H	2.17	0.42
1:A:60:PRO:HA	1:N:60:PRO:HA	2.02	0.42
1:J:29:ASN:HD21	1:J:38:GLN:NE2	2.18	0.42
1:F:124:CYS:HG	2:F:201:HEM:HHD	1.86	0.41
1:M:65:ASN:ND2	1:M:71:THR:H	2.19	0.41
1:E:84:VAL:O	1:E:89:ARG:NH1	2.55	0.40
1:M:108:GLU:OE1	1:M:108:GLU:HA	2.22	0.40
1:M:75:PRO:HB3	3:M:321:HOH:O	2.22	0.40
1:N:29:ASN:HD21	1:N:38:GLN:NE2	2.19	0.40

All (1) 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:F:108:GLU:OE1	3:J:334:HOH:O[2_645]	2.13	0.07

## 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	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	B	129/131 (98%)	128 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	F	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	I	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	J	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	M	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	N	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
All	All	1032/1048 (98%)	1021 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	92/92 (100%)	92 (100%)	0	100	100
1	B	92/92 (100%)	90 (98%)	2 (2%)	57	29
1	E	92/92 (100%)	91 (99%)	1 (1%)	78	61
1	F	92/92 (100%)	90 (98%)	2 (2%)	57	29
1	I	92/92 (100%)	91 (99%)	1 (1%)	78	61
1	J	92/92 (100%)	91 (99%)	1 (1%)	78	61
1	M	92/92 (100%)	90 (98%)	2 (2%)	57	29
1	N	92/92 (100%)	92 (100%)	0	100	100
All	All	736/736 (100%)	727 (99%)	9 (1%)	75	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	64	LYS
1	B	131	LYS
1	E	64	LYS
1	F	60	PRO

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Mol	Chain	Res	Type
1	F	64	LYS
1	I	30	LEU
1	J	123	SER
1	M	111	LYS
1	M	123	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	51	ASN
1	A	65	ASN
1	B	38	GLN
1	B	44	ASN
1	E	38	GLN
1	E	51	ASN
1	E	65	ASN
1	F	38	GLN
1	F	44	ASN
1	I	38	GLN
1	I	51	ASN
1	I	65	ASN
1	I	96	ASN
1	J	38	GLN
1	J	44	ASN
1	J	96	ASN
1	M	38	GLN
1	M	51	ASN
1	M	65	ASN
1	M	96	ASN
1	N	38	GLN
1	N	44	ASN
1	N	96	ASN

### 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](#)

8 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	HEM	A	201	1	28,50,50	1.01	1 (3%)	17,82,82	1.39	2 (11%)
2	HEM	B	201	1	28,50,50	0.88	1 (3%)	17,82,82	1.51	4 (23%)
2	HEM	E	201	1	28,50,50	0.74	0	17,82,82	1.45	2 (11%)
2	HEM	F	201	1	28,50,50	0.99	2 (7%)	17,82,82	1.50	3 (17%)
2	HEM	I	201	1	28,50,50	0.77	2 (7%)	17,82,82	1.35	3 (17%)
2	HEM	J	201	1	28,50,50	0.80	0	17,82,82	1.48	3 (17%)
2	HEM	M	201	1	28,50,50	0.87	2 (7%)	17,82,82	1.30	1 (5%)
2	HEM	N	201	1	28,50,50	0.83	1 (3%)	17,82,82	1.50	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	201	1	-	0/6/54/54	0/0/8/8
2	HEM	B	201	1	-	0/6/54/54	0/0/8/8
2	HEM	E	201	1	-	0/6/54/54	0/0/8/8
2	HEM	F	201	1	-	0/6/54/54	0/0/8/8
2	HEM	I	201	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	J	201	1	-	0/6/54/54	0/0/8/8
2	HEM	M	201	1	-	0/6/54/54	0/0/8/8
2	HEM	N	201	1	-	0/6/54/54	0/0/8/8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	HEM	C1B-NB	-2.95	1.33	1.36
2	A	201	HEM	C1B-NB	-2.73	1.33	1.36
2	F	201	HEM	C3B-C2B	-2.64	1.36	1.40
2	B	201	HEM	C1B-NB	-2.46	1.33	1.36
2	M	201	HEM	C3B-C2B	-2.36	1.37	1.40
2	M	201	HEM	C1B-NB	-2.34	1.34	1.36
2	N	201	HEM	C3B-C2B	-2.24	1.37	1.40
2	I	201	HEM	C1B-NB	-2.06	1.34	1.36
2	I	201	HEM	C3B-C2B	-2.01	1.37	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	HEM	CBD-CAD-C3D	-3.10	106.55	112.47
2	J	201	HEM	CMA-C3A-C4A	-3.10	123.70	128.46
2	N	201	HEM	CBA-CAA-C2A	-3.01	106.72	112.48
2	E	201	HEM	CMA-C3A-C4A	-2.96	123.91	128.46
2	E	201	HEM	CBD-CAD-C3D	-2.79	107.14	112.47
2	A	201	HEM	CMA-C3A-C4A	-2.58	124.49	128.46
2	B	201	HEM	CBD-CAD-C3D	-2.40	107.90	112.47
2	I	201	HEM	CBD-CAD-C3D	-2.35	107.98	112.47
2	F	201	HEM	CBA-CAA-C2A	-2.31	108.06	112.48
2	F	201	HEM	CMA-C3A-C4A	-2.31	124.91	128.46
2	A	201	HEM	CBD-CAD-C3D	-2.28	108.11	112.47
2	B	201	HEM	CBA-CAA-C2A	-2.26	108.16	112.48
2	N	201	HEM	CBD-CAD-C3D	-2.25	108.17	112.47
2	J	201	HEM	CBD-CAD-C3D	-2.24	108.19	112.47
2	I	201	HEM	CBA-CAA-C2A	-2.16	108.36	112.48
2	N	201	HEM	CMA-C3A-C4A	-2.14	125.17	128.46
2	B	201	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
2	J	201	HEM	CBA-CAA-C2A	-2.04	108.59	112.48
2	M	201	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
2	I	201	HEM	CMA-C3A-C4A	-2.00	125.39	128.46
2	N	201	HEM	CMC-C2C-C3C	2.14	128.86	124.89
2	B	201	HEM	C4A-C3A-C2A	2.21	108.53	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	HEM	10	0
2	B	201	HEM	11	0
2	E	201	HEM	11	0
2	F	201	HEM	13	0
2	I	201	HEM	11	0
2	J	201	HEM	11	0
2	M	201	HEM	11	0
2	N	201	HEM	12	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 ⓘ

### 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	131/131 (100%)	0.12	6 (4%) 33 31	12, 22, 44, 70	0
1	B	131/131 (100%)	0.04	3 (2%) 61 61	11, 20, 35, 63	0
1	E	131/131 (100%)	0.07	5 (3%) 41 40	12, 22, 43, 64	0
1	F	131/131 (100%)	0.06	4 (3%) 49 48	11, 18, 35, 56	0
1	I	131/131 (100%)	0.76	15 (11%) 5 5	17, 32, 51, 63	0
1	J	131/131 (100%)	0.19	5 (3%) 41 40	14, 23, 43, 58	0
1	M	131/131 (100%)	1.00	23 (17%) 2 1	19, 35, 60, 71	0
1	N	131/131 (100%)	0.23	4 (3%) 49 48	13, 24, 43, 61	0
All	All	1048/1048 (100%)	0.31	65 (6%) 21 20	11, 24, 49, 71	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	ALA	19.1
1	N	1	ALA	10.8
1	M	1	ALA	10.1
1	J	1	ALA	10.1
1	F	1	ALA	9.7
1	B	1	ALA	8.6
1	A	1	ALA	8.3
1	E	1	ALA	7.6
1	M	107	ALA	7.2
1	B	67	GLY	5.9
1	I	30	LEU	5.8
1	I	112	THR	5.2
1	I	2	GLY	5.0
1	M	78	PHE	4.4
1	M	112	THR	4.3
1	N	2	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	110	VAL	4.2
1	F	68	ASP	4.1
1	M	2	GLY	3.9
1	A	104	THR	3.7
1	I	68	ASP	3.6
1	J	68	ASP	3.6
1	N	67	GLY	3.5
1	A	102	ALA	3.5
1	B	68	ASP	3.5
1	M	68	ASP	3.4
1	A	131	LYS	3.3
1	M	82	GLU	3.3
1	I	67	GLY	3.3
1	M	67	GLY	3.3
1	M	28	ALA	3.3
1	I	78	PHE	3.2
1	M	99	ALA	3.2
1	M	81	MET	3.1
1	J	67	GLY	3.0
1	I	109	ALA	2.9
1	F	67	GLY	2.9
1	F	108	GLU	2.8
1	M	108	GLU	2.8
1	I	110	VAL	2.7
1	I	108	GLU	2.7
1	M	101	VAL	2.7
1	E	104	THR	2.7
1	E	131	LYS	2.7
1	E	102	ALA	2.6
1	I	60	PRO	2.6
1	N	68	ASP	2.5
1	I	113	ALA	2.5
1	J	2	GLY	2.5
1	M	114	PHE	2.5
1	M	92	VAL	2.4
1	M	61	GLY	2.4
1	M	109	ALA	2.4
1	M	33	GLU	2.4
1	M	34	TYR	2.3
1	A	107	ALA	2.3
1	M	32	GLY	2.3
1	I	104	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	66	VAL	2.2
1	E	68	ASP	2.2
1	A	68	ASP	2.2
1	M	5	PRO	2.2
1	I	116	ASP	2.2
1	J	34	TYR	2.1
1	I	107	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	B	201	43/43	0.98	0.11	0.72	10,12,18,28	0
2	HEM	F	201	43/43	0.98	0.10	0.65	11,12,20,30	0
2	HEM	N	201	43/43	0.98	0.10	0.61	10,13,16,22	0
2	HEM	A	201	43/43	0.95	0.11	0.30	12,20,29,42	0
2	HEM	E	201	43/43	0.96	0.10	0.07	16,19,27,35	0
2	HEM	J	201	43/43	0.98	0.09	-0.17	13,16,18,20	0
2	HEM	I	201	43/43	0.97	0.09	-0.51	18,21,26,35	0
2	HEM	M	201	43/43	0.97	0.09	-0.70	18,23,30,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.