



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:43 AM GMT

PDB ID : 2RGZ  
Title : Ensemble refinement of the protein crystal structure of human heme oxygenase-2 C127A (HO-2) with bound heme  
Authors : Bianchetti, C.M.; Bingman, C.A.; Bitto, E.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-10-05  
Resolution : 2.61 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

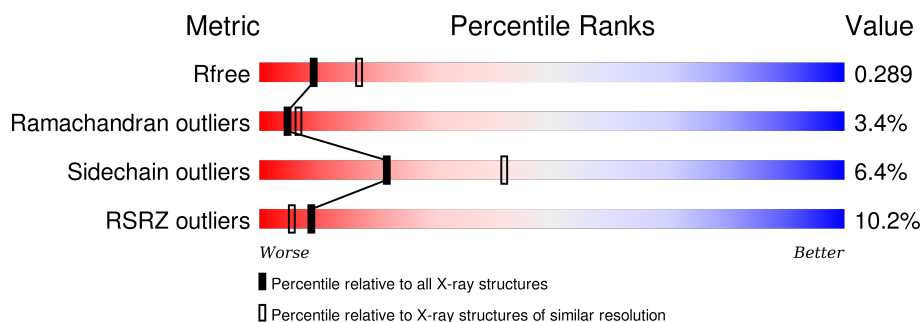
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	91344	2700 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	1-A	264	<div> <div>3%</div> <div>77%</div> <div>5%</div> <div>19%</div> </div>
1	1-B	264	<div> <div>15%</div> <div>76%</div> <div>7%</div> <div>17%</div> </div>
1	10-A	264	<div> <div>3%</div> <div>77%</div> <div>•</div> <div>19%</div> </div>
1	10-B	264	<div> <div>15%</div> <div>77%</div> <div>6%</div> <div>•</div> <div>17%</div> </div>
1	11-A	264	<div> <div>3%</div> <div>75%</div> <div>6%</div> <div>19%</div> </div>
1	11-B	264	<div> <div>15%</div> <div>77%</div> <div>6%</div> <div>17%</div> </div>
1	12-A	264	<div> <div>3%</div> <div>78%</div> <div>•</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
1	12-B	264	
1	13-A	264	
1	13-B	264	
1	14-A	264	
1	14-B	264	
1	15-A	264	
1	15-B	264	
1	16-A	264	
1	16-B	264	
1	2-A	264	
1	2-B	264	
1	3-A	264	
1	3-B	264	
1	4-A	264	
1	4-B	264	
1	5-A	264	
1	5-B	264	
1	6-A	264	
1	6-B	264	
1	7-A	264	
1	7-B	264	
1	8-A	264	
1	8-B	264	
1	9-A	264	
1	9-B	264	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58291 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 Heme oxygenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	2-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	3-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	4-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	5-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	6-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	7-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	8-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	9-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	10-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	11-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	12-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	13-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	14-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	15-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			
1	16-A	214	Total	C	N	O	S	0	0	0
			1758	1118	299	333	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	2-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	3-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	4-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	5-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	6-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	7-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	8-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	9-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	10-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	11-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	12-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	13-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	14-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	15-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			
1	16-B	219	Total	C	N	O	S	0	0	0
			1794	1140	304	342	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	CYS	ENGINEERED	UNP P30519
B	127	ALA	CYS	ENGINEERED	UNP P30519

- 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	1-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	2-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	3-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	4-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	5-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	6-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	7-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	8-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	9-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	10-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	11-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	12-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	13-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	14-A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	16-A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	1-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	2-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	3-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	4-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	5-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	6-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	7-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	8-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	9-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	10-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	11-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	12-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	13-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	14-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	15-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	16-B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	49	Total	O	0	0
			49	49		

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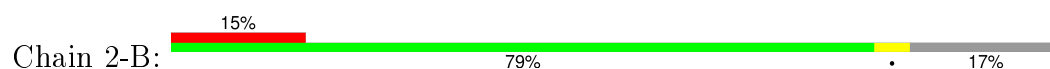
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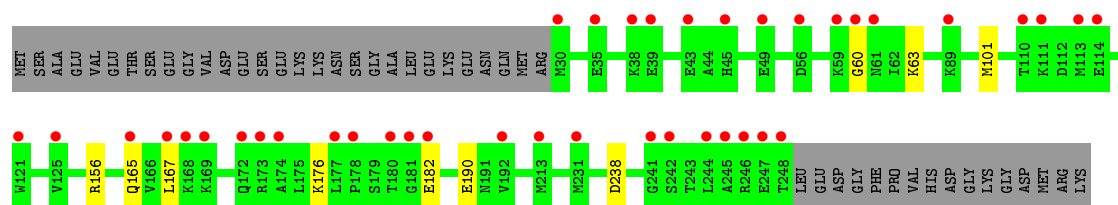
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-B	34	Total	O	0	0
			34	34		



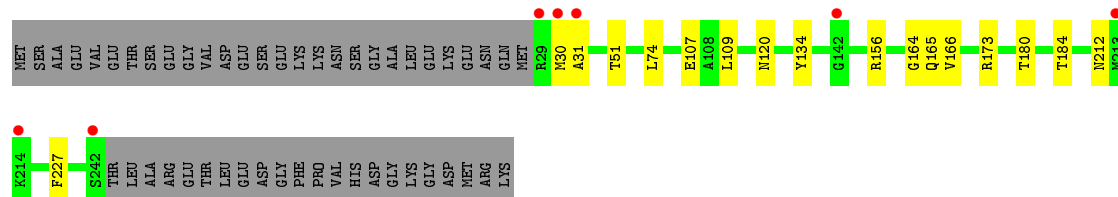
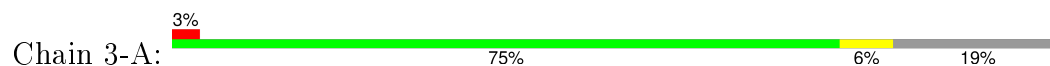


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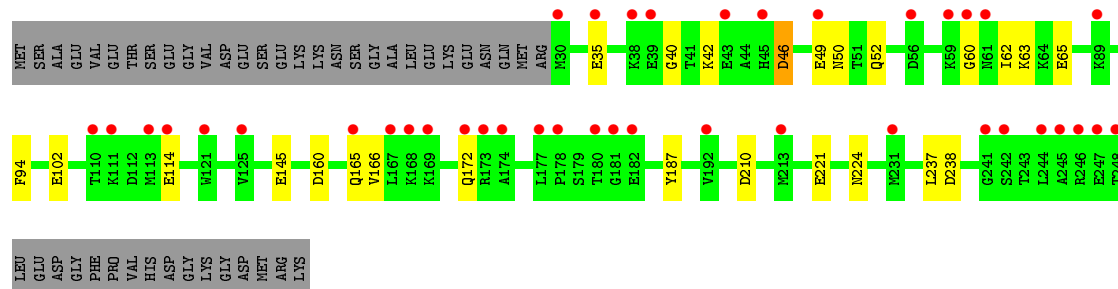
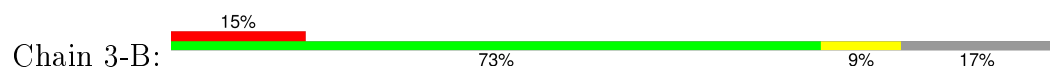




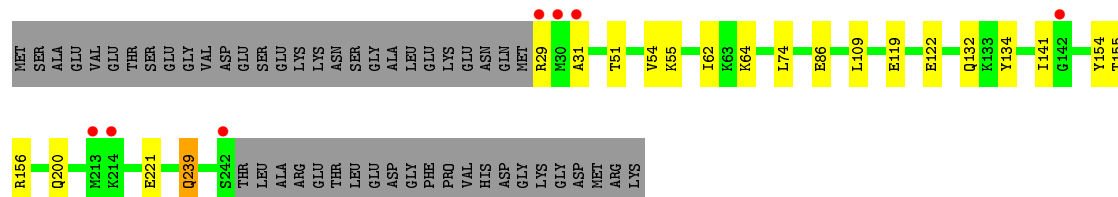
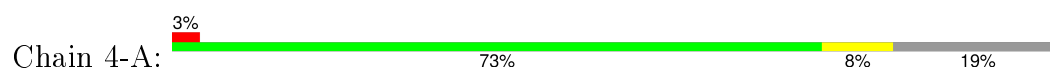
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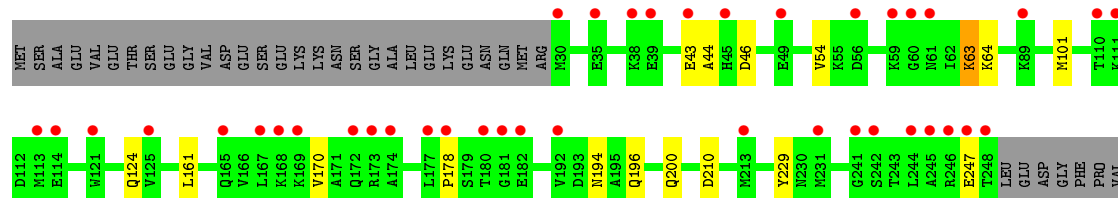
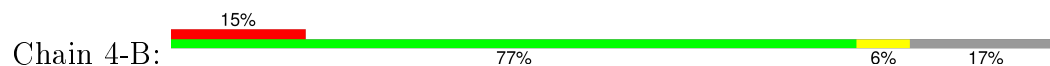
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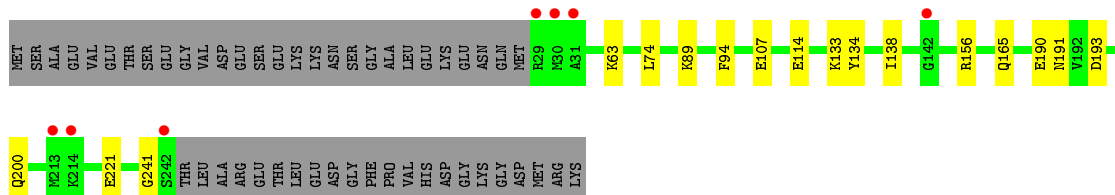
- Molecule 1: Heme oxygenase 2




HIS  
ASP  
GLY  
LYS  
GLY  
ASP  
MET  
ARG  
LYS

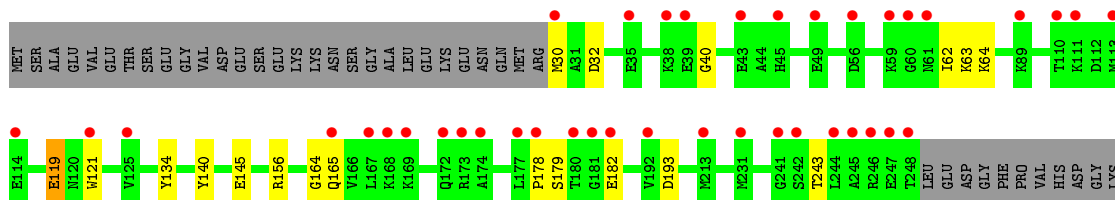
- Molecule 1: Heme oxygenase 2

Chain 5-A: 




- Molecule 1: Heme oxygenase 2

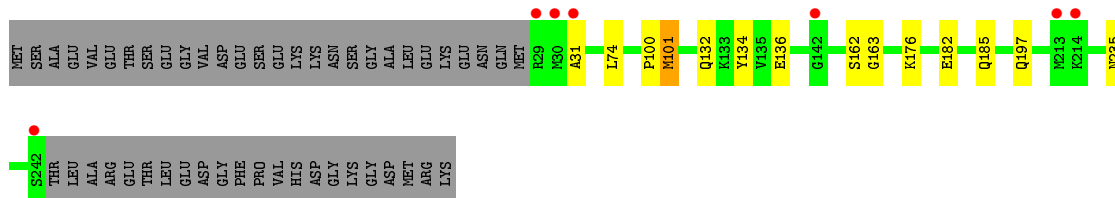
Chain 5-B: 




GLY  
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ARG  
LYS

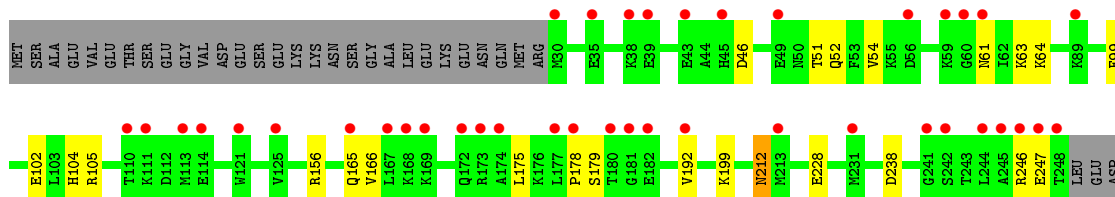
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Chain 6-A: 



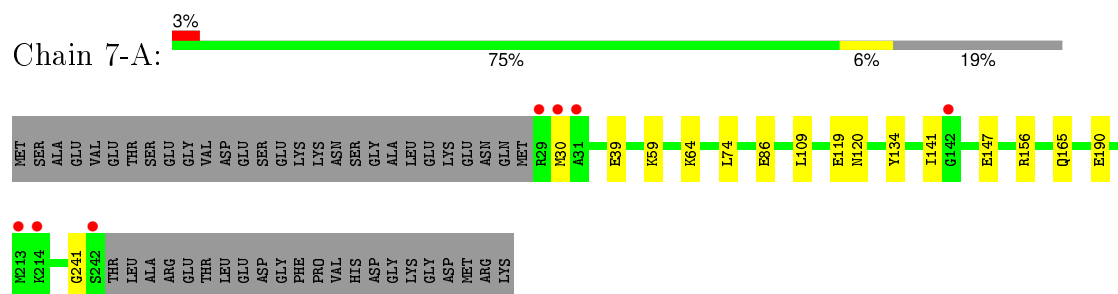
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Chain 6-B: 

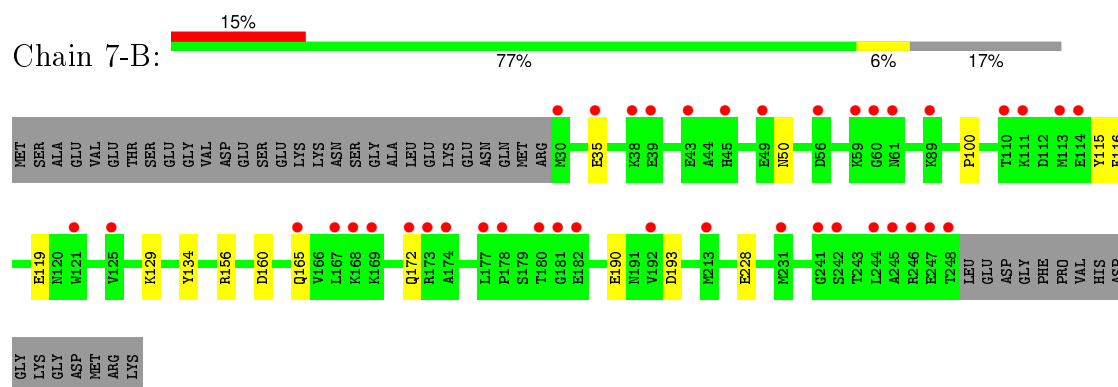


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PRO  
VAL  
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GLY  
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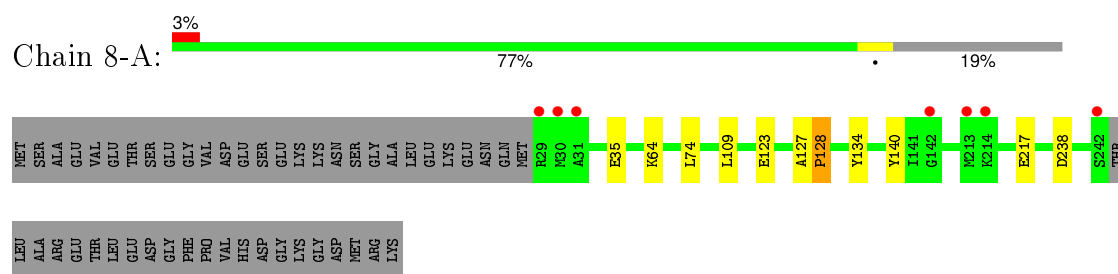
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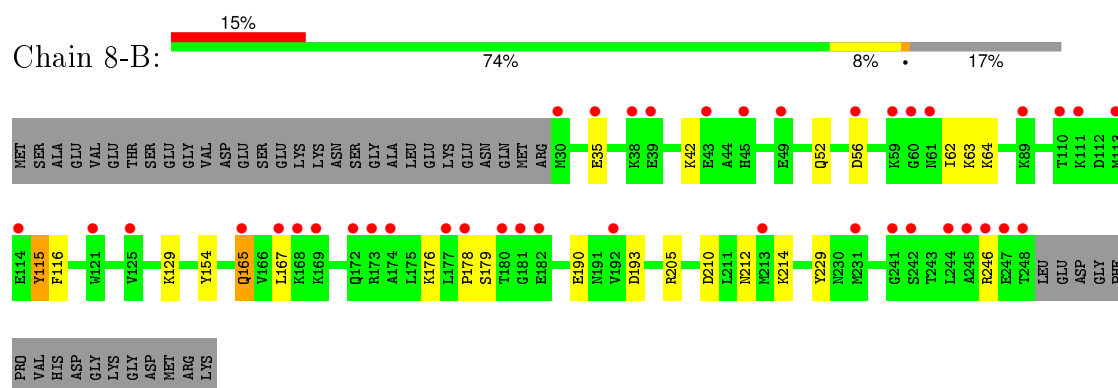
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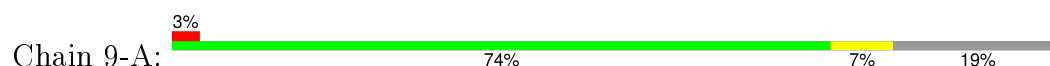
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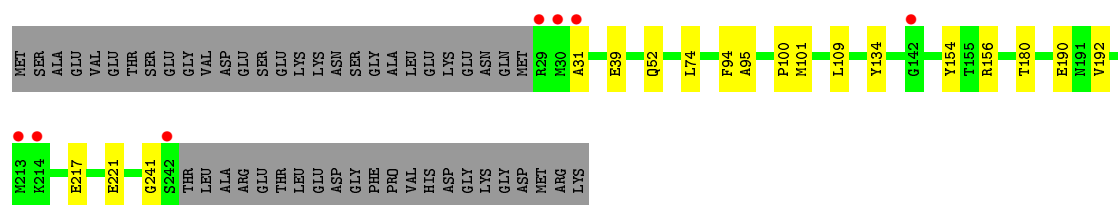


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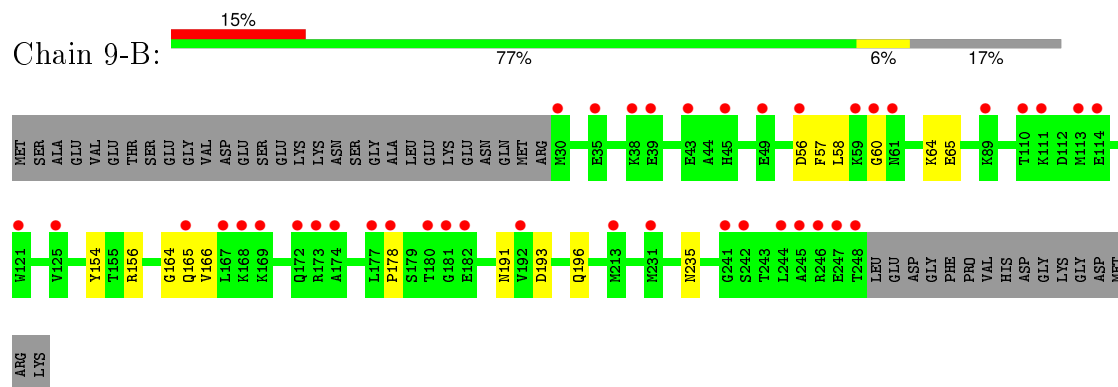


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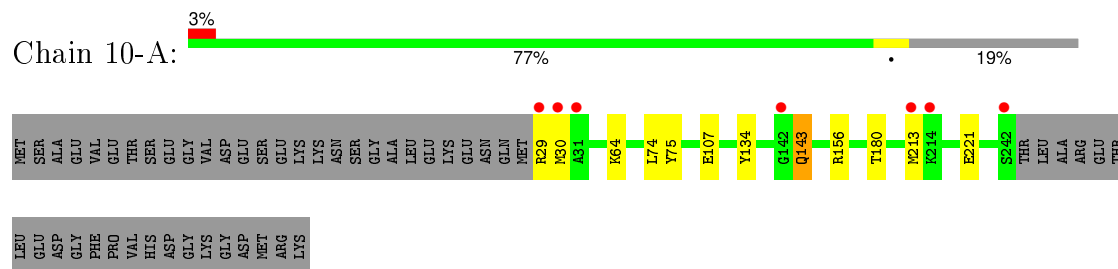




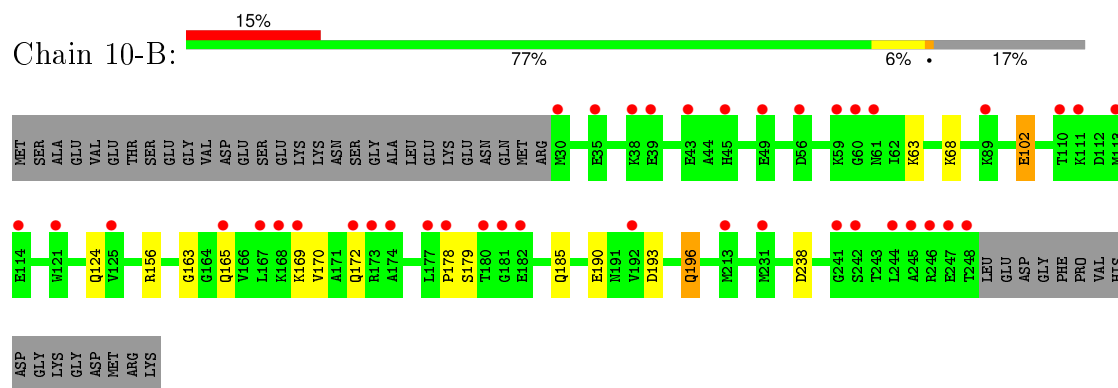
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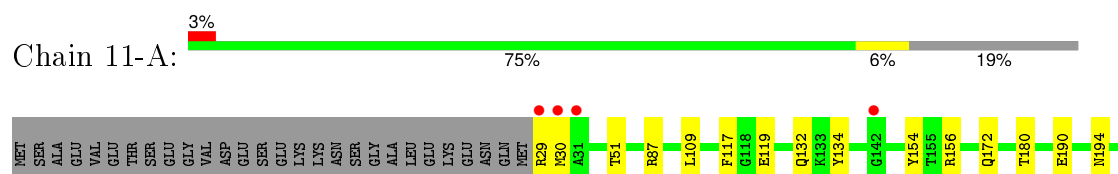
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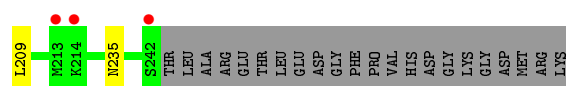


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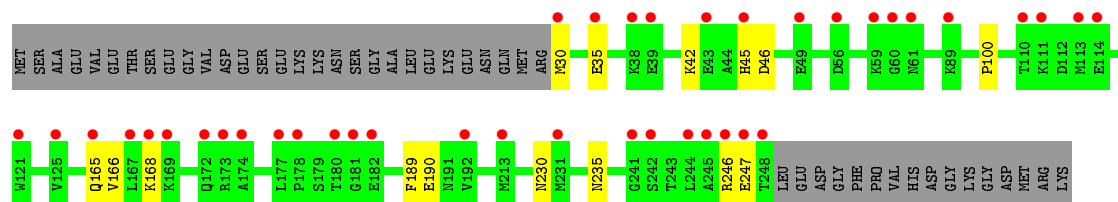
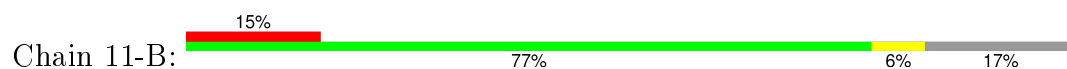


- Molecule 1: Heme oxygenase 2

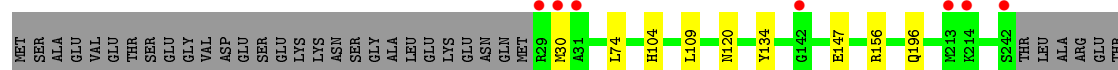
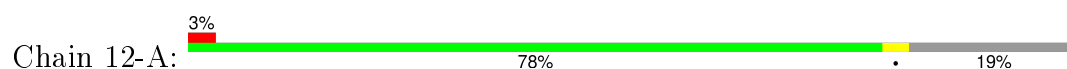




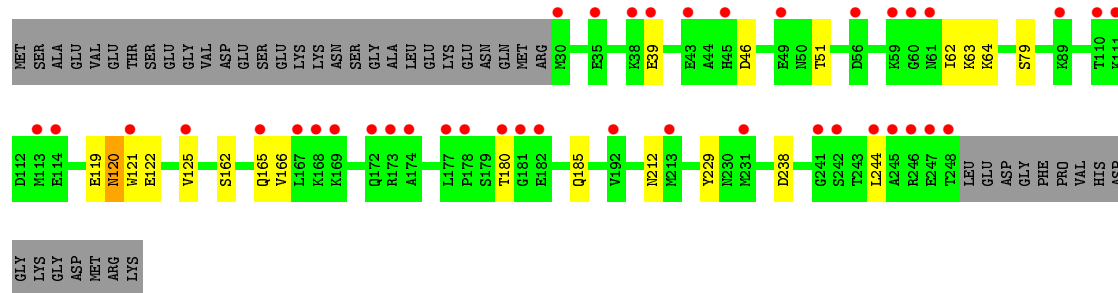
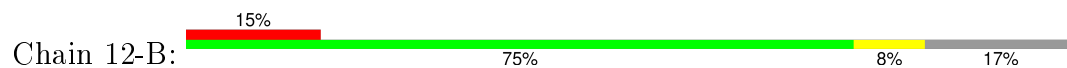
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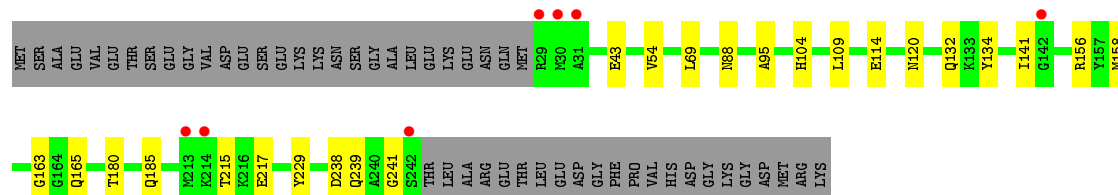
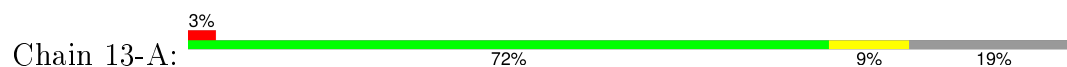
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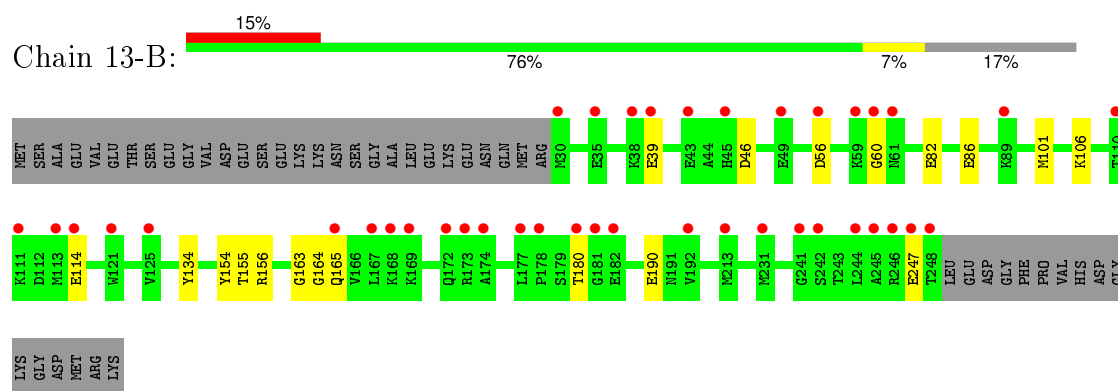
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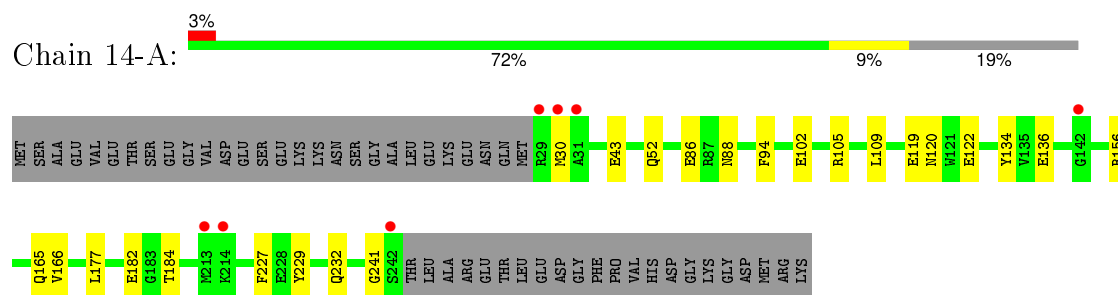
- Molecule 1: Heme oxygenase 2



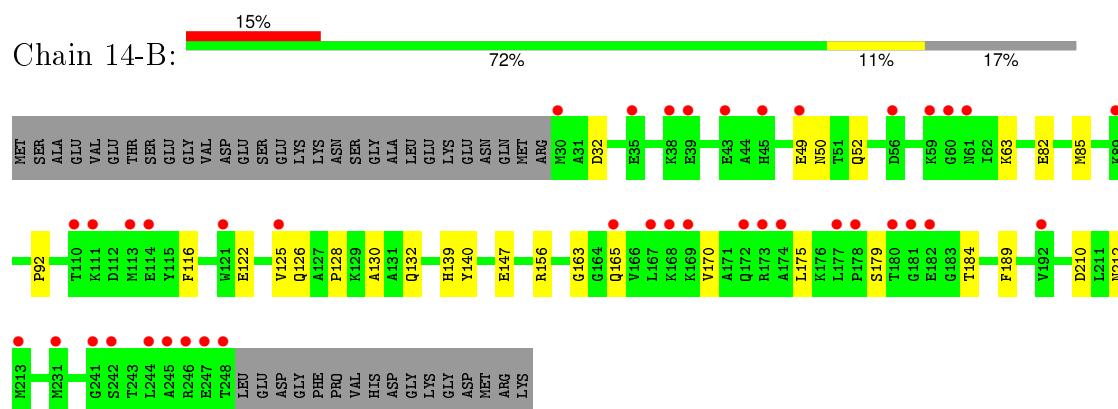
- Molecule 1: Heme oxygenase 2



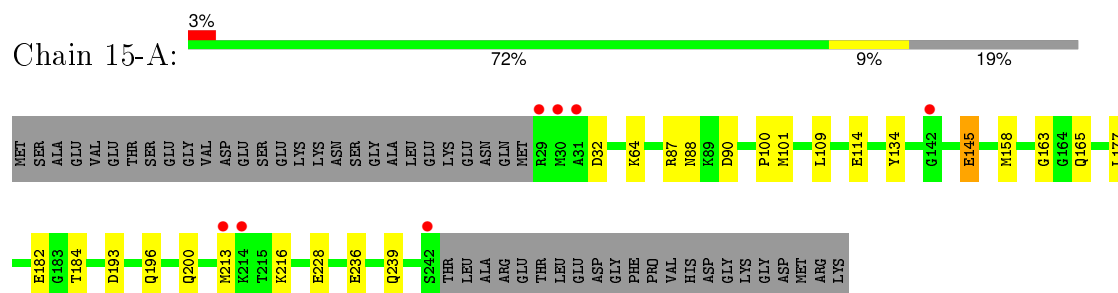
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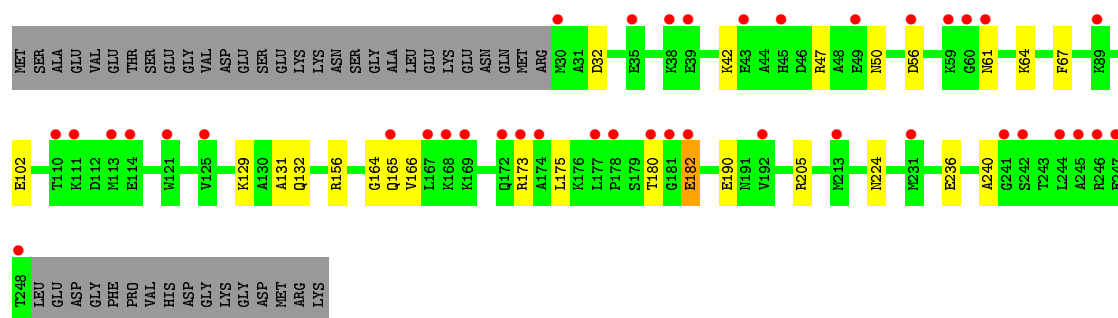


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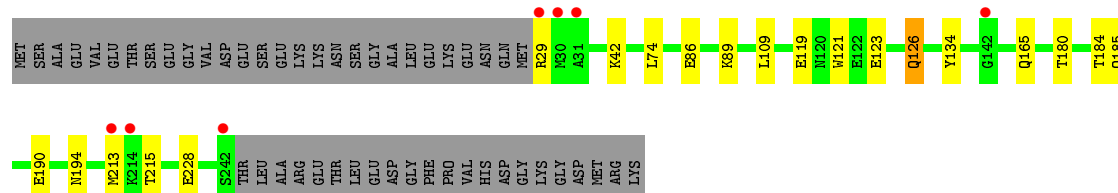
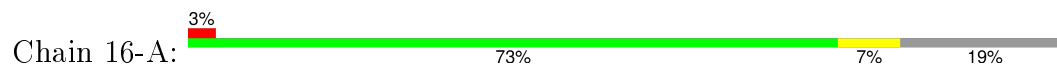


- Molecule 1: Heme oxygenase 2

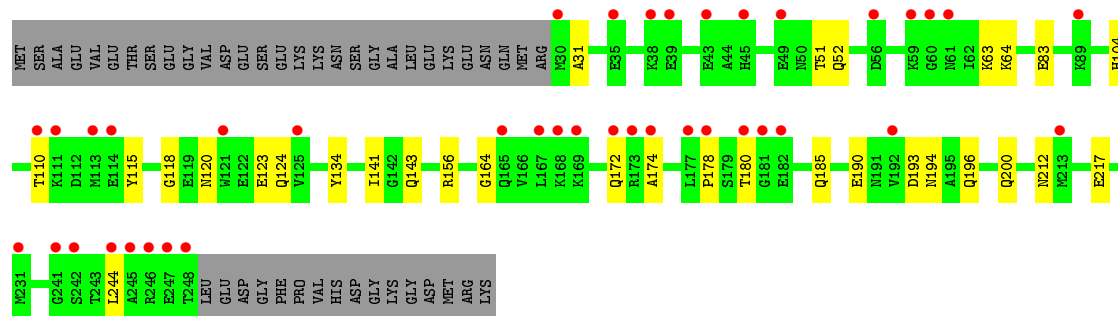
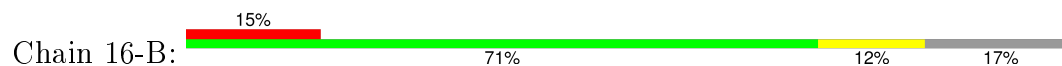




- Molecule 1: Heme oxygenase 2



- Molecule 1: Heme oxygenase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.98Å 85.09Å 97.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.02 – 2.61 39.02 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.02-2.61) 99.4 (39.02-2.61)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.161 , 0.249 0.211 , 0.289	Depositor DCC
$R_{free}$ test set	1005 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 158.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 19515 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	58291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1-A	0.43	0/1794	0.57	0/2410
1	1-B	0.39	0/1830	0.54	0/2460
1	2-A	0.43	0/1794	0.56	0/2410
1	2-B	0.40	0/1830	0.54	0/2460
1	3-A	0.43	0/1794	0.57	0/2410
1	3-B	0.39	0/1830	0.56	0/2460
1	4-A	0.44	0/1794	0.58	0/2410
1	4-B	0.39	0/1830	0.56	0/2460
1	5-A	0.43	0/1794	0.58	1/2410 (0.0%)
1	5-B	0.39	0/1830	0.54	0/2460
1	6-A	0.42	0/1794	0.56	0/2410
1	6-B	0.40	0/1830	0.55	0/2460
1	7-A	0.42	0/1794	0.57	0/2410
1	7-B	0.39	0/1830	0.54	0/2460
1	8-A	0.44	0/1794	0.57	0/2410
1	8-B	0.39	0/1830	0.55	0/2460
1	9-A	0.43	0/1794	0.57	0/2410
1	9-B	0.39	0/1830	0.54	0/2460
1	10-A	0.43	0/1794	0.57	0/2410
1	10-B	0.40	0/1830	0.55	0/2460
1	11-A	0.43	0/1794	0.56	0/2410
1	11-B	0.40	0/1830	0.55	0/2460
1	12-A	0.43	0/1794	0.55	0/2410
1	12-B	0.40	0/1830	0.55	0/2460
1	13-A	0.47	0/1794	0.63	0/2410
1	13-B	0.43	0/1830	0.55	0/2460
1	14-A	0.48	0/1794	0.61	0/2410
1	14-B	0.44	0/1830	0.58	0/2460
1	15-A	0.50	0/1794	0.64	0/2410
1	15-B	0.43	0/1830	0.60	0/2460
1	16-A	0.49	0/1794	0.64	0/2410
1	16-B	0.42	0/1830	0.57	0/2460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.42	0/57984	0.57	1/77920 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	5-A	156	ARG	NE-CZ-NH2	-5.48	117.56	120.30

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	1-A	1758	0	1717	0	0
1	1-B	1794	0	1753	0	0
1	2-A	1758	0	1717	0	0
1	2-B	1794	0	1753	0	0
1	3-A	1758	0	1717	0	0
1	3-B	1794	0	1753	0	0
1	4-A	1758	0	1717	0	0
1	4-B	1794	0	1753	0	0
1	5-A	1758	0	1717	0	0
1	5-B	1794	0	1753	0	0
1	6-A	1758	0	1717	0	0
1	6-B	1794	0	1753	0	0
1	7-A	1758	0	1717	0	0
1	7-B	1794	0	1753	0	0
1	8-A	1758	0	1717	0	0
1	8-B	1794	0	1753	0	0
1	9-A	1758	0	1717	0	0
1	9-B	1794	0	1753	0	0
1	10-A	1758	0	1717	0	0
1	10-B	1794	0	1753	0	0
1	11-A	1758	0	1717	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	11-B	1794	0	1753	0	0
1	12-A	1758	0	1717	0	0
1	12-B	1794	0	1753	0	0
1	13-A	1758	0	1717	0	0
1	13-B	1794	0	1753	0	0
1	14-A	1758	0	1717	0	0
1	14-B	1794	0	1753	0	0
1	15-A	1758	0	1717	0	0
1	15-B	1794	0	1753	0	0
1	16-A	1758	0	1717	0	0
1	16-B	1794	0	1753	0	0
2	1-A	43	0	30	0	0
2	1-B	43	0	30	0	0
2	2-A	43	0	30	0	0
2	2-B	43	0	30	0	0
2	3-A	43	0	30	0	0
2	3-B	43	0	30	0	0
2	4-A	43	0	30	0	0
2	4-B	43	0	30	0	0
2	5-A	43	0	30	0	0
2	5-B	43	0	30	0	0
2	6-A	43	0	30	0	0
2	6-B	43	0	30	0	0
2	7-A	43	0	30	0	0
2	7-B	43	0	30	0	0
2	8-A	43	0	30	0	0
2	8-B	43	0	30	0	0
2	9-A	43	0	30	0	0
2	9-B	43	0	30	0	0
2	10-A	43	0	30	0	0
2	10-B	43	0	30	0	0
2	11-A	43	0	30	0	0
2	11-B	43	0	30	0	0
2	12-A	43	0	30	0	0
2	12-B	43	0	30	0	0
2	13-A	43	0	30	0	0
2	13-B	43	0	30	0	0
2	14-A	43	0	30	0	0
2	14-B	43	0	30	0	0
2	15-A	43	0	30	0	0
2	15-B	43	0	30	0	0
2	16-A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	16-B	43	0	30	0	0
3	1-A	49	0	0	0	0
3	1-B	34	0	0	0	0
All	All	58291	0	56480	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	212/264 (80%)	185 (87%)	23 (11%)	4 (2%)	10	18
1	1-B	217/264 (82%)	190 (88%)	19 (9%)	8 (4%)	4	5
1	2-A	212/264 (80%)	184 (87%)	23 (11%)	5 (2%)	7	12
1	2-B	217/264 (82%)	183 (84%)	30 (14%)	4 (2%)	11	20
1	3-A	212/264 (80%)	192 (91%)	17 (8%)	3 (1%)	14	26
1	3-B	217/264 (82%)	174 (80%)	33 (15%)	10 (5%)	3	3
1	4-A	212/264 (80%)	188 (89%)	17 (8%)	7 (3%)	5	7
1	4-B	217/264 (82%)	175 (81%)	35 (16%)	7 (3%)	5	7
1	5-A	212/264 (80%)	189 (89%)	18 (8%)	5 (2%)	7	12
1	5-B	217/264 (82%)	186 (86%)	22 (10%)	9 (4%)	3	4
1	6-A	212/264 (80%)	181 (85%)	25 (12%)	6 (3%)	6	9
1	6-B	217/264 (82%)	167 (77%)	38 (18%)	12 (6%)	2	2
1	7-A	212/264 (80%)	182 (86%)	26 (12%)	4 (2%)	10	18
1	7-B	217/264 (82%)	183 (84%)	28 (13%)	6 (3%)	6	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-A	212/264 (80%)	187 (88%)	21 (10%)	4 (2%)	10	18
1	8-B	217/264 (82%)	183 (84%)	21 (10%)	13 (6%)	2	2
1	9-A	212/264 (80%)	179 (84%)	24 (11%)	9 (4%)	3	4
1	9-B	217/264 (82%)	184 (85%)	23 (11%)	10 (5%)	3	3
1	10-A	212/264 (80%)	189 (89%)	20 (9%)	3 (1%)	14	26
1	10-B	217/264 (82%)	185 (85%)	23 (11%)	9 (4%)	3	4
1	11-A	212/264 (80%)	185 (87%)	24 (11%)	3 (1%)	14	26
1	11-B	217/264 (82%)	184 (85%)	28 (13%)	5 (2%)	8	13
1	12-A	212/264 (80%)	198 (93%)	12 (6%)	2 (1%)	21	41
1	12-B	217/264 (82%)	174 (80%)	33 (15%)	10 (5%)	3	3
1	13-A	212/264 (80%)	186 (88%)	21 (10%)	5 (2%)	7	12
1	13-B	217/264 (82%)	182 (84%)	26 (12%)	9 (4%)	3	4
1	14-A	212/264 (80%)	176 (83%)	30 (14%)	6 (3%)	6	9
1	14-B	217/264 (82%)	165 (76%)	35 (16%)	17 (8%)	1	1
1	15-A	212/264 (80%)	176 (83%)	26 (12%)	10 (5%)	3	3
1	15-B	217/264 (82%)	171 (79%)	36 (17%)	10 (5%)	3	3
1	16-A	212/264 (80%)	177 (84%)	32 (15%)	3 (1%)	14	26
1	16-B	217/264 (82%)	172 (79%)	28 (13%)	17 (8%)	1	1
All	All	6864/8448 (81%)	5812 (85%)	817 (12%)	235 (3%)	5	7

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	64	LYS
1	2-A	64	LYS
1	3-B	46	ASP
1	3-B	52	GLN
1	3-B	65	GLU
1	4-A	154	TYR
1	4-A	239	GLN
1	4-B	44	ALA
1	5-B	62	ILE
1	5-B	64	LYS
1	5-B	119	GLU
1	6-A	31	ALA
1	6-A	100	PRO

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Mol	Chain	Res	Type
1	6-A	101	MET
1	6-B	247	GLU
1	7-A	64	LYS
1	8-A	64	LYS
1	8-A	127	ALA
1	8-A	128	PRO
1	8-B	62	ILE
1	8-B	64	LYS
1	8-B	154	TYR
1	9-A	31	ALA
1	9-A	100	PRO
1	9-A	101	MET
1	9-B	166	VAL
1	10-A	64	LYS
1	12-B	51	THR
1	12-B	64	LYS
1	12-B	120	ASN
1	12-B	166	VAL
1	14-B	50	ASN
1	15-A	100	PRO
1	15-B	164	GLY
1	15-B	182	GLU
1	16-A	121	TRP
1	16-B	31	ALA
1	16-B	64	LYS
1	16-B	120	ASN
1	16-B	124	GLN
1	16-B	193	ASP
1	1-A	125	VAL
1	1-B	52	GLN
1	1-B	193	ASP
1	2-A	94	PHE
1	2-A	155	THR
1	2-B	176	LYS
1	2-B	190	GLU
1	3-A	31	ALA
1	3-A	164	GLY
1	3-A	166	VAL
1	3-B	42	LYS
1	4-A	31	ALA
1	4-A	155	THR
1	5-A	94	PHE

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Mol	Chain	Res	Type
1	5-A	191	ASN
1	5-B	179	SER
1	6-A	162	SER
1	6-B	64	LYS
1	6-B	104	HIS
1	6-B	105	ARG
1	6-B	175	LEU
1	6-B	212	ASN
1	7-A	59	LYS
1	7-A	241	GLY
1	8-B	52	GLN
1	8-B	165	GLN
1	9-A	190	GLU
1	9-A	241	GLY
1	9-B	154	TYR
1	10-A	143	GLN
1	10-B	68	LYS
1	10-B	179	SER
1	11-B	166	VAL
1	11-B	247	GLU
1	12-B	119	GLU
1	12-B	122	GLU
1	13-A	104	HIS
1	13-B	154	TYR
1	13-B	164	GLY
1	13-B	190	GLU
1	13-B	247	GLU
1	14-A	182	GLU
1	14-B	132	GLN
1	15-A	64	LYS
1	15-B	50	ASN
1	15-B	64	LYS
1	15-B	131	ALA
1	15-B	165	GLN
1	16-B	104	HIS
1	16-B	115	TYR
1	16-B	141	ILE
1	16-B	164	GLY
1	16-B	172	GLN
1	1-A	76	PHE
1	1-A	104	HIS
1	1-A	196	GLN

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Mol	Chain	Res	Type
1	1-B	60	GLY
1	2-A	154	TYR
1	2-B	167	LEU
1	3-B	60	GLY
1	3-B	62	ILE
1	5-A	190	GLU
1	5-B	182	GLU
1	6-B	179	SER
1	7-B	172	GLN
1	8-B	42	LYS
1	8-B	179	SER
1	8-B	190	GLU
1	9-A	94	PHE
1	9-B	58	LEU
1	9-B	64	LYS
1	9-B	65	GLU
1	10-B	163	GLY
1	10-B	178	PRO
1	10-B	196	GLN
1	11-B	100	PRO
1	12-B	121	TRP
1	12-B	162	SER
1	13-A	163	GLY
1	13-A	185	GLN
1	13-B	60	GLY
1	14-B	116	PHE
1	14-B	139	HIS
1	14-B	175	LEU
1	15-A	101	MET
1	15-B	42	LYS
1	15-B	132	GLN
1	15-B	240	ALA
1	16-B	51	THR
1	16-B	118	GLY
1	16-B	174	ALA
1	16-B	180	THR
1	16-B	190	GLU
1	1-B	168	LYS
1	1-B	190	GLU
1	3-B	187	TYR
1	4-A	54	VAL
1	4-B	63	LYS

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Mol	Chain	Res	Type
1	4-B	247	GLU
1	6-B	52	GLN
1	7-A	190	GLU
1	7-B	119	GLU
1	8-B	115	TYR
1	8-B	214	LYS
1	9-A	154	TYR
1	9-B	60	GLY
1	9-B	196	GLN
1	9-B	235	ASN
1	10-B	169	LYS
1	11-A	194	ASN
1	11-B	235	ASN
1	12-A	104	HIS
1	12-A	196	GLN
1	12-B	180	THR
1	13-A	95	ALA
1	13-B	155	THR
1	13-B	180	THR
1	14-A	94	PHE
1	14-A	177	LEU
1	14-B	49	GLU
1	14-B	179	SER
1	14-B	212	ASN
1	15-A	90	ASP
1	15-A	163	GLY
1	15-A	182	GLU
1	16-A	119	GLU
1	16-B	52	GLN
1	1-B	42	LYS
1	1-B	106	LYS
1	2-A	164	GLY
1	3-B	40	GLY
1	4-A	55	LYS
1	4-A	64	LYS
1	5-A	138	ILE
1	5-B	178	PRO
1	5-B	243	THR
1	6-A	176	LYS
1	7-B	50	ASN
1	7-B	129	LYS
1	7-B	190	GLU

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Mol	Chain	Res	Type
1	8-A	140	TYR
1	8-B	116	PHE
1	8-B	176	LYS
1	10-B	170	VAL
1	11-A	209	LEU
1	11-B	168	LYS
1	14-A	136	GLU
1	14-B	85	MET
1	14-B	130	ALA
1	14-B	163	GLY
1	15-A	145	GLU
1	15-A	196	GLN
1	16-A	126	GLN
1	3-B	94	PHE
1	4-B	54	VAL
1	4-B	64	LYS
1	4-B	178	PRO
1	6-B	99	PHE
1	6-B	246	ARG
1	8-B	178	PRO
1	9-A	192	VAL
1	9-B	164	GLY
1	9-B	178	PRO
1	10-A	75	TYR
1	10-B	102	GLU
1	10-B	193	ASP
1	11-A	154	TYR
1	13-B	106	LYS
1	13-B	163	GLY
1	14-A	241	GLY
1	14-B	125	VAL
1	14-B	126	GLN
1	14-B	140	TYR
1	14-B	170	VAL
1	15-A	87	ARG
1	16-B	178	PRO
1	5-A	241	GLY
1	5-B	40	GLY
1	6-B	178	PRO
1	13-A	241	GLY
1	14-B	92	PRO
1	15-B	166	VAL

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Mol	Chain	Res	Type
1	5-B	164	GLY
1	9-A	95	ALA
1	14-B	128	PRO
1	2-B	60	GLY
1	4-B	170	VAL
1	6-B	192	VAL
1	3-B	166	VAL
1	6-A	163	GLY
1	12-B	125	VAL
1	14-A	166	VAL
1	15-A	177	LEU
1	7-B	100	PRO

### 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	1-A	182/224 (81%)	174 (96%)	8 (4%)	35	62
1	1-B	186/224 (83%)	176 (95%)	10 (5%)	27	51
1	2-A	182/224 (81%)	174 (96%)	8 (4%)	35	62
1	2-B	186/224 (83%)	180 (97%)	6 (3%)	46	74
1	3-A	182/224 (81%)	168 (92%)	14 (8%)	16	30
1	3-B	186/224 (83%)	170 (91%)	16 (9%)	13	24
1	4-A	182/224 (81%)	167 (92%)	15 (8%)	14	27
1	4-B	186/224 (83%)	175 (94%)	11 (6%)	24	46
1	5-A	182/224 (81%)	171 (94%)	11 (6%)	24	45
1	5-B	186/224 (83%)	175 (94%)	11 (6%)	24	46
1	6-A	182/224 (81%)	173 (95%)	9 (5%)	31	56
1	6-B	186/224 (83%)	173 (93%)	13 (7%)	19	36
1	7-A	182/224 (81%)	170 (93%)	12 (7%)	21	39
1	7-B	186/224 (83%)	177 (95%)	9 (5%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	182/224 (81%)	174 (96%)	8 (4%)	35	62
1	8-B	186/224 (83%)	173 (93%)	13 (7%)	19	36
1	9-A	182/224 (81%)	173 (95%)	9 (5%)	31	56
1	9-B	186/224 (83%)	180 (97%)	6 (3%)	46	74
1	10-A	182/224 (81%)	172 (94%)	10 (6%)	27	50
1	10-B	186/224 (83%)	176 (95%)	10 (5%)	27	51
1	11-A	182/224 (81%)	168 (92%)	14 (8%)	16	30
1	11-B	186/224 (83%)	176 (95%)	10 (5%)	27	51
1	12-A	182/224 (81%)	175 (96%)	7 (4%)	40	68
1	12-B	186/224 (83%)	174 (94%)	12 (6%)	21	41
1	13-A	182/224 (81%)	163 (90%)	19 (10%)	9	15
1	13-B	186/224 (83%)	176 (95%)	10 (5%)	27	51
1	14-A	182/224 (81%)	164 (90%)	18 (10%)	10	17
1	14-B	186/224 (83%)	175 (94%)	11 (6%)	24	46
1	15-A	182/224 (81%)	166 (91%)	16 (9%)	12	23
1	15-B	186/224 (83%)	170 (91%)	16 (9%)	13	24
1	16-A	182/224 (81%)	164 (90%)	18 (10%)	10	17
1	16-B	186/224 (83%)	172 (92%)	14 (8%)	17	32
All	All	5888/7168 (82%)	5514 (94%)	374 (6%)	22	42

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	29	ARG
1	1-A	30	MET
1	1-A	74	LEU
1	1-A	109	LEU
1	1-A	114	GLU
1	1-A	134	TYR
1	1-A	143	GLN
1	1-A	156	ARG
1	1-B	32	ASP
1	1-B	51	THR
1	1-B	63	LYS
1	1-B	86	GLU
1	1-B	165	GLN

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Mol	Chain	Res	Type
1	1-B	205	ARG
1	1-B	210	ASP
1	1-B	222	GLU
1	1-B	229	TYR
1	1-B	232	GLN
1	2-A	74	LEU
1	2-A	120	ASN
1	2-A	134	TYR
1	2-A	141	ILE
1	2-A	147	GLU
1	2-A	156	ARG
1	2-A	160	ASP
1	2-A	180	THR
1	2-B	63	LYS
1	2-B	101	MET
1	2-B	156	ARG
1	2-B	165	GLN
1	2-B	182	GLU
1	2-B	238	ASP
1	3-A	30	MET
1	3-A	51	THR
1	3-A	74	LEU
1	3-A	107	GLU
1	3-A	109	LEU
1	3-A	120	ASN
1	3-A	134	TYR
1	3-A	156	ARG
1	3-A	165	GLN
1	3-A	173	ARG
1	3-A	180	THR
1	3-A	184	THR
1	3-A	212	ASN
1	3-A	227	PHE
1	3-B	35	GLU
1	3-B	46	ASP
1	3-B	49	GLU
1	3-B	50	ASN
1	3-B	63	LYS
1	3-B	102	GLU
1	3-B	114	GLU
1	3-B	145	GLU
1	3-B	160	ASP

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Mol	Chain	Res	Type
1	3-B	165	GLN
1	3-B	172	GLN
1	3-B	210	ASP
1	3-B	221	GLU
1	3-B	224	ASN
1	3-B	237	LEU
1	3-B	238	ASP
1	4-A	29	ARG
1	4-A	51	THR
1	4-A	62	ILE
1	4-A	74	LEU
1	4-A	86	GLU
1	4-A	109	LEU
1	4-A	119	GLU
1	4-A	122	GLU
1	4-A	132	GLN
1	4-A	134	TYR
1	4-A	141	ILE
1	4-A	156	ARG
1	4-A	200	GLN
1	4-A	221	GLU
1	4-A	239	GLN
1	4-B	43	GLU
1	4-B	46	ASP
1	4-B	63	LYS
1	4-B	101	MET
1	4-B	124	GLN
1	4-B	161	LEU
1	4-B	194	ASN
1	4-B	196	GLN
1	4-B	200	GLN
1	4-B	210	ASP
1	4-B	229	TYR
1	5-A	63	LYS
1	5-A	74	LEU
1	5-A	89	LYS
1	5-A	107	GLU
1	5-A	114	GLU
1	5-A	133	LYS
1	5-A	134	TYR
1	5-A	165	GLN
1	5-A	193	ASP

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Mol	Chain	Res	Type
1	5-A	200	GLN
1	5-A	221	GLU
1	5-B	30	MET
1	5-B	32	ASP
1	5-B	63	LYS
1	5-B	119	GLU
1	5-B	121	TRP
1	5-B	134	TYR
1	5-B	140	TYR
1	5-B	145	GLU
1	5-B	156	ARG
1	5-B	165	GLN
1	5-B	193	ASP
1	6-A	74	LEU
1	6-A	101	MET
1	6-A	132	GLN
1	6-A	134	TYR
1	6-A	136	GLU
1	6-A	182	GLU
1	6-A	185	GLN
1	6-A	197	GLN
1	6-A	235	ASN
1	6-B	46	ASP
1	6-B	51	THR
1	6-B	54	VAL
1	6-B	61	ASN
1	6-B	63	LYS
1	6-B	102	GLU
1	6-B	156	ARG
1	6-B	165	GLN
1	6-B	166	VAL
1	6-B	199	LYS
1	6-B	212	ASN
1	6-B	228	GLU
1	6-B	238	ASP
1	7-A	30	MET
1	7-A	39	GLU
1	7-A	74	LEU
1	7-A	86	GLU
1	7-A	109	LEU
1	7-A	119	GLU
1	7-A	120	ASN

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Mol	Chain	Res	Type
1	7-A	134	TYR
1	7-A	141	ILE
1	7-A	147	GLU
1	7-A	156	ARG
1	7-A	165	GLN
1	7-B	35	GLU
1	7-B	115	TYR
1	7-B	116	PHE
1	7-B	134	TYR
1	7-B	156	ARG
1	7-B	160	ASP
1	7-B	165	GLN
1	7-B	193	ASP
1	7-B	228	GLU
1	8-A	35	GLU
1	8-A	74	LEU
1	8-A	109	LEU
1	8-A	123	GLU
1	8-A	128	PRO
1	8-A	134	TYR
1	8-A	217	GLU
1	8-A	238	ASP
1	8-B	35	GLU
1	8-B	56	ASP
1	8-B	63	LYS
1	8-B	115	TYR
1	8-B	129	LYS
1	8-B	165	GLN
1	8-B	167	LEU
1	8-B	193	ASP
1	8-B	205	ARG
1	8-B	210	ASP
1	8-B	212	ASN
1	8-B	229	TYR
1	8-B	246	ARG
1	9-A	39	GLU
1	9-A	52	GLN
1	9-A	74	LEU
1	9-A	109	LEU
1	9-A	134	TYR
1	9-A	156	ARG
1	9-A	180	THR

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Mol	Chain	Res	Type
1	9-A	217	GLU
1	9-A	221	GLU
1	9-B	56	ASP
1	9-B	57	PHE
1	9-B	156	ARG
1	9-B	165	GLN
1	9-B	191	ASN
1	9-B	193	ASP
1	10-A	29	ARG
1	10-A	30	MET
1	10-A	74	LEU
1	10-A	107	GLU
1	10-A	134	TYR
1	10-A	143	GLN
1	10-A	156	ARG
1	10-A	180	THR
1	10-A	213	MET
1	10-A	221	GLU
1	10-B	63	LYS
1	10-B	102	GLU
1	10-B	124	GLN
1	10-B	156	ARG
1	10-B	165	GLN
1	10-B	172	GLN
1	10-B	185	GLN
1	10-B	190	GLU
1	10-B	196	GLN
1	10-B	238	ASP
1	11-A	29	ARG
1	11-A	30	MET
1	11-A	51	THR
1	11-A	87	ARG
1	11-A	109	LEU
1	11-A	117	PHE
1	11-A	119	GLU
1	11-A	132	GLN
1	11-A	134	TYR
1	11-A	156	ARG
1	11-A	172	GLN
1	11-A	180	THR
1	11-A	190	GLU
1	11-A	235	ASN

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Mol	Chain	Res	Type
1	11-B	30	MET
1	11-B	35	GLU
1	11-B	42	LYS
1	11-B	45	HIS
1	11-B	46	ASP
1	11-B	165	GLN
1	11-B	189	PHE
1	11-B	190	GLU
1	11-B	230	ASN
1	11-B	246	ARG
1	12-A	30	MET
1	12-A	74	LEU
1	12-A	109	LEU
1	12-A	120	ASN
1	12-A	134	TYR
1	12-A	147	GLU
1	12-A	156	ARG
1	12-B	39	GLU
1	12-B	46	ASP
1	12-B	62	ILE
1	12-B	63	LYS
1	12-B	79	SER
1	12-B	120	ASN
1	12-B	165	GLN
1	12-B	185	GLN
1	12-B	212	ASN
1	12-B	229	TYR
1	12-B	238	ASP
1	12-B	244	LEU
1	13-A	43	GLU
1	13-A	54	VAL
1	13-A	69	LEU
1	13-A	88	ASN
1	13-A	109	LEU
1	13-A	114	GLU
1	13-A	120	ASN
1	13-A	132	GLN
1	13-A	134	TYR
1	13-A	141	ILE
1	13-A	156	ARG
1	13-A	158	MET
1	13-A	165	GLN

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Mol	Chain	Res	Type
1	13-A	180	THR
1	13-A	215	THR
1	13-A	217	GLU
1	13-A	229	TYR
1	13-A	238	ASP
1	13-A	239	GLN
1	13-B	39	GLU
1	13-B	46	ASP
1	13-B	56	ASP
1	13-B	82	GLU
1	13-B	86	GLU
1	13-B	101	MET
1	13-B	114	GLU
1	13-B	134	TYR
1	13-B	156	ARG
1	13-B	165	GLN
1	14-A	30	MET
1	14-A	43	GLU
1	14-A	52	GLN
1	14-A	86	GLU
1	14-A	88	ASN
1	14-A	102	GLU
1	14-A	105	ARG
1	14-A	109	LEU
1	14-A	119	GLU
1	14-A	120	ASN
1	14-A	122	GLU
1	14-A	134	TYR
1	14-A	156	ARG
1	14-A	165	GLN
1	14-A	184	THR
1	14-A	227	PHE
1	14-A	229	TYR
1	14-A	232	GLN
1	14-B	32	ASP
1	14-B	52	GLN
1	14-B	63	LYS
1	14-B	82	GLU
1	14-B	122	GLU
1	14-B	147	GLU
1	14-B	156	ARG
1	14-B	165	GLN

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Mol	Chain	Res	Type
1	14-B	184	THR
1	14-B	189	PHE
1	14-B	210	ASP
1	15-A	32	ASP
1	15-A	88	ASN
1	15-A	109	LEU
1	15-A	114	GLU
1	15-A	134	TYR
1	15-A	145	GLU
1	15-A	158	MET
1	15-A	165	GLN
1	15-A	184	THR
1	15-A	193	ASP
1	15-A	200	GLN
1	15-A	213	MET
1	15-A	216	LYS
1	15-A	228	GLU
1	15-A	236	GLU
1	15-A	239	GLN
1	15-B	32	ASP
1	15-B	47	ARG
1	15-B	56	ASP
1	15-B	61	ASN
1	15-B	67	PHE
1	15-B	102	GLU
1	15-B	129	LYS
1	15-B	156	ARG
1	15-B	173	ARG
1	15-B	175	LEU
1	15-B	180	THR
1	15-B	182	GLU
1	15-B	190	GLU
1	15-B	205	ARG
1	15-B	224	ASN
1	15-B	236	GLU
1	16-A	29	ARG
1	16-A	42	LYS
1	16-A	74	LEU
1	16-A	86	GLU
1	16-A	89	LYS
1	16-A	109	LEU
1	16-A	123	GLU

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Mol	Chain	Res	Type
1	16-A	126	GLN
1	16-A	134	TYR
1	16-A	165	GLN
1	16-A	180	THR
1	16-A	184	THR
1	16-A	185	GLN
1	16-A	190	GLU
1	16-A	194	ASN
1	16-A	213	MET
1	16-A	215	THR
1	16-A	228	GLU
1	16-B	63	LYS
1	16-B	83	GLU
1	16-B	110	THR
1	16-B	123	GLU
1	16-B	134	TYR
1	16-B	143	GLN
1	16-B	156	ARG
1	16-B	185	GLN
1	16-B	194	ASN
1	16-B	196	GLN
1	16-B	200	GLN
1	16-B	212	ASN
1	16-B	217	GLU
1	16-B	244	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	52	GLN
1	1-A	61	ASN
1	1-A	104	HIS
1	1-A	120	ASN
1	1-A	124	GLN
1	1-A	126	GLN
1	1-A	143	GLN
1	1-A	165	GLN
1	1-A	200	GLN
1	1-B	124	GLN
1	1-B	165	GLN
1	1-B	172	GLN
1	1-B	196	GLN

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Mol	Chain	Res	Type
1	1-B	230	ASN
1	2-A	52	GLN
1	2-A	104	HIS
1	2-A	165	GLN
1	2-B	104	HIS
1	2-B	124	GLN
1	2-B	165	GLN
1	2-B	172	GLN
1	2-B	185	GLN
1	2-B	191	ASN
1	2-B	196	GLN
1	2-B	230	ASN
1	3-A	52	GLN
1	3-A	61	ASN
1	3-A	124	GLN
1	3-A	165	GLN
1	3-A	200	GLN
1	3-A	212	ASN
1	3-A	239	GLN
1	3-B	50	ASN
1	3-B	104	HIS
1	3-B	143	GLN
1	3-B	165	GLN
1	3-B	172	GLN
1	3-B	196	GLN
1	3-B	200	GLN
1	3-B	235	ASN
1	4-A	139	HIS
1	4-A	185	GLN
1	4-B	61	ASN
1	4-B	124	GLN
1	4-B	165	GLN
1	4-B	172	GLN
1	4-B	185	GLN
1	4-B	194	ASN
1	4-B	196	GLN
1	4-B	230	ASN
1	5-A	88	ASN
1	5-A	104	HIS
1	5-A	120	ASN
1	5-A	143	GLN
1	5-A	165	GLN

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Mol	Chain	Res	Type
1	5-B	104	HIS
1	5-B	124	GLN
1	5-B	172	GLN
1	5-B	185	GLN
1	5-B	230	ASN
1	6-A	52	GLN
1	6-A	61	ASN
1	6-A	88	ASN
1	6-A	104	HIS
1	6-A	124	GLN
1	6-A	197	GLN
1	6-A	200	GLN
1	6-B	61	ASN
1	6-B	165	GLN
1	6-B	172	GLN
1	6-B	185	GLN
1	6-B	230	ASN
1	7-A	88	ASN
1	7-A	104	HIS
1	7-A	165	GLN
1	7-A	200	GLN
1	7-B	104	HIS
1	7-B	124	GLN
1	7-B	165	GLN
1	7-B	185	GLN
1	7-B	230	ASN
1	7-B	232	GLN
1	8-A	104	HIS
1	8-A	143	GLN
1	8-A	144	ASN
1	8-A	185	GLN
1	8-A	200	GLN
1	8-A	230	ASN
1	8-B	124	GLN
1	8-B	126	GLN
1	8-B	165	GLN
1	8-B	172	GLN
1	8-B	185	GLN
1	8-B	224	ASN
1	9-A	104	HIS
1	9-A	120	ASN
1	9-A	124	GLN

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Mol	Chain	Res	Type
1	9-A	143	GLN
1	9-A	196	GLN
1	9-A	200	GLN
1	9-A	235	ASN
1	9-A	239	GLN
1	9-B	104	HIS
1	9-B	124	GLN
1	9-B	165	GLN
1	9-B	172	GLN
1	9-B	191	ASN
1	9-B	194	ASN
1	9-B	200	GLN
1	9-B	230	ASN
1	10-A	52	GLN
1	10-A	104	HIS
1	10-A	143	GLN
1	10-A	165	GLN
1	10-B	120	ASN
1	10-B	124	GLN
1	10-B	143	GLN
1	10-B	165	GLN
1	10-B	172	GLN
1	10-B	185	GLN
1	10-B	194	ASN
1	10-B	230	ASN
1	10-B	232	GLN
1	11-A	61	ASN
1	11-A	104	HIS
1	11-A	143	GLN
1	11-B	50	ASN
1	11-B	124	GLN
1	11-B	165	GLN
1	11-B	172	GLN
1	11-B	196	GLN
1	11-B	224	ASN
1	12-A	52	GLN
1	12-A	143	GLN
1	12-B	61	ASN
1	12-B	120	ASN
1	12-B	165	GLN
1	12-B	172	GLN
1	12-B	185	GLN

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Mol	Chain	Res	Type
1	12-B	224	ASN
1	12-B	230	ASN
1	13-A	88	ASN
1	13-A	124	GLN
1	13-A	144	ASN
1	13-B	124	GLN
1	13-B	165	GLN
1	13-B	191	ASN
1	13-B	230	ASN
1	14-A	88	ASN
1	14-A	104	HIS
1	14-A	197	GLN
1	14-B	120	ASN
1	14-B	143	GLN
1	14-B	144	ASN
1	14-B	165	GLN
1	15-A	61	ASN
1	15-A	144	ASN
1	15-B	61	ASN
1	15-B	104	HIS
1	15-B	172	GLN
1	15-B	230	ASN
1	15-B	232	GLN
1	16-A	88	ASN
1	16-A	165	GLN
1	16-A	194	ASN
1	16-A	196	GLN
1	16-A	235	ASN
1	16-B	120	ASN
1	16-B	124	GLN
1	16-B	143	GLN
1	16-B	165	GLN
1	16-B	172	GLN
1	16-B	185	GLN
1	16-B	194	ASN
1	16-B	230	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

32 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	1-A	300	1	30,50,50	2.92	11 (36%)	24,82,82	2.06	6 (25%)
2	HEM	1-B	265	1	30,50,50	2.78	10 (33%)	24,82,82	1.99	7 (29%)
2	HEM	10-A	300	1	30,50,50	2.90	11 (36%)	24,82,82	2.06	6 (25%)
2	HEM	10-B	265	1	30,50,50	2.76	10 (33%)	24,82,82	2.00	7 (29%)
2	HEM	11-A	300	1	30,50,50	2.99	11 (36%)	24,82,82	2.04	6 (25%)
2	HEM	11-B	265	1	30,50,50	2.75	10 (33%)	24,82,82	1.96	7 (29%)
2	HEM	12-A	300	1	30,50,50	2.96	10 (33%)	24,82,82	2.03	6 (25%)
2	HEM	12-B	265	1	30,50,50	2.76	10 (33%)	24,82,82	2.00	6 (25%)
2	HEM	13-A	300	1	30,50,50	2.94	10 (33%)	24,82,82	2.03	6 (25%)
2	HEM	13-B	265	1	30,50,50	2.72	10 (33%)	24,82,82	2.00	7 (29%)
2	HEM	14-A	300	1	30,50,50	2.96	10 (33%)	24,82,82	2.07	6 (25%)
2	HEM	14-B	265	1	30,50,50	2.59	9 (30%)	24,82,82	1.97	6 (25%)
2	HEM	15-A	300	1	30,50,50	2.94	11 (36%)	24,82,82	2.07	6 (25%)
2	HEM	15-B	265	1	30,50,50	2.73	11 (36%)	24,82,82	2.02	7 (29%)
2	HEM	16-A	300	1	30,50,50	2.92	11 (36%)	24,82,82	2.06	6 (25%)
2	HEM	16-B	265	1	30,50,50	2.82	10 (33%)	24,82,82	2.06	6 (25%)
2	HEM	2-A	300	1	30,50,50	2.87	10 (33%)	24,82,82	2.05	6 (25%)
2	HEM	2-B	265	1	30,50,50	2.77	10 (33%)	24,82,82	2.01	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	3-A	300	1	30,50,50	2.93	10 (33%)	24,82,82	1.97	6 (25%)
2	HEM	3-B	265	1	30,50,50	2.73	11 (36%)	24,82,82	2.05	6 (25%)
2	HEM	4-A	300	1	30,50,50	2.91	11 (36%)	24,82,82	1.97	6 (25%)
2	HEM	4-B	265	1	30,50,50	2.77	10 (33%)	24,82,82	2.10	6 (25%)
2	HEM	5-A	300	1	30,50,50	2.90	11 (36%)	24,82,82	2.07	6 (25%)
2	HEM	5-B	265	1	30,50,50	2.72	11 (36%)	24,82,82	2.01	6 (25%)
2	HEM	6-A	300	1	30,50,50	2.97	11 (36%)	24,82,82	2.04	6 (25%)
2	HEM	6-B	265	1	30,50,50	2.73	11 (36%)	24,82,82	2.03	6 (25%)
2	HEM	7-A	300	1	30,50,50	2.93	11 (36%)	24,82,82	2.05	6 (25%)
2	HEM	7-B	265	1	30,50,50	2.73	11 (36%)	24,82,82	2.02	6 (25%)
2	HEM	8-A	300	1	30,50,50	2.91	11 (36%)	24,82,82	2.07	6 (25%)
2	HEM	8-B	265	1	30,50,50	2.82	10 (33%)	24,82,82	2.03	7 (29%)
2	HEM	9-A	300	1	30,50,50	3.02	9 (30%)	24,82,82	2.01	6 (25%)
2	HEM	9-B	265	1	30,50,50	2.78	10 (33%)	24,82,82	2.02	7 (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	HEM	1-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	1-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	10-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	10-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	11-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	11-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	12-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	12-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	13-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	13-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	14-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	14-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	15-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	15-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	16-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	16-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	2-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	2-B	265	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	3-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	3-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	4-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	4-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	5-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	5-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	6-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	6-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	7-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	7-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	8-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	8-B	265	1	-	0/10/54/54	0/0/8/8
2	HEM	9-A	300	1	-	0/10/54/54	0/0/8/8
2	HEM	9-B	265	1	-	0/10/54/54	0/0/8/8

All (333) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-A	300	HEM	C3B-C4B	-8.42	1.44	1.51
2	13-A	300	HEM	C3B-C4B	-8.09	1.44	1.51
2	9-A	300	HEM	C3B-C4B	-8.02	1.44	1.51
2	16-A	300	HEM	C3B-C4B	-7.65	1.45	1.51
2	16-B	265	HEM	C3B-C4B	-7.53	1.45	1.51
2	11-A	300	HEM	C3B-C4B	-7.48	1.45	1.51
2	12-A	300	HEM	C3B-C4B	-7.43	1.45	1.51
2	6-A	300	HEM	C3B-C4B	-7.38	1.45	1.51
2	2-A	300	HEM	C3B-C4B	-7.09	1.45	1.51
2	12-B	265	HEM	C3B-CAB	-7.08	1.38	1.51
2	1-A	300	HEM	C3B-C4B	-7.06	1.45	1.51
2	4-A	300	HEM	C3B-C4B	-6.92	1.45	1.51
2	3-A	300	HEM	C2D-C3D	-6.91	1.33	1.54
2	1-B	265	HEM	C3B-CAB	-6.88	1.38	1.51
2	9-B	265	HEM	C3B-CAB	-6.88	1.38	1.51
2	10-A	300	HEM	C3B-C4B	-6.85	1.45	1.51
2	11-B	265	HEM	C3B-CAB	-6.80	1.38	1.51
2	8-A	300	HEM	C3B-C4B	-6.78	1.45	1.51
2	9-A	300	HEM	C3C-CAC	-6.78	1.38	1.51
2	15-B	265	HEM	C3B-CAB	-6.77	1.38	1.51
2	7-B	265	HEM	C3B-CAB	-6.76	1.38	1.51
2	13-B	265	HEM	C3B-CAB	-6.75	1.38	1.51
2	10-B	265	HEM	C3B-CAB	-6.72	1.38	1.51
2	12-B	265	HEM	C3B-C4B	-6.72	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-B	265	HEM	C3C-CAC	-6.71	1.38	1.51
2	3-A	300	HEM	C3B-CAB	-6.71	1.38	1.51
2	15-A	300	HEM	C2D-C3D	-6.70	1.34	1.54
2	6-A	300	HEM	C3C-CAC	-6.69	1.38	1.51
2	7-A	300	HEM	C3B-C4B	-6.68	1.45	1.51
2	11-A	300	HEM	C3C-CAC	-6.68	1.38	1.51
2	11-A	300	HEM	C2D-C3D	-6.68	1.34	1.54
2	4-A	300	HEM	C3C-CAC	-6.66	1.38	1.51
2	6-A	300	HEM	C2D-C3D	-6.65	1.34	1.54
2	5-A	300	HEM	C2D-C3D	-6.64	1.34	1.54
2	12-A	300	HEM	C3C-CAC	-6.64	1.38	1.51
2	12-A	300	HEM	C2D-C3D	-6.63	1.34	1.54
2	4-B	265	HEM	C3B-C4B	-6.62	1.46	1.51
2	10-A	300	HEM	C2D-C3D	-6.61	1.34	1.54
2	7-A	300	HEM	C2D-C3D	-6.61	1.34	1.54
2	2-B	265	HEM	C3B-CAB	-6.60	1.38	1.51
2	15-A	300	HEM	C3B-CAB	-6.60	1.39	1.51
2	1-A	300	HEM	C2D-C3D	-6.59	1.34	1.54
2	8-A	300	HEM	C2D-C3D	-6.59	1.34	1.54
2	16-B	265	HEM	C3C-CAC	-6.57	1.39	1.51
2	10-B	265	HEM	C3C-CAC	-6.57	1.39	1.51
2	13-A	300	HEM	C3C-CAC	-6.56	1.39	1.51
2	3-A	300	HEM	C3B-C4B	-6.56	1.46	1.51
2	8-B	265	HEM	C3B-C4B	-6.55	1.46	1.51
2	4-B	265	HEM	C3C-CAC	-6.55	1.39	1.51
2	4-A	300	HEM	C2D-C3D	-6.55	1.34	1.54
2	6-B	265	HEM	C3C-CAC	-6.54	1.39	1.51
2	9-A	300	HEM	C2D-C3D	-6.52	1.35	1.54
2	2-A	300	HEM	C2D-C3D	-6.50	1.35	1.54
2	13-A	300	HEM	C2D-C3D	-6.49	1.35	1.54
2	7-B	265	HEM	C3C-CAC	-6.48	1.39	1.51
2	9-B	265	HEM	C3C-CAC	-6.48	1.39	1.51
2	15-A	300	HEM	C3D-C4D	-6.48	1.43	1.51
2	1-B	265	HEM	C3C-CAC	-6.47	1.39	1.51
2	8-B	265	HEM	C3C-CAC	-6.46	1.39	1.51
2	16-A	300	HEM	C2D-C3D	-6.46	1.35	1.54
2	14-A	300	HEM	C2D-C3D	-6.45	1.35	1.54
2	3-B	265	HEM	C3B-CAB	-6.45	1.39	1.51
2	2-B	265	HEM	C3C-CAC	-6.44	1.39	1.51
2	14-B	265	HEM	C2D-C3D	-6.44	1.35	1.54
2	5-B	265	HEM	C3C-CAC	-6.43	1.39	1.51
2	7-A	300	HEM	C3C-CAC	-6.43	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-B	265	HEM	C3B-C4B	-6.43	1.46	1.51
2	5-A	300	HEM	C3B-C4B	-6.40	1.46	1.51
2	5-A	300	HEM	C3B-CAB	-6.40	1.39	1.51
2	15-A	300	HEM	C3B-C4B	-6.39	1.46	1.51
2	11-B	265	HEM	C3C-CAC	-6.39	1.39	1.51
2	15-B	265	HEM	C3C-CAC	-6.39	1.39	1.51
2	14-A	300	HEM	C3C-CAC	-6.39	1.39	1.51
2	13-B	265	HEM	C3C-CAC	-6.30	1.39	1.51
2	8-B	265	HEM	C3B-CAB	-6.29	1.39	1.51
2	16-B	265	HEM	C3B-CAB	-6.28	1.39	1.51
2	16-A	300	HEM	C3C-CAC	-6.27	1.39	1.51
2	1-B	265	HEM	C3B-C4B	-6.22	1.46	1.51
2	9-A	300	HEM	C3B-CAB	-6.22	1.39	1.51
2	4-B	265	HEM	C3B-CAB	-6.21	1.39	1.51
2	1-A	300	HEM	C3C-CAC	-6.21	1.39	1.51
2	9-B	265	HEM	C3B-C4B	-6.20	1.46	1.51
2	6-B	265	HEM	C3B-CAB	-6.18	1.39	1.51
2	3-B	265	HEM	C3B-C4B	-6.16	1.46	1.51
2	2-A	300	HEM	C3C-CAC	-6.09	1.39	1.51
2	3-B	265	HEM	C3C-CAC	-6.09	1.39	1.51
2	5-A	300	HEM	C3D-C4D	-6.09	1.43	1.51
2	3-B	265	HEM	C2D-C3D	-6.09	1.36	1.54
2	6-B	265	HEM	C3B-C4B	-6.07	1.46	1.51
2	7-A	300	HEM	C3B-CAB	-6.07	1.39	1.51
2	4-A	300	HEM	C3B-CAB	-6.07	1.39	1.51
2	10-A	300	HEM	C3C-CAC	-6.06	1.40	1.51
2	10-B	265	HEM	C3B-C4B	-6.06	1.46	1.51
2	8-A	300	HEM	C3C-CAC	-6.05	1.40	1.51
2	11-B	265	HEM	C3B-C4B	-6.01	1.46	1.51
2	2-B	265	HEM	C2D-C3D	-6.01	1.36	1.54
2	8-A	300	HEM	C3B-CAB	-6.00	1.40	1.51
2	10-A	300	HEM	C3B-CAB	-5.99	1.40	1.51
2	9-B	265	HEM	C2D-C3D	-5.99	1.36	1.54
2	11-A	300	HEM	C3B-CAB	-5.99	1.40	1.51
2	13-A	300	HEM	C3B-CAB	-5.98	1.40	1.51
2	6-A	300	HEM	C3B-CAB	-5.98	1.40	1.51
2	1-B	265	HEM	C2D-C3D	-5.98	1.36	1.54
2	16-B	265	HEM	C2D-C3D	-5.97	1.36	1.54
2	12-A	300	HEM	C3B-CAB	-5.97	1.40	1.51
2	16-A	300	HEM	C3B-CAB	-5.94	1.40	1.51
2	8-B	265	HEM	C2D-C3D	-5.93	1.36	1.54
2	11-B	265	HEM	C2D-C3D	-5.93	1.36	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-A	300	HEM	C3B-CAB	-5.93	1.40	1.51
2	13-B	265	HEM	C3B-C4B	-5.91	1.46	1.51
2	4-B	265	HEM	C2D-C3D	-5.91	1.36	1.54
2	10-B	265	HEM	C2D-C3D	-5.89	1.36	1.54
2	5-B	265	HEM	C3B-CAB	-5.89	1.40	1.51
2	12-B	265	HEM	C2D-C3D	-5.89	1.36	1.54
2	2-A	300	HEM	C3B-CAB	-5.88	1.40	1.51
2	5-B	265	HEM	C3B-C4B	-5.88	1.46	1.51
2	5-B	265	HEM	C2D-C3D	-5.84	1.37	1.54
2	7-B	265	HEM	C2D-C3D	-5.82	1.37	1.54
2	7-A	300	HEM	C3D-C4D	-5.81	1.44	1.51
2	3-A	300	HEM	C3D-C4D	-5.80	1.44	1.51
2	8-A	300	HEM	C3D-C4D	-5.80	1.44	1.51
2	6-B	265	HEM	C2D-C3D	-5.79	1.37	1.54
2	7-B	265	HEM	C3B-C4B	-5.76	1.46	1.51
2	13-B	265	HEM	C2D-C3D	-5.76	1.37	1.54
2	14-A	300	HEM	C3B-CAB	-5.74	1.40	1.51
2	10-A	300	HEM	C3D-C4D	-5.72	1.44	1.51
2	15-B	265	HEM	C3B-C4B	-5.68	1.46	1.51
2	5-A	300	HEM	C3C-CAC	-5.67	1.40	1.51
2	1-A	300	HEM	C3D-C4D	-5.62	1.44	1.51
2	15-B	265	HEM	C2D-C3D	-5.62	1.37	1.54
2	11-A	300	HEM	C3D-C4D	-5.60	1.44	1.51
2	6-A	300	HEM	C3D-C4D	-5.55	1.44	1.51
2	3-A	300	HEM	C3C-CAC	-5.54	1.40	1.51
2	12-B	265	HEM	C3C-CAC	-5.52	1.41	1.51
2	12-A	300	HEM	C3D-C4D	-5.48	1.44	1.51
2	15-A	300	HEM	C3C-CAC	-5.37	1.41	1.51
2	2-A	300	HEM	C3D-C4D	-5.35	1.44	1.51
2	14-B	265	HEM	C3B-CAB	-5.27	1.41	1.51
2	9-A	300	HEM	C3D-C4D	-5.17	1.44	1.51
2	4-A	300	HEM	C3D-C4D	-5.16	1.45	1.51
2	16-A	300	HEM	C3D-C4D	-5.06	1.45	1.51
2	14-A	300	HEM	C3D-C4D	-4.68	1.45	1.51
2	8-B	265	HEM	C3D-C4D	-4.65	1.45	1.51
2	14-B	265	HEM	C3B-C4B	-4.56	1.47	1.51
2	13-A	300	HEM	C3D-C4D	-4.45	1.45	1.51
2	14-A	300	HEM	C2C-C1C	-4.37	1.44	1.52
2	16-A	300	HEM	C2C-C1C	-4.37	1.44	1.52
2	1-A	300	HEM	C2C-C1C	-4.28	1.44	1.52
2	11-A	300	HEM	C2C-C1C	-4.24	1.44	1.52
2	5-B	265	HEM	C3D-C4D	-4.23	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-B	265	HEM	C3D-C4D	-4.23	1.46	1.51
2	10-A	300	HEM	C2C-C1C	-4.19	1.44	1.52
2	6-A	300	HEM	C2C-C1C	-4.17	1.44	1.52
2	8-A	300	HEM	C2C-C1C	-4.16	1.44	1.52
2	9-A	300	HEM	C2C-C1C	-4.14	1.44	1.52
2	2-A	300	HEM	C2C-C1C	-4.13	1.44	1.52
2	12-A	300	HEM	C2C-C1C	-4.12	1.44	1.52
2	11-B	265	HEM	C3D-C4D	-4.09	1.46	1.51
2	7-A	300	HEM	C2C-C1C	-4.06	1.44	1.52
2	2-B	265	HEM	C3D-C4D	-4.05	1.46	1.51
2	15-B	265	HEM	C2C-C1C	-4.04	1.44	1.52
2	13-A	300	HEM	C2C-C1C	-4.04	1.44	1.52
2	4-A	300	HEM	C2C-C1C	-4.03	1.44	1.52
2	8-B	265	HEM	C2C-C1C	-4.00	1.45	1.52
2	12-B	265	HEM	C2C-C1C	-3.98	1.45	1.52
2	3-B	265	HEM	C2C-C1C	-3.95	1.45	1.52
2	9-B	265	HEM	C3D-C4D	-3.93	1.46	1.51
2	4-B	265	HEM	C2C-C1C	-3.93	1.45	1.52
2	1-B	265	HEM	C3D-C4D	-3.91	1.46	1.51
2	12-B	265	HEM	C3D-C4D	-3.91	1.46	1.51
2	5-A	300	HEM	C2C-C1C	-3.89	1.45	1.52
2	10-B	265	HEM	C3D-C4D	-3.89	1.46	1.51
2	6-B	265	HEM	C3D-C4D	-3.88	1.46	1.51
2	5-B	265	HEM	C2C-C1C	-3.88	1.45	1.52
2	13-B	265	HEM	C3D-C4D	-3.87	1.46	1.51
2	7-B	265	HEM	C2C-C1C	-3.87	1.45	1.52
2	6-B	265	HEM	C2C-C1C	-3.84	1.45	1.52
2	4-B	265	HEM	C3D-C4D	-3.82	1.46	1.51
2	3-A	300	HEM	C2C-C1C	-3.71	1.45	1.52
2	15-A	300	HEM	C2C-C1C	-3.70	1.45	1.52
2	1-B	265	HEM	C2C-C1C	-3.63	1.45	1.52
2	11-B	265	HEM	C2C-C1C	-3.62	1.45	1.52
2	7-B	265	HEM	C3D-C4D	-3.61	1.47	1.51
2	15-B	265	HEM	C3D-C4D	-3.59	1.47	1.51
2	16-B	265	HEM	C3D-C4D	-3.52	1.47	1.51
2	3-B	265	HEM	C3D-C4D	-3.52	1.47	1.51
2	10-B	265	HEM	C2C-C1C	-3.49	1.46	1.52
2	9-B	265	HEM	C2C-C1C	-3.46	1.46	1.52
2	13-B	265	HEM	C2C-C1C	-3.42	1.46	1.52
2	14-B	265	HEM	C2C-C1C	-3.35	1.46	1.52
2	16-B	265	HEM	C2C-C1C	-3.34	1.46	1.52
2	2-B	265	HEM	C2C-C1C	-3.23	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8-B	265	HEM	C2B-C1B	-2.49	1.43	1.51
2	6-B	265	HEM	C2B-C1B	-2.49	1.43	1.51
2	5-B	265	HEM	C2B-C1B	-2.44	1.43	1.51
2	4-B	265	HEM	C2B-C1B	-2.34	1.44	1.51
2	5-A	300	HEM	C2B-C1B	-2.19	1.44	1.51
2	12-B	265	HEM	C2B-C1B	-2.19	1.44	1.51
2	15-B	265	HEM	C2B-C1B	-2.19	1.44	1.51
2	3-B	265	HEM	C2B-C1B	-2.16	1.44	1.51
2	15-A	300	HEM	C2B-C1B	-2.14	1.44	1.51
2	7-A	300	HEM	C2B-C1B	-2.13	1.44	1.51
2	13-A	300	HEM	C2D-C1D	-2.09	1.45	1.51
2	14-A	300	HEM	C2D-C1D	-2.08	1.45	1.51
2	10-A	300	HEM	C2B-C1B	-2.06	1.45	1.51
2	1-A	300	HEM	C2B-C1B	-2.04	1.45	1.51
2	8-A	300	HEM	C2B-C1B	-2.04	1.45	1.51
2	4-A	300	HEM	C2D-C1D	-2.04	1.45	1.51
2	16-A	300	HEM	C2D-C1D	-2.03	1.45	1.51
2	7-B	265	HEM	C2B-C1B	-2.02	1.45	1.51
2	11-A	300	HEM	C2B-C1B	-2.00	1.45	1.51
2	6-A	300	HEM	C2B-C1B	-2.00	1.45	1.51
2	12-A	300	HEM	C4C-NC	2.03	1.38	1.36
2	6-A	300	HEM	C4C-NC	2.04	1.38	1.36
2	1-B	265	HEM	C1C-NC	2.05	1.38	1.36
2	16-A	300	HEM	C1C-NC	2.07	1.38	1.36
2	11-A	300	HEM	C4C-NC	2.08	1.38	1.36
2	3-B	265	HEM	C1C-NC	2.09	1.38	1.36
2	16-B	265	HEM	C1C-NC	2.11	1.38	1.36
2	4-A	300	HEM	C4C-NC	2.11	1.38	1.36
2	13-B	265	HEM	C1C-NC	2.14	1.38	1.36
2	10-B	265	HEM	C1C-NC	2.15	1.38	1.36
2	1-A	300	HEM	C4C-NC	2.16	1.38	1.36
2	4-B	265	HEM	C1C-NC	2.17	1.38	1.36
2	6-B	265	HEM	C1C-NC	2.18	1.38	1.36
2	2-A	300	HEM	C4C-NC	2.20	1.38	1.36
2	16-A	300	HEM	C4C-NC	2.20	1.38	1.36
2	15-A	300	HEM	C1C-NC	2.22	1.38	1.36
2	2-A	300	HEM	C1C-NC	2.22	1.38	1.36
2	7-B	265	HEM	C1C-NC	2.23	1.38	1.36
2	10-A	300	HEM	C4C-NC	2.23	1.38	1.36
2	5-A	300	HEM	C1C-NC	2.23	1.38	1.36
2	7-A	300	HEM	C4C-NC	2.24	1.38	1.36
2	12-B	265	HEM	C1C-NC	2.26	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-B	265	HEM	C1C-NC	2.28	1.38	1.36
2	10-A	300	HEM	C1C-NC	2.28	1.38	1.36
2	9-B	265	HEM	C1C-NC	2.29	1.38	1.36
2	11-B	265	HEM	C1C-NC	2.29	1.38	1.36
2	8-B	265	HEM	C4C-NC	2.29	1.38	1.36
2	8-A	300	HEM	C4C-NC	2.33	1.38	1.36
2	11-A	300	HEM	C1C-NC	2.34	1.38	1.36
2	14-A	300	HEM	C1C-NC	2.34	1.38	1.36
2	15-B	265	HEM	C1C-NC	2.36	1.38	1.36
2	8-A	300	HEM	C1C-NC	2.36	1.38	1.36
2	1-A	300	HEM	C1C-NC	2.38	1.38	1.36
2	12-A	300	HEM	C1C-NC	2.38	1.38	1.36
2	7-A	300	HEM	C1C-NC	2.39	1.39	1.36
2	2-B	265	HEM	C1C-NC	2.39	1.39	1.36
2	14-B	265	HEM	C4C-NC	2.42	1.39	1.36
2	6-A	300	HEM	C1C-NC	2.43	1.39	1.36
2	3-A	300	HEM	C1C-NC	2.43	1.39	1.36
2	9-A	300	HEM	C1C-NC	2.45	1.39	1.36
2	5-A	300	HEM	C4C-NC	2.45	1.39	1.36
2	4-A	300	HEM	C1C-NC	2.48	1.39	1.36
2	2-B	265	HEM	C4C-NC	2.53	1.39	1.36
2	11-B	265	HEM	C4C-NC	2.55	1.39	1.36
2	5-B	265	HEM	C4C-NC	2.56	1.39	1.36
2	3-B	265	HEM	C4C-NC	2.57	1.39	1.36
2	3-A	300	HEM	C4C-NC	2.59	1.39	1.36
2	13-A	300	HEM	C1C-NC	2.60	1.39	1.36
2	3-A	300	HEM	CBB-CAB	2.60	1.44	1.29
2	6-B	265	HEM	C4C-NC	2.62	1.39	1.36
2	16-B	265	HEM	C4C-NC	2.64	1.39	1.36
2	13-A	300	HEM	CBB-CAB	2.67	1.44	1.29
2	6-A	300	HEM	CBC-CAC	2.67	1.44	1.29
2	15-A	300	HEM	CBB-CAB	2.68	1.44	1.29
2	14-A	300	HEM	CBB-CAB	2.68	1.44	1.29
2	11-A	300	HEM	CBC-CAC	2.68	1.44	1.29
2	16-A	300	HEM	CBC-CAC	2.68	1.44	1.29
2	12-B	265	HEM	CBB-CAB	2.69	1.44	1.29
2	7-A	300	HEM	CBC-CAC	2.69	1.44	1.29
2	4-A	300	HEM	CBB-CAB	2.69	1.44	1.29
2	2-A	300	HEM	CBC-CAC	2.69	1.44	1.29
2	1-B	265	HEM	CBC-CAC	2.69	1.44	1.29
2	12-A	300	HEM	CBC-CAC	2.70	1.44	1.29
2	14-A	300	HEM	CBC-CAC	2.70	1.44	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-B	265	HEM	CBC-CAC	2.71	1.44	1.29
2	9-A	300	HEM	CBB-CAB	2.71	1.45	1.29
2	10-B	265	HEM	CBC-CAC	2.72	1.45	1.29
2	6-B	265	HEM	CBC-CAC	2.72	1.45	1.29
2	16-B	265	HEM	CBC-CAC	2.73	1.45	1.29
2	11-B	265	HEM	CBC-CAC	2.73	1.45	1.29
2	16-A	300	HEM	CBB-CAB	2.73	1.45	1.29
2	5-A	300	HEM	CBB-CAB	2.74	1.45	1.29
2	14-B	265	HEM	CBC-CAC	2.74	1.45	1.29
2	8-B	265	HEM	CBC-CAC	2.74	1.45	1.29
2	15-B	265	HEM	CBC-CAC	2.74	1.45	1.29
2	9-B	265	HEM	CBC-CAC	2.75	1.45	1.29
2	9-B	265	HEM	C4C-NC	2.75	1.39	1.36
2	15-A	300	HEM	C4C-NC	2.76	1.39	1.36
2	5-B	265	HEM	CBC-CAC	2.76	1.45	1.29
2	10-A	300	HEM	CBC-CAC	2.76	1.45	1.29
2	1-A	300	HEM	CBC-CAC	2.77	1.45	1.29
2	2-B	265	HEM	CBC-CAC	2.77	1.45	1.29
2	13-B	265	HEM	CBC-CAC	2.77	1.45	1.29
2	4-B	265	HEM	CBC-CAC	2.77	1.45	1.29
2	8-A	300	HEM	CBC-CAC	2.78	1.45	1.29
2	11-B	265	HEM	CBB-CAB	2.78	1.45	1.29
2	11-A	300	HEM	CBB-CAB	2.78	1.45	1.29
2	6-A	300	HEM	CBB-CAB	2.79	1.45	1.29
2	15-B	265	HEM	CBB-CAB	2.79	1.45	1.29
2	3-B	265	HEM	CBB-CAB	2.79	1.45	1.29
2	2-A	300	HEM	CBB-CAB	2.79	1.45	1.29
2	1-A	300	HEM	CBB-CAB	2.79	1.45	1.29
2	13-A	300	HEM	CBC-CAC	2.79	1.45	1.29
2	10-A	300	HEM	CBB-CAB	2.80	1.45	1.29
2	4-A	300	HEM	CBC-CAC	2.81	1.45	1.29
2	12-A	300	HEM	CBB-CAB	2.81	1.45	1.29
2	1-B	265	HEM	C4C-NC	2.81	1.39	1.36
2	15-B	265	HEM	C4C-NC	2.82	1.39	1.36
2	5-A	300	HEM	CBC-CAC	2.82	1.45	1.29
2	8-A	300	HEM	CBB-CAB	2.82	1.45	1.29
2	9-A	300	HEM	CBC-CAC	2.82	1.45	1.29
2	7-A	300	HEM	CBB-CAB	2.82	1.45	1.29
2	2-B	265	HEM	CBB-CAB	2.83	1.45	1.29
2	6-B	265	HEM	CBB-CAB	2.84	1.45	1.29
2	7-B	265	HEM	CBB-CAB	2.84	1.45	1.29
2	8-B	265	HEM	CBB-CAB	2.85	1.45	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-B	265	HEM	C4C-NC	2.86	1.39	1.36
2	5-B	265	HEM	CBB-CAB	2.87	1.45	1.29
2	1-B	265	HEM	CBB-CAB	2.88	1.45	1.29
2	15-A	300	HEM	CBC-CAC	2.88	1.46	1.29
2	16-B	265	HEM	CBB-CAB	2.89	1.46	1.29
2	9-B	265	HEM	CBB-CAB	2.90	1.46	1.29
2	10-B	265	HEM	CBB-CAB	2.92	1.46	1.29
2	3-B	265	HEM	CBC-CAC	2.93	1.46	1.29
2	13-B	265	HEM	CBB-CAB	2.93	1.46	1.29
2	3-A	300	HEM	CBC-CAC	2.95	1.46	1.29
2	4-B	265	HEM	CBB-CAB	2.95	1.46	1.29
2	10-B	265	HEM	C4C-NC	3.02	1.39	1.36
2	12-B	265	HEM	CBC-CAC	3.05	1.46	1.29
2	14-B	265	HEM	CBB-CAB	3.05	1.46	1.29
2	13-B	265	HEM	C4C-NC	3.09	1.39	1.36

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	15-B	265	HEM	C3B-CAB-CBB	-2.21	121.06	124.46
2	9-B	265	HEM	C3B-CAB-CBB	-2.15	121.16	124.46
2	1-B	265	HEM	C3B-CAB-CBB	-2.09	121.25	124.46
2	2-B	265	HEM	C3B-CAB-CBB	-2.08	121.26	124.46
2	11-B	265	HEM	C3B-CAB-CBB	-2.06	121.30	124.46
2	13-B	265	HEM	C3B-CAB-CBB	-2.05	121.30	124.46
2	8-B	265	HEM	C3B-CAB-CBB	-2.03	121.34	124.46
2	10-B	265	HEM	C3B-CAB-CBB	-2.02	121.35	124.46
2	12-B	265	HEM	C2D-C3D-C4D	2.41	105.59	101.50
2	3-B	265	HEM	C2D-C3D-C4D	2.48	105.71	101.50
2	3-A	300	HEM	CMD-C2D-C3D	2.52	125.49	114.35
2	15-A	300	HEM	CMD-C2D-C3D	2.61	125.91	114.35
2	9-B	265	HEM	CMD-C2D-C3D	2.63	126.00	114.35
2	2-B	265	HEM	CMD-C2D-C3D	2.64	126.04	114.35
2	6-B	265	HEM	CMD-C2D-C3D	2.65	126.08	114.35
2	10-B	265	HEM	CMD-C2D-C3D	2.66	126.09	114.35
2	14-B	265	HEM	C2D-C3D-C4D	2.66	106.01	101.50
2	16-B	265	HEM	CMD-C2D-C3D	2.66	126.12	114.35
2	5-A	300	HEM	CMD-C2D-C3D	2.67	126.15	114.35
2	5-B	265	HEM	CMD-C2D-C3D	2.67	126.16	114.35
2	1-B	265	HEM	CMD-C2D-C3D	2.67	126.17	114.35
2	7-A	300	HEM	CMD-C2D-C3D	2.67	126.18	114.35
2	10-A	300	HEM	CMD-C2D-C3D	2.68	126.22	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	265	HEM	CMD-C2D-C3D	2.69	126.24	114.35
2	1-A	300	HEM	CMD-C2D-C3D	2.69	126.25	114.35
2	8-A	300	HEM	CMD-C2D-C3D	2.69	126.26	114.35
2	11-A	300	HEM	CMD-C2D-C3D	2.70	126.29	114.35
2	12-A	300	HEM	CMD-C2D-C3D	2.70	126.30	114.35
2	6-A	300	HEM	CMD-C2D-C3D	2.70	126.30	114.35
2	14-B	265	HEM	CMD-C2D-C3D	2.70	126.30	114.35
2	7-B	265	HEM	CMD-C2D-C3D	2.71	126.32	114.35
2	4-B	265	HEM	CMD-C2D-C3D	2.72	126.36	114.35
2	11-B	265	HEM	C2D-C3D-C4D	2.72	106.12	101.50
2	13-B	265	HEM	CMD-C2D-C3D	2.73	126.42	114.35
2	15-B	265	HEM	CMD-C2D-C3D	2.73	126.42	114.35
2	11-B	265	HEM	CMD-C2D-C3D	2.74	126.47	114.35
2	4-A	300	HEM	CMD-C2D-C3D	2.74	126.48	114.35
2	2-B	265	HEM	C2D-C3D-C4D	2.75	106.16	101.50
2	16-A	300	HEM	CMD-C2D-C3D	2.75	126.51	114.35
2	9-A	300	HEM	CMD-C2D-C3D	2.75	126.52	114.35
2	4-B	265	HEM	C2D-C3D-C4D	2.75	106.17	101.50
2	2-A	300	HEM	CMD-C2D-C3D	2.76	126.56	114.35
2	12-B	265	HEM	CMD-C2D-C3D	2.78	126.63	114.35
2	3-B	265	HEM	CMD-C2D-C3D	2.79	126.67	114.35
2	13-A	300	HEM	CMD-C2D-C3D	2.79	126.69	114.35
2	16-B	265	HEM	C2D-C3D-C4D	2.80	106.24	101.50
2	15-B	265	HEM	C2D-C3D-C4D	2.80	106.25	101.50
2	14-A	300	HEM	CMD-C2D-C3D	2.81	126.78	114.35
2	5-B	265	HEM	C2D-C3D-C4D	2.82	106.28	101.50
2	9-B	265	HEM	C2D-C3D-C4D	2.83	106.29	101.50
2	1-B	265	HEM	C2D-C3D-C4D	2.85	106.33	101.50
2	10-B	265	HEM	C2D-C3D-C4D	2.88	106.38	101.50
2	8-B	265	HEM	C2D-C3D-C4D	2.98	106.56	101.50
2	13-B	265	HEM	C2D-C3D-C4D	2.99	106.57	101.50
2	6-B	265	HEM	C2D-C3D-C4D	3.00	106.58	101.50
2	9-A	300	HEM	C2D-C3D-C4D	3.00	106.58	101.50
2	7-B	265	HEM	C2D-C3D-C4D	3.01	106.60	101.50
2	13-A	300	HEM	C2D-C3D-C4D	3.02	106.61	101.50
2	4-A	300	HEM	C2D-C3D-C4D	3.04	106.66	101.50
2	14-A	300	HEM	C2D-C3D-C4D	3.09	106.74	101.50
2	2-A	300	HEM	C2D-C3D-C4D	3.12	106.78	101.50
2	12-A	300	HEM	C2D-C3D-C4D	3.12	106.79	101.50
2	16-A	300	HEM	C2D-C3D-C4D	3.16	106.85	101.50
2	11-A	300	HEM	C2D-C3D-C4D	3.20	106.92	101.50
2	6-A	300	HEM	C2D-C3D-C4D	3.20	106.92	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-A	300	HEM	C2D-C3D-C4D	3.21	106.93	101.50
2	3-A	300	HEM	C2D-C3D-C4D	3.22	106.95	101.50
2	7-A	300	HEM	C2D-C3D-C4D	3.22	106.95	101.50
2	1-A	300	HEM	C2D-C3D-C4D	3.23	106.97	101.50
2	8-A	300	HEM	C2D-C3D-C4D	3.29	107.08	101.50
2	5-A	300	HEM	C2D-C3D-C4D	3.30	107.09	101.50
2	15-A	300	HEM	C2D-C3D-C4D	3.41	107.28	101.50
2	15-A	300	HEM	CAD-C3D-C4D	3.67	125.40	112.47
2	11-B	265	HEM	CMC-C2C-C3C	3.73	125.85	116.53
2	10-B	265	HEM	CMC-C2C-C3C	3.75	125.90	116.53
2	13-B	265	HEM	CMC-C2C-C3C	3.76	125.91	116.53
2	5-A	300	HEM	CAD-C3D-C4D	3.77	125.77	112.47
2	2-B	265	HEM	CMC-C2C-C3C	3.77	125.95	116.53
2	9-B	265	HEM	CMC-C2C-C3C	3.78	125.98	116.53
2	10-A	300	HEM	CAD-C3D-C4D	3.80	125.88	112.47
2	8-A	300	HEM	CAD-C3D-C4D	3.81	125.90	112.47
2	4-A	300	HEM	CMB-C2B-C3B	3.82	126.06	116.53
2	1-B	265	HEM	CMC-C2C-C3C	3.82	126.08	116.53
2	7-A	300	HEM	CAD-C3D-C4D	3.83	125.98	112.47
2	16-A	300	HEM	CAD-C3D-C4D	3.84	126.03	112.47
2	11-A	300	HEM	CAD-C3D-C4D	3.85	126.04	112.47
2	1-A	300	HEM	CAD-C3D-C4D	3.85	126.05	112.47
2	8-B	265	HEM	CAD-C3D-C4D	3.85	126.06	112.47
2	14-B	265	HEM	CMB-C2B-C3B	3.86	126.16	116.53
2	6-A	300	HEM	CAD-C3D-C4D	3.86	126.08	112.47
2	7-B	265	HEM	CMC-C2C-C3C	3.86	126.17	116.53
2	5-B	265	HEM	CMC-C2C-C3C	3.86	126.17	116.53
2	14-B	265	HEM	CMC-C2C-C3C	3.86	126.17	116.53
2	2-A	300	HEM	CAD-C3D-C4D	3.86	126.10	112.47
2	12-B	265	HEM	CMB-C2B-C3B	3.88	126.22	116.53
2	12-A	300	HEM	CAD-C3D-C4D	3.90	126.23	112.47
2	6-B	265	HEM	CMC-C2C-C3C	3.90	126.28	116.53
2	3-B	265	HEM	CMB-C2B-C3B	3.91	126.30	116.53
2	15-B	265	HEM	CMC-C2C-C3C	3.92	126.32	116.53
2	8-B	265	HEM	CMC-C2C-C3C	3.93	126.34	116.53
2	16-B	265	HEM	CMC-C2C-C3C	3.95	126.39	116.53
2	4-B	265	HEM	CMC-C2C-C3C	3.95	126.40	116.53
2	11-B	265	HEM	CMB-C2B-C3B	3.96	126.41	116.53
2	3-A	300	HEM	CAD-C3D-C4D	3.96	126.44	112.47
2	14-A	300	HEM	CAD-C3D-C4D	3.96	126.44	112.47
2	9-B	265	HEM	CMB-C2B-C3B	3.97	126.44	116.53
2	1-B	265	HEM	CMB-C2B-C3B	3.98	126.46	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-A	300	HEM	CAD-C3D-C4D	3.98	126.51	112.47
2	2-B	265	HEM	CMB-C2B-C3B	3.98	126.47	116.53
2	13-B	265	HEM	CAD-C3D-C4D	3.99	126.53	112.47
2	11-B	265	HEM	CAD-C3D-C4D	3.99	126.54	112.47
2	4-A	300	HEM	CAD-C3D-C4D	3.99	126.54	112.47
2	3-A	300	HEM	CMB-C2B-C3B	4.01	126.53	116.53
2	15-B	265	HEM	CMB-C2B-C3B	4.01	126.54	116.53
2	16-B	265	HEM	CMB-C2B-C3B	4.03	126.59	116.53
2	9-A	300	HEM	CMC-C2C-C3C	4.03	126.59	116.53
2	4-A	300	HEM	CMC-C2C-C3C	4.03	126.60	116.53
2	10-B	265	HEM	CMB-C2B-C3B	4.04	126.62	116.53
2	7-B	265	HEM	CMB-C2B-C3B	4.05	126.63	116.53
2	6-B	265	HEM	CAD-C3D-C4D	4.05	126.76	112.47
2	5-B	265	HEM	CAD-C3D-C4D	4.05	126.77	112.47
2	13-A	300	HEM	CAD-C3D-C4D	4.06	126.77	112.47
2	13-B	265	HEM	CMB-C2B-C3B	4.08	126.71	116.53
2	12-A	300	HEM	CMC-C2C-C3C	4.12	126.82	116.53
2	13-A	300	HEM	CMC-C2C-C3C	4.13	126.83	116.53
2	6-B	265	HEM	CMB-C2B-C3B	4.13	126.84	116.53
2	14-A	300	HEM	CMB-C2B-C3B	4.13	126.84	116.53
2	1-B	265	HEM	CAD-C3D-C4D	4.14	127.06	112.47
2	8-B	265	HEM	CMB-C2B-C3B	4.14	126.86	116.53
2	11-A	300	HEM	CMC-C2C-C3C	4.14	126.87	116.53
2	12-B	265	HEM	CAD-C3D-C4D	4.15	127.11	112.47
2	6-A	300	HEM	CMC-C2C-C3C	4.16	126.90	116.53
2	13-A	300	HEM	CMB-C2B-C3B	4.17	126.93	116.53
2	7-B	265	HEM	CAD-C3D-C4D	4.17	127.16	112.47
2	10-B	265	HEM	CAD-C3D-C4D	4.17	127.18	112.47
2	7-A	300	HEM	CMC-C2C-C3C	4.17	126.94	116.53
2	3-A	300	HEM	CAD-C3D-C2D	4.18	125.23	113.22
2	9-A	300	HEM	CMB-C2B-C3B	4.19	127.00	116.53
2	3-B	265	HEM	CMC-C2C-C3C	4.19	127.00	116.53
2	14-B	265	HEM	CAD-C3D-C4D	4.20	127.28	112.47
2	12-B	265	HEM	CMC-C2C-C3C	4.20	127.02	116.53
2	15-A	300	HEM	CMB-C2B-C3B	4.21	127.04	116.53
2	15-B	265	HEM	CAD-C3D-C4D	4.22	127.34	112.47
2	9-B	265	HEM	CAD-C3D-C4D	4.22	127.37	112.47
2	2-B	265	HEM	CAD-C3D-C4D	4.23	127.38	112.47
2	16-A	300	HEM	CMB-C2B-C3B	4.23	127.09	116.53
2	12-A	300	HEM	CMB-C2B-C3B	4.24	127.11	116.53
2	5-B	265	HEM	CMB-C2B-C3B	4.25	127.14	116.53
2	4-B	265	HEM	CAD-C3D-C4D	4.28	127.56	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-A	300	HEM	CMB-C2B-C3B	4.30	127.26	116.53
2	11-A	300	HEM	CMB-C2B-C3B	4.30	127.28	116.53
2	6-A	300	HEM	CMB-C2B-C3B	4.31	127.28	116.53
2	5-A	300	HEM	CMB-C2B-C3B	4.31	127.30	116.53
2	16-B	265	HEM	CAD-C3D-C4D	4.32	127.70	112.47
2	8-A	300	HEM	CMB-C2B-C3B	4.34	127.37	116.53
2	3-B	265	HEM	CAD-C3D-C4D	4.35	127.80	112.47
2	7-A	300	HEM	CMB-C2B-C3B	4.36	127.40	116.53
2	1-A	300	HEM	CMB-C2B-C3B	4.37	127.44	116.53
2	10-A	300	HEM	CMB-C2B-C3B	4.37	127.45	116.53
2	3-A	300	HEM	CMC-C2C-C3C	4.39	127.48	116.53
2	8-A	300	HEM	CMC-C2C-C3C	4.39	127.50	116.53
2	1-A	300	HEM	CMC-C2C-C3C	4.40	127.50	116.53
2	4-B	265	HEM	CMB-C2B-C3B	4.40	127.52	116.53
2	10-A	300	HEM	CMC-C2C-C3C	4.41	127.53	116.53
2	14-A	300	HEM	CMC-C2C-C3C	4.43	127.59	116.53
2	5-A	300	HEM	CMC-C2C-C3C	4.45	127.64	116.53
2	16-B	265	HEM	CAD-C3D-C2D	4.46	126.04	113.22
2	15-A	300	HEM	CMC-C2C-C3C	4.48	127.71	116.53
2	2-A	300	HEM	CMC-C2C-C3C	4.48	127.72	116.53
2	4-B	265	HEM	CAD-C3D-C2D	4.49	126.13	113.22
2	7-B	265	HEM	CAD-C3D-C2D	4.51	126.17	113.22
2	16-A	300	HEM	CMC-C2C-C3C	4.51	127.80	116.53
2	11-B	265	HEM	CAD-C3D-C2D	4.52	126.21	113.22
2	9-B	265	HEM	CAD-C3D-C2D	4.55	126.29	113.22
2	15-B	265	HEM	CAD-C3D-C2D	4.55	126.31	113.22
2	2-B	265	HEM	CAD-C3D-C2D	4.56	126.33	113.22
2	1-B	265	HEM	CAD-C3D-C2D	4.58	126.39	113.22
2	10-B	265	HEM	CAD-C3D-C2D	4.60	126.44	113.22
2	14-B	265	HEM	CAD-C3D-C2D	4.60	126.44	113.22
2	3-B	265	HEM	CAD-C3D-C2D	4.61	126.47	113.22
2	4-A	300	HEM	CAD-C3D-C2D	4.63	126.52	113.22
2	13-B	265	HEM	CAD-C3D-C2D	4.63	126.54	113.22
2	13-A	300	HEM	CAD-C3D-C2D	4.64	126.56	113.22
2	9-A	300	HEM	CAD-C3D-C2D	4.65	126.57	113.22
2	6-B	265	HEM	CAD-C3D-C2D	4.67	126.64	113.22
2	16-A	300	HEM	CAD-C3D-C2D	4.71	126.77	113.22
2	14-A	300	HEM	CAD-C3D-C2D	4.72	126.78	113.22
2	12-B	265	HEM	CAD-C3D-C2D	4.73	126.80	113.22
2	5-B	265	HEM	CAD-C3D-C2D	4.73	126.82	113.22
2	2-A	300	HEM	CAD-C3D-C2D	4.77	126.92	113.22
2	1-A	300	HEM	CAD-C3D-C2D	4.78	126.95	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12-A	300	HEM	CAD-C3D-C2D	4.78	126.95	113.22
2	6-A	300	HEM	CAD-C3D-C2D	4.78	126.95	113.22
2	8-A	300	HEM	CAD-C3D-C2D	4.78	126.95	113.22
2	11-A	300	HEM	CAD-C3D-C2D	4.78	126.97	113.22
2	7-A	300	HEM	CAD-C3D-C2D	4.80	127.02	113.22
2	5-A	300	HEM	CAD-C3D-C2D	4.83	127.09	113.22
2	10-A	300	HEM	CAD-C3D-C2D	4.83	127.11	113.22
2	8-B	265	HEM	CAD-C3D-C2D	4.83	127.11	113.22
2	15-A	300	HEM	CAD-C3D-C2D	4.87	127.22	113.22

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	1-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	1-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	2-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	2-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	3-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	3-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	4-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	4-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	5-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	5-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	6-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	6-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	7-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	7-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	8-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	8-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	9-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	9-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	10-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	10-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	11-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	11-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)
1	12-A	214/264 (81%)	0.12	7 (3%)	50	43	29, 50, 62, 67	214 (100%)
1	12-B	219/264 (82%)	0.72	40 (18%)	2	1	34, 59, 81, 91	219 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13-A	214/264 (81%)	0.12	7 (3%) 50 43	29, 50, 62, 67	214 (100%)
1	13-B	219/264 (82%)	0.72	40 (18%) 2 1	34, 59, 81, 91	219 (100%)
1	14-A	214/264 (81%)	0.12	7 (3%) 50 43	29, 50, 62, 67	214 (100%)
1	14-B	219/264 (82%)	0.72	40 (18%) 2 1	34, 59, 81, 91	219 (100%)
1	15-A	214/264 (81%)	0.12	7 (3%) 50 43	29, 50, 62, 67	214 (100%)
1	15-B	219/264 (82%)	0.72	40 (18%) 2 1	34, 59, 81, 91	219 (100%)
1	16-A	214/264 (81%)	0.12	7 (3%) 50 43	29, 50, 62, 67	214 (100%)
1	16-B	219/264 (82%)	0.72	40 (18%) 2 1	34, 59, 81, 91	219 (100%)
All	All	6928/8448 (82%)	0.42	752 (10%) 9 4	29, 53, 78, 91	6928 (100%)

All (752) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	29	ARG	10.8
1	2-A	29	ARG	10.8
1	3-A	29	ARG	10.8
1	4-A	29	ARG	10.8
1	5-A	29	ARG	10.8
1	6-A	29	ARG	10.8
1	7-A	29	ARG	10.8
1	8-A	29	ARG	10.8
1	9-A	29	ARG	10.8
1	10-A	29	ARG	10.8
1	11-A	29	ARG	10.8
1	12-A	29	ARG	10.8
1	13-A	29	ARG	10.8
1	14-A	29	ARG	10.8
1	15-A	29	ARG	10.8
1	16-A	29	ARG	10.8
1	1-B	168	LYS	10.0
1	2-B	168	LYS	10.0
1	3-B	168	LYS	10.0
1	4-B	168	LYS	10.0
1	5-B	168	LYS	10.0
1	6-B	168	LYS	10.0
1	7-B	168	LYS	10.0
1	8-B	168	LYS	10.0
1	9-B	168	LYS	10.0
1	10-B	168	LYS	10.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	11-B	168	LYS	10.0
1	12-B	168	LYS	10.0
1	13-B	168	LYS	10.0
1	14-B	168	LYS	10.0
1	15-B	168	LYS	10.0
1	16-B	168	LYS	10.0
1	1-B	245	ALA	8.0
1	2-B	245	ALA	8.0
1	3-B	245	ALA	8.0
1	4-B	245	ALA	8.0
1	5-B	245	ALA	8.0
1	6-B	245	ALA	8.0
1	7-B	245	ALA	8.0
1	8-B	245	ALA	8.0
1	9-B	245	ALA	8.0
1	10-B	245	ALA	8.0
1	11-B	245	ALA	8.0
1	12-B	245	ALA	8.0
1	13-B	245	ALA	8.0
1	14-B	245	ALA	8.0
1	15-B	245	ALA	8.0
1	16-B	245	ALA	8.0
1	1-A	30	MET	7.9
1	2-A	30	MET	7.9
1	3-A	30	MET	7.9
1	4-A	30	MET	7.9
1	5-A	30	MET	7.9
1	6-A	30	MET	7.9
1	7-A	30	MET	7.9
1	8-A	30	MET	7.9
1	9-A	30	MET	7.9
1	10-A	30	MET	7.9
1	11-A	30	MET	7.9
1	12-A	30	MET	7.9
1	13-A	30	MET	7.9
1	14-A	30	MET	7.9
1	15-A	30	MET	7.9
1	16-A	30	MET	7.9
1	1-B	165	GLN	7.4
1	2-B	165	GLN	7.4
1	3-B	165	GLN	7.4
1	4-B	165	GLN	7.4

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Mol	Chain	Res	Type	RSRZ
1	5-B	165	GLN	7.4
1	6-B	165	GLN	7.4
1	7-B	165	GLN	7.4
1	8-B	165	GLN	7.4
1	9-B	165	GLN	7.4
1	10-B	165	GLN	7.4
1	11-B	165	GLN	7.4
1	12-B	165	GLN	7.4
1	13-B	165	GLN	7.4
1	14-B	165	GLN	7.4
1	15-B	165	GLN	7.4
1	16-B	165	GLN	7.4
1	1-A	31	ALA	7.0
1	2-A	31	ALA	7.0
1	3-A	31	ALA	7.0
1	4-A	31	ALA	7.0
1	5-A	31	ALA	7.0
1	6-A	31	ALA	7.0
1	7-A	31	ALA	7.0
1	8-A	31	ALA	7.0
1	9-A	31	ALA	7.0
1	10-A	31	ALA	7.0
1	11-A	31	ALA	7.0
1	12-A	31	ALA	7.0
1	13-A	31	ALA	7.0
1	14-A	31	ALA	7.0
1	15-A	31	ALA	7.0
1	16-A	31	ALA	7.0
1	1-B	169	LYS	6.5
1	2-B	169	LYS	6.5
1	3-B	169	LYS	6.5
1	4-B	169	LYS	6.5
1	5-B	169	LYS	6.5
1	6-B	169	LYS	6.5
1	7-B	169	LYS	6.5
1	8-B	169	LYS	6.5
1	9-B	169	LYS	6.5
1	10-B	169	LYS	6.5
1	11-B	169	LYS	6.5
1	12-B	169	LYS	6.5
1	13-B	169	LYS	6.5
1	14-B	169	LYS	6.5

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Mol	Chain	Res	Type	RSRZ
1	15-B	169	LYS	6.5
1	16-B	169	LYS	6.5
1	1-B	247	GLU	6.2
1	2-B	247	GLU	6.2
1	3-B	247	GLU	6.2
1	4-B	247	GLU	6.2
1	5-B	247	GLU	6.2
1	6-B	247	GLU	6.2
1	7-B	247	GLU	6.2
1	8-B	247	GLU	6.2
1	9-B	247	GLU	6.2
1	10-B	247	GLU	6.2
1	11-B	247	GLU	6.2
1	12-B	247	GLU	6.2
1	13-B	247	GLU	6.2
1	14-B	247	GLU	6.2
1	15-B	247	GLU	6.2
1	16-B	247	GLU	6.2
1	1-B	30	MET	6.1
1	2-B	30	MET	6.1
1	3-B	30	MET	6.1
1	4-B	30	MET	6.1
1	5-B	30	MET	6.1
1	6-B	30	MET	6.1
1	7-B	30	MET	6.1
1	8-B	30	MET	6.1
1	9-B	30	MET	6.1
1	10-B	30	MET	6.1
1	11-B	30	MET	6.1
1	12-B	30	MET	6.1
1	13-B	30	MET	6.1
1	14-B	30	MET	6.1
1	15-B	30	MET	6.1
1	16-B	30	MET	6.1
1	1-B	246	ARG	6.1
1	2-B	246	ARG	6.1
1	3-B	246	ARG	6.1
1	4-B	246	ARG	6.1
1	5-B	246	ARG	6.1
1	6-B	246	ARG	6.1
1	7-B	246	ARG	6.1
1	8-B	246	ARG	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	9-B	246	ARG	6.1
1	10-B	246	ARG	6.1
1	11-B	246	ARG	6.1
1	12-B	246	ARG	6.1
1	13-B	246	ARG	6.1
1	14-B	246	ARG	6.1
1	15-B	246	ARG	6.1
1	16-B	246	ARG	6.1
1	1-B	60	GLY	5.8
1	2-B	60	GLY	5.8
1	3-B	60	GLY	5.8
1	4-B	60	GLY	5.8
1	5-B	60	GLY	5.8
1	6-B	60	GLY	5.8
1	7-B	60	GLY	5.8
1	8-B	60	GLY	5.8
1	9-B	60	GLY	5.8
1	10-B	60	GLY	5.8
1	11-B	60	GLY	5.8
1	12-B	60	GLY	5.8
1	13-B	60	GLY	5.8
1	14-B	60	GLY	5.8
1	15-B	60	GLY	5.8
1	16-B	60	GLY	5.8
1	1-B	182	GLU	5.3
1	2-B	182	GLU	5.3
1	3-B	182	GLU	5.3
1	4-B	182	GLU	5.3
1	5-B	182	GLU	5.3
1	6-B	182	GLU	5.3
1	7-B	182	GLU	5.3
1	8-B	182	GLU	5.3
1	9-B	182	GLU	5.3
1	10-B	182	GLU	5.3
1	11-B	182	GLU	5.3
1	12-B	182	GLU	5.3
1	13-B	182	GLU	5.3
1	14-B	182	GLU	5.3
1	15-B	182	GLU	5.3
1	16-B	182	GLU	5.3
1	1-A	213	MET	5.2
1	2-A	213	MET	5.2

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Mol	Chain	Res	Type	RSRZ
1	3-A	213	MET	5.2
1	4-A	213	MET	5.2
1	5-A	213	MET	5.2
1	6-A	213	MET	5.2
1	7-A	213	MET	5.2
1	8-A	213	MET	5.2
1	9-A	213	MET	5.2
1	10-A	213	MET	5.2
1	11-A	213	MET	5.2
1	12-A	213	MET	5.2
1	13-A	213	MET	5.2
1	14-A	213	MET	5.2
1	15-A	213	MET	5.2
1	16-A	213	MET	5.2
1	1-B	181	GLY	4.7
1	2-B	181	GLY	4.7
1	3-B	181	GLY	4.7
1	4-B	181	GLY	4.7
1	5-B	181	GLY	4.7
1	6-B	181	GLY	4.7
1	7-B	181	GLY	4.7
1	8-B	181	GLY	4.7
1	9-B	181	GLY	4.7
1	10-B	181	GLY	4.7
1	11-B	181	GLY	4.7
1	12-B	181	GLY	4.7
1	13-B	181	GLY	4.7
1	14-B	181	GLY	4.7
1	15-B	181	GLY	4.7
1	16-B	181	GLY	4.7
1	1-B	213	MET	4.7
1	2-B	213	MET	4.7
1	3-B	213	MET	4.7
1	4-B	213	MET	4.7
1	5-B	213	MET	4.7
1	6-B	213	MET	4.7
1	7-B	213	MET	4.7
1	8-B	213	MET	4.7
1	9-B	213	MET	4.7
1	10-B	213	MET	4.7
1	11-B	213	MET	4.7
1	12-B	213	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	13-B	213	MET	4.7
1	14-B	213	MET	4.7
1	15-B	213	MET	4.7
1	16-B	213	MET	4.7
1	1-B	177	LEU	4.4
1	2-B	177	LEU	4.4
1	3-B	177	LEU	4.4
1	4-B	177	LEU	4.4
1	5-B	177	LEU	4.4
1	6-B	177	LEU	4.4
1	7-B	177	LEU	4.4
1	8-B	177	LEU	4.4
1	9-B	177	LEU	4.4
1	10-B	177	LEU	4.4
1	11-B	177	LEU	4.4
1	12-B	177	LEU	4.4
1	13-B	177	LEU	4.4
1	14-B	177	LEU	4.4
1	15-B	177	LEU	4.4
1	16-B	177	LEU	4.4
1	1-B	244	LEU	4.2
1	2-B	244	LEU	4.2
1	3-B	244	LEU	4.2
1	4-B	244	LEU	4.2
1	5-B	244	LEU	4.2
1	6-B	244	LEU	4.2
1	7-B	244	LEU	4.2
1	8-B	244	LEU	4.2
1	9-B	244	LEU	4.2
1	10-B	244	LEU	4.2
1	11-B	244	LEU	4.2
1	12-B	244	LEU	4.2
1	13-B	244	LEU	4.2
1	14-B	244	LEU	4.2
1	15-B	244	LEU	4.2
1	16-B	244	LEU	4.2
1	1-B	174	ALA	4.2
1	2-B	174	ALA	4.2
1	3-B	174	ALA	4.2
1	4-B	174	ALA	4.2
1	5-B	174	ALA	4.2
1	6-B	174	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	7-B	174	ALA	4.2
1	8-B	174	ALA	4.2
1	9-B	174	ALA	4.2
1	10-B	174	ALA	4.2
1	11-B	174	ALA	4.2
1	12-B	174	ALA	4.2
1	13-B	174	ALA	4.2
1	14-B	174	ALA	4.2
1	15-B	174	ALA	4.2
1	16-B	174	ALA	4.2
1	1-B	167	LEU	4.0
1	2-B	167	LEU	4.0
1	3-B	167	LEU	4.0
1	4-B	167	LEU	4.0
1	5-B	167	LEU	4.0
1	6-B	167	LEU	4.0
1	7-B	167	LEU	4.0
1	8-B	167	LEU	4.0
1	9-B	167	LEU	4.0
1	10-B	167	LEU	4.0
1	11-B	167	LEU	4.0
1	12-B	167	LEU	4.0
1	13-B	167	LEU	4.0
1	14-B	167	LEU	4.0
1	15-B	167	LEU	4.0
1	16-B	167	LEU	4.0
1	1-B	248	THR	4.0
1	2-B	248	THR	4.0
1	3-B	248	THR	4.0
1	4-B	248	THR	4.0
1	5-B	248	THR	4.0
1	6-B	248	THR	4.0
1	7-B	248	THR	4.0
1	8-B	248	THR	4.0
1	9-B	248	THR	4.0
1	10-B	248	THR	4.0
1	11-B	248	THR	4.0
1	12-B	248	THR	4.0
1	13-B	248	THR	4.0
1	14-B	248	THR	4.0
1	15-B	248	THR	4.0
1	16-B	248	THR	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1-B	180	THR	3.7
1	2-B	180	THR	3.7
1	3-B	180	THR	3.7
1	4-B	180	THR	3.7
1	5-B	180	THR	3.7
1	6-B	180	THR	3.7
1	7-B	180	THR	3.7
1	8-B	180	THR	3.7
1	9-B	180	THR	3.7
1	10-B	180	THR	3.7
1	11-B	180	THR	3.7
1	12-B	180	THR	3.7
1	13-B	180	THR	3.7
1	14-B	180	THR	3.7
1	15-B	180	THR	3.7
1	16-B	180	THR	3.7
1	1-B	39	GLU	3.6
1	2-B	39	GLU	3.6
1	3-B	39	GLU	3.6
1	4-B	39	GLU	3.6
1	5-B	39	GLU	3.6
1	6-B	39	GLU	3.6
1	7-B	39	GLU	3.6
1	8-B	39	GLU	3.6
1	9-B	39	GLU	3.6
1	10-B	39	GLU	3.6
1	11-B	39	GLU	3.6
1	12-B	39	GLU	3.6
1	13-B	39	GLU	3.6
1	14-B	39	GLU	3.6
1	15-B	39	GLU	3.6
1	16-B	39	GLU	3.6
1	1-B	241	GLY	3.5
1	2-B	241	GLY	3.5
1	3-B	241	GLY	3.5
1	4-B	241	GLY	3.5
1	5-B	241	GLY	3.5
1	6-B	241	GLY	3.5
1	7-B	241	GLY	3.5
1	8-B	241	GLY	3.5
1	9-B	241	GLY	3.5
1	10-B	241	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	11-B	241	GLY	3.5
1	12-B	241	GLY	3.5
1	13-B	241	GLY	3.5
1	14-B	241	GLY	3.5
1	15-B	241	GLY	3.5
1	16-B	241	GLY	3.5
1	1-B	61	ASN	3.4
1	2-B	61	ASN	3.4
1	3-B	61	ASN	3.4
1	4-B	61	ASN	3.4
1	5-B	61	ASN	3.4
1	6-B	61	ASN	3.4
1	7-B	61	ASN	3.4
1	8-B	61	ASN	3.4
1	9-B	61	ASN	3.4
1	10-B	61	ASN	3.4
1	11-B	61	ASN	3.4
1	12-B	61	ASN	3.4
1	13-B	61	ASN	3.4
1	14-B	61	ASN	3.4
1	15-B	61	ASN	3.4
1	16-B	61	ASN	3.4
1	1-B	178	PRO	3.4
1	2-B	178	PRO	3.4
1	3-B	178	PRO	3.4
1	4-B	178	PRO	3.4
1	5-B	178	PRO	3.4
1	6-B	178	PRO	3.4
1	7-B	178	PRO	3.4
1	8-B	178	PRO	3.4
1	9-B	178	PRO	3.4
1	10-B	178	PRO	3.4
1	11-B	178	PRO	3.4
1	12-B	178	PRO	3.4
1	13-B	178	PRO	3.4
1	14-B	178	PRO	3.4
1	15-B	178	PRO	3.4
1	16-B	178	PRO	3.4
1	1-B	172	GLN	3.2
1	2-B	172	GLN	3.2
1	3-B	172	GLN	3.2
1	4-B	172	GLN	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	5-B	172	GLN	3.2
1	6-B	172	GLN	3.2
1	7-B	172	GLN	3.2
1	8-B	172	GLN	3.2
1	9-B	172	GLN	3.2
1	10-B	172	GLN	3.2
1	11-B	172	GLN	3.2
1	12-B	172	GLN	3.2
1	13-B	172	GLN	3.2
1	14-B	172	GLN	3.2
1	15-B	172	GLN	3.2
1	16-B	172	GLN	3.2
1	1-A	214	LYS	3.0
1	2-A	214	LYS	3.0
1	3-A	214	LYS	3.0
1	4-A	214	LYS	3.0
1	5-A	214	LYS	3.0
1	6-A	214	LYS	3.0
1	7-A	214	LYS	3.0
1	8-A	214	LYS	3.0
1	9-A	214	LYS	3.0
1	10-A	214	LYS	3.0
1	11-A	214	LYS	3.0
1	12-A	214	LYS	3.0
1	13-A	214	LYS	3.0
1	14-A	214	LYS	3.0
1	15-A	214	LYS	3.0
1	16-A	214	LYS	3.0
1	1-B	114	GLU	2.9
1	2-B	114	GLU	2.9
1	3-B	114	GLU	2.9
1	4-B	114	GLU	2.9
1	5-B	114	GLU	2.9
1	6-B	114	GLU	2.9
1	7-B	114	GLU	2.9
1	8-B	114	GLU	2.9
1	9-B	114	GLU	2.9
1	10-B	114	GLU	2.9
1	11-B	114	GLU	2.9
1	12-B	114	GLU	2.9
1	13-B	114	GLU	2.9
1	14-B	114	GLU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	15-B	114	GLU	2.9
1	16-B	114	GLU	2.9
1	1-B	121	TRP	2.8
1	2-B	121	TRP	2.8
1	3-B	121	TRP	2.8
1	4-B	121	TRP	2.8
1	5-B	121	TRP	2.8
1	6-B	121	TRP	2.8
1	7-B	121	TRP	2.8
1	8-B	121	TRP	2.8
1	9-B	121	TRP	2.8
1	10-B	121	TRP	2.8
1	11-B	121	TRP	2.8
1	12-B	121	TRP	2.8
1	13-B	121	TRP	2.8
1	14-B	121	TRP	2.8
1	15-B	121	TRP	2.8
1	16-B	121	TRP	2.8
1	1-B	49	GLU	2.7
1	2-B	49	GLU	2.7
1	3-B	49	GLU	2.7
1	4-B	49	GLU	2.7
1	5-B	49	GLU	2.7
1	6-B	49	GLU	2.7
1	7-B	49	GLU	2.7
1	8-B	49	GLU	2.7
1	9-B	49	GLU	2.7
1	10-B	49	GLU	2.7
1	11-B	49	GLU	2.7
1	12-B	49	GLU	2.7
1	13-B	49	GLU	2.7
1	14-B	49	GLU	2.7
1	15-B	49	GLU	2.7
1	16-B	49	GLU	2.7
1	1-B	38	LYS	2.6
1	2-B	38	LYS	2.6
1	3-B	38	LYS	2.6
1	4-B	38	LYS	2.6
1	5-B	38	LYS	2.6
1	6-B	38	LYS	2.6
1	7-B	38	LYS	2.6
1	8-B	38	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	9-B	38	LYS	2.6
1	10-B	38	LYS	2.6
1	11-B	38	LYS	2.6
1	12-B	38	LYS	2.6
1	13-B	38	LYS	2.6
1	14-B	38	LYS	2.6
1	15-B	38	LYS	2.6
1	16-B	38	LYS	2.6
1	1-B	59	LYS	2.6
1	2-B	59	LYS	2.6
1	3-B	59	LYS	2.6
1	4-B	59	LYS	2.6
1	5-B	59	LYS	2.6
1	6-B	59	LYS	2.6
1	7-B	59	LYS	2.6
1	8-B	59	LYS	2.6
1	9-B	59	LYS	2.6
1	10-B	59	LYS	2.6
1	11-B	59	LYS	2.6
1	12-B	59	LYS	2.6
1	13-B	59	LYS	2.6
1	14-B	59	LYS	2.6
1	15-B	59	LYS	2.6
1	16-B	59	LYS	2.6
1	1-B	125	VAL	2.6
1	2-B	125	VAL	2.6
1	3-B	125	VAL	2.6
1	4-B	125	VAL	2.6
1	5-B	125	VAL	2.6
1	6-B	125	VAL	2.6
1	7-B	125	VAL	2.6
1	8-B	125	VAL	2.6
1	9-B	125	VAL	2.6
1	10-B	125	VAL	2.6
1	11-B	125	VAL	2.6
1	12-B	125	VAL	2.6
1	13-B	125	VAL	2.6
1	14-B	125	VAL	2.6
1	15-B	125	VAL	2.6
1	16-B	125	VAL	2.6
1	1-B	110	THR	2.5
1	2-B	110	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	3-B	110	THR	2.5
1	4-B	110	THR	2.5
1	5-B	110	THR	2.5
1	6-B	110	THR	2.5
1	7-B	110	THR	2.5
1	8-B	110	THR	2.5
1	9-B	110	THR	2.5
1	10-B	110	THR	2.5
1	11-B	110	THR	2.5
1	12-B	110	THR	2.5
1	13-B	110	THR	2.5
1	14-B	110	THR	2.5
1	15-B	110	THR	2.5
1	16-B	110	THR	2.5
1	1-B	56	ASP	2.5
1	2-B	56	ASP	2.5
1	3-B	56	ASP	2.5
1	4-B	56	ASP	2.5
1	5-B	56	ASP	2.5
1	6-B	56	ASP	2.5
1	7-B	56	ASP	2.5
1	8-B	56	ASP	2.5
1	9-B	56	ASP	2.5
1	10-B	56	ASP	2.5
1	11-B	56	ASP	2.5
1	12-B	56	ASP	2.5
1	13-B	56	ASP	2.5
1	14-B	56	ASP	2.5
1	15-B	56	ASP	2.5
1	16-B	56	ASP	2.5
1	1-A	142	GLY	2.4
1	2-A	142	GLY	2.4
1	3-A	142	GLY	2.4
1	4-A	142	GLY	2.4
1	5-A	142	GLY	2.4
1	6-A	142	GLY	2.4
1	7-A	142	GLY	2.4
1	8-A	142	GLY	2.4
1	9-A	142	GLY	2.4
1	10-A	142	GLY	2.4
1	11-A	142	GLY	2.4
1	12-A	142	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	13-A	142	GLY	2.4
1	14-A	142	GLY	2.4
1	15-A	142	GLY	2.4
1	16-A	142	GLY	2.4
1	1-B	113	MET	2.4
1	2-B	113	MET	2.4
1	3-B	113	MET	2.4
1	4-B	113	MET	2.4
1	5-B	113	MET	2.4
1	6-B	113	MET	2.4
1	7-B	113	MET	2.4
1	8-B	113	MET	2.4
1	9-B	113	MET	2.4
1	10-B	113	MET	2.4
1	11-B	113	MET	2.4
1	12-B	113	MET	2.4
1	13-B	113	MET	2.4
1	14-B	113	MET	2.4
1	15-B	113	MET	2.4
1	16-B	113	MET	2.4
1	1-B	35	GLU	2.4
1	2-B	35	GLU	2.4
1	3-B	35	GLU	2.4
1	4-B	35	GLU	2.4
1	5-B	35	GLU	2.4
1	6-B	35	GLU	2.4
1	7-B	35	GLU	2.4
1	8-B	35	GLU	2.4
1	9-B	35	GLU	2.4
1	10-B	35	GLU	2.4
1	11-B	35	GLU	2.4
1	12-B	35	GLU	2.4
1	13-B	35	GLU	2.4
1	14-B	35	GLU	2.4
1	15-B	35	GLU	2.4
1	16-B	35	GLU	2.4
1	1-B	43	GLU	2.4
1	2-B	43	GLU	2.4
1	3-B	43	GLU	2.4
1	4-B	43	GLU	2.4
1	5-B	43	GLU	2.4
1	6-B	43	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	7-B	43	GLU	2.4
1	8-B	43	GLU	2.4
1	9-B	43	GLU	2.4
1	10-B	43	GLU	2.4
1	11-B	43	GLU	2.4
1	12-B	43	GLU	2.4
1	13-B	43	GLU	2.4
1	14-B	43	GLU	2.4
1	15-B	43	GLU	2.4
1	16-B	43	GLU	2.4
1	1-B	242	SER	2.4
1	2-B	242	SER	2.4
1	3-B	242	SER	2.4
1	4-B	242	SER	2.4
1	5-B	242	SER	2.4
1	6-B	242	SER	2.4
1	7-B	242	SER	2.4
1	8-B	242	SER	2.4
1	9-B	242	SER	2.4
1	10-B	242	SER	2.4
1	11-B	242	SER	2.4
1	12-B	242	SER	2.4
1	13-B	242	SER	2.4
1	14-B	242	SER	2.4
1	15-B	242	SER	2.4
1	16-B	242	SER	2.4
1	1-B	89	LYS	2.3
1	2-B	89	LYS	2.3
1	3-B	89	LYS	2.3
1	4-B	89	LYS	2.3
1	5-B	89	LYS	2.3
1	6-B	89	LYS	2.3
1	7-B	89	LYS	2.3
1	8-B	89	LYS	2.3
1	9-B	89	LYS	2.3
1	10-B	89	LYS	2.3
1	11-B	89	LYS	2.3
1	12-B	89	LYS	2.3
1	13-B	89	LYS	2.3
1	14-B	89	LYS	2.3
1	15-B	89	LYS	2.3
1	16-B	89	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	242	SER	2.3
1	2-A	242	SER	2.3
1	3-A	242	SER	2.3
1	4-A	242	SER	2.3
1	5-A	242	SER	2.3
1	6-A	242	SER	2.3
1	7-A	242	SER	2.3
1	8-A	242	SER	2.3
1	9-A	242	SER	2.3
1	10-A	242	SER	2.3
1	11-A	242	SER	2.3
1	12-A	242	SER	2.3
1	13-A	242	SER	2.3
1	14-A	242	SER	2.3
1	15-A	242	SER	2.3
1	16-A	242	SER	2.3
1	1-B	45	HIS	2.3
1	2-B	45	HIS	2.3
1	3-B	45	HIS	2.3
1	4-B	45	HIS	2.3
1	5-B	45	HIS	2.3
1	6-B	45	HIS	2.3
1	7-B	45	HIS	2.3
1	8-B	45	HIS	2.3
1	9-B	45	HIS	2.3
1	10-B	45	HIS	2.3
1	11-B	45	HIS	2.3
1	12-B	45	HIS	2.3
1	13-B	45	HIS	2.3
1	14-B	45	HIS	2.3
1	15-B	45	HIS	2.3
1	16-B	45	HIS	2.3
1	1-B	111	LYS	2.2
1	2-B	111	LYS	2.2
1	3-B	111	LYS	2.2
1	4-B	111	LYS	2.2
1	5-B	111	LYS	2.2
1	6-B	111	LYS	2.2
1	7-B	111	LYS	2.2
1	8-B	111	LYS	2.2
1	9-B	111	LYS	2.2
1	10-B	111	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	11-B	111	LYS	2.2
1	12-B	111	LYS	2.2
1	13-B	111	LYS	2.2
1	14-B	111	LYS	2.2
1	15-B	111	LYS	2.2
1	16-B	111	LYS	2.2
1	1-B	192	VAL	2.2
1	2-B	192	VAL	2.2
1	3-B	192	VAL	2.2
1	4-B	192	VAL	2.2
1	5-B	192	VAL	2.2
1	6-B	192	VAL	2.2
1	7-B	192	VAL	2.2
1	8-B	192	VAL	2.2
1	9-B	192	VAL	2.2
1	10-B	192	VAL	2.2
1	11-B	192	VAL	2.2
1	12-B	192	VAL	2.2
1	13-B	192	VAL	2.2
1	14-B	192	VAL	2.2
1	15-B	192	VAL	2.2
1	16-B	192	VAL	2.2
1	1-B	231	MET	2.1
1	2-B	231	MET	2.1
1	3-B	231	MET	2.1
1	4-B	231	MET	2.1
1	5-B	231	MET	2.1
1	6-B	231	MET	2.1
1	7-B	231	MET	2.1
1	8-B	231	MET	2.1
1	9-B	231	MET	2.1
1	10-B	231	MET	2.1
1	11-B	231	MET	2.1
1	12-B	231	MET	2.1
1	13-B	231	MET	2.1
1	14-B	231	MET	2.1
1	15-B	231	MET	2.1
1	16-B	231	MET	2.1
1	1-B	173	ARG	2.1
1	2-B	173	ARG	2.1
1	3-B	173	ARG	2.1
1	4-B	173	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	5-B	173	ARG	2.1
1	6-B	173	ARG	2.1
1	7-B	173	ARG	2.1
1	8-B	173	ARG	2.1
1	9-B	173	ARG	2.1
1	10-B	173	ARG	2.1
1	11-B	173	ARG	2.1
1	12-B	173	ARG	2.1
1	13-B	173	ARG	2.1
1	14-B	173	ARG	2.1
1	15-B	173	ARG	2.1
1	16-B	173	ARG	2.1

## 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( $\text{\AA}^2$ )	Q<0.9
2	HEM	16-B	265	43/43	0.89	0.21	0.34	54,61,63,64	43
2	HEM	5-B	265	43/43	0.89	0.21	0.15	56,64,66,67	43
2	HEM	10-B	265	43/43	0.89	0.21	0.15	59,64,66,67	43
2	HEM	6-B	265	43/43	0.89	0.21	0.13	57,64,66,68	43
2	HEM	15-B	265	43/43	0.89	0.21	0.12	54,63,65,66	43
2	HEM	14-B	265	43/43	0.89	0.21	0.10	50,60,64,66	43
2	HEM	2-B	265	43/43	0.89	0.21	0.10	57,62,64,64	43
2	HEM	1-B	265	43/43	0.89	0.21	0.06	57,64,65,65	43
2	HEM	11-B	265	43/43	0.89	0.21	0.06	57,62,64,65	43

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	8-B	265	43/43	0.89	0.21	0.05	55,64,65,66	43
2	HEM	4-B	265	43/43	0.89	0.21	0.03	59,63,65,66	43
2	HEM	13-B	265	43/43	0.89	0.21	0.01	56,63,65,67	43
2	HEM	7-B	265	43/43	0.89	0.21	-0.02	58,64,65,66	43
2	HEM	9-B	265	43/43	0.89	0.21	-0.02	54,63,65,65	43
2	HEM	3-B	265	43/43	0.89	0.21	-0.02	44,62,64,65	43
2	HEM	12-B	265	43/43	0.89	0.21	-0.10	56,62,65,65	43
2	HEM	14-A	300	43/43	0.94	0.16	-0.52	44,50,53,56	43
2	HEM	15-A	300	43/43	0.94	0.16	-0.54	41,51,59,62	43
2	HEM	13-A	300	43/43	0.94	0.16	-0.59	44,49,53,55	43
2	HEM	9-A	300	43/43	0.94	0.16	-0.60	45,50,52,53	43
2	HEM	4-A	300	43/43	0.94	0.16	-0.60	43,49,53,57	43
2	HEM	6-A	300	43/43	0.94	0.16	-0.61	47,53,59,60	43
2	HEM	10-A	300	43/43	0.94	0.16	-0.61	47,53,59,60	43
2	HEM	5-A	300	43/43	0.94	0.16	-0.61	47,53,60,61	43
2	HEM	3-A	300	43/43	0.94	0.16	-0.65	42,51,53,54	43
2	HEM	2-A	300	43/43	0.94	0.16	-0.66	47,52,56,56	43
2	HEM	1-A	300	43/43	0.94	0.16	-0.66	47,53,59,60	43
2	HEM	16-A	300	43/43	0.94	0.16	-0.66	44,51,55,56	43
2	HEM	8-A	300	43/43	0.94	0.16	-0.66	47,52,55,56	43
2	HEM	11-A	300	43/43	0.94	0.16	-0.66	47,53,58,60	43
2	HEM	12-A	300	43/43	0.94	0.16	-0.66	47,53,59,60	43
2	HEM	7-A	300	43/43	0.94	0.16	-0.66	48,53,59,60	43

## 6.5 Other polymers

There are no such residues in this entry.