



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:33 PM GMT

PDB ID : 4DVQ  
Title : Structure of human aldosterone synthase, CYP11B2, in complex with deoxy-corticosterone  
Authors : Strushkevich, N.; Shen, L.; Tempel, W.; Arrowsmith, C.; Edwards, A.; Usanov, S.A.; Park, H.-W.  
Deposited on : 2012-02-23  
Resolution : 2.49 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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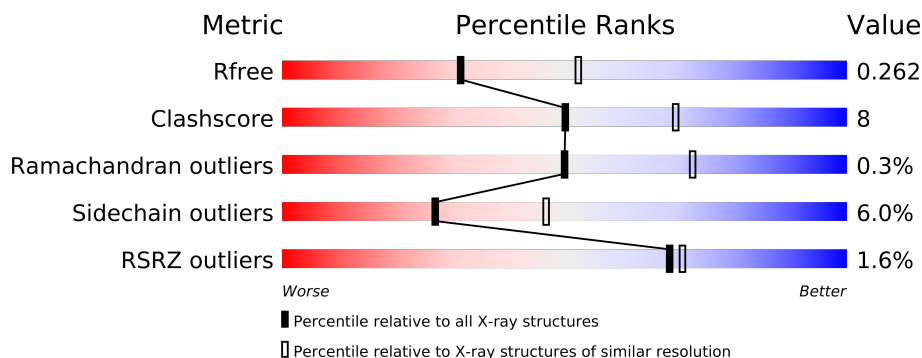
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.49 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	483	
1	B	483	
1	C	483	
1	D	483	
1	E	483	
1	F	483	
1	G	483	
1	H	483	
1	I	483	
1	J	483	
1	K	483	
1	L	483	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46194 atoms, of which 0 are hydrogen and 0 are deuterium.

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 P450 11B2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3758	2431	662	645	20			
1	B	463	Total	C	N	O	S	0	0	0
			3758	2431	662	645	20			
1	C	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	D	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	E	470	Total	C	N	O	S	0	0	0
			3826	2469	683	654	20			
1	F	469	Total	C	N	O	S	0	0	0
			3818	2465	681	652	20			
1	G	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	H	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	I	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	J	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	K	460	Total	C	N	O	S	0	0	0
			3734	2415	659	640	20			
1	L	454	Total	C	N	O	S	0	0	0
			3691	2387	650	634	20			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	EXPRESSION TAG	UNP P19099
A	28	ALA	-	EXPRESSION TAG	UNP P19099
A	29	LYS	-	EXPRESSION TAG	UNP P19099
A	30	LYS	-	EXPRESSION TAG	UNP P19099
A	31	THR	-	EXPRESSION TAG	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	-	EXPRESSION TAG	UNP P19099
A	33	SER	-	EXPRESSION TAG	UNP P19099
A	504	HIS	-	EXPRESSION TAG	UNP P19099
A	505	HIS	-	EXPRESSION TAG	UNP P19099
A	506	HIS	-	EXPRESSION TAG	UNP P19099
A	507	HIS	-	EXPRESSION TAG	UNP P19099
A	508	HIS	-	EXPRESSION TAG	UNP P19099
A	509	HIS	-	EXPRESSION TAG	UNP P19099
B	27	MET	-	EXPRESSION TAG	UNP P19099
B	28	ALA	-	EXPRESSION TAG	UNP P19099
B	29	LYS	-	EXPRESSION TAG	UNP P19099
B	30	LYS	-	EXPRESSION TAG	UNP P19099
B	31	THR	-	EXPRESSION TAG	UNP P19099
B	32	SER	-	EXPRESSION TAG	UNP P19099
B	33	SER	-	EXPRESSION TAG	UNP P19099
B	504	HIS	-	EXPRESSION TAG	UNP P19099
B	505	HIS	-	EXPRESSION TAG	UNP P19099
B	506	HIS	-	EXPRESSION TAG	UNP P19099
B	507	HIS	-	EXPRESSION TAG	UNP P19099
B	508	HIS	-	EXPRESSION TAG	UNP P19099
B	509	HIS	-	EXPRESSION TAG	UNP P19099
C	27	MET	-	EXPRESSION TAG	UNP P19099
C	28	ALA	-	EXPRESSION TAG	UNP P19099
C	29	LYS	-	EXPRESSION TAG	UNP P19099
C	30	LYS	-	EXPRESSION TAG	UNP P19099
C	31	THR	-	EXPRESSION TAG	UNP P19099
C	32	SER	-	EXPRESSION TAG	UNP P19099
C	33	SER	-	EXPRESSION TAG	UNP P19099
C	504	HIS	-	EXPRESSION TAG	UNP P19099
C	505	HIS	-	EXPRESSION TAG	UNP P19099
C	506	HIS	-	EXPRESSION TAG	UNP P19099
C	507	HIS	-	EXPRESSION TAG	UNP P19099
C	508	HIS	-	EXPRESSION TAG	UNP P19099
C	509	HIS	-	EXPRESSION TAG	UNP P19099
D	27	MET	-	EXPRESSION TAG	UNP P19099
D	28	ALA	-	EXPRESSION TAG	UNP P19099
D	29	LYS	-	EXPRESSION TAG	UNP P19099
D	30	LYS	-	EXPRESSION TAG	UNP P19099
D	31	THR	-	EXPRESSION TAG	UNP P19099
D	32	SER	-	EXPRESSION TAG	UNP P19099
D	33	SER	-	EXPRESSION TAG	UNP P19099
D	504	HIS	-	EXPRESSION TAG	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
D	505	HIS	-	EXPRESSION TAG	UNP P19099
D	506	HIS	-	EXPRESSION TAG	UNP P19099
D	507	HIS	-	EXPRESSION TAG	UNP P19099
D	508	HIS	-	EXPRESSION TAG	UNP P19099
D	509	HIS	-	EXPRESSION TAG	UNP P19099
E	27	MET	-	EXPRESSION TAG	UNP P19099
E	28	ALA	-	EXPRESSION TAG	UNP P19099
E	29	LYS	-	EXPRESSION TAG	UNP P19099
E	30	LYS	-	EXPRESSION TAG	UNP P19099
E	31	THR	-	EXPRESSION TAG	UNP P19099
E	32	SER	-	EXPRESSION TAG	UNP P19099
E	33	SER	-	EXPRESSION TAG	UNP P19099
E	504	HIS	-	EXPRESSION TAG	UNP P19099
E	505	HIS	-	EXPRESSION TAG	UNP P19099
E	506	HIS	-	EXPRESSION TAG	UNP P19099
E	507	HIS	-	EXPRESSION TAG	UNP P19099
E	508	HIS	-	EXPRESSION TAG	UNP P19099
E	509	HIS	-	EXPRESSION TAG	UNP P19099
F	27	MET	-	EXPRESSION TAG	UNP P19099
F	28	ALA	-	EXPRESSION TAG	UNP P19099
F	29	LYS	-	EXPRESSION TAG	UNP P19099
F	30	LYS	-	EXPRESSION TAG	UNP P19099
F	31	THR	-	EXPRESSION TAG	UNP P19099
F	32	SER	-	EXPRESSION TAG	UNP P19099
F	33	SER	-	EXPRESSION TAG	UNP P19099
F	504	HIS	-	EXPRESSION TAG	UNP P19099
F	505	HIS	-	EXPRESSION TAG	UNP P19099
F	506	HIS	-	EXPRESSION TAG	UNP P19099
F	507	HIS	-	EXPRESSION TAG	UNP P19099
F	508	HIS	-	EXPRESSION TAG	UNP P19099
F	509	HIS	-	EXPRESSION TAG	UNP P19099
G	27	MET	-	EXPRESSION TAG	UNP P19099
G	28	ALA	-	EXPRESSION TAG	UNP P19099
G	29	LYS	-	EXPRESSION TAG	UNP P19099
G	30	LYS	-	EXPRESSION TAG	UNP P19099
G	31	THR	-	EXPRESSION TAG	UNP P19099
G	32	SER	-	EXPRESSION TAG	UNP P19099
G	33	SER	-	EXPRESSION TAG	UNP P19099
G	504	HIS	-	EXPRESSION TAG	UNP P19099
G	505	HIS	-	EXPRESSION TAG	UNP P19099
G	506	HIS	-	EXPRESSION TAG	UNP P19099
G	507	HIS	-	EXPRESSION TAG	UNP P19099

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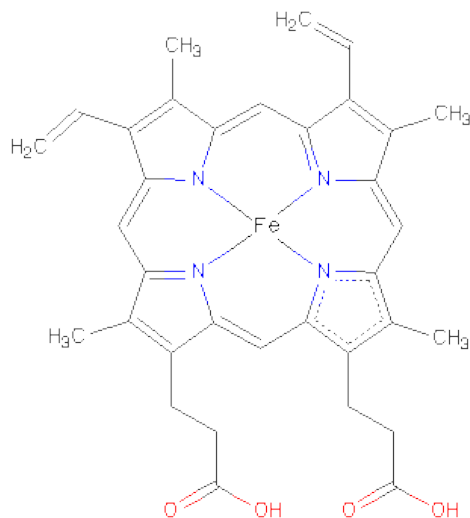
Chain	Residue	Modelled	Actual	Comment	Reference
G	508	HIS	-	EXPRESSION TAG	UNP P19099
G	509	HIS	-	EXPRESSION TAG	UNP P19099
H	27	MET	-	EXPRESSION TAG	UNP P19099
H	28	ALA	-	EXPRESSION TAG	UNP P19099
H	29	LYS	-	EXPRESSION TAG	UNP P19099
H	30	LYS	-	EXPRESSION TAG	UNP P19099
H	31	THR	-	EXPRESSION TAG	UNP P19099
H	32	SER	-	EXPRESSION TAG	UNP P19099
H	33	SER	-	EXPRESSION TAG	UNP P19099
H	504	HIS	-	EXPRESSION TAG	UNP P19099
H	505	HIS	-	EXPRESSION TAG	UNP P19099
H	506	HIS	-	EXPRESSION TAG	UNP P19099
H	507	HIS	-	EXPRESSION TAG	UNP P19099
H	508	HIS	-	EXPRESSION TAG	UNP P19099
H	509	HIS	-	EXPRESSION TAG	UNP P19099
I	27	MET	-	EXPRESSION TAG	UNP P19099
I	28	ALA	-	EXPRESSION TAG	UNP P19099
I	29	LYS	-	EXPRESSION TAG	UNP P19099
I	30	LYS	-	EXPRESSION TAG	UNP P19099
I	31	THR	-	EXPRESSION TAG	UNP P19099
I	32	SER	-	EXPRESSION TAG	UNP P19099
I	33	SER	-	EXPRESSION TAG	UNP P19099
I	504	HIS	-	EXPRESSION TAG	UNP P19099
I	505	HIS	-	EXPRESSION TAG	UNP P19099
I	506	HIS	-	EXPRESSION TAG	UNP P19099
I	507	HIS	-	EXPRESSION TAG	UNP P19099
I	508	HIS	-	EXPRESSION TAG	UNP P19099
I	509	HIS	-	EXPRESSION TAG	UNP P19099
J	27	MET	-	EXPRESSION TAG	UNP P19099
J	28	ALA	-	EXPRESSION TAG	UNP P19099
J	29	LYS	-	EXPRESSION TAG	UNP P19099
J	30	LYS	-	EXPRESSION TAG	UNP P19099
J	31	THR	-	EXPRESSION TAG	UNP P19099
J	32	SER	-	EXPRESSION TAG	UNP P19099
J	33	SER	-	EXPRESSION TAG	UNP P19099
J	504	HIS	-	EXPRESSION TAG	UNP P19099
J	505	HIS	-	EXPRESSION TAG	UNP P19099
J	506	HIS	-	EXPRESSION TAG	UNP P19099
J	507	HIS	-	EXPRESSION TAG	UNP P19099
J	508	HIS	-	EXPRESSION TAG	UNP P19099
J	509	HIS	-	EXPRESSION TAG	UNP P19099
K	27	MET	-	EXPRESSION TAG	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
K	28	ALA	-	EXPRESSION TAG	UNP P19099
K	29	LYS	-	EXPRESSION TAG	UNP P19099
K	30	LYS	-	EXPRESSION TAG	UNP P19099
K	31	THR	-	EXPRESSION TAG	UNP P19099
K	32	SER	-	EXPRESSION TAG	UNP P19099
K	33	SER	-	EXPRESSION TAG	UNP P19099
K	504	HIS	-	EXPRESSION TAG	UNP P19099
K	505	HIS	-	EXPRESSION TAG	UNP P19099
K	506	HIS	-	EXPRESSION TAG	UNP P19099
K	507	HIS	-	EXPRESSION TAG	UNP P19099
K	508	HIS	-	EXPRESSION TAG	UNP P19099
K	509	HIS	-	EXPRESSION TAG	UNP P19099
L	27	MET	-	EXPRESSION TAG	UNP P19099
L	28	ALA	-	EXPRESSION TAG	UNP P19099
L	29	LYS	-	EXPRESSION TAG	UNP P19099
L	30	LYS	-	EXPRESSION TAG	UNP P19099
L	31	THR	-	EXPRESSION TAG	UNP P19099
L	32	SER	-	EXPRESSION TAG	UNP P19099
L	33	SER	-	EXPRESSION TAG	UNP P19099
L	504	HIS	-	EXPRESSION TAG	UNP P19099
L	505	HIS	-	EXPRESSION TAG	UNP P19099
L	506	HIS	-	EXPRESSION TAG	UNP P19099
L	507	HIS	-	EXPRESSION TAG	UNP P19099
L	508	HIS	-	EXPRESSION TAG	UNP P19099
L	509	HIS	-	EXPRESSION TAG	UNP P19099

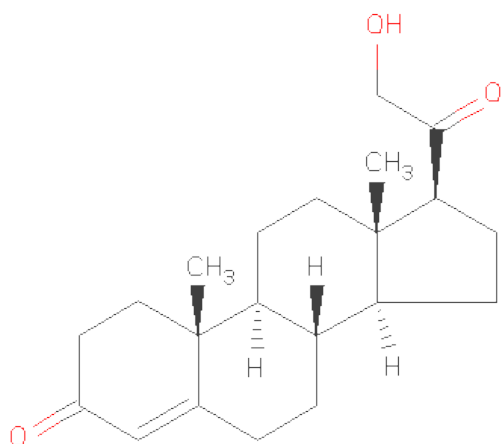
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

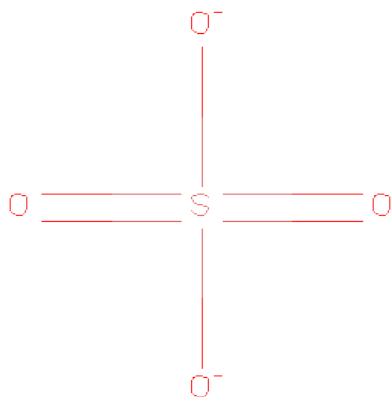
- Molecule 3 is DESOXYCORTICOSTERONE (three-letter code: 1CA) (formula: C<sub>21</sub>H<sub>30</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	21	3		
3	B	1	Total	C	O	0	0
			24	21	3		
3	C	1	Total	C	O	0	0
			24	21	3		
3	D	1	Total	C	O	0	0
			24	21	3		
3	E	1	Total	C	O	0	0
			24	21	3		
3	F	1	Total	C	O	0	0
			24	21	3		
3	G	1	Total	C	O	0	0
			24	21	3		
3	H	1	Total	C	O	0	0
			24	21	3		
3	I	1	Total	C	O	0	0
			24	21	3		
3	J	1	Total	C	O	0	0
			24	21	3		
3	K	1	Total	C	O	0	0
			24	21	3		
3	L	1	Total	C	O	0	0
			24	21	3		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	14	Total	O	0	0
			14	14		
5	C	31	Total	O	0	0
			31	31		

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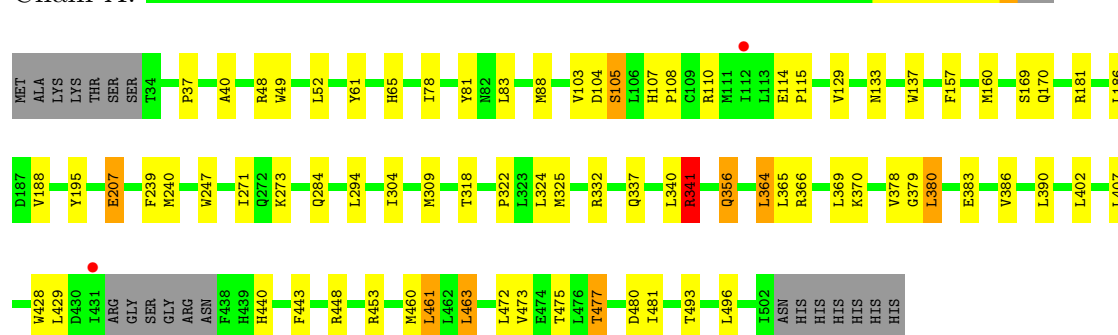
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	34	Total 34	O 34	0	0
5	E	30	Total 30	O 30	0	0
5	F	33	Total 33	O 33	0	0
5	G	18	Total 18	O 18	0	0
5	H	25	Total 25	O 25	0	0
5	I	6	Total 6	O 6	0	0
5	J	6	Total 6	O 6	0	0
5	K	13	Total 13	O 13	0	0
5	L	19	Total 19	O 19	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

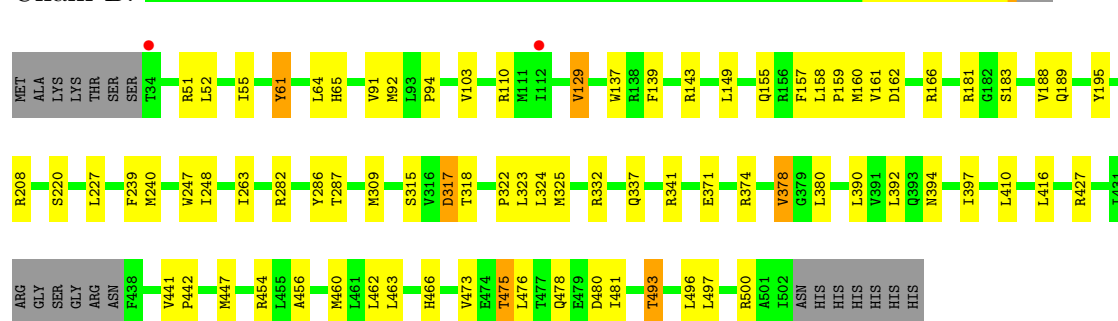
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain A:



- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain B:



- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain C:



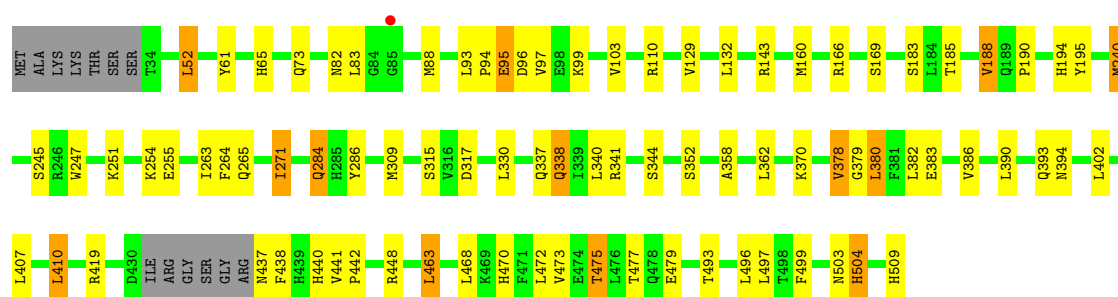
- Molecule 1: Cytochrome P450 11B2, mitochondrial

## Chain D:



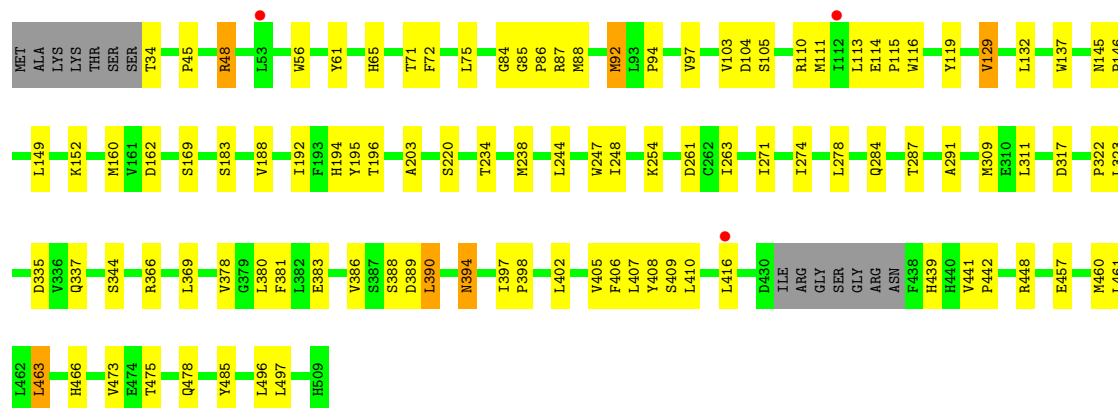
- Molecule 1: Cytochrome P450 11B2, mitochondrial

## Chain E:



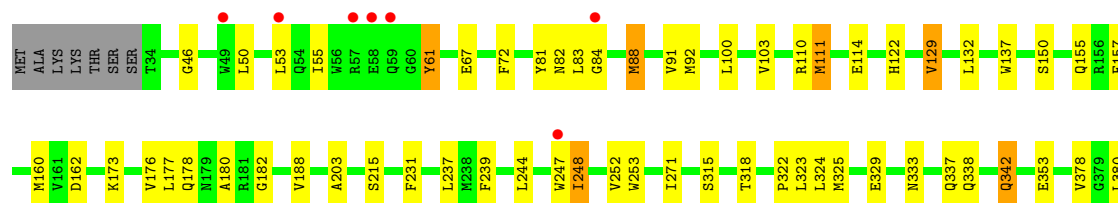
- Molecule 1: Cytochrome P450 11B2, mitochondrial

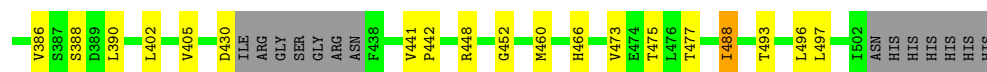
## Chain F:



- Molecule 1: Cytochrome P450 11B2, mitochondrial

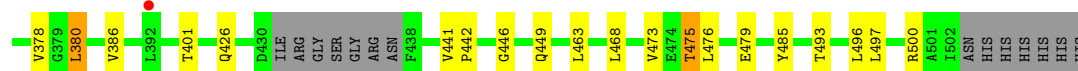
## Chain G:





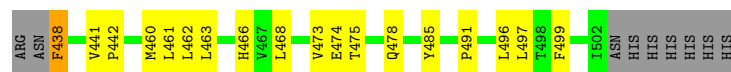
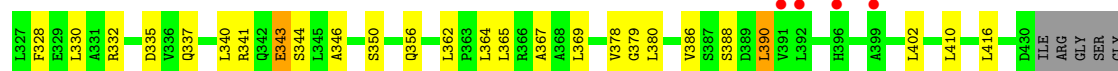
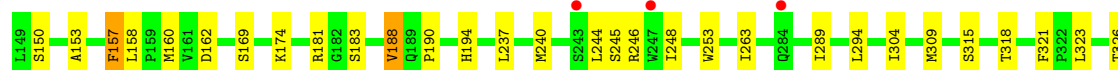
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain H:



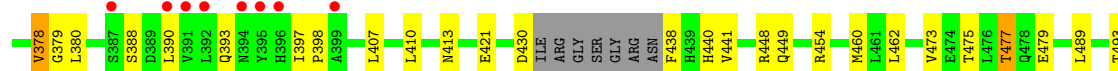
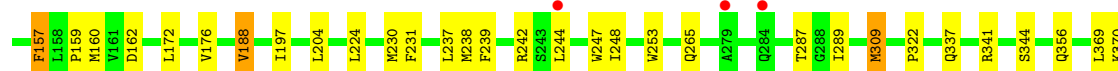
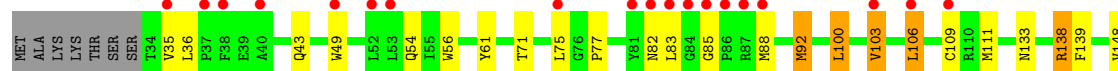
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain I:



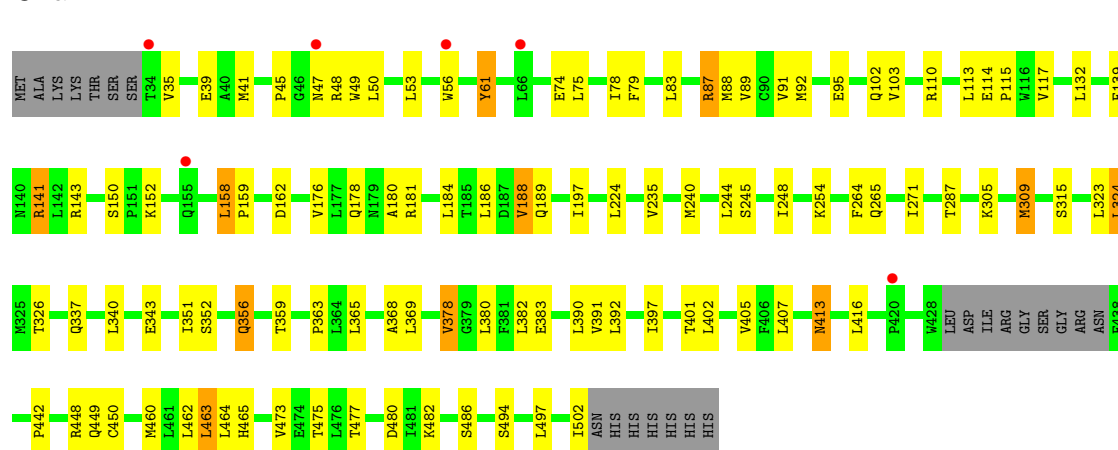
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain J:



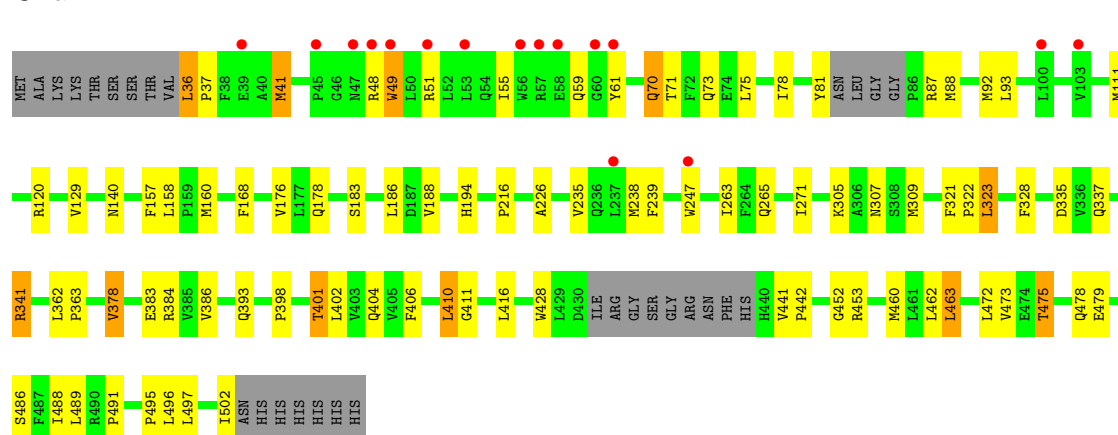
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain K:



- Molecule 1: Cytochrome P450 11B2, mitochondrial

## Chain L:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.35Å 199.63Å 150.15Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	48.07 – 2.49 48.07 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.07-2.49) 99.2 (48.07-2.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.204 , 0.263 0.205 , 0.262	Depositor DCC
$R_{free}$ test set	12220 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 23.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 245705 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	46194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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 42.03 % 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 2.1639e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 1CA, SO4

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	0.68	3/3858 (0.1%)	0.69	2/5235 (0.0%)
1	B	0.63	1/3858 (0.0%)	0.66	0/5235
1	C	0.67	2/3850 (0.1%)	0.68	0/5224
1	D	0.67	2/3850 (0.1%)	0.68	0/5224
1	E	0.67	1/3932 (0.0%)	0.68	0/5336
1	F	0.66	1/3924 (0.0%)	0.66	0/5325
1	G	0.62	0/3850	0.65	0/5224
1	H	0.64	0/3850	0.67	0/5224
1	I	0.62	2/3850 (0.1%)	0.63	0/5224
1	J	0.61	3/3850 (0.1%)	0.62	1/5224 (0.0%)
1	K	0.62	1/3834 (0.0%)	0.64	0/5202
1	L	0.63	3/3788 (0.1%)	0.65	0/5137
All	All	0.64	19/46294 (0.0%)	0.66	3/62814 (0.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	TRP	CD2-CE2	5.77	1.48	1.41
1	A	247	TRP	CD2-CE2	5.71	1.48	1.41
1	E	247	TRP	CD2-CE2	5.57	1.48	1.41
1	L	428	TRP	CD2-CE2	5.45	1.47	1.41
1	J	56	TRP	CD2-CE2	5.34	1.47	1.41
1	A	49	TRP	CD2-CE2	5.26	1.47	1.41
1	F	56	TRP	CD2-CE2	5.24	1.47	1.41
1	D	247	TRP	CD2-CE2	5.22	1.47	1.41
1	I	49	TRP	CD2-CE2	5.20	1.47	1.41
1	L	49	TRP	CD2-CE2	5.20	1.47	1.41
1	C	253	TRP	CD2-CE2	5.18	1.47	1.41
1	L	247	TRP	CD2-CE2	5.18	1.47	1.41
1	J	49	TRP	CD2-CE2	5.17	1.47	1.41
1	D	49	TRP	CD2-CE2	5.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	49	TRP	CD2-CE2	5.13	1.47	1.41
1	A	428	TRP	CD2-CE2	5.11	1.47	1.41
1	C	49	TRP	CD2-CE2	5.11	1.47	1.41
1	J	247	TRP	CD2-CE2	5.08	1.47	1.41
1	I	56	TRP	CD2-CE2	5.00	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	J	454	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	104	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3758	0	3796	48	0
1	B	3758	0	3796	55	0
1	C	3750	0	3785	51	0
1	D	3750	0	3785	52	0
1	E	3826	0	3839	54	0
1	F	3818	0	3833	67	0
1	G	3750	0	3785	57	0
1	H	3750	0	3785	52	0
1	I	3750	0	3785	62	0
1	J	3750	0	3785	51	0
1	K	3734	0	3770	80	0
1	L	3691	0	3730	55	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	2	0
2	E	43	0	30	7	0
2	F	43	0	30	4	0
2	G	43	0	30	5	0
2	H	43	0	30	2	0
2	I	43	0	30	4	0
2	J	43	0	30	0	0
2	K	43	0	30	3	0
2	L	43	0	30	9	0
3	A	24	0	30	0	0
3	B	24	0	30	0	0
3	C	24	0	30	1	0
3	D	24	0	30	0	0
3	E	24	0	30	0	0
3	F	24	0	30	0	0
3	G	24	0	30	0	0
3	H	24	0	30	0	0
3	I	24	0	30	1	0
3	J	24	0	30	0	0
3	K	24	0	30	0	0
3	L	24	0	30	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	K	5	0	0	0	0
4	L	5	0	0	0	0
5	A	31	0	0	0	0
5	B	14	0	0	1	0
5	C	31	0	0	0	0
5	D	34	0	0	1	0
5	E	30	0	0	0	0
5	F	33	0	0	2	0
5	G	18	0	0	0	0
5	H	25	0	0	0	0
5	I	6	0	0	0	0
5	J	6	0	0	0	0
5	K	13	0	0	1	0
5	L	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	46194	0	46194	691	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (691) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:475:THR:CG2	1:I:497:LEU:HD23	1.87	1.04
1:J:369:LEU:HD22	1:J:460:MET:HE2	1.38	1.03
1:G:337:GLN:HE22	1:G:473:VAL:H	1.04	1.01
1:H:475:THR:HG22	1:H:496:LEU:O	1.62	0.99
1:F:475:THR:HG22	1:F:496:LEU:O	1.61	0.98
1:F:369:LEU:HD22	1:F:460:MET:HE2	1.42	0.98
1:L:398:PRO:O	1:L:401:THR:HG23	1.64	0.97
1:A:481:ILE:HG23	1:A:493:THR:HG22	1.44	0.95
1:H:475:THR:HG23	1:H:497:LEU:HD23	1.46	0.95
1:K:356:GLN:HE21	1:K:356:GLN:H	1.17	0.92
1:H:475:THR:CG2	1:H:497:LEU:HD23	2.01	0.91
1:B:158:LEU:CD1	1:B:462:LEU:HD11	2.00	0.91
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	1.99	0.89
1:D:337:GLN:HE22	1:D:473:VAL:H	1.16	0.89
1:I:337:GLN:HE22	1:I:473:VAL:H	1.17	0.89
1:K:475:THR:CG2	1:K:497:LEU:HD22	2.04	0.88
1:D:475:THR:HG23	1:D:496:LEU:O	1.74	0.87
1:L:378:VAL:CG1	2:L:601:HEM:HMB2	2.05	0.86
1:H:337:GLN:HE22	1:H:473:VAL:H	1.20	0.85
1:K:475:THR:HG21	1:K:497:LEU:CD2	2.06	0.85
1:F:475:THR:CG2	1:F:497:LEU:HD23	2.06	0.83
1:F:475:THR:HG23	1:F:497:LEU:HD23	1.58	0.83
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.58	0.83
1:B:337:GLN:HE22	1:B:473:VAL:H	1.24	0.83
1:I:475:THR:HG21	1:I:497:LEU:HD23	1.59	0.83
1:D:47:ASN:HD21	1:D:50:LEU:HD12	1.43	0.83
1:B:475:THR:HG23	1:B:497:LEU:HD23	1.62	0.81
1:B:158:LEU:HD12	1:B:462:LEU:HD11	1.60	0.80
1:E:83:LEU:HD22	1:E:88:MET:HE1	1.62	0.80
1:A:83:LEU:HD13	1:A:88:MET:HE1	1.63	0.79
1:A:475:THR:HG23	1:A:496:LEU:O	1.82	0.79
1:A:337:GLN:HE22	1:A:473:VAL:H	1.29	0.78
1:B:322:PRO:HB2	1:B:460:MET:HE3	1.66	0.78
1:K:337:GLN:HE22	1:K:473:VAL:H	1.31	0.78
1:A:157:PHE:HA	1:A:160:MET:HE2	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:369:LEU:HD22	1:I:460:MET:HE2	1.66	0.78
1:K:475:THR:CG2	1:K:497:LEU:CD2	2.61	0.77
1:G:315:SER:HB3	2:G:601:HEM:HBC2	1.65	0.77
1:E:337:GLN:HE22	1:E:473:VAL:H	1.32	0.77
1:A:356:GLN:HE21	1:A:356:GLN:H	1.32	0.77
1:J:103:VAL:HG11	1:J:390:LEU:HD13	1.64	0.77
1:L:378:VAL:CG1	2:L:601:HEM:CMB	2.61	0.77
1:C:158:LEU:CD2	1:C:462:LEU:HD11	2.14	0.77
1:L:140:ASN:HD22	1:L:307:ASN:HD21	1.30	0.77
1:E:378:VAL:CG2	2:E:601:HEM:HMB2	2.15	0.77
2:F:601:HEM:HBC2	2:F:601:HEM:HMC2	1.67	0.76
1:F:337:GLN:HE22	1:F:473:VAL:H	1.30	0.76
1:K:323:LEU:HD21	1:K:463:LEU:CD2	2.16	0.76
1:B:263:ILE:HG22	1:B:309:MET:HE1	1.66	0.76
1:H:240:MET:CE	1:H:248:ILE:HD12	2.16	0.76
1:F:94:PRO:HG3	1:F:416:LEU:HD11	1.68	0.75
1:F:386:VAL:HG11	1:F:390:LEU:CD2	2.17	0.75
1:L:475:THR:HG23	1:L:497:LEU:HD23	1.69	0.74
1:D:160:MET:HE3	1:D:203:ALA:HA	1.70	0.73
1:I:263:ILE:HG22	1:I:309:MET:HE1	1.69	0.73
1:L:263:ILE:HG22	1:L:309:MET:HE1	1.69	0.73
1:H:240:MET:HE3	1:H:248:ILE:HD12	1.70	0.73
1:I:337:GLN:HE21	1:I:341:ARG:HH22	1.36	0.72
1:K:323:LEU:HD21	1:K:463:LEU:HD22	1.72	0.72
1:G:475:THR:OG1	1:G:497:LEU:HD23	1.88	0.72
1:L:337:GLN:HE22	1:L:473:VAL:H	1.35	0.72
1:L:55:ILE:HD11	1:L:239:PHE:HD1	1.54	0.72
1:I:475:THR:HG23	1:I:497:LEU:HD23	1.71	0.71
1:J:380:LEU:HD13	1:J:489:LEU:HD22	1.72	0.71
1:A:81:TYR:HB3	1:A:88:MET:HE2	1.71	0.71
1:J:337:GLN:HE22	1:J:473:VAL:H	1.38	0.71
1:L:383:GLU:HG2	1:L:402:LEU:HD11	1.72	0.71
1:A:364:LEU:HD13	1:A:429:LEU:HD11	1.71	0.71
2:A:601:HEM:HMC2	2:A:601:HEM:CBC	2.21	0.71
1:C:337:GLN:HE22	1:C:473:VAL:H	1.38	0.71
1:G:55:ILE:HD11	1:G:239:PHE:HD1	1.56	0.71
1:L:41:MET:HE1	1:L:78:ILE:HG12	1.71	0.70
1:A:356:GLN:NE2	1:A:356:GLN:H	1.88	0.70
1:D:158:LEU:HD22	1:D:356:GLN:HA	1.74	0.70
1:B:322:PRO:HB2	1:B:460:MET:CE	2.20	0.70
1:L:410:LEU:HD12	1:L:410:LEU:C	2.11	0.69
1:E:337:GLN:HE21	1:E:341:ARG:HH22	1.40	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:47:ASN:ND2	1:D:50:LEU:HD12	2.07	0.69
1:I:475:THR:CG2	1:I:497:LEU:CD2	2.67	0.69
1:I:475:THR:HG22	1:I:496:LEU:O	1.92	0.68
1:F:311:LEU:HD23	2:F:601:HEM:HAC	1.76	0.68
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.75	0.68
1:C:154:VAL:HG21	1:C:454:ARG:HD3	1.74	0.68
1:F:369:LEU:HD22	1:F:460:MET:CE	2.19	0.68
1:E:503:ASN:O	1:E:504:HIS:HB2	1.94	0.68
1:H:244:LEU:HD21	1:K:53:LEU:HD13	1.76	0.67
1:B:181:ARG:HG2	1:F:287:THR:HG21	1.76	0.67
1:E:83:LEU:HD13	1:E:88:MET:HE1	1.77	0.67
1:K:186:LEU:HD21	1:K:188:VAL:HG13	1.77	0.66
1:C:158:LEU:HD23	1:C:462:LEU:HD11	1.77	0.65
1:H:323:LEU:HD11	1:H:463:LEU:HD13	1.78	0.65
1:L:140:ASN:ND2	1:L:307:ASN:HD21	1.94	0.65
1:J:43:GLN:HE22	1:J:82:ASN:HD22	1.43	0.65
1:J:100:LEU:O	1:J:100:LEU:HD12	1.97	0.65
1:D:240:MET:CE	1:D:248:ILE:HD12	2.27	0.65
1:D:240:MET:HE3	1:D:248:ILE:HD12	1.79	0.65
1:E:386:VAL:HG11	1:E:390:LEU:HD22	1.78	0.65
1:K:369:LEU:HD22	1:K:460:MET:HE2	1.77	0.65
1:G:475:THR:HG22	1:G:477:THR:H	1.60	0.65
1:E:378:VAL:CG2	2:E:601:HEM:CMB	2.75	0.65
1:K:309:MET:HE3	1:K:309:MET:HA	1.78	0.64
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.26	0.64
1:G:111:MET:HE1	1:G:402:LEU:HD22	1.79	0.64
1:I:475:THR:HG23	1:I:497:LEU:CD2	2.27	0.64
1:J:204:LEU:HD23	1:J:289:ILE:HD12	1.78	0.64
1:C:322:PRO:HB2	1:C:460:MET:CE	2.28	0.64
1:J:157:PHE:HA	1:J:160:MET:HE2	1.80	0.64
1:J:337:GLN:HE21	1:J:341:ARG:HH22	1.44	0.64
1:F:103:VAL:HG12	1:F:103:VAL:O	1.96	0.64
1:A:52:LEU:HD22	1:A:239:PHE:O	1.98	0.64
1:A:386:VAL:HG21	1:A:390:LEU:HD22	1.79	0.63
1:B:332:ARG:NH1	1:B:480:ASP:OD1	2.31	0.63
1:I:245:SER:HA	1:I:248:ILE:HG22	1.80	0.63
1:A:337:GLN:HE21	1:A:341:ARG:HH22	1.45	0.63
1:K:114:GLU:HG2	1:K:115:PRO:HD3	1.81	0.63
1:K:41:MET:HE1	1:K:78:ILE:HG12	1.80	0.62
1:L:322:PRO:HB2	1:L:460:MET:HE3	1.80	0.62
1:G:315:SER:HB3	2:G:601:HEM:CBC	2.29	0.62
1:E:110:ARG:NH1	2:E:601:HEM:O1A	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:53:LEU:HD13	1:K:244:LEU:HD11	1.80	0.62
1:L:157:PHE:HA	1:L:160:MET:HE2	1.82	0.62
1:H:157:PHE:HA	1:H:160:MET:HE1	1.80	0.62
1:C:410:LEU:O	1:C:410:LEU:HD12	1.99	0.61
1:F:113:LEU:HD23	1:F:116:TRP:CG	2.36	0.61
1:D:103:VAL:HG12	1:D:103:VAL:O	2.00	0.61
1:A:366:ARG:HG3	1:A:461:LEU:HD21	1.83	0.61
1:I:94:PRO:HG2	1:I:416:LEU:HD13	1.82	0.61
1:B:157:PHE:HA	1:B:160:MET:HE2	1.83	0.61
1:F:194:HIS:CE1	1:F:220:SER:OG	2.54	0.61
1:K:87:ARG:HB2	1:K:401:THR:HG23	1.82	0.61
1:J:475:THR:OG1	1:J:497:LEU:HD23	2.01	0.60
1:E:378:VAL:HG21	2:E:601:HEM:HMB2	1.84	0.60
1:B:456:ALA:O	1:B:460:MET:HG3	2.01	0.60
1:C:322:PRO:HG3	1:C:378:VAL:CG2	2.31	0.60
1:J:477:THR:HG23	1:J:479:GLU:OE2	2.02	0.60
1:L:235:VAL:HA	1:L:238:MET:HE2	1.83	0.60
1:G:72:PHE:HB3	1:G:92:MET:CE	2.32	0.60
1:G:337:GLN:HE22	1:G:473:VAL:N	1.87	0.60
1:E:475:THR:HG23	1:E:497:LEU:HD23	1.83	0.60
1:B:129:VAL:HG22	1:B:137:TRP:CD1	2.37	0.60
1:G:160:MET:HE1	1:G:203:ALA:HA	1.83	0.60
1:H:112:ILE:HG23	1:H:117:VAL:HG21	1.83	0.60
1:C:52:LEU:HD22	1:C:240:MET:HB3	1.84	0.60
1:L:383:GLU:CG	1:L:402:LEU:HD11	2.31	0.60
1:K:392:LEU:HB2	1:K:397:ILE:HD11	1.84	0.60
1:G:188:VAL:HG23	1:G:324:LEU:CD1	2.32	0.60
1:G:103:VAL:HG21	1:G:390:LEU:HD13	1.84	0.60
1:J:369:LEU:HD22	1:J:460:MET:CE	2.24	0.59
1:H:240:MET:HE1	1:H:245:SER:HA	1.84	0.59
1:J:475:THR:HG23	1:J:496:LEU:O	2.02	0.59
1:K:356:GLN:NE2	1:K:356:GLN:H	1.94	0.59
1:E:315:SER:HA	2:E:601:HEM:HMC2	1.85	0.59
1:K:41:MET:HE1	1:K:89:VAL:HG13	1.82	0.59
1:F:45:PRO:HD3	1:F:75:LEU:HD11	1.84	0.59
1:K:240:MET:HE1	1:K:245:SER:HA	1.85	0.59
1:J:287:THR:HG22	1:K:180:ALA:HB1	1.83	0.59
1:K:47:ASN:HD22	1:K:50:LEU:HD12	1.67	0.59
1:H:263:ILE:HG22	1:H:309:MET:HE1	1.85	0.59
1:G:475:THR:HG1	1:G:497:LEU:HD23	1.67	0.59
2:F:601:HEM:CMC	2:F:601:HEM:HBC2	2.31	0.59
1:G:475:THR:OG1	1:G:497:LEU:CD2	2.51	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:102:GLN:HE21	1:C:102:GLN:N	2.01	0.59
1:L:378:VAL:HG13	2:L:601:HEM:CMB	2.33	0.58
1:L:322:PRO:HB2	1:L:460:MET:CE	2.31	0.58
1:G:180:ALA:HB1	1:K:287:THR:HG22	1.84	0.58
1:H:446:GLY:O	1:H:449:GLN:NE2	2.35	0.58
1:I:340:LEU:CD2	1:I:364:LEU:HD23	2.33	0.58
1:F:475:THR:CG2	1:F:496:LEU:O	2.45	0.58
1:A:83:LEU:HD13	1:A:88:MET:CE	2.34	0.58
1:G:111:MET:CE	1:G:402:LEU:HD22	2.34	0.58
1:E:263:ILE:HG22	1:E:309:MET:HE1	1.85	0.58
1:I:340:LEU:HD21	1:I:364:LEU:HD23	1.86	0.58
1:L:378:VAL:HG13	2:L:601:HEM:HMB1	1.85	0.58
1:J:43:GLN:NE2	1:J:82:ASN:HD22	2.02	0.58
1:D:76:GLY:HA2	1:I:139:PHE:CE1	2.38	0.58
1:D:339:ILE:HG22	1:D:364:LEU:HD13	1.86	0.58
1:H:475:THR:CG2	1:H:496:LEU:O	2.47	0.58
1:H:323:LEU:CD1	1:H:463:LEU:HD13	2.34	0.58
1:B:240:MET:CE	1:B:248:ILE:HD12	2.34	0.58
1:J:83:LEU:HD13	1:J:88:MET:HE3	1.85	0.57
1:D:475:THR:CG2	1:D:496:LEU:O	2.51	0.57
1:L:475:THR:HG22	1:L:496:LEU:O	2.04	0.57
1:A:133:ASN:OD1	1:A:448:ARG:NH2	2.37	0.57
1:E:103:VAL:O	1:E:103:VAL:HG12	2.05	0.57
1:D:356:GLN:HE21	1:D:356:GLN:H	1.53	0.57
1:I:148:VAL:HG22	1:I:289:ILE:HG21	1.87	0.57
1:K:113:LEU:O	1:K:117:VAL:HG23	2.04	0.57
1:E:195:TYR:CD2	1:E:463:LEU:HD13	2.39	0.57
1:I:146:PRO:O	1:I:150:SER:OG	2.22	0.57
1:B:52:LEU:HD22	1:B:239:PHE:O	2.05	0.57
1:F:244:LEU:HD12	1:F:247:TRP:CZ2	2.39	0.57
1:B:240:MET:HE1	1:B:248:ILE:HD12	1.87	0.57
1:B:158:LEU:HD11	1:B:462:LEU:HD11	1.87	0.57
1:I:323:LEU:HD22	1:I:463:LEU:HD22	1.87	0.57
1:C:158:LEU:HD22	1:C:462:LEU:HD11	1.87	0.56
1:C:475:THR:HG23	1:C:496:LEU:O	2.05	0.56
1:C:158:LEU:HD23	1:C:462:LEU:CD1	2.35	0.56
1:G:103:VAL:O	1:G:103:VAL:HG12	2.05	0.56
1:B:475:THR:CG2	1:B:497:LEU:HD23	2.35	0.56
1:A:364:LEU:HD13	1:A:429:LEU:CD1	2.34	0.56
1:B:315:SER:HA	2:B:601:HEM:HMC2	1.87	0.56
1:E:94:PRO:O	1:E:95:GLU:C	2.42	0.56
1:G:91:VAL:HG23	1:G:405:VAL:HG22	1.85	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:340:LEU:HD22	1:K:365:LEU:HA	1.86	0.56
1:D:337:GLN:HE22	1:D:473:VAL:N	1.95	0.56
1:D:176:VAL:HG13	1:D:183:SER:HA	1.87	0.56
1:K:392:LEU:HD12	1:K:397:ILE:HD13	1.88	0.56
1:E:52:LEU:HD21	1:E:240:MET:HB3	1.88	0.56
1:K:41:MET:HE2	1:K:79:PHE:C	2.25	0.56
1:L:378:VAL:HG12	2:L:601:HEM:HMB2	1.84	0.56
1:D:383:GLU:HG3	1:D:402:LEU:HD11	1.87	0.56
1:J:172:LEU:O	1:J:176:VAL:HG23	2.06	0.56
1:H:195:TYR:CD2	1:H:463:LEU:HD12	2.41	0.55
1:A:332:ARG:NH1	1:A:480:ASP:OD1	2.34	0.55
1:G:157:PHE:HA	1:G:160:MET:HE2	1.88	0.55
1:E:83:LEU:HD13	1:E:88:MET:CE	2.37	0.55
1:C:83:LEU:HD22	1:C:88:MET:HB2	1.88	0.55
1:G:237:LEU:HD11	1:G:252:VAL:HG12	1.89	0.55
1:B:337:GLN:NE2	1:B:473:VAL:H	2.01	0.55
1:C:94:PRO:HD3	1:C:410:LEU:HD13	1.87	0.55
1:I:369:LEU:HD22	1:I:460:MET:CE	2.36	0.55
1:F:416:LEU:HD22	1:F:439:HIS:NE2	2.22	0.55
1:L:475:THR:CG2	1:L:497:LEU:HD23	2.35	0.55
1:I:315:SER:HA	2:I:601:HEM:HMC2	1.89	0.55
1:H:176:VAL:HG22	1:H:184:LEU:N	2.22	0.55
1:D:443:PHE:CG	1:D:453:ARG:HG3	2.42	0.55
1:H:83:LEU:HD22	1:H:86:PRO:HG2	1.88	0.55
1:B:227:LEU:HD13	1:B:317:ASP:OD1	2.07	0.55
1:K:315:SER:HA	2:K:601:HEM:HMC2	1.88	0.55
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.88	0.55
1:C:337:GLN:HE21	1:C:341:ARG:HH22	1.54	0.55
2:D:601:HEM:HBC2	2:D:601:HEM:CMC	2.36	0.55
1:D:149:LEU:HD12	1:D:454:ARG:HG3	1.89	0.55
1:F:386:VAL:HG12	1:F:388:SER:H	1.72	0.55
1:J:197:ILE:HD11	1:J:224:LEU:HD21	1.89	0.55
1:H:47:ASN:ND2	1:H:50:LEU:HD13	2.22	0.55
1:I:83:LEU:HD23	1:I:86:PRO:HG2	1.89	0.54
1:B:189:GLN:HA	1:B:324:LEU:HD21	1.90	0.54
1:A:322:PRO:HG3	1:A:378:VAL:CG2	2.37	0.54
1:B:475:THR:HG22	1:B:496:LEU:O	2.07	0.54
1:H:240:MET:HE3	1:H:244:LEU:HB3	1.88	0.54
1:F:94:PRO:CG	1:F:416:LEU:HD11	2.35	0.54
1:C:240:MET:HE3	1:C:245:SER:HA	1.90	0.54
1:B:103:VAL:CG1	1:B:103:VAL:O	2.55	0.54
1:E:284:GLN:H	1:E:284:GLN:CD	2.11	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:463:LEU:HD23	1:H:463:LEU:C	2.27	0.54
1:J:475:THR:HG22	1:J:477:THR:H	1.71	0.54
1:J:148:VAL:HG22	1:J:289:ILE:HG21	1.89	0.54
1:K:158:LEU:HD13	1:K:462:LEU:HD11	1.90	0.54
1:L:475:THR:CG2	1:L:496:LEU:O	2.55	0.54
1:E:240:MET:HE2	1:E:245:SER:HB3	1.90	0.54
1:D:263:ILE:HG22	1:D:309:MET:HE1	1.89	0.54
1:L:55:ILE:HD11	1:L:239:PHE:CD1	2.41	0.54
1:C:110:ARG:NH2	2:C:601:HEM:O2D	2.40	0.54
1:L:384:ARG:NH2	2:L:601:HEM:O1A	2.41	0.53
1:J:83:LEU:HD13	1:J:88:MET:CE	2.38	0.53
1:D:322:PRO:HB2	1:D:460:MET:HE3	1.90	0.53
1:L:337:GLN:HE21	1:L:341:ARG:HH22	1.56	0.53
1:G:110:ARG:NH1	2:G:601:HEM:O1A	2.42	0.53
1:E:475:THR:HG22	1:E:496:LEU:O	2.08	0.53
1:I:318:THR:HA	1:I:378:VAL:HG11	1.89	0.53
1:L:321:PHE:CD2	1:L:491:PRO:HD2	2.43	0.53
1:K:326:THR:HG21	1:K:464:LEU:CD1	2.38	0.53
1:I:475:THR:HG21	1:I:497:LEU:CD2	2.33	0.53
1:D:160:MET:CE	1:D:203:ALA:HA	2.37	0.53
1:K:365:LEU:O	1:K:368:ALA:HB3	2.09	0.53
1:A:325:MET:HA	1:A:325:MET:CE	2.38	0.53
1:C:102:GLN:CA	1:C:102:GLN:HE21	2.21	0.53
1:D:443:PHE:CD2	1:D:453:ARG:HG3	2.43	0.53
1:A:318:THR:HA	1:A:378:VAL:HG11	1.91	0.53
1:G:173:LYS:HE3	1:G:177:LEU:HD11	1.91	0.53
1:I:328:PHE:CE2	1:I:332:ARG:HD2	2.42	0.53
1:E:475:THR:CG2	1:E:496:LEU:O	2.57	0.53
1:G:237:LEU:HD22	1:G:253:TRP:CE2	2.44	0.53
1:D:424:ASN:O	1:D:427:ARG:HG2	2.08	0.53
1:E:94:PRO:O	1:E:97:VAL:N	2.42	0.53
1:K:158:LEU:CD1	1:K:462:LEU:HD11	2.39	0.53
1:K:326:THR:HG21	1:K:464:LEU:HD11	1.91	0.53
1:C:148:VAL:HG22	1:C:289:ILE:CG2	2.39	0.53
1:K:383:GLU:CG	1:K:402:LEU:HD11	2.39	0.53
1:I:441:VAL:N	1:I:442:PRO:CD	2.72	0.53
1:F:441:VAL:N	1:F:442:PRO:CD	2.72	0.52
1:L:93:LEU:HD12	1:L:393:GLN:NE2	2.24	0.52
1:E:382:LEU:HG	1:E:407:LEU:HD21	1.91	0.52
1:G:244:LEU:O	1:G:248:ILE:HG23	2.09	0.52
1:I:157:PHE:HA	1:I:160:MET:HE2	1.92	0.52
1:H:240:MET:HE1	1:H:248:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:263:ILE:CG2	1:H:309:MET:HE1	2.39	0.52
1:F:244:LEU:HD11	1:F:248:ILE:HD11	1.91	0.52
1:D:410:LEU:C	1:D:410:LEU:HD23	2.30	0.52
1:I:386:VAL:HG12	1:I:388:SER:H	1.74	0.52
1:K:41:MET:CE	1:K:89:VAL:HG13	2.39	0.52
1:J:287:THR:HG21	1:K:181:ARG:HG2	1.92	0.52
1:B:287:THR:HG21	1:D:181:ARG:HG2	1.90	0.52
1:G:160:MET:CE	1:G:203:ALA:HA	2.39	0.52
1:D:322:PRO:HG3	1:D:378:VAL:HG22	1.92	0.52
1:B:337:GLN:HE21	1:B:341:ARG:HH22	1.57	0.52
1:H:240:MET:CE	1:H:244:LEU:HB3	2.40	0.52
1:K:47:ASN:HD22	1:K:50:LEU:CD1	2.23	0.52
2:I:601:HEM:CMB	2:I:601:HEM:HBB2	2.39	0.52
1:I:328:PHE:CZ	1:I:332:ARG:HD2	2.45	0.52
1:F:160:MET:HE3	1:F:203:ALA:HA	1.91	0.52
1:K:378:VAL:CG2	2:K:601:HEM:HMB2	2.39	0.51
1:K:103:VAL:HG12	1:K:103:VAL:O	2.10	0.51
1:I:343:GLU:OE1	1:I:362:LEU:HA	2.10	0.51
1:I:103:VAL:O	1:I:103:VAL:HG12	2.10	0.51
1:G:55:ILE:HD11	1:G:239:PHE:CD1	2.42	0.51
1:C:322:PRO:HB2	1:C:460:MET:HE1	1.92	0.51
1:I:386:VAL:HG11	1:I:390:LEU:HD22	1.91	0.51
1:K:382:LEU:CD2	1:K:407:LEU:HD11	2.40	0.51
1:K:475:THR:HG22	1:K:497:LEU:HA	1.92	0.51
1:K:413:ASN:HD21	1:K:416:LEU:HB2	1.76	0.51
1:F:263:ILE:HG22	1:F:309:MET:CE	2.40	0.51
1:E:83:LEU:CD2	1:E:88:MET:HE1	2.35	0.51
1:G:110:ARG:NH2	2:G:601:HEM:O2D	2.44	0.51
1:D:356:GLN:NE2	1:D:356:GLN:H	2.09	0.51
1:C:94:PRO:HG2	1:C:416:LEU:HD21	1.91	0.51
1:F:416:LEU:HD13	1:F:439:HIS:CD2	2.45	0.51
1:F:390:LEU:HG	1:F:397:ILE:HB	1.93	0.51
1:C:410:LEU:C	1:C:410:LEU:HD12	2.31	0.51
1:K:240:MET:CE	1:K:248:ILE:HD11	2.41	0.50
1:I:386:VAL:HG11	1:I:390:LEU:CD2	2.41	0.50
1:E:160:MET:HE2	1:E:286:TYR:HE2	1.75	0.50
1:H:52:LEU:HD22	1:H:240:MET:HB3	1.92	0.50
1:K:413:ASN:O	1:K:413:ASN:ND2	2.44	0.50
1:B:481:ILE:HG23	1:B:493:THR:HG22	1.92	0.50
1:L:378:VAL:HG11	2:L:601:HEM:HMB2	1.89	0.50
1:D:101:GLN:HE21	1:D:438:PHE:HZ	1.59	0.50
1:A:443:PHE:CG	1:A:453:ARG:HG3	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:404:GLN:HE21	1:L:406:PHE:HE1	1.58	0.50
1:C:441:VAL:N	1:C:442:PRO:CD	2.75	0.50
1:B:160:MET:HE2	1:B:286:TYR:HE2	1.76	0.50
1:D:416:LEU:HD21	1:D:439:HIS:CE1	2.47	0.50
1:H:157:PHE:HA	1:H:160:MET:CE	2.42	0.50
1:D:441:VAL:N	1:D:442:PRO:CD	2.73	0.50
1:K:41:MET:CE	1:K:78:ILE:HG12	2.41	0.50
1:J:475:THR:HG22	1:J:477:THR:N	2.26	0.50
1:H:110:ARG:NH1	2:H:601:HEM:O1A	2.45	0.50
1:F:65:HIS:HB3	1:F:380:LEU:HD11	1.93	0.50
1:K:337:GLN:NE2	1:K:473:VAL:H	2.05	0.49
1:G:322:PRO:HB2	1:G:460:MET:HE3	1.94	0.49
1:F:406:PHE:CZ	1:F:408:TYR:HB3	2.46	0.49
1:J:35:VAL:HG12	1:J:36:LEU:N	2.27	0.49
1:F:244:LEU:CD1	1:F:247:TRP:CZ2	2.95	0.49
1:I:88:MET:HE1	1:I:402:LEU:HD23	1.93	0.49
1:E:65:HIS:HB3	1:E:380:LEU:HD11	1.93	0.49
1:I:365:LEU:HD23	1:I:461:LEU:HD12	1.94	0.49
1:A:103:VAL:CG1	1:A:103:VAL:O	2.60	0.49
1:F:94:PRO:CB	1:F:416:LEU:HD11	2.42	0.49
1:F:194:HIS:HE1	1:F:220:SER:OG	1.94	0.49
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.94	0.49
1:F:271:ILE:HA	1:F:274:ILE:HG22	1.93	0.49
1:E:410:LEU:C	1:E:410:LEU:HD12	2.32	0.49
1:J:370:LYS:HG2	1:J:440:HIS:CE1	2.48	0.49
1:L:488:ILE:HG22	3:L:602:1CA:H152	1.94	0.49
1:H:65:HIS:HB3	1:H:380:LEU:HD11	1.94	0.49
1:J:397:ILE:N	1:J:397:ILE:HD12	2.27	0.49
1:D:227:LEU:HD13	1:D:317:ASP:OD1	2.13	0.49
1:C:242:ARG:O	1:C:246:ARG:HB2	2.12	0.49
1:J:244:LEU:O	1:J:248:ILE:HG22	2.12	0.49
1:F:129:VAL:HG22	1:F:137:TRP:CD1	2.48	0.49
1:G:475:THR:HG23	1:G:496:LEU:O	2.13	0.49
1:H:475:THR:HG21	1:H:497:LEU:HD23	1.88	0.49
1:B:322:PRO:HG3	1:B:378:VAL:HG22	1.95	0.49
1:G:72:PHE:HB3	1:G:92:MET:HE3	1.94	0.49
1:K:141:ARG:NH1	1:K:449:GLN:O	2.35	0.49
1:H:126:LYS:NZ	1:H:136:GLU:OE2	2.30	0.49
1:F:103:VAL:O	1:F:103:VAL:CG1	2.59	0.48
1:C:475:THR:HG22	1:C:477:THR:H	1.77	0.48
1:J:322:PRO:HD3	1:J:378:VAL:CG2	2.43	0.48
1:L:81:TYR:CG	1:L:88:MET:HE1	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:47:ASN:ND2	1:K:50:LEU:HD12	2.28	0.48
1:E:379:GLY:O	1:E:407:LEU:HD12	2.13	0.48
1:G:318:THR:HA	1:G:378:VAL:HG11	1.94	0.48
1:I:244:LEU:O	1:I:244:LEU:HD23	2.13	0.48
1:K:158:LEU:N	1:K:159:PRO:HD2	2.28	0.48
1:K:103:VAL:HG21	1:K:390:LEU:HD13	1.95	0.48
1:K:47:ASN:HB2	1:K:50:LEU:HD12	1.96	0.48
1:I:39:GLU:O	1:I:80:ARG:NH2	2.46	0.48
1:E:88:MET:HA	1:E:402:LEU:O	2.14	0.48
1:B:166:ARG:HG3	1:B:466:HIS:CE1	2.48	0.48
1:L:71:THR:HG22	1:L:75:LEU:HD12	1.96	0.48
1:F:48:ARG:CZ	1:F:84:GLY:HA2	2.44	0.48
1:B:61:TYR:CE1	1:B:64:LEU:HD13	2.48	0.48
1:B:51:ARG:O	1:B:55:ILE:HD12	2.12	0.48
1:I:321:PHE:CD2	1:I:491:PRO:HD2	2.48	0.48
1:F:475:THR:HG23	1:F:497:LEU:CD2	2.37	0.48
1:K:41:MET:HE1	1:K:78:ILE:CG1	2.44	0.48
1:K:83:LEU:HD22	1:K:88:MET:HG2	1.94	0.48
1:K:176:VAL:HG22	1:K:184:LEU:N	2.29	0.48
1:I:240:MET:CG	1:I:245:SER:HB3	2.45	0.47
1:G:46:GLY:HA3	1:G:50:LEU:HD12	1.95	0.47
1:B:371:GLU:CD	1:B:374:ARG:HH11	2.17	0.47
1:H:158:LEU:HD23	1:H:158:LEU:C	2.34	0.47
2:C:601:HEM:CMB	2:C:601:HEM:HBB2	2.44	0.47
1:K:45:PRO:HD3	1:K:75:LEU:HD11	1.95	0.47
1:J:92:MET:O	1:J:410:LEU:HD13	2.14	0.47
1:J:188:VAL:CG2	1:J:497:LEU:HD12	2.43	0.47
1:A:105:SER:HB2	1:A:107:HIS:H	1.79	0.47
1:F:263:ILE:HG22	1:F:309:MET:HE1	1.96	0.47
1:J:493:THR:CG2	1:J:494:SER:N	2.77	0.47
1:F:145:ASN:HB2	1:F:146:PRO:HD3	1.97	0.47
1:B:65:HIS:HB3	1:B:380:LEU:HD21	1.96	0.47
1:C:322:PRO:HB2	1:C:460:MET:HE3	1.95	0.47
1:F:192:ILE:O	1:F:196:THR:HG23	2.14	0.47
1:J:230:MET:HE1	1:J:231:PHE:CE1	2.50	0.47
1:F:234:THR:O	1:F:238:MET:HB2	2.14	0.47
1:D:236:GLN:HB2	1:D:252:VAL:HG11	1.97	0.47
1:A:370:LYS:HG2	1:A:440:HIS:CE1	2.49	0.47
1:B:162:ASP:CA	1:B:462:LEU:HD13	2.44	0.47
1:G:475:THR:HG22	1:G:477:THR:N	2.29	0.47
1:L:271:ILE:HD13	1:L:305:LYS:HG3	1.97	0.47
1:D:162:ASP:HA	1:D:462:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:34:THR:O	1:F:394:ASN:ND2	2.48	0.47
1:A:78:ILE:HG23	1:A:78:ILE:O	2.14	0.47
1:D:240:MET:HE1	1:D:248:ILE:HB	1.96	0.47
1:F:406:PHE:HE2	1:F:409:SER:HG	1.62	0.47
1:L:71:THR:CG2	1:L:75:LEU:HD12	2.45	0.47
1:I:379:GLY:HA2	3:I:602:1CA:H162	1.96	0.47
1:L:410:LEU:C	1:L:410:LEU:CD1	2.81	0.47
1:I:441:VAL:N	1:I:442:PRO:HD3	2.30	0.47
1:G:338:GLN:HE21	1:G:342:GLN:HE21	1.63	0.47
1:I:462:LEU:HD23	1:I:462:LEU:HA	1.80	0.47
1:G:132:LEU:O	1:G:448:ARG:NH2	2.45	0.47
1:E:441:VAL:N	1:E:442:PRO:CD	2.77	0.47
1:K:271:ILE:HG21	1:K:305:LYS:HG2	1.97	0.47
1:L:441:VAL:N	1:L:442:PRO:HD3	2.30	0.46
1:F:162:ASP:OD1	1:F:466:HIS:HE1	1.98	0.46
1:C:235:VAL:HG21	1:C:486:SER:HA	1.97	0.46
1:E:370:LYS:HG2	1:E:440:HIS:CE1	2.51	0.46
1:A:37:PRO:HD2	1:A:40:ALA:HB2	1.98	0.46
1:H:274:ILE:HD12	1:I:181:ARG:NH1	2.31	0.46
1:E:132:LEU:O	1:E:448:ARG:NH2	2.45	0.46
1:C:322:PRO:HG3	1:C:378:VAL:HG22	1.97	0.46
1:H:113:LEU:O	1:H:117:VAL:HG23	2.14	0.46
1:F:113:LEU:HD23	1:F:116:TRP:CD1	2.50	0.46
1:A:114:GLU:N	1:A:115:PRO:CD	2.78	0.46
1:G:188:VAL:HG23	1:G:324:LEU:HD11	1.96	0.46
1:G:91:VAL:CG2	1:G:405:VAL:HG22	2.45	0.46
1:H:315:SER:HA	2:H:601:HEM:HMC2	1.97	0.46
1:K:475:THR:HG21	1:K:497:LEU:HD23	1.95	0.46
1:L:452:GLY:HA3	2:L:601:HEM:C3C	2.51	0.46
1:F:322:PRO:HG3	1:F:378:VAL:CG2	2.46	0.46
1:I:438:PHE:HD2	1:I:438:PHE:O	1.98	0.46
1:A:157:PHE:CA	1:A:160:MET:HE2	2.41	0.46
1:D:103:VAL:CG1	1:D:103:VAL:O	2.64	0.46
1:C:52:LEU:CD1	1:C:244:LEU:HD23	2.46	0.46
1:I:188:VAL:HG11	1:I:499:PHE:CZ	2.51	0.46
1:F:149:LEU:O	1:F:149:LEU:HD12	2.16	0.46
1:H:52:LEU:HD13	1:H:240:MET:SD	2.56	0.46
1:C:110:ARG:NH1	2:C:601:HEM:O1A	2.49	0.46
1:F:441:VAL:HA	5:F:701:HOH:O	2.16	0.46
1:D:162:ASP:CA	1:D:462:LEU:HD13	2.46	0.46
1:G:176:VAL:HG13	1:G:182:GLY:C	2.36	0.46
1:E:83:LEU:CD1	1:E:88:MET:HE1	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:103:VAL:CG1	1:J:390:LEU:HD13	2.42	0.46
1:J:159:PRO:HG3	1:J:356:GLN:HE21	1.80	0.46
1:H:190:PRO:O	1:H:194:HIS:HD2	1.99	0.45
1:L:70:GLN:HA	1:L:73:GLN:HG2	1.97	0.45
1:J:204:LEU:HD23	1:J:289:ILE:CD1	2.44	0.45
1:K:114:GLU:CG	1:K:115:PRO:HD3	2.44	0.45
1:C:72:PHE:CD2	1:C:92:MET:HG2	2.51	0.45
1:E:166:ARG:HH22	1:E:352:SER:HA	1.80	0.45
1:G:72:PHE:CG	1:G:92:MET:HE2	2.51	0.45
1:F:441:VAL:N	1:F:442:PRO:HD3	2.31	0.45
1:K:91:VAL:CG2	1:K:405:VAL:HG22	2.47	0.45
1:K:88:MET:CE	1:K:402:LEU:HD23	2.46	0.45
1:K:132:LEU:O	1:K:448:ARG:NH2	2.41	0.45
1:B:183:SER:HB3	1:B:500:ARG:HA	1.99	0.45
1:A:383:GLU:CG	1:A:402:LEU:HD11	2.47	0.45
1:A:284:GLN:N	1:A:284:GLN:CD	2.70	0.45
1:I:114:GLU:N	1:I:115:PRO:CD	2.79	0.45
1:K:369:LEU:CD2	1:K:460:MET:HE2	2.45	0.45
1:A:108:PRO:HB2	1:A:448:ARG:HG3	1.99	0.45
1:J:133:ASN:OD1	1:J:448:ARG:NH2	2.49	0.45
1:K:235:VAL:HG21	1:K:486:SER:HA	1.99	0.45
1:B:392:LEU:HB2	1:B:397:ILE:HD11	1.99	0.45
1:B:282:ARG:NH1	5:B:712:HOH:O	2.49	0.45
1:C:393:GLN:HA	1:C:393:GLN:NE2	2.32	0.45
1:K:35:VAL:HG11	1:K:391:VAL:HG22	1.99	0.45
1:I:341:ARG:HD3	1:I:468:LEU:O	2.17	0.45
1:C:94:PRO:O	1:C:95:GLU:C	2.55	0.45
1:B:94:PRO:HD3	1:B:410:LEU:CD1	2.47	0.45
1:I:326:THR:O	1:I:330:LEU:HG	2.17	0.45
1:E:470:HIS:CE1	1:E:509:HIS:HB3	2.52	0.45
1:J:309:MET:HE3	1:J:309:MET:HA	1.99	0.45
1:I:162:ASP:OD1	1:I:466:HIS:HE1	2.00	0.45
1:A:341:ARG:CZ	1:A:472:LEU:HD23	2.47	0.45
1:H:329:GLU:OE1	1:H:332:ARG:HD3	2.17	0.45
1:B:149:LEU:HD12	1:B:454:ARG:HG3	1.97	0.45
1:C:273:LYS:HG2	1:E:185:THR:HB	1.99	0.45
1:B:161:VAL:HG12	1:B:462:LEU:HD12	2.00	0.45
1:A:340:LEU:HD23	1:A:364:LEU:HB3	1.99	0.45
1:I:294:LEU:HD23	1:I:304:ILE:HD13	1.98	0.45
1:C:89:VAL:HG21	1:C:397:ILE:HD12	1.99	0.45
1:B:318:THR:HA	1:B:378:VAL:HG11	1.98	0.44
2:F:601:HEM:HBB2	2:F:601:HEM:CMB	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.47	0.44
1:I:119:TYR:O	1:I:123:ARG:HG2	2.17	0.44
1:G:441:VAL:N	1:G:442:PRO:CD	2.80	0.44
1:A:129:VAL:HG22	1:A:137:TRP:CD1	2.52	0.44
1:H:386:VAL:HG22	1:H:401:THR:O	2.18	0.44
1:C:154:VAL:HG21	1:C:454:ARG:CD	2.45	0.44
1:E:103:VAL:HG11	1:E:386:VAL:HG13	2.00	0.44
1:K:110:ARG:NH1	5:K:704:HOH:O	2.50	0.44
1:A:195:TYR:CD2	1:A:463:LEU:HD13	2.52	0.44
1:D:337:GLN:HE21	1:D:341:ARG:HH22	1.65	0.44
1:H:341:ARG:HD3	1:H:468:LEU:O	2.17	0.44
1:H:189:GLN:HB3	1:H:190:PRO:HD3	2.00	0.44
1:D:202:LEU:HD22	1:D:208:ARG:HD3	1.98	0.44
1:C:129:VAL:HG22	1:C:137:TRP:CD1	2.51	0.44
1:B:441:VAL:N	1:B:442:PRO:CD	2.80	0.44
1:B:325:MET:CE	1:B:325:MET:HA	2.47	0.44
1:B:325:MET:HA	1:B:325:MET:HE2	1.99	0.44
1:J:103:VAL:HG13	1:J:103:VAL:O	2.17	0.44
1:L:226:ALA:HB1	1:L:263:ILE:HG13	2.00	0.44
1:B:392:LEU:HG	1:B:397:ILE:HD13	2.00	0.44
1:J:379:GLY:O	1:J:407:LEU:HD12	2.18	0.44
1:E:378:VAL:HG23	2:E:601:HEM:HMB1	1.99	0.44
1:K:56:TRP:HD1	1:K:248:ILE:HD12	1.82	0.44
1:I:237:LEU:HD13	1:I:253:TRP:CE2	2.53	0.44
1:E:358:ALA:HB1	1:E:362:LEU:HD12	2.00	0.44
1:L:384:ARG:HH22	2:L:601:HEM:CGA	2.31	0.44
1:G:452:GLY:HA3	2:G:601:HEM:C3C	2.53	0.44
1:A:369:LEU:HD22	1:A:460:MET:HE3	1.98	0.44
1:I:113:LEU:HD23	1:I:116:TRP:CG	2.52	0.44
1:K:186:LEU:CD2	1:K:188:VAL:HG13	2.44	0.44
1:E:386:VAL:HG11	1:E:390:LEU:CD2	2.44	0.44
1:D:407:LEU:CD2	1:D:441:VAL:HG23	2.48	0.44
1:K:343:GLU:OE1	1:K:363:PRO:HD2	2.18	0.44
1:G:386:VAL:CG1	1:G:388:SER:O	2.66	0.44
1:F:94:PRO:HB3	1:F:416:LEU:HD11	2.00	0.44
1:F:380:LEU:HD12	1:F:485:TYR:CD1	2.52	0.44
1:A:475:THR:HG22	1:A:477:THR:H	1.82	0.43
1:H:380:LEU:HD12	1:H:485:TYR:CD1	2.53	0.43
1:H:274:ILE:HD11	1:H:291:ALA:HB2	2.00	0.43
1:A:207:GLU:CD	1:A:273:LYS:NZ	2.72	0.43
1:B:332:ARG:NH1	1:B:480:ASP:HA	2.33	0.43
1:E:94:PRO:O	1:E:96:ASP:N	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:410:LEU:C	1:I:410:LEU:HD23	2.38	0.43
1:H:337:GLN:HE21	1:H:341:ARG:HH22	1.66	0.43
1:G:88:MET:HB2	1:G:402:LEU:HB3	2.01	0.43
1:C:339:ILE:HG22	1:C:364:LEU:HD13	2.00	0.43
1:L:410:LEU:HD12	1:L:411:GLY:N	2.32	0.43
1:I:110:ARG:NH1	2:I:601:HEM:O1A	2.47	0.43
1:D:87:ARG:HB3	1:D:401:THR:HG23	2.00	0.43
1:E:271:ILE:HD13	1:E:271:ILE:HA	1.84	0.43
1:H:114:GLU:N	1:H:115:PRO:HD2	2.34	0.43
1:G:231:PHE:CE2	1:G:488:ILE:HD13	2.53	0.43
1:K:264:PHE:HA	1:K:309:MET:SD	2.58	0.43
1:H:309:MET:O	1:H:309:MET:HE3	2.17	0.43
1:E:264:PHE:HA	1:E:309:MET:SD	2.57	0.43
1:I:190:PRO:O	1:I:194:HIS:HD2	2.00	0.43
1:K:475:THR:CG2	1:K:497:LEU:HD23	2.46	0.43
1:D:240:MET:HG3	1:D:245:SER:HB3	2.00	0.43
1:F:366:ARG:HG2	1:F:461:LEU:HD13	2.01	0.43
1:G:81:TYR:HB3	1:G:88:MET:HG2	2.01	0.43
1:L:362:LEU:N	1:L:363:PRO:CD	2.82	0.43
1:A:379:GLY:O	1:A:407:LEU:HD12	2.18	0.43
1:F:475:THR:HG21	1:F:497:LEU:HD23	1.93	0.43
1:F:94:PRO:HA	1:F:97:VAL:HG23	2.00	0.43
1:D:155:GLN:OE1	1:D:356:GLN:HB3	2.18	0.43
1:J:148:VAL:HG22	1:J:289:ILE:CG2	2.49	0.43
1:G:188:VAL:HG23	1:G:324:LEU:HD12	2.00	0.43
1:A:294:LEU:HD23	1:A:304:ILE:HD13	2.00	0.43
1:D:414:ALA:HB2	1:D:420:PRO:HG3	2.00	0.43
1:E:93:LEU:HD12	1:E:393:GLN:HE22	1.83	0.43
1:A:309:MET:HE2	1:A:309:MET:HB3	1.42	0.43
1:G:83:LEU:HD13	1:G:88:MET:HE3	2.00	0.43
1:J:322:PRO:HD3	1:J:378:VAL:HG21	2.00	0.43
1:H:234:THR:O	1:H:238:MET:HG3	2.19	0.43
1:J:237:LEU:HD22	1:J:253:TRP:NE1	2.34	0.43
1:C:271:ILE:HD12	1:C:305:LYS:HA	2.00	0.43
1:I:150:SER:O	1:I:153:ALA:HB3	2.19	0.42
1:D:267:GLY:HA3	1:D:309:MET:SD	2.59	0.42
1:G:325:MET:CE	1:G:325:MET:HA	2.49	0.42
1:I:148:VAL:HG22	1:I:289:ILE:CG2	2.48	0.42
1:E:330:LEU:HD21	1:E:340:LEU:HD12	2.01	0.42
1:H:44:HIS:HD2	1:H:71:THR:HG21	1.84	0.42
1:C:48:ARG:NH2	1:C:84:GLY:HA3	2.34	0.42
1:H:237:LEU:HD22	1:H:253:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:475:THR:HG21	1:K:497:LEU:HD22	1.75	0.42
1:J:103:VAL:CG2	1:J:388:SER:HB2	2.49	0.42
1:K:61:TYR:H	1:K:235:VAL:HG11	1.83	0.42
1:H:231:PHE:O	1:H:234:THR:HB	2.19	0.42
1:C:160:MET:HE3	1:C:203:ALA:HA	2.01	0.42
1:D:240:MET:HE1	1:D:248:ILE:HD12	2.02	0.42
1:H:160:MET:HE1	1:H:286:TYR:CE2	2.54	0.42
1:J:244:LEU:C	1:J:244:LEU:HD23	2.40	0.42
1:J:106:LEU:HD23	1:J:138:ARG:HD2	2.01	0.42
1:C:176:VAL:HG13	1:C:183:SER:HA	2.00	0.42
1:I:380:LEU:HD22	1:I:485:TYR:CD1	2.54	0.42
1:A:443:PHE:CD2	1:A:453:ARG:HG3	2.55	0.42
1:C:337:GLN:HE22	1:C:473:VAL:N	2.12	0.42
1:B:181:ARG:CG	1:F:287:THR:HG21	2.45	0.42
1:I:158:LEU:HD22	1:I:356:GLN:HA	2.01	0.42
1:B:195:TYR:CD2	1:B:463:LEU:HD13	2.55	0.42
1:B:158:LEU:N	1:B:159:PRO:CD	2.83	0.42
1:C:148:VAL:HG22	1:C:289:ILE:HG21	2.02	0.42
1:B:94:PRO:HG2	1:B:416:LEU:HD13	2.00	0.42
1:G:329:GLU:O	1:G:333:ASN:ND2	2.35	0.42
1:F:407:LEU:HD21	1:F:441:VAL:HG23	2.01	0.42
1:L:158:LEU:CD2	1:L:462:LEU:HD11	2.50	0.42
1:D:68:MET:HB3	1:D:68:MET:HE3	1.95	0.42
1:B:158:LEU:HD12	1:B:158:LEU:O	2.20	0.42
1:K:340:LEU:CD2	1:K:365:LEU:HA	2.50	0.42
1:J:309:MET:HE3	1:J:309:MET:CA	2.50	0.42
1:K:351:ILE:HD12	1:K:465:HIS:CE1	2.54	0.42
1:B:392:LEU:CG	1:B:397:ILE:HD13	2.50	0.41
1:A:65:HIS:HB3	1:A:380:LEU:HD11	2.00	0.41
1:F:92:MET:HE2	1:F:92:MET:HB2	1.87	0.41
1:L:88:MET:HG3	1:L:402:LEU:HD23	2.01	0.41
1:K:56:TRP:CD1	1:K:248:ILE:HD12	2.55	0.41
1:D:72:PHE:HB3	1:D:92:MET:HE3	2.01	0.41
1:C:472:LEU:HD12	1:C:500:ARG:HD2	2.03	0.41
1:B:161:VAL:CG1	1:B:462:LEU:HD12	2.50	0.41
1:E:83:LEU:HD22	1:E:88:MET:CE	2.41	0.41
1:A:341:ARG:NH1	1:A:472:LEU:HD23	2.35	0.41
1:K:309:MET:HA	1:K:309:MET:CE	2.48	0.41
1:C:441:VAL:N	1:C:442:PRO:HD3	2.36	0.41
1:F:119:TYR:OH	1:F:261:ASP:OD1	2.35	0.41
1:L:472:LEU:HD23	1:L:502:ILE:HD11	2.01	0.41
1:F:85:GLY:N	1:F:86:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:365:LEU:HD23	1:A:461:LEU:CD1	2.51	0.41
1:F:71:THR:CG2	1:F:75:LEU:HD12	2.50	0.41
1:I:88:MET:CE	1:I:402:LEU:HD23	2.49	0.41
1:G:129:VAL:HG22	1:G:137:TRP:CD1	2.56	0.41
1:E:188:VAL:HG11	1:E:499:PHE:CE1	2.56	0.41
1:L:81:TYR:CD1	1:L:88:MET:HE1	2.55	0.41
1:E:190:PRO:O	1:E:194:HIS:HD2	2.03	0.41
1:F:88:MET:HB2	1:F:402:LEU:HB3	2.03	0.41
1:F:132:LEU:O	1:F:448:ARG:NH2	2.45	0.41
1:E:341:ARG:NH1	1:E:472:LEU:HD23	2.35	0.41
1:L:41:MET:CE	1:L:78:ILE:HG12	2.46	0.41
1:A:325:MET:HA	1:A:325:MET:HE2	2.03	0.41
1:L:323:LEU:HD21	1:L:463:LEU:HD23	2.02	0.41
1:L:194:HIS:CE1	1:L:216:PRO:HB3	2.55	0.41
1:F:381:PHE:HA	1:F:405:VAL:O	2.20	0.41
1:E:315:SER:HA	2:E:601:HEM:CMC	2.50	0.41
1:G:88:MET:HE2	1:G:402:LEU:HD23	2.01	0.41
1:E:475:THR:CG2	1:E:497:LEU:HD23	2.48	0.41
1:K:407:LEU:HD22	1:K:442:PRO:HA	2.03	0.41
1:G:46:GLY:CA	1:G:50:LEU:HD12	2.51	0.41
1:F:278:LEU:HD11	1:F:291:ALA:HA	2.03	0.41
1:J:238:MET:CE	1:J:239:PHE:CE1	3.04	0.41
1:F:114:GLU:N	1:F:115:PRO:CD	2.83	0.41
1:J:162:ASP:HB2	1:J:462:LEU:HD13	2.02	0.41
1:C:94:PRO:HG2	1:C:416:LEU:CD2	2.51	0.41
1:K:315:SER:HA	2:K:601:HEM:CMC	2.51	0.41
1:L:168:PHE:CD2	1:L:463:LEU:HD11	2.56	0.41
1:C:197:ILE:HD11	1:C:224:LEU:HD21	2.01	0.41
1:K:189:GLN:HA	1:K:324:LEU:HD11	2.03	0.41
1:G:61:TYR:OH	1:G:67:GLU:OE2	2.26	0.41
1:D:148:VAL:HG11	1:D:451:LEU:HG	2.02	0.41
1:G:178:GLN:OE1	1:G:178:GLN:N	2.53	0.41
1:C:296:LYS:O	1:C:297:ALA:C	2.58	0.41
1:E:338:GLN:NE2	1:E:341:ARG:HE	2.19	0.41
1:J:475:THR:OG1	1:J:497:LEU:CD2	2.68	0.41
2:I:601:HEM:HMB2	2:I:601:HEM:HBB2	2.03	0.41
1:L:176:VAL:HG13	1:L:183:SER:HA	2.02	0.41
1:L:328:PHE:CD1	1:L:495:PRO:HG3	2.55	0.41
1:F:195:TYR:CD2	1:F:463:LEU:HD13	2.56	0.41
1:G:162:ASP:OD1	1:G:466:HIS:HE1	2.03	0.41
1:G:82:ASN:C	1:G:84:GLY:H	2.25	0.41
1:J:103:VAL:HG21	1:J:388:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:322:PRO:CG	1:C:378:VAL:CG2	2.99	0.40
1:I:343:GLU:O	1:I:346:ALA:HB3	2.21	0.40
1:J:71:THR:HG22	1:J:75:LEU:HD12	2.02	0.40
1:A:186:LEU:N	1:A:186:LEU:HD23	2.36	0.40
1:D:357:LYS:HB3	1:D:361:GLU:HG3	2.03	0.40
2:A:601:HEM:HBC2	2:A:601:HEM:HMC3	1.94	0.40
2:B:601:HEM:CBC	2:B:601:HEM:CMC	3.00	0.40
1:K:162:ASP:OD2	1:K:462:LEU:HD22	2.20	0.40
1:D:420:PRO:HD2	5:D:703:HOH:O	2.20	0.40
1:B:139:PHE:CE1	1:B:143:ARG:CZ	3.04	0.40
1:L:36:LEU:N	1:L:37:PRO:CD	2.84	0.40
1:F:389:ASP:OD1	1:F:398:PRO:HA	2.21	0.40
1:H:441:VAL:N	1:H:442:PRO:CD	2.85	0.40
1:C:338:GLN:HE21	1:C:342:GLN:HE21	1.68	0.40
1:D:41:MET:HA	1:D:42:PRO:HD3	1.97	0.40
1:I:364:LEU:O	1:I:367:ALA:HB3	2.20	0.40
1:B:315:SER:HA	2:B:601:HEM:CMC	2.52	0.40
1:L:158:LEU:HD23	1:L:158:LEU:O	2.22	0.40
1:K:197:ILE:HD11	1:K:224:LEU:HD21	2.03	0.40
1:G:122:HIS:CG	1:G:122:HIS:O	2.74	0.40
3:C:602:1CA:H211	3:C:602:1CA:H121	2.03	0.40
1:F:335:ASP:HB2	5:F:703:HOH:O	2.20	0.40
1:E:341:ARG:HD3	1:E:468:LEU:O	2.21	0.40
1:A:103:VAL:HG12	1:A:103:VAL:O	2.21	0.40
1:F:72:PHE:CG	1:F:92:MET:HG2	2.57	0.40
1:D:242:ARG:O	1:D:246:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	459/483 (95%)	444 (97%)	14 (3%)	1 (0%)	56 79
1	B	459/483 (95%)	437 (95%)	21 (5%)	1 (0%)	56 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	458/483 (95%)	444 (97%)	13 (3%)	1 (0%)	56	79
1	D	458/483 (95%)	435 (95%)	23 (5%)	0	100	100
1	E	466/483 (96%)	445 (96%)	16 (3%)	5 (1%)	21	34
1	F	465/483 (96%)	449 (97%)	15 (3%)	1 (0%)	56	79
1	G	458/483 (95%)	439 (96%)	19 (4%)	0	100	100
1	H	458/483 (95%)	439 (96%)	18 (4%)	1 (0%)	56	79
1	I	458/483 (95%)	429 (94%)	29 (6%)	0	100	100
1	J	458/483 (95%)	435 (95%)	18 (4%)	5 (1%)	21	34
1	K	456/483 (94%)	433 (95%)	21 (5%)	2 (0%)	43	66
1	L	448/483 (93%)	434 (97%)	13 (3%)	1 (0%)	56	79
All	All	5501/5796 (95%)	5263 (96%)	220 (4%)	18 (0%)	50	73

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	504	HIS
1	B	427	ARG
1	F	48	ARG
1	J	477	THR
1	A	477	THR
1	E	477	THR
1	H	82	ASN
1	C	95	GLU
1	E	95	GLU
1	J	85	GLY
1	J	413	ASN
1	K	74	GLU
1	E	82	ASN
1	E	438	PHE
1	K	450	CYS
1	L	48	ARG
1	J	398	PRO
1	J	77	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	A	408/425 (96%)	390 (96%)	18 (4%)	39	64
1	B	408/425 (96%)	389 (95%)	19 (5%)	36	61
1	C	407/425 (96%)	382 (94%)	25 (6%)	26	46
1	D	407/425 (96%)	385 (95%)	22 (5%)	31	53
1	E	415/425 (98%)	385 (93%)	30 (7%)	21	36
1	F	414/425 (97%)	390 (94%)	24 (6%)	28	49
1	G	407/425 (96%)	387 (95%)	20 (5%)	35	59
1	H	407/425 (96%)	380 (93%)	27 (7%)	24	41
1	I	407/425 (96%)	385 (95%)	22 (5%)	31	53
1	J	407/425 (96%)	384 (94%)	23 (6%)	29	50
1	K	405/425 (95%)	374 (92%)	31 (8%)	18	33
1	L	401/425 (94%)	370 (92%)	31 (8%)	18	33
All	All	4893/5100 (96%)	4601 (94%)	292 (6%)	27	47

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	61	TYR
1	A	105	SER
1	A	110	ARG
1	A	169	SER
1	A	170	GLN
1	A	181	ARG
1	A	188	VAL
1	A	207	GLU
1	A	240	MET
1	A	271	ILE
1	A	324	LEU
1	A	341	ARG
1	A	356	GLN
1	A	364	LEU
1	A	380	LEU
1	A	461	LEU
1	A	463	LEU
1	B	61	TYR

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Mol	Chain	Res	Type
1	B	91	VAL
1	B	92	MET
1	B	110	ARG
1	B	129	VAL
1	B	155	GLN
1	B	188	VAL
1	B	208	ARG
1	B	220	SER
1	B	317	ASP
1	B	323	LEU
1	B	378	VAL
1	B	390	LEU
1	B	394	ASN
1	B	447	MET
1	B	475	THR
1	B	476	LEU
1	B	478	GLN
1	B	493	THR
1	C	48	ARG
1	C	61	TYR
1	C	83	LEU
1	C	102	GLN
1	C	120	ARG
1	C	121	GLN
1	C	126	LYS
1	C	129	VAL
1	C	138	ARG
1	C	157	PHE
1	C	169	SER
1	C	183	SER
1	C	242	ARG
1	C	251	LYS
1	C	254	LYS
1	C	271	ILE
1	C	284	GLN
1	C	324	LEU
1	C	356	GLN
1	C	386	VAL
1	C	393	GLN
1	C	410	LEU
1	C	422	ARG
1	C	463	LEU

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Mol	Chain	Res	Type
1	C	475	THR
1	D	34	THR
1	D	47	ASN
1	D	83	LEU
1	D	92	MET
1	D	110	ARG
1	D	111	MET
1	D	155	GLN
1	D	188	VAL
1	D	242	ARG
1	D	251	LYS
1	D	255	GLU
1	D	323	LEU
1	D	324	LEU
1	D	350	SER
1	D	353	GLU
1	D	356	GLN
1	D	380	LEU
1	D	386	VAL
1	D	427	ARG
1	D	438	PHE
1	D	475	THR
1	D	478	GLN
1	E	52	LEU
1	E	61	TYR
1	E	73	GLN
1	E	99	LYS
1	E	129	VAL
1	E	143	ARG
1	E	169	SER
1	E	183	SER
1	E	188	VAL
1	E	240	MET
1	E	251	LYS
1	E	254	LYS
1	E	255	GLU
1	E	265	GLN
1	E	271	ILE
1	E	284	GLN
1	E	317	ASP
1	E	338	GLN
1	E	344	SER

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Mol	Chain	Res	Type
1	E	378	VAL
1	E	380	LEU
1	E	383	GLU
1	E	394	ASN
1	E	410	LEU
1	E	419	ARG
1	E	437	ASN
1	E	463	LEU
1	E	475	THR
1	E	479	GLU
1	E	493	THR
1	F	61	TYR
1	F	87	ARG
1	F	92	MET
1	F	104	ASP
1	F	105	SER
1	F	110	ARG
1	F	111	MET
1	F	129	VAL
1	F	152	LYS
1	F	169	SER
1	F	183	SER
1	F	188	VAL
1	F	254	LYS
1	F	284	GLN
1	F	317	ASP
1	F	323	LEU
1	F	344	SER
1	F	383	GLU
1	F	390	LEU
1	F	394	ASN
1	F	410	LEU
1	F	457	GLU
1	F	463	LEU
1	F	478	GLN
1	G	53	LEU
1	G	61	TYR
1	G	88	MET
1	G	100	LEU
1	G	111	MET
1	G	114	GLU
1	G	129	VAL

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Mol	Chain	Res	Type
1	G	150	SER
1	G	155	GLN
1	G	215	SER
1	G	247	TRP
1	G	248	ILE
1	G	271	ILE
1	G	323	LEU
1	G	342	GLN
1	G	353	GLU
1	G	380	LEU
1	G	430	ASP
1	G	488	ILE
1	G	493	THR
1	H	39	GLU
1	H	47	ASN
1	H	52	LEU
1	H	83	LEU
1	H	92	MET
1	H	103	VAL
1	H	122	HIS
1	H	129	VAL
1	H	173	LYS
1	H	188	VAL
1	H	215	SER
1	H	246	ARG
1	H	284	GLN
1	H	323	LEU
1	H	335	ASP
1	H	342	GLN
1	H	344	SER
1	H	352	SER
1	H	361	GLU
1	H	378	VAL
1	H	380	LEU
1	H	426	GLN
1	H	475	THR
1	H	476	LEU
1	H	479	GLU
1	H	493	THR
1	H	500	ARG
1	I	34	THR
1	I	61	TYR

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Mol	Chain	Res	Type
1	I	87	ARG
1	I	92	MET
1	I	109	CYS
1	I	110	ARG
1	I	111	MET
1	I	129	VAL
1	I	157	PHE
1	I	169	SER
1	I	174	LYS
1	I	183	SER
1	I	188	VAL
1	I	246	ARG
1	I	335	ASP
1	I	343	GLU
1	I	344	SER
1	I	350	SER
1	I	390	LEU
1	I	438	PHE
1	I	474	GLU
1	I	478	GLN
1	J	54	GLN
1	J	61	TYR
1	J	92	MET
1	J	100	LEU
1	J	103	VAL
1	J	106	LEU
1	J	109	CYS
1	J	111	MET
1	J	138	ARG
1	J	139	PHE
1	J	157	PHE
1	J	188	VAL
1	J	242	ARG
1	J	265	GLN
1	J	309	MET
1	J	344	SER
1	J	378	VAL
1	J	393	GLN
1	J	421	GLU
1	J	430	ASP
1	J	438	PHE
1	J	441	VAL

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Mol	Chain	Res	Type
1	J	449	GLN
1	K	39	GLU
1	K	48	ARG
1	K	61	TYR
1	K	87	ARG
1	K	92	MET
1	K	95	GLU
1	K	102	GLN
1	K	139	PHE
1	K	141	ARG
1	K	143	ARG
1	K	150	SER
1	K	152	LYS
1	K	158	LEU
1	K	178	GLN
1	K	188	VAL
1	K	254	LYS
1	K	265	GLN
1	K	309	MET
1	K	324	LEU
1	K	352	SER
1	K	356	GLN
1	K	359	THR
1	K	378	VAL
1	K	380	LEU
1	K	413	ASN
1	K	463	LEU
1	K	477	THR
1	K	480	ASP
1	K	482	LYS
1	K	494	SER
1	K	502	ILE
1	L	36	LEU
1	L	41	MET
1	L	49	TRP
1	L	51	ARG
1	L	59	GLN
1	L	61	TYR
1	L	70	GLN
1	L	87	ARG
1	L	92	MET
1	L	111	MET

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Mol	Chain	Res	Type
1	L	120	ARG
1	L	129	VAL
1	L	178	GLN
1	L	186	LEU
1	L	188	VAL
1	L	265	GLN
1	L	323	LEU
1	L	335	ASP
1	L	341	ARG
1	L	378	VAL
1	L	386	VAL
1	L	401	THR
1	L	410	LEU
1	L	416	LEU
1	L	453	ARG
1	L	463	LEU
1	L	475	THR
1	L	478	GLN
1	L	479	GLU
1	L	486	SER
1	L	489	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	65	HIS
1	A	337	GLN
1	A	356	GLN
1	A	394	ASN
1	A	404	GLN
1	A	440	HIS
1	A	466	HIS
1	A	470	HIS
1	B	54	GLN
1	B	65	HIS
1	B	194	HIS
1	B	256	HIS
1	B	337	GLN
1	B	342	GLN
1	B	356	GLN
1	B	404	GLN

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Mol	Chain	Res	Type
1	B	478	GLN
1	C	65	HIS
1	C	102	GLN
1	C	155	GLN
1	C	337	GLN
1	C	342	GLN
1	C	393	GLN
1	C	404	GLN
1	D	47	ASN
1	D	65	HIS
1	D	101	GLN
1	D	121	GLN
1	D	170	GLN
1	D	194	HIS
1	D	272	GLN
1	D	337	GLN
1	D	356	GLN
1	D	394	ASN
1	D	404	GLN
1	D	439	HIS
1	E	54	GLN
1	E	73	GLN
1	E	194	HIS
1	E	337	GLN
1	E	338	GLN
1	E	393	GLN
1	E	394	ASN
1	E	404	GLN
1	E	440	HIS
1	E	505	HIS
1	F	47	ASN
1	F	54	GLN
1	F	59	GLN
1	F	65	HIS
1	F	102	GLN
1	F	155	GLN
1	F	194	HIS
1	F	284	GLN
1	F	337	GLN
1	F	394	ASN
1	F	466	HIS
1	F	470	HIS

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Mol	Chain	Res	Type
1	F	505	HIS
1	G	65	HIS
1	G	101	GLN
1	G	194	HIS
1	G	337	GLN
1	G	342	GLN
1	G	404	GLN
1	G	440	HIS
1	H	47	ASN
1	H	65	HIS
1	H	121	GLN
1	H	194	HIS
1	H	337	GLN
1	H	404	GLN
1	H	440	HIS
1	H	466	HIS
1	I	47	ASN
1	I	54	GLN
1	I	194	HIS
1	I	337	GLN
1	I	356	GLN
1	I	404	GLN
1	I	466	HIS
1	J	43	GLN
1	J	65	HIS
1	J	337	GLN
1	J	342	GLN
1	J	356	GLN
1	J	404	GLN
1	J	440	HIS
1	K	47	ASN
1	K	54	GLN
1	K	101	GLN
1	K	102	GLN
1	K	170	GLN
1	K	337	GLN
1	K	356	GLN
1	K	393	GLN
1	K	413	ASN
1	K	424	ASN
1	K	440	HIS
1	K	470	HIS

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Mol	Chain	Res	Type
1	L	47	ASN
1	L	65	HIS
1	L	140	ASN
1	L	236	GLN
1	L	337	GLN
1	L	356	GLN
1	L	393	GLN
1	L	394	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

33 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	601	1	49,50,50	2.31	16 (32%)	46,82,82	2.01	10 (21%)
3	1CA	A	602	-	27,27,27	0.79	0	43,43,43	1.30	8 (18%)
4	SO4	A	603	-	4,4,4	0.46	0	6,6,6	0.37	0
2	HEM	B	601	1	49,50,50	1.95	11 (22%)	46,82,82	1.83	10 (21%)
3	1CA	B	602	-	27,27,27	0.71	0	43,43,43	1.20	5 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	B	603	-	4,4,4	0.50	0	6,6,6	0.35	0
2	HEM	C	601	1	49,50,50	2.64	12 (24%)	46,82,82	1.90	12 (26%)
3	1CA	C	602	-	27,27,27	0.97	3 (11%)	43,43,43	1.65	12 (27%)
4	SO4	C	603	-	4,4,4	0.50	0	6,6,6	0.25	0
2	HEM	D	601	1	49,50,50	2.04	10 (20%)	46,82,82	1.78	9 (19%)
3	1CA	D	602	-	27,27,27	0.83	0	43,43,43	1.40	7 (16%)
4	SO4	D	603	-	4,4,4	0.53	0	6,6,6	0.18	0
2	HEM	E	601	1	49,50,50	2.37	13 (26%)	46,82,82	1.70	5 (10%)
3	1CA	E	602	-	27,27,27	0.79	0	43,43,43	1.53	10 (23%)
4	SO4	E	603	-	4,4,4	0.51	0	6,6,6	0.39	0
2	HEM	F	601	1	49,50,50	2.04	11 (22%)	46,82,82	2.05	9 (19%)
3	1CA	F	602	-	27,27,27	0.98	1 (3%)	43,43,43	1.31	8 (18%)
4	SO4	F	603	-	4,4,4	0.48	0	6,6,6	0.23	0
2	HEM	G	601	1	49,50,50	2.08	15 (30%)	46,82,82	2.06	10 (21%)
3	1CA	G	602	-	27,27,27	0.87	0	43,43,43	1.24	3 (6%)
4	SO4	G	603	-	4,4,4	0.42	0	6,6,6	0.57	0
2	HEM	H	601	1	49,50,50	2.21	13 (26%)	46,82,82	1.92	8 (17%)
3	1CA	H	602	-	27,27,27	0.81	1 (3%)	43,43,43	1.13	6 (13%)
2	HEM	I	601	1	49,50,50	2.14	11 (22%)	46,82,82	1.67	5 (10%)
3	1CA	I	602	-	27,27,27	0.80	0	43,43,43	1.51	6 (13%)
2	HEM	J	601	1	49,50,50	2.33	13 (26%)	46,82,82	2.03	11 (23%)
3	1CA	J	602	-	27,27,27	0.81	0	43,43,43	1.40	9 (20%)
2	HEM	K	601	1	49,50,50	2.24	14 (28%)	46,82,82	2.00	8 (17%)
3	1CA	K	602	-	27,27,27	0.59	0	43,43,43	1.55	9 (20%)
4	SO4	K	603	-	4,4,4	0.43	0	6,6,6	0.46	0
2	HEM	L	601	1	49,50,50	2.27	14 (28%)	46,82,82	2.08	9 (19%)
3	1CA	L	602	-	27,27,27	0.64	0	43,43,43	1.30	3 (6%)
4	SO4	L	603	-	4,4,4	0.43	0	6,6,6	0.28	0

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	601	1	-	0/14/114/114	0/0/8/8
3	1CA	A	602	-	-	0/6/64/64	0/0/4/4
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	601	1	-	0/14/114/114	0/0/8/8
3	1CA	B	602	-	-	0/6/64/64	0/0/4/4
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0
2	HEM	C	601	1	-	0/14/114/114	0/0/8/8
3	1CA	C	602	-	-	0/6/64/64	0/0/4/4
4	SO4	C	603	-	-	0/0/0/0	0/0/0/0
2	HEM	D	601	1	-	0/14/114/114	0/0/8/8
3	1CA	D	602	-	-	0/6/64/64	0/0/4/4
4	SO4	D	603	-	-	0/0/0/0	0/0/0/0
2	HEM	E	601	1	-	0/14/114/114	0/0/8/8
3	1CA	E	602	-	-	0/6/64/64	0/0/4/4
4	SO4	E	603	-	-	0/0/0/0	0/0/0/0
2	HEM	F	601	1	-	0/14/114/114	0/0/8/8
3	1CA	F	602	-	-	0/6/64/64	0/0/4/4
4	SO4	F	603	-	-	0/0/0/0	0/0/0/0
2	HEM	G	601	1	-	0/14/114/114	0/0/8/8
3	1CA	G	602	-	-	0/6/64/64	0/0/4/4
4	SO4	G	603	-	-	0/0/0/0	0/0/0/0
2	HEM	H	601	1	-	0/14/114/114	0/0/8/8
3	1CA	H	602	-	-	0/6/64/64	0/0/4/4
2	HEM	I	601	1	-	0/14/114/114	0/0/8/8
3	1CA	I	602	-	-	0/6/64/64	0/0/4/4
2	HEM	J	601	1	-	0/14/114/114	0/0/8/8
3	1CA	J	602	-	-	0/6/64/64	0/0/4/4
2	HEM	K	601	1	-	0/14/114/114	0/0/8/8
3	1CA	K	602	-	-	0/6/64/64	0/0/4/4
4	SO4	K	603	-	-	0/0/0/0	0/0/0/0
2	HEM	L	601	1	-	0/14/114/114	0/0/8/8
3	1CA	L	602	-	-	0/6/64/64	0/0/4/4
4	SO4	L	603	-	-	0/0/0/0	0/0/0/0

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C3D-C4D	-8.91	1.42	1.44
2	E	601	HEM	C2B-C1B	7.78	1.46	1.44
2	J	601	HEM	C3D-C4D	-7.48	1.42	1.44
2	I	601	HEM	C3C-C2C	-6.97	1.31	1.43
2	A	601	HEM	C3C-C2C	-6.85	1.31	1.43
2	A	601	HEM	C3D-C4D	6.64	1.46	1.44
2	B	601	HEM	C3C-C2C	-6.44	1.32	1.43
2	E	601	HEM	C3C-C2C	-6.43	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C2B-C1B	6.41	1.46	1.44
2	J	601	HEM	C3C-C2C	-6.37	1.32	1.43
2	C	601	HEM	C3B-C2B	-6.21	1.32	1.43
2	E	601	HEM	C3B-C2B	-6.05	1.33	1.43
2	K	601	HEM	C3C-C2C	-6.00	1.33	1.43
2	F	601	HEM	C3B-C2B	-5.99	1.33	1.43
2	H	601	HEM	C2B-C1B	5.92	1.46	1.44
2	G	601	HEM	C3C-C2C	-5.92	1.33	1.43
2	L	601	HEM	C3C-C2C	-5.67	1.33	1.43
2	A	601	HEM	C3B-C2B	-5.67	1.33	1.43
2	I	601	HEM	C3B-C2B	-5.64	1.33	1.43
2	C	601	HEM	C3C-C2C	-5.63	1.33	1.43
2	D	601	HEM	C3B-C2B	-5.63	1.33	1.43
2	F	601	HEM	C3C-C2C	-5.58	1.34	1.43
2	H	601	HEM	C3C-C2C	-5.47	1.34	1.43
2	K	601	HEM	C2D-C1D	5.46	1.45	1.44
2	L	601	HEM	C3B-C2B	-5.36	1.34	1.43
2	D	601	HEM	C3C-C2C	-5.35	1.34	1.43
2	J	601	HEM	C3B-C2B	-5.34	1.34	1.43
2	H	601	HEM	C3B-C2B	-5.26	1.34	1.43
2	G	601	HEM	C3B-C2B	-5.17	1.34	1.43
2	L	601	HEM	C3D-C2D	5.12	1.52	1.43
2	B	601	HEM	C3B-C2B	-5.09	1.34	1.43
2	H	601	HEM	C3D-C2D	5.05	1.52	1.43
2	K	601	HEM	C3D-C2D	5.04	1.52	1.43
2	D	601	HEM	C3D-C2D	5.01	1.52	1.43
2	J	601	HEM	C3C-CAC	4.82	1.55	1.40
2	K	601	HEM	C3B-C2B	-4.82	1.35	1.43
2	C	601	HEM	C3B-CAB	4.62	1.54	1.40
2	L	601	HEM	C3B-CAB	4.61	1.54	1.40
2	F	601	HEM	C3D-C2D	4.61	1.51	1.43
2	D	601	HEM	C3C-CAC	4.60	1.54	1.40
2	J	601	HEM	C3B-CAB	4.55	1.54	1.40
2	I	601	HEM	C3D-C2D	4.53	1.51	1.43
2	H	601	HEM	C3B-CAB	4.48	1.54	1.40
2	L	601	HEM	C3C-CAC	4.47	1.54	1.40
2	J	601	HEM	C4A-C3A	4.44	1.45	1.40
2	I	601	HEM	C3B-CAB	4.38	1.54	1.40
2	I	601	HEM	C3C-CAC	4.37	1.54	1.40
2	A	601	HEM	C3D-C2D	4.37	1.51	1.43
2	C	601	HEM	C3D-C2D	4.30	1.51	1.43
2	C	601	HEM	C4A-C3A	4.29	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	HEM	C3C-CAC	4.29	1.53	1.40
2	H	601	HEM	C3C-CAC	4.28	1.53	1.40
2	L	601	HEM	FE-ND	4.24	2.13	1.97
2	E	601	HEM	C3C-CAC	4.21	1.53	1.40
2	B	601	HEM	C3B-CAB	4.20	1.53	1.40
2	G	601	HEM	C4A-C3A	4.12	1.45	1.40
2	K	601	HEM	C3B-CAB	4.10	1.53	1.40
2	E	601	HEM	C3B-CAB	4.10	1.53	1.40
2	E	601	HEM	C3D-C2D	4.09	1.50	1.43
2	C	601	HEM	C3C-CAC	4.07	1.53	1.40
2	K	601	HEM	C3C-CAC	4.07	1.53	1.40
2	D	601	HEM	C3B-CAB	4.07	1.53	1.40
2	K	601	HEM	C4A-C3A	4.06	1.45	1.40
2	G	601	HEM	C3B-CAB	4.05	1.53	1.40
2	F	601	HEM	C3B-CAB	4.04	1.53	1.40
2	G	601	HEM	C3D-C2D	4.00	1.50	1.43
2	C	601	HEM	FE-ND	3.97	2.12	1.97
2	F	601	HEM	C3C-CAC	3.97	1.52	1.40
2	B	601	HEM	C3C-CAC	3.88	1.52	1.40
2	A	601	HEM	C3B-CAB	3.87	1.52	1.40
2	E	601	HEM	C4A-C3A	3.82	1.44	1.40
2	B	601	HEM	C3D-C2D	3.78	1.50	1.43
2	L	601	HEM	C4A-C3A	3.76	1.44	1.40
2	A	601	HEM	C3C-CAC	3.70	1.52	1.40
2	I	601	HEM	C3D-C4D	3.70	1.45	1.44
2	L	601	HEM	C2B-C1B	3.64	1.45	1.44
2	I	601	HEM	C4A-C3A	3.60	1.44	1.40
2	H	601	HEM	C4A-C3A	3.51	1.44	1.40
2	F	601	HEM	C3D-C4D	-3.49	1.43	1.44
2	F	601	HEM	C4A-C3A	3.41	1.44	1.40
2	K	601	HEM	FE-ND	3.34	2.10	1.97
2	L	601	HEM	C2D-C1D	3.34	1.45	1.44
2	J	601	HEM	C2D-C1D	-3.28	1.43	1.44
2	J	601	HEM	C3D-C2D	3.27	1.49	1.43
2	D	601	HEM	CMC-C2C	3.21	1.57	1.47
2	D	601	HEM	C4A-C3A	3.16	1.44	1.40
2	E	601	HEM	FE-NA	3.11	2.05	1.92
2	A	601	HEM	C4A-C3A	3.00	1.43	1.40
2	L	601	HEM	FE-NB	2.90	2.08	1.97
2	L	601	HEM	CMB-C2B	2.83	1.56	1.47
2	K	601	HEM	FE-NA	2.82	2.04	1.92
3	F	602	1CA	C13-C17	-2.81	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	601	HEM	C2B-C1B	2.81	1.45	1.44
2	A	601	HEM	C2D-C1D	2.80	1.45	1.44
2	J	601	HEM	FE-NA	2.77	2.04	1.92
2	G	601	HEM	CMB-C2B	2.76	1.56	1.47
2	C	601	HEM	CMB-C2B	2.75	1.56	1.47
2	H	601	HEM	CMC-C2C	2.75	1.55	1.47
2	A	601	HEM	CMC-C2C	2.74	1.55	1.47
2	L	601	HEM	CMC-C2C	2.68	1.55	1.47
2	H	601	HEM	FE-ND	2.66	2.07	1.97
2	G	601	HEM	CMC-C2C	2.66	1.55	1.47
2	K	601	HEM	CMB-C2B	2.66	1.55	1.47
2	D	601	HEM	C2B-C1B	-2.63	1.43	1.44
2	A	601	HEM	FE-NC	2.62	2.07	1.97
2	D	601	HEM	CMB-C2B	2.59	1.55	1.47
2	K	601	HEM	C3D-C4D	2.59	1.45	1.44
2	B	601	HEM	C4A-C3A	2.54	1.43	1.40
2	F	601	HEM	C2D-C1D	-2.54	1.43	1.44
2	F	601	HEM	CMB-C2B	2.54	1.55	1.47
2	B	601	HEM	CMB-C2B	2.52	1.55	1.47
2	A	601	HEM	CMB-C2B	2.51	1.55	1.47
2	H	601	HEM	FE-NA	2.51	2.03	1.92
2	E	601	HEM	CMB-C2B	2.51	1.55	1.47
2	G	601	HEM	C2D-C1D	2.49	1.45	1.44
2	B	601	HEM	CMC-C2C	2.48	1.55	1.47
2	G	601	HEM	FE-NA	2.47	2.03	1.92
2	E	601	HEM	CMD-C2D	2.47	1.55	1.47
2	B	601	HEM	C3D-C4D	2.46	1.45	1.44
2	E	601	HEM	CMC-C2C	2.45	1.55	1.47
2	L	601	HEM	CMD-C2D	2.41	1.54	1.47
2	A	601	HEM	C2B-C1B	-2.39	1.44	1.44
2	C	601	HEM	FE-NB	2.37	2.06	1.97
2	E	601	HEM	C1A-C2A	2.37	1.47	1.43
2	F	601	HEM	CMC-C2C	2.37	1.54	1.47
2	G	601	HEM	C2B-C1B	2.36	1.45	1.44
2	C	601	HEM	CMC-C2C	2.36	1.54	1.47
2	A	601	HEM	CMD-C2D	2.29	1.54	1.47
2	H	601	HEM	CMB-C2B	2.30	1.54	1.47
2	J	601	HEM	CMC-C2C	2.29	1.54	1.47
2	A	601	HEM	CAA-C2A	2.29	1.56	1.52
2	G	601	HEM	FE-NC	2.24	2.06	1.97
2	K	601	HEM	FE-NC	2.22	2.06	1.97
2	G	601	HEM	C3D-C4D	-2.19	1.44	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	HEM	C3B-C4B	2.19	1.47	1.44
3	C	602	1CA	O3-C3	-2.16	1.19	1.23
2	G	601	HEM	CMD-C2D	2.16	1.54	1.47
3	H	602	1CA	C13-C14	-2.16	1.50	1.55
2	J	601	HEM	CAA-C2A	2.16	1.55	1.52
2	B	601	HEM	FE-NC	2.16	2.05	1.97
2	I	601	HEM	CMC-C2C	2.15	1.54	1.47
2	K	601	HEM	CMA-C3A	2.14	1.56	1.51
2	A	601	HEM	CHA-C4D	2.14	1.38	1.35
2	I	601	HEM	C2B-C1B	2.14	1.45	1.44
2	A	601	HEM	FE-NA	2.13	2.01	1.92
2	F	601	HEM	C4A-NA	2.13	1.40	1.36
3	C	602	1CA	C13-C17	-2.13	1.52	1.56
2	B	601	HEM	FE-NA	2.13	2.01	1.92
2	J	601	HEM	CMB-C2B	2.11	1.53	1.47
2	I	601	HEM	CMD-C2D	2.11	1.53	1.47
2	I	601	HEM	FE-NA	2.08	2.01	1.92
2	D	601	HEM	C2D-C1D	2.07	1.45	1.44
2	L	601	HEM	FE-NA	2.06	2.01	1.92
2	E	601	HEM	CAA-C2A	2.06	1.55	1.52
2	H	601	HEM	FE-NB	2.05	2.05	1.97
2	G	601	HEM	CAA-C2A	2.05	1.55	1.52
3	C	602	1CA	C10-C9	-2.04	1.52	1.56
2	J	601	HEM	CMD-C2D	2.00	1.53	1.47

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	HEM	C3B-C4B-NB	-8.91	107.63	114.00
2	J	601	HEM	C3B-C4B-NB	-8.84	107.67	114.00
2	F	601	HEM	C3B-C4B-NB	-8.48	107.93	114.00
2	A	601	HEM	C3B-C4B-NB	-8.41	107.98	114.00
2	K	601	HEM	C3B-C4B-NB	-8.38	108.00	114.00
2	H	601	HEM	C3B-C4B-NB	-7.67	108.51	114.00
2	L	601	HEM	C3B-C4B-NB	-7.63	108.54	114.00
2	I	601	HEM	C3B-C4B-NB	-7.53	108.61	114.00
2	B	601	HEM	C3B-C4B-NB	-7.29	108.78	114.00
2	E	601	HEM	C3B-C4B-NB	-7.08	108.94	114.00
2	D	601	HEM	C3B-C4B-NB	-7.01	108.99	114.00
2	L	601	HEM	C4D-ND-C1D	6.60	111.92	105.16
2	K	601	HEM	C4D-ND-C1D	5.70	110.99	105.16
2	C	601	HEM	C3B-C4B-NB	-5.43	110.11	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	HEM	C4D-ND-C1D	5.14	110.42	105.16
2	G	601	HEM	C4D-ND-C1D	5.11	110.39	105.16
2	F	601	HEM	C4D-ND-C1D	4.83	110.10	105.16
2	C	601	HEM	C4D-ND-C1D	4.56	109.83	105.16
2	J	601	HEM	C4D-ND-C1D	4.49	109.75	105.16
2	A	601	HEM	C4D-ND-C1D	4.43	109.69	105.16
2	C	601	HEM	CBA-CAA-C2A	-4.16	105.36	112.69
2	B	601	HEM	C4D-ND-C1D	4.09	109.34	105.16
2	E	601	HEM	CBA-CAA-C2A	-4.08	105.50	112.69
2	L	601	HEM	C2D-C1D-ND	-4.08	108.11	112.93
3	K	602	1CA	C6-C5-C4	-3.83	116.12	120.93
2	F	601	HEM	CBA-CAA-C2A	-3.82	105.95	112.69
2	L	601	HEM	CBA-CAA-C2A	-3.78	106.03	112.69
2	A	601	HEM	CHC-C4B-NB	3.77	127.72	124.58
2	C	601	HEM	C1A-CHA-C4D	-3.76	122.52	127.47
2	I	601	HEM	C4D-ND-C1D	3.75	109.00	105.16
3	C	602	1CA	O3-C3-C2	-3.72	115.99	121.58
2	C	601	HEM	CHD-C4C-NC	3.66	127.91	124.73
2	A	601	HEM	CBD-CAD-C3D	-3.63	106.45	114.37
3	I	602	1CA	C6-C7-C8	3.60	117.72	111.71
2	H	601	HEM	CBA-CAA-C2A	-3.60	106.35	112.69
2	D	601	HEM	CHD-C4C-NC	3.52	127.79	124.73
2	D	601	HEM	C4D-ND-C1D	3.46	108.70	105.16
3	H	602	1CA	C9-C10-C5	-3.45	104.29	109.67
3	C	602	1CA	C5-C4-C3	-3.44	119.53	123.77
2	E	601	HEM	C4D-ND-C1D	3.43	108.67	105.16
3	D	602	1CA	C2-C3-C4	3.43	121.99	116.76
2	J	601	HEM	CHC-C4B-NB	3.42	127.42	124.58
3	I	602	1CA	C14-C8-C9	-3.40	104.52	109.04
3	D	602	1CA	C2-C1-C10	3.38	118.14	113.39
2	K	601	HEM	CHC-C4B-NB	3.35	127.37	124.58
2	K	601	HEM	C2D-C1D-ND	-3.35	108.98	112.93
2	G	601	HEM	CBA-CAA-C2A	-3.32	106.84	112.69
2	J	601	HEM	C4A-CHB-C1B	-3.32	123.11	127.47
3	I	602	1CA	C7-C8-C9	3.30	114.51	110.47
2	D	601	HEM	CBA-CAA-C2A	-3.30	106.87	112.69
2	A	601	HEM	CBA-CAA-C2A	-3.29	106.89	112.69
2	C	601	HEM	C4A-C3A-C2A	3.21	109.23	107.00
3	G	602	1CA	C5-C4-C3	-3.16	119.88	123.77
2	F	601	HEM	CBD-CAD-C3D	-3.15	107.50	114.37
2	H	601	HEM	CHD-C4C-NC	3.14	127.46	124.73
2	J	601	HEM	CHA-C4D-ND	3.12	128.60	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	601	HEM	C4A-CHB-C1B	-3.09	123.41	127.47
2	H	601	HEM	C2D-C1D-ND	-3.07	109.30	112.93
2	B	601	HEM	CBA-CAA-C2A	-3.05	107.31	112.69
2	L	601	HEM	C4C-NC-C1C	3.03	108.68	105.53
3	K	602	1CA	C6-C5-C10	3.02	120.08	116.69
3	C	602	1CA	C19-C10-C5	3.01	113.21	108.39
3	L	602	1CA	C6-C5-C4	-2.98	117.19	120.93
2	G	601	HEM	C1B-NB-C4B	2.98	108.21	105.16
3	E	602	1CA	C21-C20-C17	2.95	121.51	116.36
3	B	602	1CA	C9-C10-C5	-2.93	105.11	109.67
3	C	602	1CA	C2-C3-C4	2.90	121.18	116.76
3	G	602	1CA	O3-C3-C2	-2.90	117.22	121.58
2	G	601	HEM	CBD-CAD-C3D	-2.89	108.07	114.37
2	F	601	HEM	C4A-CHB-C1B	-2.86	123.71	127.47
3	E	602	1CA	C5-C4-C3	-2.82	120.29	123.77
2	H	601	HEM	C4C-NC-C1C	2.82	108.47	105.53
2	B	601	HEM	CAD-C3D-C4D	2.81	129.58	124.53
2	G	601	HEM	C2D-C1D-ND	-2.80	109.62	112.93
3	E	602	1CA	C9-C10-C5	-2.77	105.36	109.67
2	C	601	HEM	C2D-C1D-ND	-2.76	109.67	112.93
2	F	601	HEM	C2D-C1D-ND	-2.75	109.68	112.93
2	B	601	HEM	CHC-C4B-NB	2.73	126.85	124.58
2	E	601	HEM	CHD-C4C-NC	2.73	127.10	124.73
3	C	602	1CA	C7-C8-C14	-2.70	107.40	112.00
3	L	602	1CA	C7-C8-C14	-2.69	107.41	112.00
2	C	601	HEM	C3A-C4A-NA	-2.69	107.38	109.41
3	D	602	1CA	C6-C5-C4	-2.69	117.56	120.93
3	B	602	1CA	C1-C10-C5	2.68	113.83	108.81
2	C	601	HEM	CBD-CAD-C3D	-2.68	108.53	114.37
2	D	601	HEM	C1A-CHA-C4D	-2.67	123.95	127.47
3	E	602	1CA	C16-C17-C13	-2.66	101.39	104.14
3	I	602	1CA	O3-C3-C2	-2.66	117.58	121.58
2	L	601	HEM	C1B-NB-C4B	2.66	107.88	105.16
3	C	602	1CA	C6-C5-C4	-2.64	117.62	120.93
3	J	602	1CA	C2-C1-C10	2.63	117.09	113.39
3	J	602	1CA	O3-C3-C2	-2.63	117.62	121.58
3	E	602	1CA	C7-C6-C5	-2.62	107.09	111.90
3	D	602	1CA	C1-C10-C5	2.61	113.69	108.81
2	L	601	HEM	CHD-C4C-NC	2.60	127.00	124.73
2	G	601	HEM	C4C-NC-C1C	2.60	108.24	105.53
2	J	601	HEM	CBA-CAA-C2A	-2.60	108.11	112.69
3	G	602	1CA	C2-C3-C4	2.59	120.71	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	HEM	CHC-C4B-NB	2.58	126.73	124.58
2	K	601	HEM	CBA-CAA-C2A	-2.58	108.15	112.69
2	I	601	HEM	CBA-CAA-C2A	-2.55	108.19	112.69
2	I	601	HEM	CHC-C4B-NB	2.55	126.71	124.58
2	K	601	HEM	C4C-NC-C1C	2.55	108.19	105.53
2	J	601	HEM	CBD-CAD-C3D	-2.55	108.82	114.37
2	K	601	HEM	C1B-NB-C4B	2.54	107.76	105.16
2	A	601	HEM	C4A-CHB-C1B	-2.51	124.17	127.47
3	F	602	1CA	C21-C20-C17	2.50	120.72	116.36
3	A	602	1CA	C16-C17-C13	-2.49	101.57	104.14
2	D	601	HEM	CBD-CAD-C3D	-2.45	109.02	114.37
2	B	601	HEM	CHD-C4C-NC	2.45	126.86	124.73
3	F	602	1CA	C9-C10-C5	-2.43	105.88	109.67
3	K	602	1CA	C21-C20-C17	2.43	120.60	116.36
2	A	601	HEM	CHD-C4C-NC	2.42	126.83	124.73
2	L	601	HEM	CAD-C3D-C4D	2.41	128.86	124.53
3	E	602	1CA	C1-C10-C9	-2.40	105.40	108.60
3	A	602	1CA	C12-C11-C9	2.40	117.15	113.15
2	E	601	HEM	CHC-C4B-NB	2.39	126.57	124.58
3	C	602	1CA	C7-C8-C9	2.37	113.37	110.47
3	E	602	1CA	C6-C5-C4	-2.35	117.97	120.93
3	A	602	1CA	C12-C13-C14	2.35	111.21	107.28
3	J	602	1CA	C2-C3-C4	2.35	120.35	116.76
3	K	602	1CA	C7-C8-C14	-2.34	108.01	112.00
2	J	601	HEM	C2D-C1D-ND	-2.34	110.17	112.93
3	A	602	1CA	C2-C1-C10	2.34	116.68	113.39
2	A	601	HEM	CMA-C3A-C4A	-2.34	125.03	128.62
3	J	602	1CA	C1-C10-C9	-2.34	105.49	108.60
3	I	602	1CA	C7-C6-C5	2.32	116.15	111.90
2	F	601	HEM	CHD-C1D-ND	2.32	126.51	124.58
3	E	602	1CA	C7-C8-C14	-2.31	108.06	112.00
2	F	601	HEM	CMA-C3A-C4A	-2.31	125.06	128.62
3	H	602	1CA	C14-C8-C9	-2.31	105.97	109.04
2	G	601	HEM	CAD-C3D-C4D	2.30	128.66	124.53
2	D	601	HEM	CHC-C4B-NB	2.30	126.50	124.58
3	H	602	1CA	C5-C4-C3	-2.30	120.94	123.77
3	B	602	1CA	C2-C1-C10	2.29	116.61	113.39
2	C	601	HEM	CHB-C4A-NA	2.29	128.40	124.58
3	J	602	1CA	C21-C20-C17	2.28	120.35	116.36
2	G	601	HEM	CHC-C4B-NB	2.28	126.48	124.58
3	B	602	1CA	C6-C5-C4	-2.27	118.08	120.93
3	C	602	1CA	C1-C10-C9	-2.27	105.58	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	602	1CA	C19-C10-C5	2.26	112.01	108.39
2	B	601	HEM	CBD-CAD-C3D	-2.25	109.47	114.37
3	F	602	1CA	C11-C9-C8	-2.24	108.49	111.73
3	J	602	1CA	C5-C4-C3	-2.23	121.02	123.77
2	L	601	HEM	CHC-C1C-NC	2.22	126.66	124.73
3	D	602	1CA	C9-C10-C5	-2.21	106.23	109.67
2	C	601	HEM	CHA-C1A-NA	2.21	128.26	124.58
3	J	602	1CA	C6-C5-C4	-2.20	118.17	120.93
3	H	602	1CA	C1-C10-C5	2.20	112.92	108.81
3	A	602	1CA	C7-C8-C14	-2.19	108.26	112.00
3	K	602	1CA	C12-C11-C9	-2.19	109.49	113.15
3	K	602	1CA	C2-C3-C4	2.18	120.09	116.76
3	F	602	1CA	C6-C5-C4	-2.17	118.20	120.93
3	K	602	1CA	C14-C8-C9	-2.18	106.15	109.04
2	B	601	HEM	C2D-C1D-ND	-2.17	110.36	112.93
2	K	601	HEM	CBD-CAD-C3D	-2.16	109.66	114.37
3	B	602	1CA	C11-C9-C8	-2.16	108.62	111.73
3	A	602	1CA	C1-C10-C9	-2.16	105.73	108.60
3	K	602	1CA	C19-C10-C5	2.15	111.84	108.39
3	F	602	1CA	O20-C20-C17	-2.14	118.26	122.25
3	E	602	1CA	C2-C3-C4	2.14	120.03	116.76
2	D	601	HEM	C4A-CHB-C1B	-2.14	124.66	127.47
2	B	601	HEM	C1A-CHA-C4D	-2.14	124.66	127.47
2	H	601	HEM	O2D-CGD-CBD	2.14	121.77	114.22
3	I	602	1CA	C6-C5-C10	2.13	119.08	116.69
3	C	602	1CA	C9-C10-C5	-2.12	106.36	109.67
2	G	601	HEM	CHD-C4C-NC	2.12	126.58	124.73
3	D	602	1CA	C7-C8-C14	-2.12	108.39	112.00
3	E	602	1CA	C1-C10-C5	2.12	112.77	108.81
3	F	602	1CA	C2-C1-C10	2.11	116.36	113.39
3	K	602	1CA	C9-C10-C5	-2.10	106.39	109.67
3	F	602	1CA	C2-C3-C4	2.10	119.97	116.76
3	C	602	1CA	C14-C8-C9	-2.10	106.25	109.04
3	L	602	1CA	C5-C4-C3	-2.08	121.21	123.77
2	J	601	HEM	C1B-NB-C4B	2.07	107.28	105.16
2	A	601	HEM	CAD-C3D-C4D	2.07	128.25	124.53
2	J	601	HEM	CHB-C1B-NB	2.06	127.14	124.31
2	H	601	HEM	CAD-C3D-C4D	2.06	128.24	124.53
2	C	601	HEM	CAD-C3D-C4D	2.06	128.23	124.53
3	C	602	1CA	C6-C7-C8	2.05	115.13	111.71
2	J	601	HEM	CAD-CBD-CGD	-2.05	107.10	113.48
3	D	602	1CA	C6-C5-C10	2.04	118.98	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	1CA	C21-C20-C17	2.04	119.92	116.36
3	J	602	1CA	C14-C8-C9	-2.04	106.32	109.04
2	D	601	HEM	CAD-C3D-C4D	2.04	128.19	124.53
3	F	602	1CA	C5-C4-C3	-2.02	121.28	123.77
3	C	602	1CA	C2-C1-C10	2.02	116.23	113.39
3	A	602	1CA	C6-C5-C4	-2.02	118.40	120.93
2	B	601	HEM	C4C-NC-C1C	2.02	107.63	105.53
3	H	602	1CA	C2-C1-C10	2.01	116.22	113.39
2	A	601	HEM	O2D-CGD-CBD	2.01	121.32	114.22
3	H	602	1CA	C2-C3-C4	2.01	119.83	116.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	A	463/483 (95%)	-0.16	2 (0%)	90 92	26, 42, 64, 113	0
1	B	463/483 (95%)	-0.07	2 (0%)	90 92	32, 50, 76, 107	0
1	C	462/483 (95%)	-0.18	3 (0%)	86 88	26, 43, 68, 95	0
1	D	462/483 (95%)	-0.23	1 (0%)	93 94	26, 44, 69, 88	0
1	E	470/483 (97%)	-0.17	1 (0%)	93 94	28, 44, 66, 97	0
1	F	469/483 (97%)	-0.08	3 (0%)	86 88	29, 47, 80, 123	0
1	G	462/483 (95%)	-0.08	7 (1%)	70 72	32, 50, 91, 147	0
1	H	462/483 (95%)	-0.10	3 (0%)	86 88	31, 48, 78, 106	0
1	I	462/483 (95%)	0.18	17 (3%)	39 41	35, 60, 101, 121	0
1	J	462/483 (95%)	0.20	30 (6%)	18 18	37, 59, 101, 119	0
1	K	460/483 (95%)	-0.02	6 (1%)	74 76	38, 60, 85, 112	0
1	L	454/483 (93%)	0.01	16 (3%)	42 43	36, 55, 95, 154	0
All	All	5551/5796 (95%)	-0.06	91 (1%)	68 71	26, 50, 84, 154	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	86	PRO	5.2
1	G	247	TRP	5.0
1	L	49	TRP	4.7
1	I	53	LEU	4.4
1	L	56	TRP	4.1
1	A	431	ILE	4.0
1	I	106	LEU	4.0
1	H	247	TRP	3.8
1	J	52	LEU	3.7
1	L	247	TRP	3.5
1	L	58	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	279	ALA	3.5
1	I	391	VAL	3.5
1	L	61	TYR	3.5
1	J	391	VAL	3.5
1	K	155	GLN	3.4
1	L	60	GLY	3.4
1	B	34	THR	3.4
1	J	392	LEU	3.4
1	G	59	GLN	3.3
1	I	103	VAL	3.3
1	I	50	LEU	3.2
1	I	284	GLN	3.2
1	J	103	VAL	3.1
1	I	399	ALA	3.1
1	J	84	GLY	3.1
1	J	53	LEU	3.1
1	I	247	TRP	3.1
1	I	392	LEU	3.1
1	E	85	GLY	3.1
1	G	58	GLU	3.0
1	J	284	GLN	3.0
1	G	49	TRP	2.9
1	L	48	ARG	2.8
1	A	112	ILE	2.8
1	I	85	GLY	2.8
1	J	49	TRP	2.8
1	J	82	ASN	2.7
1	J	396	HIS	2.6
1	J	85	GLY	2.6
1	L	103	VAL	2.6
1	F	416	LEU	2.6
1	L	47	ASN	2.6
1	J	38	PHE	2.6
1	L	57	ARG	2.6
1	J	83	LEU	2.5
1	J	390	LEU	2.5
1	D	34	THR	2.5
1	K	34	THR	2.5
1	I	49	TRP	2.5
1	J	81	TYR	2.4
1	I	38	PHE	2.4
1	K	47	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	244	LEU	2.4
1	L	45	PRO	2.4
1	L	39	GLU	2.3
1	F	53	LEU	2.3
1	G	57	ARG	2.3
1	G	84	GLY	2.3
1	J	387	SER	2.3
1	J	394	ASN	2.2
1	G	53	LEU	2.2
1	K	56	TRP	2.2
1	J	88	MET	2.2
1	K	66	LEU	2.2
1	C	122	HIS	2.2
1	I	81	TYR	2.2
1	H	392	LEU	2.1
1	I	396	HIS	2.1
1	J	106	LEU	2.1
1	I	55	ILE	2.1
1	J	40	ALA	2.1
1	J	87	ARG	2.1
1	J	35	VAL	2.1
1	J	399	ALA	2.1
1	I	83	LEU	2.1
1	J	75	LEU	2.1
1	L	53	LEU	2.1
1	L	100	LEU	2.1
1	I	243	SER	2.1
1	J	395	TYR	2.1
1	B	112	ILE	2.1
1	K	420	PRO	2.0
1	H	35	VAL	2.0
1	C	112	ILE	2.0
1	F	112	ILE	2.0
1	J	37	PRO	2.0
1	L	51	ARG	2.0
1	C	56	TRP	2.0
1	L	237	LEU	2.0
1	J	109	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	I	601	43/43	0.18	0.54	36,46,57,62	0
3	1CA	L	602	24/24	0.16	0.46	42,46,52,57	0
3	1CA	B	602	24/24	0.17	0.36	34,36,39,44	0
2	HEM	J	601	43/43	0.17	0.32	35,41,53,57	0
3	1CA	A	602	24/24	0.16	0.27	29,35,38,38	0
3	1CA	K	602	24/24	0.16	0.25	43,45,52,55	0
2	HEM	C	601	43/43	0.14	0.23	25,30,35,38	0
3	1CA	F	602	24/24	0.16	0.23	35,38,43,49	0
2	HEM	E	601	43/43	0.15	0.22	25,29,41,42	0
3	1CA	I	602	24/24	0.17	0.20	41,45,52,59	0
2	HEM	H	601	43/43	0.15	0.15	30,35,38,41	0
3	1CA	J	602	24/24	0.15	-0.02	42,46,52,57	0
2	HEM	G	601	43/43	0.15	-0.04	32,35,39,43	0
3	1CA	E	602	24/24	0.14	-0.06	31,33,39,40	0
2	HEM	D	601	43/43	0.14	-0.13	27,31,39,44	0
2	HEM	L	601	43/43	0.14	-0.35	38,45,51,56	0
2	HEM	K	601	43/43	0.13	-0.43	36,45,52,55	0
3	1CA	H	602	24/24	0.14	-0.45	33,36,39,40	0
2	HEM	F	601	43/43	0.14	-0.60	30,33,39,41	0
2	HEM	B	601	43/43	0.14	-0.62	30,35,47,51	0
3	1CA	C	602	24/24	0.13	-0.67	32,35,39,41	0
2	HEM	A	601	43/43	0.13	-0.70	25,29,34,38	0
3	1CA	G	602	24/24	0.13	-0.90	34,38,39,41	0
4	SO4	E	603	5/5	0.11	-1.08	59,61,70,71	0
3	1CA	D	602	24/24	0.12	-1.59	30,34,38,43	0
4	SO4	L	603	5/5	0.10	-1.83	60,66,69,75	0
4	SO4	C	603	5/5	0.11	-2.14	72,73,76,77	0
4	SO4	F	603	5/5	0.10	-2.15	63,65,70,71	0
4	SO4	K	603	5/5	0.09	-2.23	64,71,73,75	0
4	SO4	D	603	5/5	0.09	-2.94	67,76,78,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	603	5/5	0.11	-3.26	74,74,76,80	0
4	SO4	A	603	5/5	0.08	-3.77	55,55,56,58	0
4	SO4	G	603	5/5	0.10	-3.81	58,63,64,64	0

## 6.5 Other polymers

There are no such residues in this entry.