



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:58 am GMT

PDB ID : 2QJY  
Title : Crystal structure of rhodobacter sphaeroides double mutant with stigmatellin and UQ2  
Authors : Esser, L.; Xia, D.  
Deposited on : 2007-07-09  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28683
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

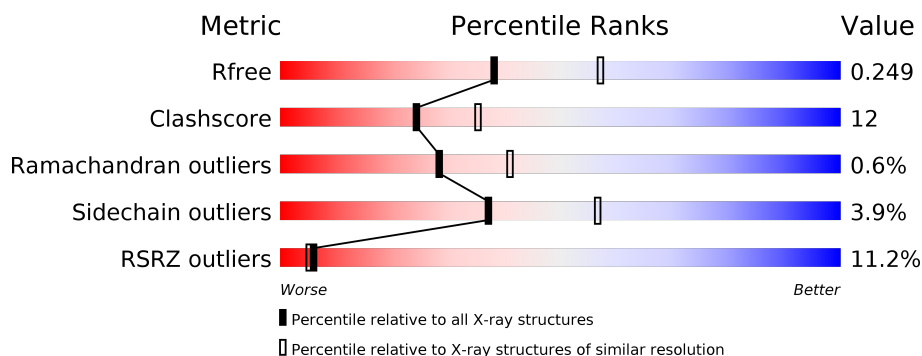
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	D	445	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	G	445	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	J	445	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	M	445	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	P	445	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	269	
2	E	269	
2	H	269	
2	K	269	
2	N	269	
2	Q	269	
3	C	187	
3	F	187	
3	I	187	
3	L	187	
3	O	187	
3	R	187	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	LOP	D	1022	-	-	-	X
10	LOP	G	1023	-	-	-	X
10	LOP	J	1024	-	-	-	X
10	LOP	P	1026	-	-	-	X
11	UQ2	A	1101	-	-	-	X
11	UQ2	D	1102	-	-	-	X
11	UQ2	G	1103	-	-	-	X
11	UQ2	J	1104	-	-	-	X
11	UQ2	M	1105	-	-	-	X
11	UQ2	P	1106	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 42656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	D	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	G	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	J	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	M	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	P	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	ARG	SER	ENGINEERED	UNP Q02761
D	287	ARG	SER	ENGINEERED	UNP Q02761
G	287	ARG	SER	ENGINEERED	UNP Q02761
J	287	ARG	SER	ENGINEERED	UNP Q02761
M	287	ARG	SER	ENGINEERED	UNP Q02761
P	287	ARG	SER	ENGINEERED	UNP Q02761

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	E	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	H	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	N	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	Q	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	265	HIS	-	EXPRESSION TAG	UNP Q3IY11

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	269	HIS	-	EXPRESSION TAG	UNP Q3IY11

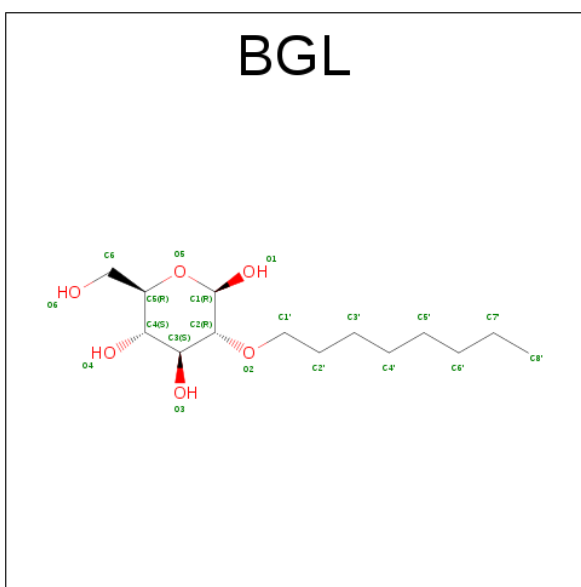
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	F	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	I	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	L	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	O	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	R	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135	SER	VAL	ENGINEERED	UNP Q02762
F	135	SER	VAL	ENGINEERED	UNP Q02762
I	135	SER	VAL	ENGINEERED	UNP Q02762
L	135	SER	VAL	ENGINEERED	UNP Q02762
O	135	SER	VAL	ENGINEERED	UNP Q02762
R	135	SER	VAL	ENGINEERED	UNP Q02762

- Molecule 4 is beta-octyl glucopyranoside (three-letter code: BGL) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			20	14	6		
4	E	1	Total	C	O	0	0
			20	14	6		
4	G	1	Total	C	O	0	0
			20	14	6		
4	K	1	Total	C	O	0	0
			20	14	6		
4	N	1	Total	C	O	0	0
			20	14	6		
4	P	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Sr	0	0
			1	1		
5	Q	1	Total	Sr	0	0
			1	1		
5	K	1	Total	Sr	0	0
			1	1		
5	E	1	Total	Sr	0	0
			1	1		
5	H	1	Total	Sr	0	0
			1	1		
5	B	1	Total	Sr	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Sr	0	0
			1	1		
5	N	1	Total	Sr	0	0
			1	1		
5	M	1	Total	Sr	0	0
			1	1		

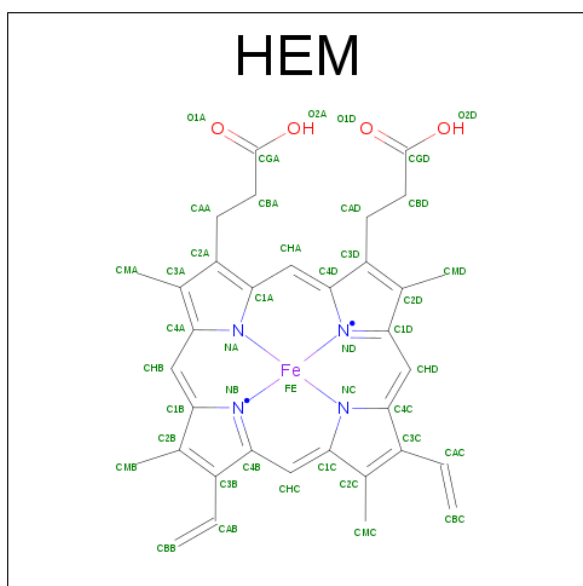
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total	Cl	0	0
			1	1		
6	I	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	R	1	Total	Na	0	0
			1	1		

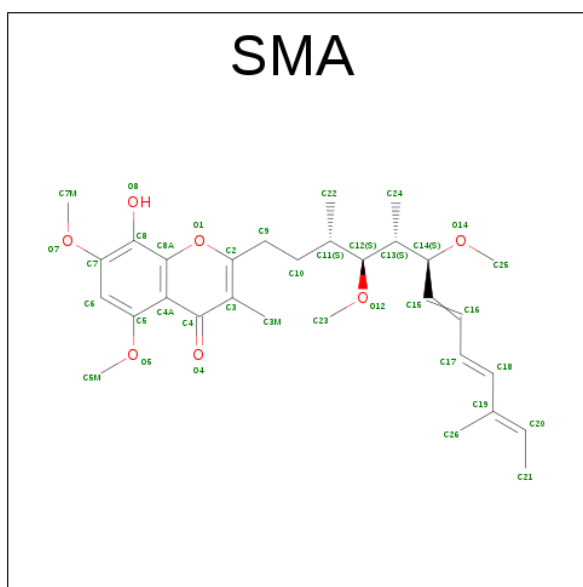
- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





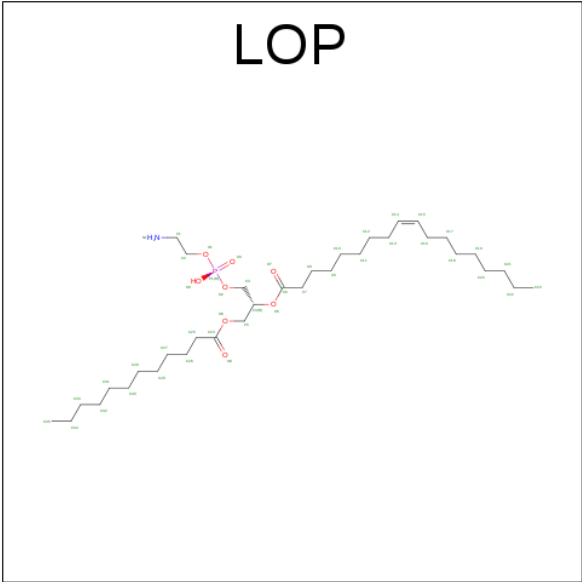
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 9 is STIGMATELLIN A (three-letter code: SMA) (formula: C<sub>30</sub>H<sub>42</sub>O<sub>7</sub>).



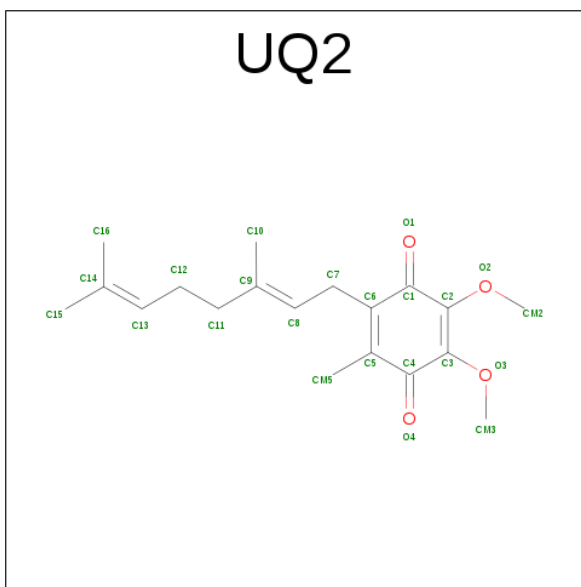
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			37	30	7		
9	D	1	Total	C	O	0	0
			37	30	7		
9	G	1	Total	C	O	0	0
			37	30	7		
9	J	1	Total	C	O	0	0
			37	30	7		
9	M	1	Total	C	O	0	0
			37	30	7		
9	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 10 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C<sub>35</sub>H<sub>68</sub>NO<sub>8</sub>P).



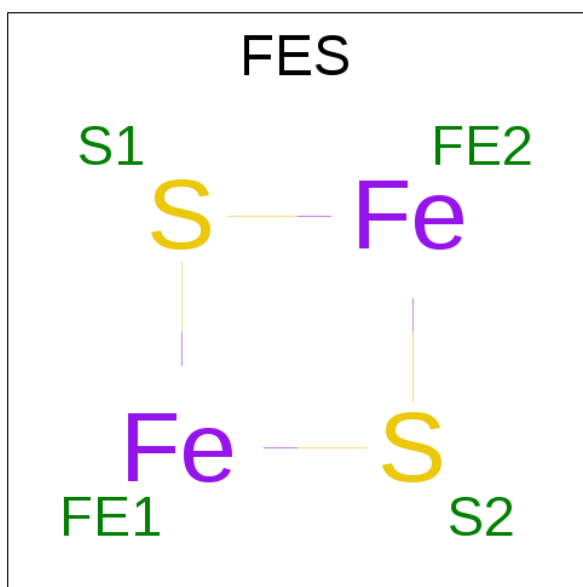
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	M	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 11 is UBIQUINONE-2 (three-letter code: UQ2) (formula: C<sub>19</sub>H<sub>26</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			23	19	4		
11	D	1	Total	C	O	0	0
			23	19	4		
11	G	1	Total	C	O	0	0
			23	19	4		
11	J	1	Total	C	O	0	0
			23	19	4		
11	M	1	Total	C	O	0	0
			23	19	4		
11	P	1	Total	C	O	0	0
			23	19	4		

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	Fe	S	0	0
			4	2	2		
12	F	1	Total	Fe	S	0	0
			4	2	2		
12	I	1	Total	Fe	S	0	0
			4	2	2		
12	L	1	Total	Fe	S	0	0
			4	2	2		
12	O	1	Total	Fe	S	0	0
			4	2	2		
12	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	73	Total	O	0	0
			73	73		
13	B	19	Total	O	0	0
			19	19		
13	C	47	Total	O	0	0
			47	47		
13	D	64	Total	O	0	0
			64	64		
13	E	14	Total	O	0	0
			14	14		
13	F	36	Total	O	0	0
			36	36		

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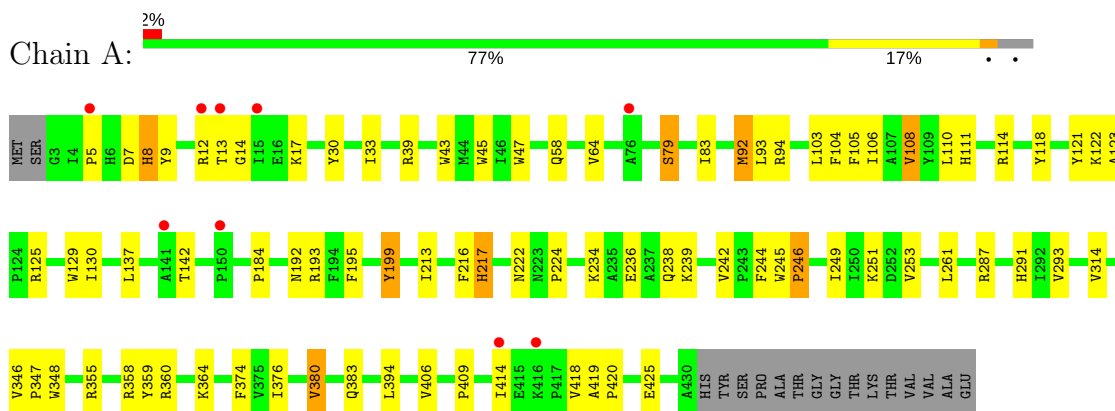
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	G	68	Total 68	O 68	0	0
13	H	35	Total 35	O 35	0	0
13	I	42	Total 42	O 42	0	0
13	J	55	Total 55	O 55	0	0
13	K	17	Total 17	O 17	0	0
13	L	42	Total 42	O 42	0	0
13	M	34	Total 34	O 34	0	0
13	N	11	Total 11	O 11	0	0
13	O	41	Total 41	O 41	0	0
13	P	60	Total 60	O 60	0	0
13	Q	16	Total 16	O 16	0	0
13	R	24	Total 24	O 24	0	0

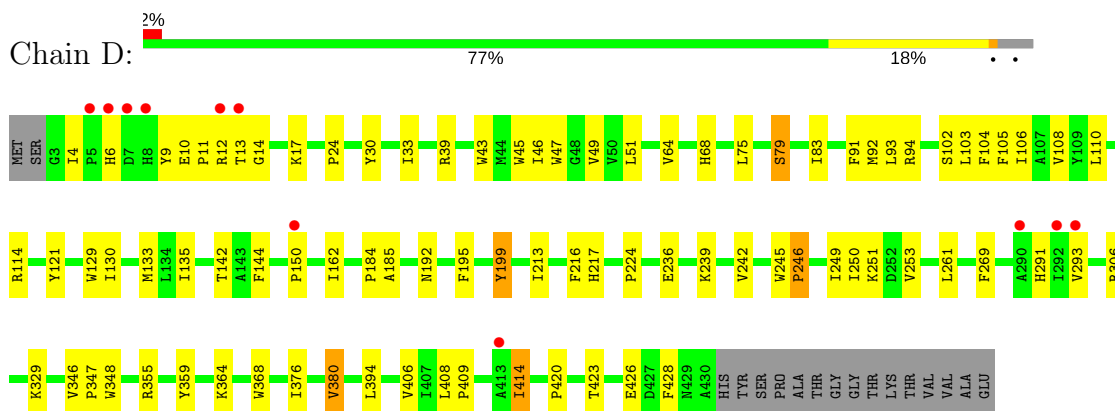
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

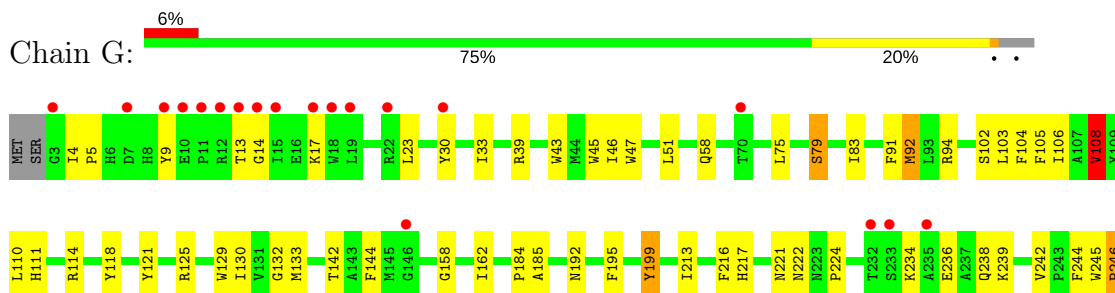
#### • Molecule 1: Cytochrome b

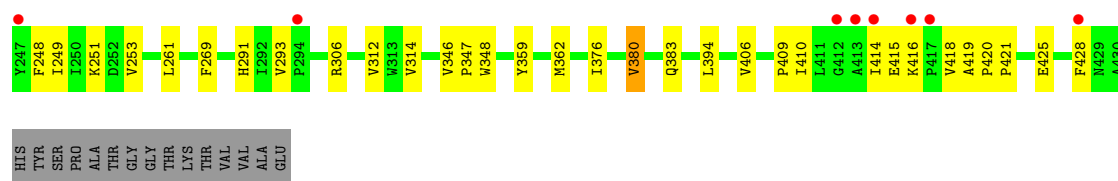


#### • Molecule 1: Cytochrome b

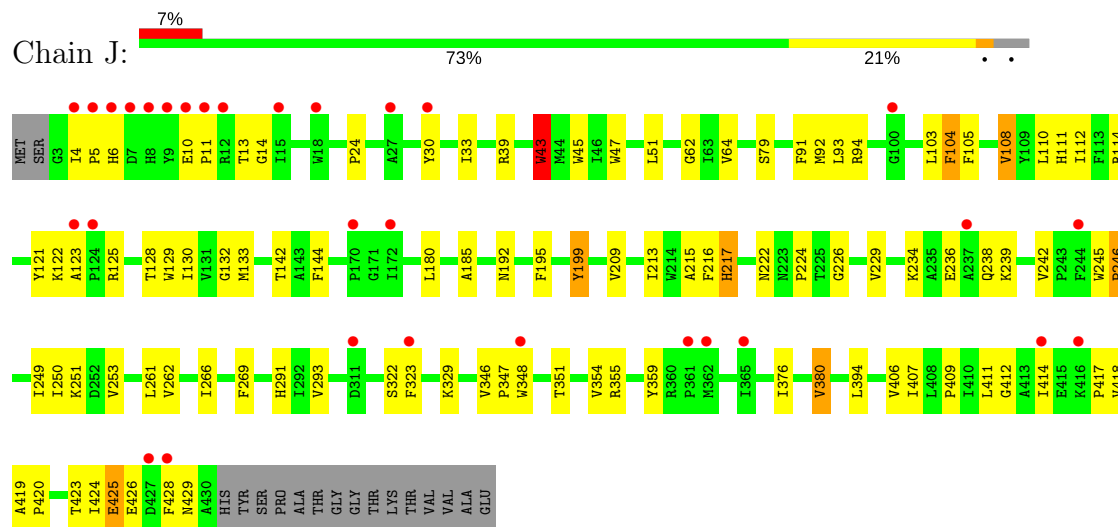


#### • Molecule 1: Cytochrome b

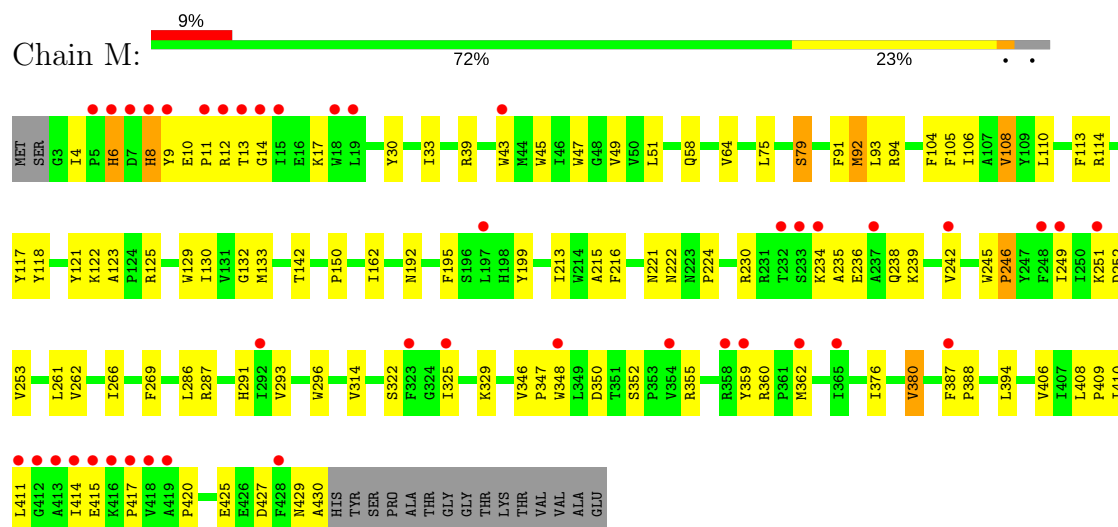




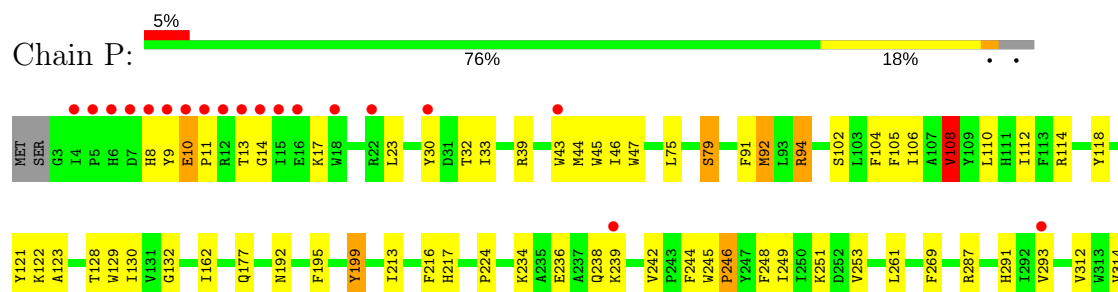
• Molecule 1: Cytochrome b



• Molecule 1: Cytochrome b



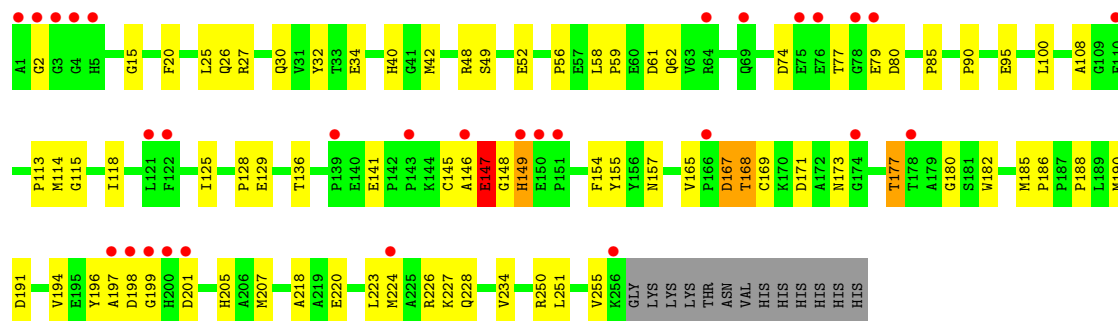
• Molecule 1: Cytochrome b



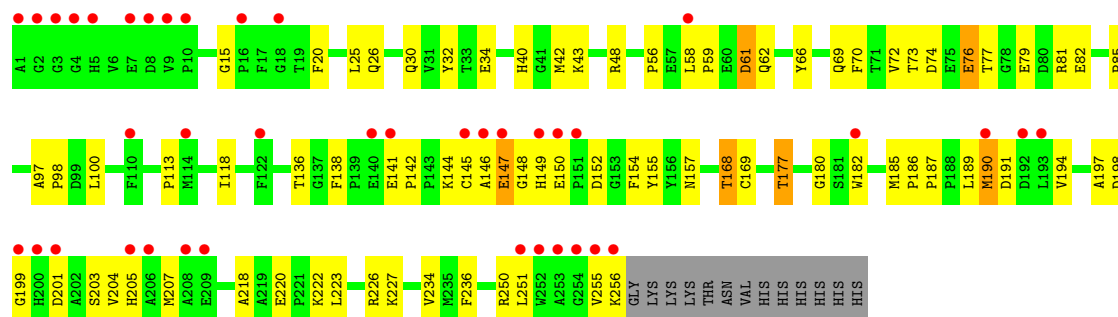




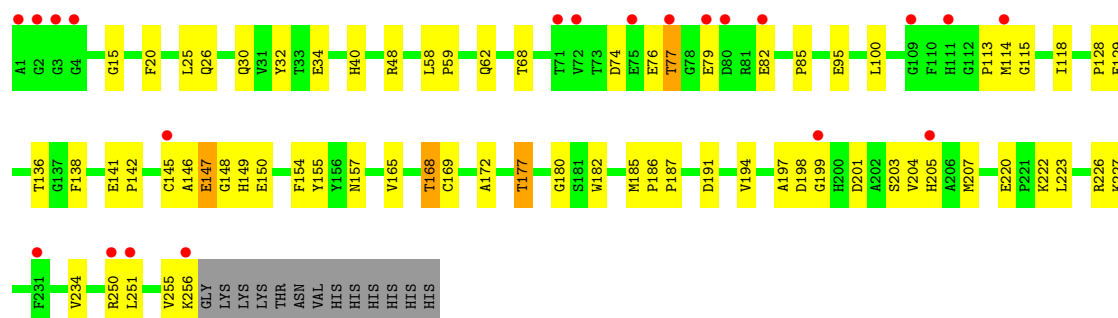
• Molecule 2: Cytochrome c1



• Molecule 2: Cytochrome c1

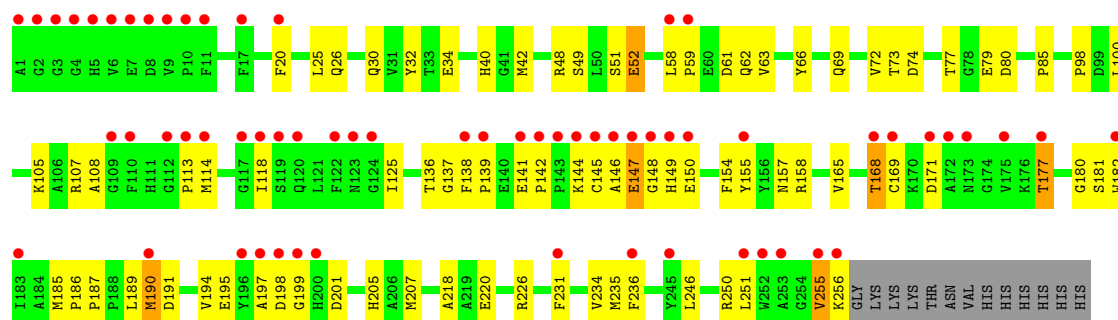


• Molecule 2: Cytochrome c1

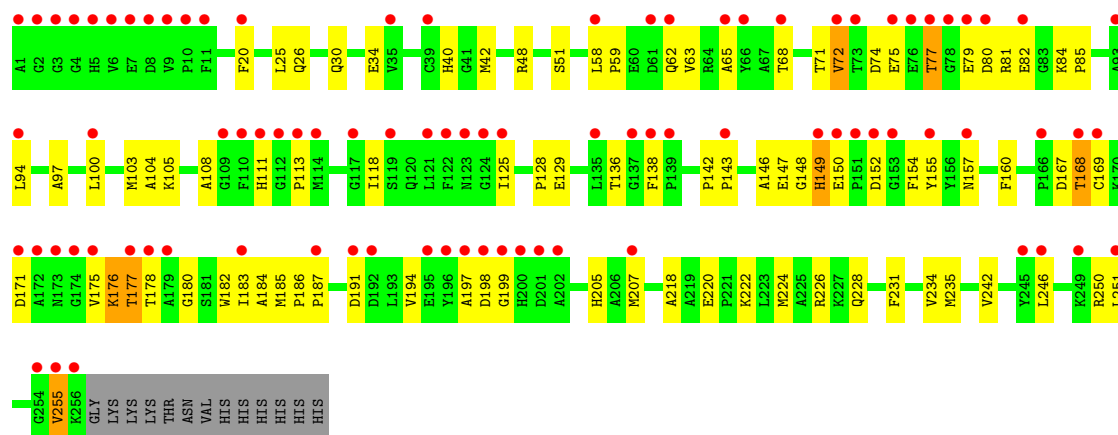


• Molecule 2: Cytochrome c1

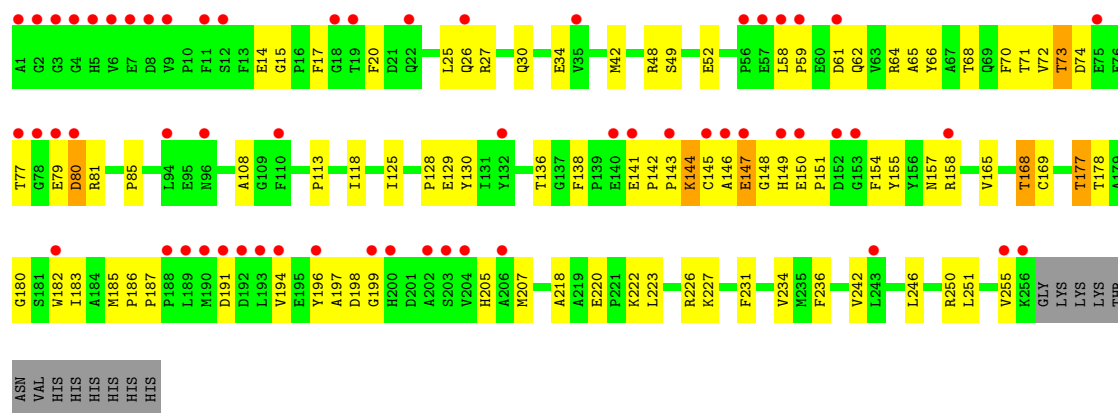




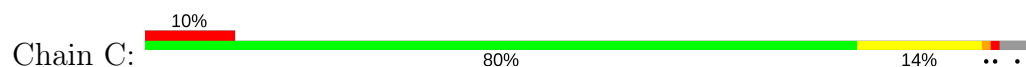
• Molecule 2: Cytochrome c1

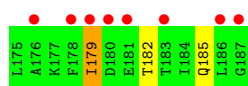


• Molecule 2: Cytochrome c1

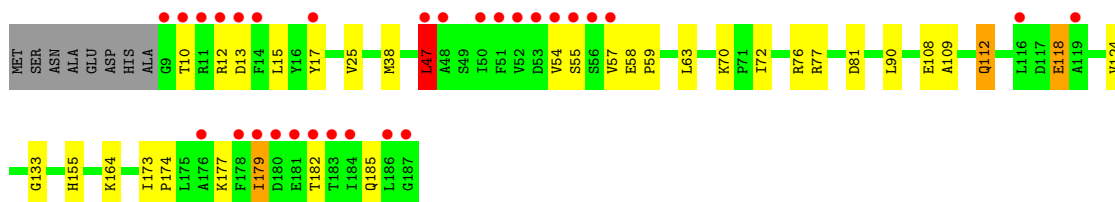


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

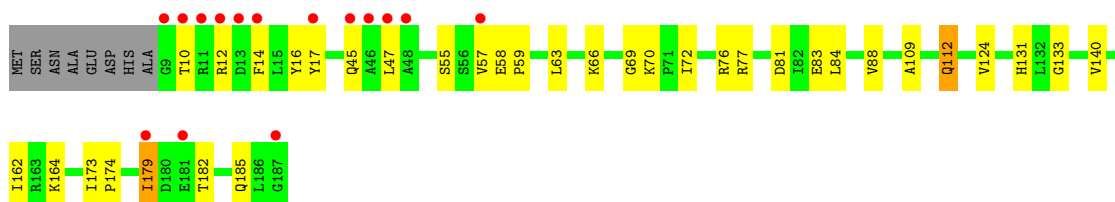
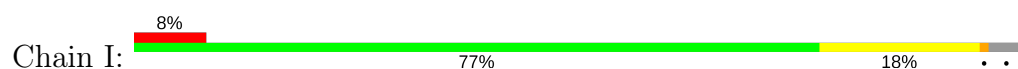




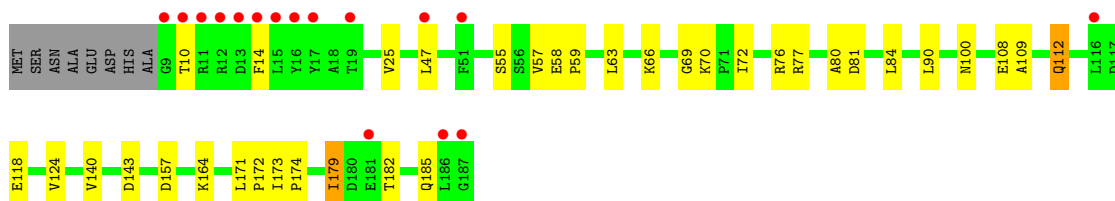
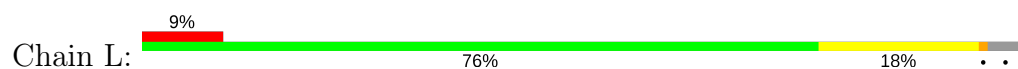
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



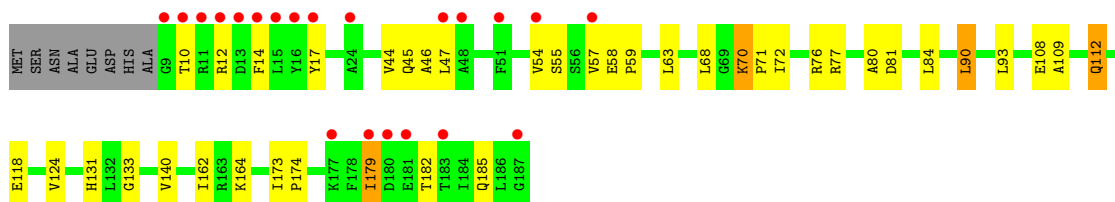
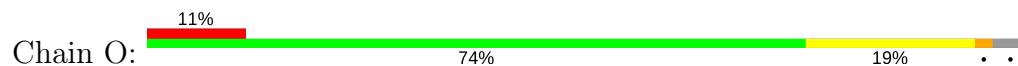
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



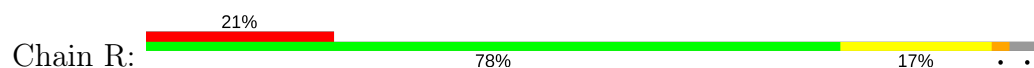
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

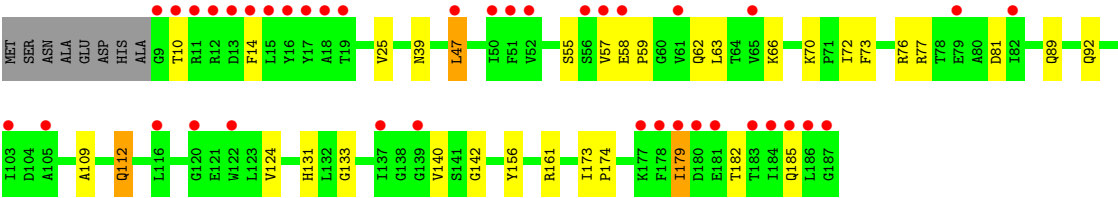


- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	351.89Å 147.04Å 161.31Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	18.00 – 2.40 47.10 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.7 (18.00-2.40) 91.9 (47.10-2.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.251 0.231 , 0.249	Depositor DCC
$R_{free}$ test set	4928 reflections (1.72%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	42656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SR, BGL, LOP, FES, NA, HEM, UQ2, SMA

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	0.39	0/3570	0.66	0/4897
1	D	0.39	0/3570	0.66	0/4897
1	G	0.38	0/3570	0.66	1/4897 (0.0%)
1	J	0.40	0/3570	0.66	0/4897
1	M	0.38	0/3570	0.65	0/4897
1	P	0.38	0/3570	0.65	1/4897 (0.0%)
2	B	0.37	0/2010	0.67	0/2733
2	E	0.36	0/2010	0.68	0/2733
2	H	0.37	0/2010	0.68	0/2733
2	K	0.36	0/2010	0.67	0/2733
2	N	0.36	0/2010	0.67	0/2733
2	Q	0.35	0/2010	0.66	0/2733
3	C	0.38	0/1370	0.74	1/1866 (0.1%)
3	F	0.39	0/1370	0.74	2/1866 (0.1%)
3	I	0.39	0/1370	0.76	1/1866 (0.1%)
3	L	0.38	0/1370	0.72	1/1866 (0.1%)
3	O	0.38	0/1370	0.72	1/1866 (0.1%)
3	R	0.38	0/1370	0.73	2/1866 (0.1%)
All	All	0.38	0/41700	0.68	10/56976 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	47	LEU	CA-CB-CG	7.62	132.83	115.30
3	R	47	LEU	CA-CB-CG	7.10	131.63	115.30
3	C	47	LEU	CA-CB-CG	6.99	131.38	115.30
3	L	47	LEU	CA-CB-CG	6.49	130.22	115.30
1	P	108	VAL	CB-CA-C	-5.59	100.78	111.40
1	G	108	VAL	CB-CA-C	-5.29	101.34	111.40
3	O	133	GLY	N-CA-C	5.21	126.12	113.10
3	R	133	GLY	N-CA-C	5.13	125.94	113.10
3	I	133	GLY	N-CA-C	5.12	125.89	113.10
3	F	133	GLY	N-CA-C	5.00	125.60	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TYR	Sidechain
2	E	32	TYR	Sidechain
2	H	32	TYR	Sidechain
2	K	32	TYR	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3428	70	0
1	D	3440	0	3428	81	0
1	G	3440	0	3428	91	0
1	J	3440	0	3428	96	0
1	M	3440	0	3428	95	0
1	P	3440	0	3428	78	0
2	B	1953	0	1848	65	0
2	E	1953	0	1848	89	0
2	H	1953	0	1848	71	0
2	K	1953	0	1848	70	0
2	N	1953	0	1848	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1953	0	1848	78	0
3	C	1340	0	1303	26	0
3	F	1340	0	1303	27	0
3	I	1340	0	1303	27	0
3	L	1340	0	1303	25	0
3	O	1340	0	1303	27	0
3	R	1340	0	1303	26	0
4	B	20	0	28	1	0
4	E	20	0	28	3	0
4	G	20	0	28	2	0
4	K	20	0	28	2	0
4	N	20	0	28	1	0
4	P	20	0	28	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	Q	1	0	0	0	0
6	I	1	0	0	0	0
6	R	1	0	0	0	0
7	R	1	0	0	0	0
8	A	86	0	60	7	0
8	B	43	0	30	1	0
8	D	86	0	60	8	0
8	E	43	0	30	1	0
8	G	86	0	60	9	0
8	H	43	0	30	1	0
8	J	86	0	60	15	0
8	K	43	0	30	2	0
8	M	86	0	60	8	0
8	N	43	0	30	3	0
8	P	86	0	60	7	0
8	Q	43	0	30	2	0
9	A	37	0	42	0	0
9	D	37	0	42	0	0
9	G	37	0	42	0	0
9	J	37	0	42	1	0
9	M	37	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	37	0	42	1	0
10	A	45	0	67	6	0
10	D	45	0	67	1	0
10	G	45	0	67	3	0
10	J	45	0	67	1	0
10	M	45	0	67	3	0
10	P	45	0	67	2	0
11	A	23	0	26	2	0
11	D	23	0	26	2	0
11	G	23	0	26	3	0
11	J	23	0	26	1	0
11	M	23	0	26	2	0
11	P	23	0	26	4	0
12	C	4	0	0	0	0
12	F	4	0	0	0	0
12	I	4	0	0	0	0
12	L	4	0	0	0	0
12	O	4	0	0	0	0
12	R	4	0	0	0	0
13	A	73	0	0	1	0
13	B	19	0	0	2	0
13	C	47	0	0	0	0
13	D	64	0	0	4	0
13	E	14	0	0	1	0
13	F	36	0	0	0	0
13	G	68	0	0	2	0
13	H	35	0	0	3	0
13	I	42	0	0	0	0
13	J	55	0	0	3	0
13	K	17	0	0	0	0
13	L	42	0	0	1	0
13	M	34	0	0	1	0
13	N	11	0	0	1	0
13	O	41	0	0	1	0
13	P	60	0	0	1	0
13	Q	16	0	0	1	0
13	R	24	0	0	2	0
All	All	42656	0	40992	1025	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1025) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:144:LYS:HZ3	2:Q:144:LYS:HA	1.06	1.14
2:K:139:PRO:HG3	2:K:158:ARG:HH11	1.14	1.12
2:N:77:THR:HG22	2:N:79:GLU:H	1.25	1.02
2:Q:144:LYS:NZ	2:Q:144:LYS:HA	1.75	1.01
2:B:250:ARG:HD3	3:C:12:ARG:HG2	1.41	1.01
2:K:74:ASP:HB3	2:K:77:THR:HB	1.42	0.99
2:K:144:LYS:O	2:K:147:GLU:HG3	1.66	0.95
2:Q:223:LEU:HD21	2:Q:227:LYS:HE3	1.45	0.95
2:N:74:ASP:HB3	2:N:77:THR:HB	1.48	0.94
1:D:142:THR:HG21	8:D:502:HEM:HBB2	1.50	0.94
1:A:195:PHE:HE2	1:D:195:PHE:HE2	1.18	0.92
2:E:144:LYS:O	2:E:147:GLU:HG3	1.71	0.90
1:M:329:LYS:HE3	3:R:131:HIS:O	1.70	0.90
2:H:77:THR:HG22	2:H:79:GLU:H	1.36	0.89
2:N:138:PHE:CD2	2:N:187:PRO:HG3	2.07	0.89
2:E:236:PHE:HE2	3:F:25:VAL:HG12	1.37	0.88
1:M:410:ILE:HG23	1:M:414:ILE:HD12	1.57	0.87
1:M:12:ARG:O	1:M:17:LYS:HE2	1.74	0.86
1:A:142:THR:HG21	8:A:502:HEM:HBB2	1.55	0.86
1:M:195:PHE:HE2	1:P:195:PHE:HE2	1.20	0.85
2:N:142:PRO:HG2	2:N:150:GLU:OE2	1.77	0.85
2:E:223:LEU:HD21	2:E:227:LYS:HE3	1.58	0.85
2:B:250:ARG:HG2	3:C:12:ARG:HD3	1.58	0.85
1:J:424:ILE:HG13	13:J:1157:HOH:O	1.76	0.84
1:G:410:ILE:HG23	1:G:414:ILE:HD12	1.58	0.84
1:G:195:PHE:HE2	1:J:195:PHE:HE2	1.22	0.84
1:G:248:PHE:CD1	1:G:251:LYS:HD3	2.13	0.83
2:K:139:PRO:HG3	2:K:158:ARG:NH1	1.92	0.83
2:Q:149:HIS:CD2	2:Q:168:THR:HG21	2.13	0.83
2:E:149:HIS:CD2	2:E:168:THR:HG21	2.14	0.83
2:E:236:PHE:CE2	3:F:25:VAL:HG12	2.14	0.82
2:N:77:THR:HG22	2:N:79:GLU:N	1.95	0.82
1:D:135:ILE:HG21	8:D:501:HEM:HAB	1.61	0.81
1:G:9:TYR:HB2	1:G:30:TYR:CD2	2.14	0.81
2:E:15:GLY:H	4:E:1042:BGL:H5	1.46	0.81
1:D:246:PRO:HG2	2:E:251:LEU:HD21	1.63	0.80
2:E:138:PHE:CD2	2:E:187:PRO:HG3	2.18	0.79
2:K:138:PHE:CD2	2:K:187:PRO:HG3	2.17	0.79
1:G:248:PHE:HD1	1:G:251:LYS:HD3	1.46	0.79
2:K:149:HIS:CD2	2:K:168:THR:HG21	2.18	0.79
2:H:95:GLU:HG2	13:H:327:HOH:O	1.82	0.78
2:E:74:ASP:HB3	2:E:77:THR:HB	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:250:ARG:HG3	2:E:250:ARG:HH11	1.45	0.78
1:J:4:ILE:N	1:J:4:ILE:HD12	1.99	0.78
2:N:74:ASP:CB	2:N:77:THR:HB	2.14	0.77
2:Q:77:THR:HG22	2:Q:79:GLU:HB2	1.65	0.77
2:K:77:THR:HG22	2:K:79:GLU:H	1.50	0.77
3:O:131:HIS:O	1:P:329:LYS:HE3	1.84	0.77
2:H:250:ARG:NH1	3:I:12:ARG:HB2	2.00	0.76
2:H:77:THR:HG22	2:H:79:GLU:N	2.00	0.76
2:N:231:PHE:O	2:N:235:MET:HG2	1.84	0.76
1:P:239:LYS:HE2	1:P:425:GLU:OE2	1.86	0.75
1:M:13:THR:O	1:M:17:LYS:HG3	1.87	0.75
2:N:183:ILE:HG23	2:N:185:MET:H	1.52	0.75
2:H:250:ARG:CZ	3:I:12:ARG:HB2	2.17	0.75
1:M:105:PHE:HA	1:M:108:VAL:HG22	1.69	0.74
1:G:239:LYS:HE2	1:G:425:GLU:OE2	1.87	0.74
1:G:261:LEU:HD11	2:H:234:VAL:HG13	1.69	0.74
1:D:12:ARG:O	1:D:17:LYS:HE2	1.88	0.74
1:P:9:TYR:HB2	1:P:30:TYR:CD2	2.23	0.74
1:M:4:ILE:H	1:M:4:ILE:HD12	1.53	0.74
2:N:40:HIS:ND1	2:N:97:ALA:HB1	2.03	0.73
1:G:4:ILE:H	1:G:4:ILE:HD12	1.49	0.73
1:A:9:TYR:HB2	1:A:30:TYR:CD2	2.23	0.73
2:E:77:THR:CG2	2:E:79:GLU:HB2	2.19	0.73
2:Q:223:LEU:CD2	2:Q:227:LYS:HE3	2.18	0.73
2:Q:138:PHE:CD2	2:Q:187:PRO:HG3	2.24	0.73
1:J:4:ILE:H	1:J:4:ILE:HD12	1.53	0.72
1:M:91:PHE:CD1	2:N:222:LYS:HG2	2.24	0.72
1:J:428:PHE:CE1	2:K:256:LYS:HD2	2.24	0.72
1:M:9:TYR:HB2	1:M:30:TYR:CD2	2.24	0.72
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.25	0.72
1:G:142:THR:HG21	8:G:502:HEM:HBB2	1.70	0.72
1:P:213:ILE:HA	1:P:216:PHE:CE2	2.25	0.72
1:P:287:ARG:HG2	1:P:287:ARG:HH11	1.53	0.72
1:M:213:ILE:HA	1:M:216:PHE:CE2	2.26	0.71
2:N:194:VAL:HB	2:N:207:MET:CE	2.21	0.71
1:J:213:ILE:HA	1:J:216:PHE:CE2	2.25	0.71
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.26	0.71
3:C:47:LEU:O	3:C:47:LEU:HD23	1.91	0.71
1:G:213:ILE:HA	1:G:216:PHE:CE2	2.26	0.70
2:Q:59:PRO:HD2	2:Q:62:GLN:NE2	2.06	0.70
2:N:59:PRO:HD2	2:N:62:GLN:NE2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:LYS:HE2	1:J:425:GLU:OE1	1.90	0.70
1:D:92:MET:HE1	2:E:226:ARG:HG3	1.72	0.70
1:G:130:ILE:HD11	1:G:348:TRP:HH2	1.57	0.70
1:G:246:PRO:HG2	2:H:251:LEU:HD21	1.74	0.70
1:A:261:LEU:HD11	2:B:234:VAL:HG13	1.71	0.70
1:D:261:LEU:HD11	2:E:234:VAL:HG13	1.73	0.70
2:Q:194:VAL:HB	2:Q:207:MET:CE	2.22	0.70
3:C:84:LEU:HD23	3:L:84:LEU:HD23	1.74	0.70
1:M:376:ILE:O	1:M:380:VAL:HG22	1.92	0.70
2:N:194:VAL:HB	2:N:207:MET:HE3	1.72	0.69
3:F:47:LEU:O	3:F:47:LEU:HD23	1.92	0.69
2:H:59:PRO:HD2	2:H:62:GLN:NE2	2.07	0.69
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.27	0.69
1:P:130:ILE:HD11	1:P:348:TRP:HH2	1.57	0.69
2:H:194:VAL:HB	2:H:207:MET:CE	2.23	0.69
2:K:59:PRO:HD2	2:K:62:GLN:NE2	2.06	0.69
1:M:269:PHE:HB3	4:N:1045:BGL:H1'2	1.75	0.69
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.56	0.69
2:E:59:PRO:HD2	2:E:62:GLN:NE2	2.07	0.69
1:J:130:ILE:HD11	1:J:348:TRP:HH2	1.57	0.69
2:K:194:VAL:HB	2:K:207:MET:CE	2.23	0.69
3:F:112:GLN:H	3:F:112:GLN:NE2	1.91	0.69
1:M:8:HIS:H	1:M:8:HIS:CD2	2.09	0.69
1:A:287:ARG:HH11	1:A:287:ARG:HG2	1.57	0.69
2:B:59:PRO:HD2	2:B:62:GLN:NE2	2.07	0.69
1:P:91:PHE:CD1	2:Q:222:LYS:HG2	2.28	0.69
2:E:77:THR:HG22	2:E:79:GLU:H	1.58	0.69
8:A:501:HEM:HBC2	8:A:501:HEM:HMC2	1.75	0.68
1:A:374:PHE:HD2	10:A:1021:LOP:H321	1.57	0.68
2:N:40:HIS:CE1	2:N:97:ALA:HB1	2.28	0.68
1:A:376:ILE:O	1:A:380:VAL:HG22	1.93	0.68
1:D:130:ILE:HD11	1:D:348:TRP:HH2	1.57	0.68
1:J:376:ILE:O	1:J:380:VAL:HG22	1.92	0.68
1:P:376:ILE:O	1:P:380:VAL:HG22	1.92	0.68
1:P:261:LEU:HD11	2:Q:234:VAL:HG13	1.76	0.68
1:D:376:ILE:O	1:D:380:VAL:HG22	1.93	0.68
1:G:376:ILE:O	1:G:380:VAL:HG22	1.93	0.68
2:K:49:SER:HA	2:K:52:GLU:HG3	1.76	0.68
1:M:130:ILE:HD11	1:M:348:TRP:HH2	1.57	0.68
1:A:105:PHE:HA	1:A:108:VAL:HG22	1.76	0.67
3:C:70:LYS:HE3	1:D:184:PRO:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:194:VAL:HB	2:E:207:MET:CE	2.24	0.67
1:J:104:PHE:O	1:J:108:VAL:HG22	1.94	0.67
1:G:103:LEU:HD13	10:G:1023:LOP:H211	1.76	0.67
2:H:250:ARG:CZ	3:I:12:ARG:CB	2.72	0.67
1:M:230:ARG:HA	13:M:528:HOH:O	1.94	0.67
1:P:43:TRP:CZ3	1:P:251:LYS:HE3	2.30	0.67
2:B:74:ASP:HB3	2:B:77:THR:HB	1.76	0.66
1:M:118:TYR:OH	10:M:1025:LOP:H31	1.96	0.66
2:N:138:PHE:HD2	2:N:187:PRO:HG3	1.56	0.66
2:B:194:VAL:HB	2:B:207:MET:CE	2.24	0.66
1:A:246:PRO:HG2	2:B:251:LEU:HD21	1.76	0.66
1:M:261:LEU:HD11	2:N:234:VAL:HG13	1.78	0.66
2:E:77:THR:HG22	2:E:79:GLU:N	2.11	0.65
3:L:112:GLN:NE2	3:L:112:GLN:H	1.93	0.65
1:M:142:THR:HG21	8:M:502:HEM:HBB2	1.76	0.65
1:A:125:ARG:CZ	1:A:222:ASN:HB2	2.25	0.65
2:N:224:MET:O	2:N:228:GLN:HG3	1.95	0.65
1:D:39:ARG:HH12	2:E:255:VAL:CG1	2.09	0.65
2:K:105:LYS:HD3	2:K:220:GLU:HG2	1.78	0.65
1:J:199:TYR:HA	8:J:502:HEM:HBC2	1.78	0.65
2:Q:20:PHE:HB3	2:Q:25:LEU:HD11	1.78	0.65
2:B:26:GLN:HG2	2:B:58:LEU:HD21	1.79	0.65
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.79	0.65
1:M:39:ARG:HG2	1:M:242:VAL:HG13	1.79	0.65
1:D:39:ARG:HG2	1:D:242:VAL:HG13	1.78	0.65
2:E:26:GLN:HG2	2:E:58:LEU:HD21	1.79	0.65
1:J:24:PRO:HA	13:J:1105:HOH:O	1.96	0.65
1:P:39:ARG:HG2	1:P:242:VAL:HG13	1.78	0.65
3:R:112:GLN:H	3:R:112:GLN:NE2	1.95	0.65
2:K:26:GLN:HG2	2:K:58:LEU:HD21	1.79	0.65
3:C:112:GLN:H	3:C:112:GLN:NE2	1.95	0.64
1:G:105:PHE:HA	1:G:108:VAL:HG22	1.78	0.64
1:J:105:PHE:HA	1:J:108:VAL:HG23	1.78	0.64
2:Q:128:PRO:HG2	2:Q:129:GLU:OE1	1.98	0.64
2:H:74:ASP:HB3	2:H:77:THR:HB	1.80	0.64
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.80	0.64
1:M:105:PHE:HA	1:M:108:VAL:CG2	2.26	0.64
1:J:180:LEU:HD22	9:J:1004:SMA:H26	1.78	0.64
2:N:20:PHE:HB3	2:N:25:LEU:HD11	1.78	0.64
2:N:26:GLN:HG2	2:N:58:LEU:HD21	1.80	0.64
1:D:103:LEU:HD13	10:D:1022:LOP:H201	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:GLN:HG2	2:H:58:LEU:HD21	1.80	0.64
1:P:217:HIS:NE2	11:P:1106:UQ2:O4	2.31	0.64
2:Q:61:ASP:HA	2:Q:64:ARG:NH1	2.12	0.64
3:I:112:GLN:H	3:I:112:GLN:NE2	1.96	0.64
1:G:39:ARG:HG2	1:G:242:VAL:HG13	1.78	0.64
1:A:33:ILE:HG13	1:A:245:TRP:HB2	1.79	0.64
2:Q:26:GLN:HG2	2:Q:58:LEU:HD21	1.80	0.63
1:J:125:ARG:CZ	1:J:222:ASN:HB2	2.28	0.63
1:J:428:PHE:HZ	2:K:256:LYS:HB2	1.63	0.63
1:J:39:ARG:HG2	1:J:242:VAL:HG13	1.78	0.63
1:P:246:PRO:HG2	2:Q:251:LEU:HD21	1.80	0.63
1:A:39:ARG:HG2	1:A:242:VAL:HG13	1.79	0.63
1:D:33:ILE:HG13	1:D:245:TRP:HB2	1.79	0.63
1:G:33:ILE:HG13	1:G:245:TRP:HB2	1.80	0.63
2:K:142:PRO:HG2	2:K:150:GLU:OE2	1.98	0.63
3:O:118:GLU:H	3:O:118:GLU:CD	2.02	0.63
2:E:250:ARG:HD3	3:F:12:ARG:HB3	1.80	0.63
2:E:20:PHE:HB3	2:E:25:LEU:HD11	1.81	0.63
1:P:33:ILE:HG13	1:P:245:TRP:HB2	1.81	0.63
2:H:142:PRO:HG2	2:H:150:GLU:OE2	1.98	0.63
3:I:131:HIS:O	1:J:329:LYS:HE3	1.99	0.63
2:K:66:TYR:O	2:K:69:GLN:HG2	1.98	0.63
1:P:39:ARG:HH12	2:Q:255:VAL:CG1	2.11	0.62
1:M:117:TYR:CE2	10:M:1025:LOP:H32	2.34	0.62
1:G:39:ARG:HH12	2:H:255:VAL:CG1	2.11	0.62
1:J:33:ILE:HG13	1:J:245:TRP:HB2	1.80	0.62
1:J:103:LEU:HD13	10:J:1024:LOP:H211	1.82	0.62
1:G:269:PHE:HB3	4:G:1043:BGL:H1'2	1.81	0.62
1:J:4:ILE:H	1:J:4:ILE:CD1	2.12	0.62
2:B:20:PHE:HB3	2:B:25:LEU:HD11	1.81	0.62
1:D:43:TRP:CZ3	1:D:251:LYS:HG2	2.35	0.62
1:D:269:PHE:HB3	4:E:1042:BGL:H1'2	1.80	0.62
1:J:62:GLY:C	8:J:502:HEM:HAC	2.20	0.61
2:K:108:ALA:HA	2:K:125:ILE:HG22	1.83	0.61
1:A:374:PHE:CD2	10:A:1021:LOP:H321	2.35	0.61
1:G:199:TYR:CD2	8:G:502:HEM:HBC1	2.35	0.61
1:D:24:PRO:HA	13:D:1103:HOH:O	2.01	0.61
1:D:10:GLU:OE2	1:D:11:PRO:HD2	2.00	0.61
1:M:33:ILE:HG13	1:M:245:TRP:HB2	1.81	0.61
2:K:194:VAL:HB	2:K:207:MET:HE1	1.81	0.61
3:O:118:GLU:CD	3:O:118:GLU:N	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:47:LEU:O	3:O:47:LEU:HD23	2.00	0.61
2:E:72:VAL:HG12	2:E:73:THR:N	2.16	0.61
2:N:171:ASP:OD2	2:N:175:VAL:HB	2.01	0.61
2:B:167:ASP:OD1	2:B:167:ASP:N	2.28	0.61
3:C:83:GLU:OE1	3:C:83:GLU:HA	2.00	0.61
2:H:256:LYS:HG2	2:H:256:LYS:O	2.00	0.61
2:K:189:LEU:O	2:K:190:MET:HB2	2.00	0.60
1:P:105:PHE:HA	1:P:108:VAL:HG22	1.82	0.60
2:B:129:GLU:OE1	2:B:129:GLU:N	2.27	0.60
1:A:39:ARG:HH12	2:B:255:VAL:CG1	2.15	0.60
1:D:91:PHE:CE2	1:D:92:MET:HE3	2.37	0.60
2:N:142:PRO:CG	2:N:150:GLU:OE2	2.49	0.60
3:O:112:GLN:H	3:O:112:GLN:NE2	1.99	0.60
2:B:149:HIS:CD2	2:B:168:THR:HG21	2.37	0.60
1:G:306:ARG:HG3	13:G:1156:HOH:O	2.01	0.60
3:L:80:ALA:O	3:L:84:LEU:HG	2.01	0.60
2:B:250:ARG:HD3	3:C:12:ARG:CG	2.26	0.60
2:N:71:THR:CG2	2:N:80:ASP:HB3	2.32	0.59
2:H:77:THR:HG21	2:H:79:GLU:HB2	1.83	0.59
2:H:194:VAL:HB	2:H:207:MET:HE1	1.83	0.59
1:A:103:LEU:HD13	10:A:1021:LOP:H211	1.84	0.59
1:J:425:GLU:HG3	1:J:429:ASN:HD21	1.67	0.59
1:P:406:VAL:O	1:P:409:PRO:HD2	2.01	0.59
1:A:287:ARG:NH1	1:A:287:ARG:HG2	2.16	0.59
2:B:194:VAL:HB	2:B:207:MET:HE3	1.85	0.59
2:Q:194:VAL:HB	2:Q:207:MET:HE1	1.83	0.59
2:B:56:PRO:HD2	13:B:1044:HOH:O	2.01	0.59
2:E:223:LEU:CD2	2:E:227:LYS:HE3	2.30	0.59
2:K:42:MET:HE2	2:K:218:ALA:HB1	1.85	0.59
2:Q:129:GLU:OE1	2:Q:129:GLU:N	2.36	0.59
2:K:77:THR:HG22	2:K:79:GLU:N	2.16	0.59
11:P:1106:UQ2:H5M1	11:P:1106:UQ2:C8	2.33	0.59
2:E:144:LYS:HA	2:E:144:LYS:HE2	1.84	0.59
1:J:144:PHE:HD1	13:J:1113:HOH:O	1.86	0.58
2:Q:77:THR:CG2	2:Q:79:GLU:HB2	2.33	0.58
2:Q:194:VAL:HB	2:Q:207:MET:HE3	1.84	0.58
1:D:91:PHE:HE2	1:D:92:MET:HE3	1.68	0.58
1:G:406:VAL:O	1:G:409:PRO:HD2	2.02	0.58
2:Q:42:MET:HE2	2:Q:218:ALA:HB1	1.85	0.58
1:M:221:ASN:HD21	11:M:1105:UQ2:H3M1	1.68	0.58
1:M:4:ILE:N	1:M:4:ILE:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:10:THR:O	3:O:10:THR:HG22	2.04	0.58
1:A:92:MET:CE	2:B:226:ARG:HG3	2.33	0.58
1:D:249:ILE:O	1:D:253:VAL:HG23	2.04	0.58
1:D:68:HIS:ND1	13:D:1105:HOH:O	2.32	0.58
3:I:55:SER:HB3	3:I:182:THR:OG1	2.04	0.58
3:R:10:THR:O	3:R:10:THR:HG22	2.04	0.58
1:A:249:ILE:O	1:A:253:VAL:HG23	2.04	0.57
1:D:43:TRP:CH2	1:D:251:LYS:HG2	2.39	0.57
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.04	0.57
2:E:194:VAL:HB	2:E:207:MET:HE1	1.85	0.57
3:L:55:SER:HB3	3:L:182:THR:OG1	2.04	0.57
3:O:55:SER:HB3	3:O:182:THR:OG1	2.04	0.57
1:A:92:MET:HE1	2:B:226:ARG:HG3	1.86	0.57
3:F:55:SER:HB3	3:F:182:THR:OG1	2.04	0.57
1:M:39:ARG:HH12	2:N:255:VAL:CG1	2.17	0.57
2:B:42:MET:HE2	2:B:218:ALA:HB1	1.86	0.57
3:C:55:SER:HB3	3:C:182:THR:OG1	2.05	0.57
3:F:10:THR:HG22	3:F:10:THR:O	2.04	0.57
1:M:132:GLY:C	8:M:501:HEM:HBC2	2.25	0.57
2:K:51:SER:OG	2:K:63:VAL:HG21	2.05	0.57
1:D:105:PHE:HA	1:D:108:VAL:HG22	1.86	0.57
1:J:105:PHE:HA	1:J:108:VAL:CG2	2.35	0.57
1:J:261:LEU:HD11	2:K:234:VAL:HG13	1.87	0.57
2:N:71:THR:HG22	2:N:80:ASP:HB3	1.87	0.57
2:E:42:MET:HE2	2:E:218:ALA:HB1	1.86	0.57
1:G:199:TYR:CE2	8:G:502:HEM:HBC1	2.40	0.57
2:Q:49:SER:HA	2:Q:52:GLU:HG3	1.87	0.56
3:R:55:SER:HB3	3:R:182:THR:OG1	2.05	0.56
1:M:411:LEU:O	1:M:415:GLU:HG2	2.04	0.56
2:B:42:MET:HE1	2:B:218:ALA:CB	2.35	0.56
2:N:138:PHE:CE1	2:N:157:ASN:ND2	2.73	0.56
1:A:5:PRO:HB2	1:A:234:LYS:HA	1.87	0.56
3:C:10:THR:HG22	3:C:10:THR:O	2.05	0.56
1:D:406:VAL:O	1:D:409:PRO:HD2	2.05	0.56
1:G:158:GLY:O	1:G:162:ILE:HD12	2.04	0.56
1:G:248:PHE:HA	1:G:251:LYS:HG2	1.87	0.56
3:I:10:THR:O	3:I:10:THR:HG22	2.04	0.56
3:L:10:THR:O	3:L:10:THR:HG22	2.05	0.56
2:H:77:THR:CG2	2:H:79:GLU:HB2	2.36	0.56
1:J:5:PRO:HB2	1:J:234:LYS:HA	1.86	0.56
1:J:246:PRO:HG2	2:K:251:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:125:ARG:CZ	1:M:222:ASN:HB2	2.35	0.56
2:Q:72:VAL:HG12	2:Q:73:THR:N	2.21	0.56
1:D:217:HIS:NE2	11:D:1102:UQ2:O4	2.26	0.56
1:P:351:THR:OG1	1:P:412:GLY:HA3	2.05	0.56
1:A:12:ARG:O	1:A:17:LYS:HE2	2.05	0.56
1:A:359:TYR:CD2	1:A:420:PRO:HB3	2.41	0.56
2:B:145:CYS:O	2:B:168:THR:OG1	2.21	0.56
2:N:42:MET:HE2	2:N:218:ALA:HB1	1.88	0.56
2:N:220:GLU:OE2	2:N:226:ARG:NH1	2.39	0.56
1:G:184:PRO:O	3:L:70:LYS:HE3	2.05	0.56
2:Q:81:ARG:HH11	2:Q:81:ARG:HG3	1.70	0.56
3:C:131:HIS:O	1:D:329:LYS:HE3	2.06	0.56
1:P:43:TRP:HZ3	1:P:251:LYS:HE3	1.69	0.56
1:G:383:GLN:HE22	2:H:115:GLY:HA3	1.71	0.56
1:J:249:ILE:O	1:J:253:VAL:HG23	2.06	0.55
1:P:236:GLU:HA	1:P:239:LYS:CD	2.36	0.55
1:J:199:TYR:CD2	8:J:502:HEM:HBC1	2.42	0.55
1:D:144:PHE:CD1	1:D:162:ILE:HD12	2.40	0.55
2:E:194:VAL:HB	2:E:207:MET:HE3	1.88	0.55
2:K:114:MET:HG2	2:K:114:MET:O	2.05	0.55
1:A:358:ARG:HH21	10:A:1021:LOP:H21	1.71	0.55
1:G:4:ILE:N	1:G:4:ILE:HD12	2.19	0.55
2:K:194:VAL:HB	2:K:207:MET:HE3	1.89	0.55
1:P:199:TYR:CD2	8:P:502:HEM:HBC1	2.41	0.55
2:E:56:PRO:HD2	13:E:1045:HOH:O	2.06	0.55
1:A:58:GLN:CB	8:A:502:HEM:HAB	2.37	0.55
2:E:42:MET:HE1	2:E:218:ALA:CB	2.37	0.55
2:B:250:ARG:CD	3:C:12:ARG:HG2	2.28	0.55
1:D:13:THR:HG22	1:D:14:GLY:N	2.22	0.55
1:P:287:ARG:NH1	1:P:287:ARG:HG2	2.21	0.55
2:B:27:ARG:HD2	2:B:196:TYR:CE2	2.42	0.55
1:A:195:PHE:CE2	1:D:195:PHE:HE2	2.10	0.55
2:H:194:VAL:HB	2:H:207:MET:HE3	1.87	0.55
2:Q:246:LEU:O	2:Q:250:ARG:HG2	2.07	0.55
1:D:92:MET:CE	2:E:226:ARG:HG3	2.35	0.55
1:G:92:MET:HE2	1:G:92:MET:HA	1.89	0.55
2:B:194:VAL:HB	2:B:207:MET:HE1	1.88	0.54
1:M:246:PRO:HG2	2:N:251:LEU:HD21	1.88	0.54
1:P:244:PHE:CE1	11:P:1106:UQ2:H2M2	2.42	0.54
3:R:89:GLN:O	3:R:92:GLN:HB2	2.07	0.54
2:Q:66:TYR:CE1	2:Q:70:PHE:HE2	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:TYR:CD2	1:D:420:PRO:HB3	2.43	0.54
2:E:169:CYS:O	2:E:177:THR:HB	2.06	0.54
2:E:142:PRO:HG2	2:E:150:GLU:OE2	2.07	0.54
2:H:146:ALA:O	2:H:148:GLY:N	2.41	0.54
1:J:226:GLY:HA2	1:J:355:ARG:HD2	1.89	0.54
1:M:249:ILE:O	1:M:253:VAL:HG23	2.07	0.54
2:B:141:GLU:HG3	2:B:141:GLU:O	2.07	0.54
2:B:42:MET:CE	2:B:218:ALA:CB	2.85	0.54
1:D:13:THR:HG22	1:D:14:GLY:H	1.72	0.54
2:E:250:ARG:CD	3:F:12:ARG:HB3	2.36	0.54
1:G:185:ALA:HB2	3:L:70:LYS:HG3	1.87	0.54
1:G:249:ILE:O	1:G:253:VAL:HG23	2.06	0.54
1:P:269:PHE:HB3	4:P:1046:BGL:H1'2	1.89	0.54
2:Q:169:CYS:O	2:Q:177:THR:HB	2.08	0.54
2:B:169:CYS:O	2:B:177:THR:HB	2.08	0.54
1:M:362:MET:CB	1:M:411:LEU:HD21	2.38	0.54
1:A:13:THR:HG22	1:A:14:GLY:N	2.22	0.54
1:A:5:PRO:HB3	1:A:234:LYS:HG2	1.90	0.54
2:N:128:PRO:HG2	2:N:129:GLU:OE1	2.08	0.54
1:G:13:THR:HG22	1:G:14:GLY:H	1.73	0.54
1:M:8:HIS:CD2	1:M:8:HIS:N	2.73	0.54
1:P:249:ILE:O	1:P:253:VAL:HG23	2.07	0.54
2:Q:236:PHE:CE1	3:R:25:VAL:CG1	2.90	0.54
2:E:66:TYR:O	2:E:69:GLN:HG2	2.07	0.54
1:A:195:PHE:HE2	1:D:195:PHE:CE2	2.10	0.53
2:B:128:PRO:HG2	2:B:129:GLU:OE1	2.08	0.53
1:D:346:VAL:HG12	1:D:347:PRO:HD3	1.90	0.53
1:A:13:THR:O	1:A:17:LYS:HG3	2.08	0.53
2:B:149:HIS:CE1	2:B:168:THR:HG21	2.43	0.53
1:G:13:THR:HG22	1:G:14:GLY:N	2.23	0.53
1:J:91:PHE:CE2	1:J:92:MET:HE2	2.43	0.53
2:N:146:ALA:O	2:N:148:GLY:N	2.40	0.53
3:O:90:LEU:HD11	3:O:108:GLU:HB3	1.90	0.53
1:P:112:ILE:HG12	8:P:501:HEM:HAC	1.90	0.53
1:A:217:HIS:NE2	11:A:1101:UQ2:O4	2.40	0.53
2:K:146:ALA:O	2:K:148:GLY:N	2.41	0.53
1:M:13:THR:HG22	1:M:14:GLY:N	2.24	0.53
1:M:234:LYS:O	1:M:238:GLN:HG3	2.09	0.53
2:Q:146:ALA:O	2:Q:148:GLY:N	2.41	0.53
1:A:13:THR:HG22	1:A:14:GLY:H	1.72	0.53
1:J:13:THR:HG22	1:J:14:GLY:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ALA:O	2:B:148:GLY:N	2.41	0.53
2:B:49:SER:HA	2:B:52:GLU:HG3	1.89	0.53
2:E:66:TYR:CE1	2:E:70:PHE:HE2	2.26	0.53
1:M:346:VAL:HG12	1:M:347:PRO:HD3	1.91	0.53
1:M:362:MET:HB2	1:M:411:LEU:HD21	1.91	0.53
2:E:81:ARG:HG3	2:E:81:ARG:HH11	1.74	0.53
1:G:58:GLN:CB	8:G:502:HEM:HAB	2.38	0.53
1:J:13:THR:HG22	1:J:14:GLY:H	1.73	0.53
2:K:42:MET:CE	2:K:218:ALA:HB1	2.38	0.53
2:Q:77:THR:C	2:Q:79:GLU:H	2.11	0.53
2:Q:144:LYS:HZ3	2:Q:144:LYS:CA	1.97	0.53
1:D:39:ARG:NH1	2:E:255:VAL:CG1	2.72	0.53
1:A:184:PRO:O	3:F:70:LYS:HE3	2.08	0.53
1:G:33:ILE:HG13	1:G:245:TRP:CB	2.39	0.53
2:N:169:CYS:O	2:N:177:THR:HB	2.08	0.53
1:P:199:TYR:CE2	8:P:502:HEM:HBC1	2.44	0.53
2:Q:142:PRO:HB3	2:Q:150:GLU:OE2	2.09	0.53
1:D:199:TYR:CZ	8:D:502:HEM:HBC1	2.43	0.52
1:D:9:TYR:HB2	1:D:30:TYR:CD2	2.44	0.52
2:K:169:CYS:O	2:K:177:THR:HB	2.09	0.52
1:J:428:PHE:CZ	2:K:256:LYS:HD2	2.43	0.52
2:E:40:HIS:ND1	2:E:97:ALA:HB1	2.23	0.52
2:H:128:PRO:HG2	2:H:129:GLU:OE1	2.09	0.52
1:J:346:VAL:HG12	1:J:347:PRO:HD3	1.90	0.52
2:K:77:THR:HG22	2:K:79:GLU:CB	2.40	0.52
1:P:13:THR:HG22	1:P:14:GLY:N	2.23	0.52
1:P:33:ILE:HG13	1:P:245:TRP:CB	2.39	0.52
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.43	0.52
2:E:189:LEU:O	2:E:190:MET:HB2	2.10	0.52
1:J:234:LYS:O	1:J:238:GLN:HG3	2.09	0.52
1:M:13:THR:HG22	1:M:14:GLY:H	1.74	0.52
1:M:352:SER:HB2	1:M:415:GLU:OE2	2.09	0.52
1:A:33:ILE:HG13	1:A:245:TRP:CB	2.39	0.52
2:E:146:ALA:O	2:E:148:GLY:N	2.43	0.52
2:K:74:ASP:HB3	2:K:77:THR:CB	2.29	0.52
1:P:346:VAL:HG12	1:P:347:PRO:HD3	1.90	0.52
3:C:84:LEU:CD2	3:L:84:LEU:HD23	2.39	0.52
1:D:33:ILE:HG13	1:D:245:TRP:CB	2.39	0.52
1:G:217:HIS:NE2	11:G:1103:UQ2:O4	2.36	0.52
1:G:144:PHE:CD1	1:G:162:ILE:HD13	2.43	0.52
1:J:199:TYR:CE2	8:J:502:HEM:HBC1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:33:ILE:HG13	1:M:245:TRP:CB	2.39	0.52
3:C:70:LYS:HG3	1:D:185:ALA:HB2	1.92	0.52
1:D:150:PRO:HG3	8:D:502:HEM:O2D	2.10	0.52
2:E:74:ASP:CB	2:E:77:THR:HB	2.35	0.52
1:J:229:VAL:HG22	1:J:424:ILE:HD12	1.92	0.52
3:O:80:ALA:O	3:O:84:LEU:HG	2.09	0.52
1:P:32:THR:HG23	1:P:217:HIS:HE1	1.74	0.52
1:A:114:ARG:HD2	1:A:114:ARG:C	2.30	0.52
2:B:171:ASP:OD1	2:B:173:ASN:N	2.37	0.52
2:E:250:ARG:CZ	3:F:12:ARG:HG2	2.40	0.52
1:J:269:PHE:HB3	4:K:1044:BGL:H1'2	1.92	0.52
2:K:185:MET:HB2	8:K:301:HEM:C1D	2.45	0.52
1:P:13:THR:HG22	1:P:14:GLY:H	1.74	0.52
1:G:346:VAL:HG12	1:G:347:PRO:HD3	1.91	0.52
1:J:114:ARG:HD2	1:J:114:ARG:C	2.31	0.52
1:J:132:GLY:C	8:J:501:HEM:HBC2	2.31	0.52
1:M:236:GLU:HA	1:M:239:LYS:CD	2.40	0.52
1:M:236:GLU:HA	1:M:239:LYS:HD3	1.92	0.52
1:M:58:GLN:CB	8:M:502:HEM:HAB	2.39	0.52
1:P:114:ARG:C	1:P:114:ARG:HD2	2.31	0.52
1:P:39:ARG:NH1	2:Q:255:VAL:CG1	2.72	0.52
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.91	0.51
2:H:114:MET:O	2:H:114:MET:HG2	2.10	0.51
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.13	0.51
1:J:33:ILE:HG13	1:J:245:TRP:CB	2.39	0.51
1:M:114:ARG:HD2	1:M:114:ARG:C	2.31	0.51
2:N:160:PHE:CE2	2:N:183:ILE:HG13	2.44	0.51
2:E:77:THR:HG22	2:E:79:GLU:HB2	1.92	0.51
1:J:142:THR:HG21	8:J:502:HEM:HBB2	1.92	0.51
1:G:114:ARG:HD2	1:G:114:ARG:C	2.30	0.51
2:B:224:MET:O	2:B:228:GLN:HG3	2.11	0.51
1:G:125:ARG:NE	1:G:222:ASN:HB2	2.25	0.51
2:H:250:ARG:CZ	3:I:12:ARG:HB3	2.40	0.51
1:D:114:ARG:HD2	1:D:114:ARG:C	2.31	0.51
2:E:42:MET:CE	2:E:218:ALA:CB	2.89	0.51
8:D:501:HEM:CMB	8:D:501:HEM:HBB2	2.41	0.51
2:H:169:CYS:O	2:H:177:THR:HB	2.11	0.51
2:K:40:HIS:HE1	2:K:98:PRO:HD2	1.76	0.51
2:K:42:MET:HE1	2:K:218:ALA:CB	2.41	0.51
1:G:125:ARG:HD2	13:G:1118:HOH:O	2.11	0.50
1:M:92:MET:CE	2:N:226:ARG:HG3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:66:TYR:CE1	2:Q:70:PHE:CE2	3.00	0.50
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.44	0.50
2:H:250:ARG:NH1	3:I:12:ARG:CB	2.73	0.50
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.25	0.50
1:M:133:MET:N	8:M:501:HEM:HBC2	2.27	0.50
1:G:5:PRO:HB3	1:G:234:LYS:HG2	1.93	0.50
1:A:383:GLN:HE22	2:B:115:GLY:HA3	1.76	0.50
1:D:91:PHE:CD1	2:E:222:LYS:HG2	2.46	0.50
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.93	0.50
2:N:176:LYS:HD3	2:N:176:LYS:O	2.11	0.50
3:C:57:VAL:HG22	3:C:63:LEU:HD13	1.94	0.50
2:E:66:TYR:CE1	2:E:70:PHE:CE2	2.99	0.50
1:P:312:VAL:HG12	1:P:314:VAL:HG12	1.94	0.50
3:I:70:LYS:HE3	1:J:185:ALA:HB2	1.92	0.50
1:M:125:ARG:NH1	1:M:222:ASN:HB2	2.27	0.50
2:N:149:HIS:CD2	2:N:168:THR:HG21	2.46	0.50
2:Q:236:PHE:CE1	3:R:25:VAL:HG12	2.46	0.50
2:E:42:MET:CE	2:E:218:ALA:HB1	2.42	0.50
2:H:149:HIS:CE1	2:H:168:THR:HG21	2.47	0.50
1:P:11:PRO:HB2	1:P:17:LYS:HG2	1.94	0.50
1:G:236:GLU:HA	1:G:239:LYS:HG3	1.92	0.49
2:H:154:PHE:HB3	2:H:182:TRP:HB3	1.94	0.49
3:L:157:ASP:HB2	13:L:505:HOH:O	2.12	0.49
2:E:40:HIS:CE1	2:E:97:ALA:HB1	2.47	0.49
2:Q:220:GLU:OE2	2:Q:226:ARG:NH1	2.45	0.49
3:R:70:LYS:NZ	3:R:70:LYS:HB2	2.27	0.49
1:G:5:PRO:CB	1:G:234:LYS:HG2	2.42	0.49
1:P:128:THR:HG21	8:P:501:HEM:HBD1	1.94	0.49
1:P:406:VAL:C	1:P:409:PRO:HD2	2.33	0.49
1:J:236:GLU:HA	1:J:239:LYS:CD	2.41	0.49
2:K:236:PHE:CE1	3:L:25:VAL:HG12	2.47	0.49
2:N:143:PRO:HG3	2:N:178:THR:CG2	2.42	0.49
1:P:248:PHE:CD1	1:P:251:LYS:HD3	2.48	0.49
1:P:354:VAL:HG21	1:P:417:PRO:CB	2.42	0.49
3:C:59:PRO:HD3	3:C:76:ARG:NH1	2.28	0.49
2:K:154:PHE:HB3	2:K:182:TRP:HB3	1.94	0.49
2:N:149:HIS:CG	2:N:168:THR:HG21	2.47	0.49
2:Q:151:PRO:HD2	2:Q:182:TRP:CD1	2.47	0.49
1:D:43:TRP:CE3	1:D:43:TRP:HA	2.48	0.49
1:D:92:MET:HE1	2:E:226:ARG:CG	2.41	0.49
1:M:122:LYS:O	1:M:123:ALA:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:ALA:O	1:M:239:LYS:HG3	2.13	0.49
2:N:183:ILE:HG23	2:N:185:MET:N	2.24	0.49
3:F:57:VAL:HG22	3:F:63:LEU:HD13	1.95	0.49
3:R:59:PRO:HD3	3:R:76:ARG:NH1	2.28	0.49
2:K:49:SER:HA	2:K:52:GLU:CG	2.43	0.49
1:G:362:MET:N	1:G:415:GLU:OE2	2.45	0.49
2:K:231:PHE:O	2:K:235:MET:HG2	2.13	0.49
1:D:39:ARG:HH12	2:E:255:VAL:HG12	1.76	0.48
1:P:32:THR:HG23	1:P:217:HIS:CE1	2.48	0.48
1:D:102:SER:O	1:D:106:ILE:HG13	2.13	0.48
2:H:250:ARG:NH1	3:I:16:TYR:CZ	2.81	0.48
1:M:406:VAL:O	1:M:409:PRO:HD2	2.12	0.48
1:D:4:ILE:HD12	1:D:4:ILE:N	2.28	0.48
11:G:1103:UQ2:C8	11:G:1103:UQ2:H5M1	2.43	0.48
3:I:59:PRO:HD3	3:I:76:ARG:NH1	2.28	0.48
2:Q:130:TYR:OH	8:Q:301:HEM:O2A	2.17	0.48
3:R:57:VAL:HG22	3:R:63:LEU:HD13	1.94	0.48
4:G:1043:BGL:H5	2:H:15:GLY:H	1.77	0.48
1:G:125:ARG:CZ	1:G:222:ASN:HB2	2.43	0.48
2:N:184:ALA:HB3	8:N:301:HEM:HBD2	1.95	0.48
2:N:72:VAL:O	2:N:80:ASP:HA	2.13	0.48
2:B:149:HIS:NE2	2:B:168:THR:HG21	2.28	0.48
3:F:47:LEU:O	3:F:47:LEU:CD2	2.61	0.48
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.76	0.48
1:G:105:PHE:HA	1:G:108:VAL:CG2	2.44	0.48
1:G:58:GLN:HB3	8:G:502:HEM:HAB	1.95	0.48
1:J:355:ARG:HG3	1:J:355:ARG:HH11	1.79	0.48
1:J:91:PHE:HE2	1:J:92:MET:CE	2.26	0.48
3:L:57:VAL:HG22	3:L:63:LEU:HD13	1.94	0.48
2:N:154:PHE:HB3	2:N:182:TRP:HB3	1.95	0.48
3:F:90:LEU:HD11	3:F:108:GLU:HB3	1.95	0.48
1:M:51:LEU:HB3	8:M:501:HEM:HMB1	1.96	0.48
2:N:42:MET:CE	2:N:218:ALA:CB	2.91	0.48
2:Q:73:THR:HG23	2:Q:80:ASP:OD1	2.13	0.48
1:G:312:VAL:HG12	1:G:314:VAL:HG12	1.96	0.48
1:M:346:VAL:CG1	1:M:347:PRO:HD3	2.44	0.48
2:E:72:VAL:CG1	2:E:73:THR:N	2.76	0.48
3:I:57:VAL:HG22	3:I:63:LEU:HD13	1.95	0.48
3:L:90:LEU:HD11	3:L:108:GLU:HB3	1.96	0.48
3:L:59:PRO:HD3	3:L:76:ARG:NH1	2.29	0.48
2:N:108:ALA:HA	2:N:125:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:185:MET:HB2	8:Q:301:HEM:C1D	2.49	0.48
2:B:77:THR:C	2:B:79:GLU:H	2.16	0.47
1:D:43:TRP:O	1:D:46:ILE:HG12	2.14	0.47
1:J:51:LEU:HB3	8:J:501:HEM:HMB1	1.96	0.47
3:O:59:PRO:HD3	3:O:76:ARG:NH1	2.29	0.47
1:P:92:MET:HE2	1:P:92:MET:HA	1.96	0.47
2:Q:141:GLU:H	2:Q:141:GLU:HG2	1.49	0.47
2:Q:81:ARG:HG3	2:Q:81:ARG:NH1	2.29	0.47
1:A:236:GLU:HA	1:A:239:LYS:HD3	1.97	0.47
1:G:346:VAL:CG1	1:G:347:PRO:HD3	2.44	0.47
1:M:425:GLU:O	1:M:429:ASN:ND2	2.47	0.47
1:M:4:ILE:H	1:M:4:ILE:CD1	2.24	0.47
1:P:43:TRP:HA	1:P:43:TRP:CE3	2.49	0.47
2:E:142:PRO:CG	2:E:150:GLU:OE2	2.62	0.47
1:D:246:PRO:CG	2:E:251:LEU:HD21	2.41	0.47
3:F:59:PRO:HD3	3:F:76:ARG:NH1	2.30	0.47
1:G:248:PHE:CE1	1:G:251:LYS:HD3	2.48	0.47
3:I:66:LYS:HE2	3:I:69:GLY:HA2	1.96	0.47
1:J:91:PHE:CE2	1:J:92:MET:CE	2.97	0.47
1:P:346:VAL:CG1	1:P:347:PRO:HD3	2.44	0.47
1:A:346:VAL:CG1	1:A:347:PRO:HD3	2.45	0.47
2:E:40:HIS:HE1	2:E:98:PRO:HD2	1.79	0.47
3:I:84:LEU:O	3:I:88:VAL:HG23	2.14	0.47
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.48	0.47
1:M:43:TRP:CZ3	1:M:251:LYS:HE2	2.50	0.47
3:O:57:VAL:HG22	3:O:63:LEU:HD13	1.95	0.47
3:R:62:GLN:NE2	3:R:73:PHE:CD1	2.83	0.47
1:A:360:ARG:O	1:A:364:LYS:HG3	2.14	0.47
2:B:205:HIS:ND1	2:B:205:HIS:C	2.68	0.47
1:M:10:GLU:HA	1:M:11:PRO:HD3	1.70	0.47
1:P:177:GLN:NE2	13:P:611:HOH:O	2.40	0.47
1:A:43:TRP:CZ3	1:A:251:LYS:HE3	2.50	0.47
1:D:346:VAL:CG1	1:D:347:PRO:HD3	2.44	0.47
1:J:407:ILE:O	1:J:411:LEU:HG	2.14	0.47
1:M:113:PHE:HB3	10:M:1025:LOP:H261	1.95	0.47
1:M:92:MET:HE1	2:N:226:ARG:HG3	1.97	0.47
2:Q:236:PHE:CE1	3:R:25:VAL:HG11	2.49	0.47
1:A:199:TYR:CD2	8:A:502:HEM:HBC1	2.50	0.47
1:G:39:ARG:HD3	1:G:428:PHE:CD2	2.50	0.47
1:J:346:VAL:CG1	1:J:347:PRO:HD3	2.44	0.47
1:J:217:HIS:NE2	11:J:1104:UQ2:O4	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:414:ILE:CG2	1:J:414:ILE:O	2.62	0.47
1:A:118:TYR:OH	10:A:1021:LOP:H32	2.15	0.47
1:D:423:THR:OG1	1:D:426:GLU:HB2	2.14	0.47
2:E:77:THR:C	2:E:79:GLU:H	2.17	0.47
2:N:157:ASN:O	2:N:180:GLY:HA3	2.15	0.47
1:J:128:THR:HG21	8:J:501:HEM:HBD1	1.97	0.47
1:M:195:PHE:HE2	1:P:195:PHE:CE2	2.12	0.47
1:M:92:MET:HA	1:M:92:MET:CE	2.45	0.47
2:Q:157:ASN:O	2:Q:180:GLY:HA3	2.15	0.47
2:Q:226:ARG:HD3	13:Q:672:HOH:O	2.14	0.47
1:A:123:ALA:O	1:A:355:ARG:NH1	2.48	0.47
8:A:501:HEM:CBC	8:A:501:HEM:HMC2	2.43	0.47
1:G:43:TRP:HA	1:G:43:TRP:CE3	2.50	0.47
2:E:185:MET:HB2	8:E:301:HEM:C1D	2.50	0.46
2:K:77:THR:HG22	2:K:79:GLU:HG3	1.97	0.46
3:L:66:LYS:HD3	3:L:69:GLY:HA2	1.96	0.46
1:M:30:TYR:HA	1:M:33:ILE:HG22	1.97	0.46
2:N:205:HIS:C	2:N:205:HIS:ND1	2.69	0.46
3:O:47:LEU:HG	3:O:68:LEU:HD21	1.97	0.46
2:E:205:HIS:C	2:E:205:HIS:ND1	2.68	0.46
1:G:30:TYR:HA	1:G:33:ILE:HG22	1.98	0.46
2:H:205:HIS:C	2:H:205:HIS:ND1	2.69	0.46
1:J:30:TYR:HA	1:J:33:ILE:HG22	1.97	0.46
1:M:106:ILE:HG13	1:M:296:TRP:CH2	2.50	0.46
1:M:410:ILE:HG23	1:M:414:ILE:CD1	2.37	0.46
2:Q:145:CYS:O	2:Q:168:THR:OG1	2.26	0.46
1:A:234:LYS:O	1:A:238:GLN:HG3	2.16	0.46
2:B:147:GLU:OE1	2:B:147:GLU:HA	2.14	0.46
2:B:42:MET:CE	2:B:218:ALA:HB1	2.45	0.46
1:A:39:ARG:NH1	2:B:255:VAL:CG1	2.79	0.46
1:G:132:GLY:C	8:G:501:HEM:HBC2	2.35	0.46
1:M:49:VAL:HG21	1:M:252:ASP:OD2	2.15	0.46
2:N:81:ARG:NH1	2:N:84:LYS:HG3	2.30	0.46
4:P:1046:BGL:H5	2:Q:15:GLY:H	1.81	0.46
3:R:39:ASN:HB3	13:R:676:HOH:O	2.14	0.46
1:D:30:TYR:HA	1:D:33:ILE:HG22	1.98	0.46
1:D:269:PHE:HB3	4:E:1042:BGL:O1	2.15	0.46
2:N:155:TYR:CZ	2:N:186:PRO:HB3	2.50	0.46
1:A:30:TYR:HA	1:A:33:ILE:HG22	1.98	0.46
2:B:155:TYR:CZ	2:B:186:PRO:HB3	2.51	0.46
1:J:354:VAL:HG21	1:J:417:PRO:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:VAL:CG1	2:B:169:CYS:HB2	2.46	0.46
1:D:51:LEU:CD2	1:D:108:VAL:HG13	2.46	0.46
1:D:4:ILE:O	1:D:6:HIS:HD2	1.99	0.46
1:G:244:PHE:CE1	11:G:1103:UQ2:H2M2	2.51	0.46
2:H:165:VAL:CG1	2:H:169:CYS:HB2	2.45	0.46
2:K:155:TYR:CZ	2:K:186:PRO:HB3	2.51	0.46
1:M:359:TYR:CD2	1:M:420:PRO:HB3	2.51	0.46
2:B:90:PRO:HA	13:B:1046:HOH:O	2.15	0.46
1:G:111:HIS:CD2	8:G:501:HEM:NC	2.84	0.46
1:G:234:LYS:O	1:G:238:GLN:HG3	2.15	0.46
2:N:194:VAL:HB	2:N:207:MET:HE1	1.94	0.46
2:Q:154:PHE:HB3	2:Q:182:TRP:HB3	1.98	0.46
11:P:1106:UQ2:H5M1	11:P:1106:UQ2:H8	1.98	0.46
2:Q:223:LEU:HD21	2:Q:227:LYS:CE	2.32	0.46
2:E:144:LYS:CA	2:E:144:LYS:HE2	2.46	0.46
1:G:43:TRP:CZ3	1:G:251:LYS:HE3	2.49	0.46
2:H:113:PRO:O	2:H:114:MET:HB3	2.16	0.46
3:I:131:HIS:O	1:J:329:LYS:CE	2.64	0.46
1:J:236:GLU:HA	1:J:239:LYS:HD3	1.98	0.46
1:J:322:SER:O	1:J:323:PHE:HB2	2.16	0.46
2:K:157:ASN:O	2:K:180:GLY:HA3	2.16	0.46
2:K:246:LEU:O	2:K:250:ARG:HG2	2.16	0.46
2:K:77:THR:HG22	2:K:79:GLU:CG	2.46	0.46
1:M:58:GLN:HB3	8:M:502:HEM:HAB	1.96	0.46
2:Q:72:VAL:CG1	2:Q:73:THR:N	2.79	0.46
2:H:149:HIS:CD2	2:H:149:HIS:N	2.83	0.46
2:K:77:THR:CG2	2:K:79:GLU:HB2	2.46	0.46
1:P:92:MET:HE2	1:P:92:MET:CA	2.44	0.46
2:Q:27:ARG:HD2	2:Q:196:TYR:CE2	2.51	0.46
3:C:90:LEU:HB2	2:H:172:ALA:HB1	1.98	0.45
1:P:30:TYR:HA	1:P:33:ILE:HG22	1.98	0.45
2:E:155:TYR:CZ	2:E:186:PRO:HB3	2.51	0.45
2:H:155:TYR:CZ	2:H:186:PRO:HB3	2.51	0.45
1:J:291:HIS:O	1:J:293:VAL:HG23	2.16	0.45
1:P:291:HIS:O	1:P:293:VAL:HG23	2.16	0.45
2:Q:155:TYR:CZ	2:Q:186:PRO:HB3	2.51	0.45
2:Q:205:HIS:ND1	2:Q:205:HIS:C	2.69	0.45
1:A:244:PHE:CE1	11:A:1101:UQ2:H2M3	2.51	0.45
1:A:291:HIS:O	1:A:293:VAL:HG23	2.16	0.45
2:E:145:CYS:O	2:E:168:THR:OG1	2.27	0.45
2:E:40:HIS:HB3	2:E:100:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:205:HIS:C	2:K:205:HIS:ND1	2.68	0.45
2:B:77:THR:HG22	2:B:79:GLU:CG	2.47	0.45
2:E:250:ARG:HG3	2:E:250:ARG:NH1	2.23	0.45
2:E:250:ARG:NH2	3:F:15:LEU:HD22	2.31	0.45
2:H:250:ARG:NH1	3:I:16:TYR:CE1	2.84	0.45
1:M:150:PRO:HG3	8:M:502:HEM:O2D	2.16	0.45
1:P:94:ARG:C	1:P:94:ARG:HD3	2.37	0.45
2:Q:236:PHE:HE1	3:R:25:VAL:HG11	1.81	0.45
1:A:58:GLN:HB3	8:A:502:HEM:HAB	1.98	0.45
2:E:141:GLU:O	2:E:141:GLU:HG3	2.16	0.45
2:E:157:ASN:O	2:E:180:GLY:HA3	2.16	0.45
1:G:418:VAL:CG1	1:G:419:ALA:N	2.80	0.45
1:G:428:PHE:CE1	2:H:256:LYS:HD3	2.51	0.45
2:H:157:ASN:O	2:H:180:GLY:HA3	2.16	0.45
2:H:185:MET:HB2	8:H:301:HEM:C1D	2.52	0.45
1:G:23:LEU:HD13	1:J:215:ALA:HA	1.98	0.45
1:J:209:VAL:HG22	8:J:501:HEM:HBB2	1.98	0.45
1:M:291:HIS:O	1:M:293:VAL:HG23	2.16	0.45
2:N:48:ARG:HB3	2:N:85:PRO:O	2.17	0.45
2:B:77:THR:HG22	2:B:79:GLU:HB2	1.99	0.45
2:H:68:THR:HG23	2:H:82:GLU:OE1	2.16	0.45
1:M:415:GLU:O	1:M:417:PRO:HD3	2.17	0.45
2:N:250:ARG:HH11	3:O:12:ARG:HA	1.80	0.45
2:N:77:THR:CG2	2:N:79:GLU:HB2	2.46	0.45
1:P:118:TYR:OH	10:P:1026:LOP:H32	2.17	0.45
1:D:51:LEU:HD21	1:D:108:VAL:HG13	1.98	0.45
2:H:48:ARG:HB3	2:H:85:PRO:O	2.17	0.45
1:P:162:ILE:CG2	9:P:1006:SMA:H21	2.46	0.45
2:Q:42:MET:HE2	2:Q:218:ALA:CB	2.46	0.45
3:R:142:GLY:HA3	13:R:691:HOH:O	2.16	0.45
2:B:157:ASN:O	2:B:180:GLY:HA3	2.17	0.45
2:B:171:ASP:OD1	2:B:171:ASP:C	2.56	0.45
1:G:13:THR:O	1:G:17:LYS:HG3	2.17	0.45
1:G:291:HIS:O	1:G:293:VAL:HG23	2.16	0.45
2:E:250:ARG:CG	2:E:250:ARG:HH11	2.19	0.45
3:F:118:GLU:CD	3:F:118:GLU:N	2.70	0.45
1:G:118:TYR:OH	10:G:1023:LOP:H32	2.15	0.45
2:H:76:GLU:O	2:H:77:THR:C	2.55	0.45
2:N:42:MET:HE1	2:N:218:ALA:CB	2.47	0.45
2:N:51:SER:OG	2:N:63:VAL:HG21	2.17	0.45
3:O:140:VAL:HG12	3:O:140:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:HIS:O	1:D:293:VAL:HG23	2.16	0.44
1:G:47:TRP:CZ2	1:G:110:LEU:HD13	2.53	0.44
1:P:102:SER:O	1:P:106:ILE:HG13	2.16	0.44
1:G:121:TYR:HB3	1:G:129:TRP:CE3	2.53	0.44
1:G:416:LYS:HA	1:G:416:LYS:HD3	1.63	0.44
1:D:47:TRP:CZ2	1:D:110:LEU:HD13	2.53	0.44
1:G:106:ILE:HD12	10:G:1023:LOP:H212	1.99	0.44
1:A:418:VAL:CG1	1:A:419:ALA:N	2.80	0.44
2:B:223:LEU:CD2	2:B:227:LYS:HD2	2.46	0.44
2:H:138:PHE:CD2	2:H:187:PRO:HG3	2.51	0.44
3:I:14:PHE:O	3:I:17:TYR:HB3	2.17	0.44
1:J:130:ILE:HD11	1:J:348:TRP:CH2	2.46	0.44
1:J:209:VAL:CG2	8:J:501:HEM:HBB2	2.48	0.44
3:R:140:VAL:HG12	3:R:140:VAL:O	2.16	0.44
1:A:47:TRP:CZ2	1:A:110:LEU:HD13	2.53	0.44
1:G:428:PHE:CZ	2:H:256:LYS:HB3	2.52	0.44
1:J:406:VAL:O	1:J:409:PRO:HD2	2.18	0.44
1:M:39:ARG:NH1	2:N:255:VAL:CG1	2.80	0.44
1:P:427:ASP:O	1:P:430:ALA:HB3	2.18	0.44
2:Q:17:PHE:CE1	2:Q:231:PHE:CZ	3.04	0.44
2:K:236:PHE:HE1	3:L:25:VAL:CG1	2.30	0.44
1:P:132:GLY:C	8:P:501:HEM:HBC2	2.38	0.44
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.52	0.44
1:G:133:MET:SD	8:G:501:HEM:HBC1	2.58	0.44
3:O:47:LEU:CD2	3:O:47:LEU:O	2.64	0.44
2:Q:48:ARG:HB3	2:Q:85:PRO:O	2.17	0.44
1:A:8:HIS:CD2	1:A:8:HIS:H	2.36	0.44
2:B:113:PRO:HD2	2:B:118:ILE:HB	1.99	0.44
1:D:49:VAL:HG23	11:D:1102:UQ2:H2M3	1.99	0.44
2:K:144:LYS:HA	2:K:147:GLU:HG3	1.99	0.44
3:L:143:ASP:OD2	3:L:164:LYS:NZ	2.51	0.44
1:M:387:PHE:CE1	1:M:388:PRO:HB3	2.53	0.44
2:N:197:ALA:C	2:N:199:GLY:H	2.22	0.44
2:Q:74:ASP:HB3	2:Q:77:THR:HB	2.00	0.44
1:D:121:TYR:HB3	1:D:129:TRP:CE3	2.53	0.43
2:H:222:LYS:HB2	13:H:347:HOH:O	2.18	0.43
1:M:425:GLU:HG2	1:M:429:ASN:HD21	1.82	0.43
1:A:106:ILE:HD12	10:A:1021:LOP:H212	1.99	0.43
2:B:15:GLY:H	4:B:1041:BGL:H1	1.82	0.43
2:E:113:PRO:HD2	2:E:118:ILE:HB	2.00	0.43
3:I:12:ARG:H	3:I:12:ARG:HG2	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:226:GLY:CA	1:J:355:ARG:HD2	2.49	0.43
2:N:111:HIS:HE1	13:N:552:HOH:O	2.00	0.43
1:P:10:GLU:HA	1:P:11:PRO:HD3	1.69	0.43
1:P:248:PHE:HD1	1:P:251:LYS:HD3	1.82	0.43
3:R:77:ARG:HB3	3:R:81:ASP:HB2	2.00	0.43
1:G:406:VAL:C	1:G:409:PRO:HD2	2.38	0.43
2:H:223:LEU:HD21	2:H:227:LYS:CE	2.49	0.43
1:J:43:TRP:HA	1:J:43:TRP:HE3	1.83	0.43
2:E:34:GLU:OE1	2:E:194:VAL:HG22	2.19	0.43
1:G:92:MET:CE	1:G:92:MET:HA	2.47	0.43
1:J:262:VAL:HG13	4:K:1044:BGL:H8'1	1.99	0.43
2:K:48:ARG:HB3	2:K:85:PRO:O	2.17	0.43
1:P:105:PHE:HA	1:P:108:VAL:CG2	2.48	0.43
1:M:195:PHE:CE2	1:P:195:PHE:HE2	2.12	0.43
8:P:502:HEM:HHD	8:P:502:HEM:CBC	2.48	0.43
3:C:84:LEU:HD23	3:C:84:LEU:HA	1.81	0.43
1:D:355:ARG:CD	13:D:1155:HOH:O	2.66	0.43
3:I:179:ILE:HA	3:I:179:ILE:HD13	1.74	0.43
2:K:141:GLU:HA	2:K:142:PRO:HD3	1.76	0.43
2:K:40:HIS:HB3	2:K:100:LEU:HG	2.00	0.43
1:P:43:TRP:HA	1:P:43:TRP:HE3	1.84	0.43
1:P:44:MET:CE	10:P:1026:LOP:H92	2.48	0.43
3:R:10:THR:O	3:R:14:PHE:HB3	2.18	0.43
3:R:62:GLN:NE2	3:R:73:PHE:CG	2.87	0.43
1:A:92:MET:HE2	1:A:92:MET:HA	2.01	0.43
2:H:141:GLU:HG2	13:H:338:HOH:O	2.19	0.43
2:N:149:HIS:CD2	2:N:168:THR:OG1	2.70	0.43
1:P:359:TYR:CD2	1:P:420:PRO:HB3	2.53	0.43
2:H:77:THR:HG23	2:H:79:GLU:OE2	2.19	0.43
1:J:43:TRP:HA	1:J:43:TRP:CE3	2.54	0.43
11:M:1105:UQ2:H3M3	11:M:1105:UQ2:H2M2	2.01	0.43
1:P:47:TRP:CZ2	1:P:110:LEU:HD13	2.53	0.43
2:Q:144:LYS:NZ	2:Q:147:GLU:OE1	2.51	0.43
2:Q:197:ALA:C	2:Q:199:GLY:H	2.21	0.43
1:A:105:PHE:HA	1:A:108:VAL:CG2	2.45	0.43
2:B:155:TYR:N	2:B:155:TYR:CD1	2.87	0.43
2:B:34:GLU:OE1	2:B:194:VAL:HG22	2.18	0.43
1:J:359:TYR:CD2	1:J:420:PRO:HB3	2.54	0.43
2:K:155:TYR:CD1	2:K:155:TYR:N	2.87	0.43
2:K:165:VAL:CG1	2:K:169:CYS:HB2	2.48	0.43
2:K:42:MET:CE	2:K:218:ALA:CB	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:427:ASP:O	1:M:430:ALA:HB3	2.18	0.43
2:N:74:ASP:CG	2:N:77:THR:HB	2.39	0.43
1:P:360:ARG:O	1:P:364:LYS:HG3	2.19	0.43
1:A:45:TRP:CZ3	1:A:224:PRO:HG3	2.53	0.43
3:C:14:PHE:O	3:C:17:TYR:HB3	2.18	0.43
2:E:144:LYS:HD3	2:E:147:GLU:OE2	2.18	0.43
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.52	0.43
1:G:45:TRP:CZ3	1:G:224:PRO:HG3	2.54	0.43
2:H:155:TYR:CD1	2:H:155:TYR:N	2.87	0.43
1:J:47:TRP:CZ2	1:J:110:LEU:HD13	2.53	0.43
1:J:121:TYR:HB3	1:J:129:TRP:CE3	2.53	0.43
2:K:113:PRO:HD2	2:K:118:ILE:HB	2.01	0.43
3:L:77:ARG:HB3	3:L:81:ASP:HB2	2.01	0.43
1:M:92:MET:HA	1:M:92:MET:HE2	2.00	0.43
1:P:45:TRP:CZ3	1:P:224:PRO:HG3	2.54	0.43
1:A:406:VAL:O	1:A:409:PRO:HD2	2.19	0.43
1:G:306:ARG:NH2	1:G:383:GLN:O	2.40	0.43
1:J:111:HIS:CD2	8:J:501:HEM:NC	2.87	0.43
1:J:45:TRP:CZ3	1:J:224:PRO:HG3	2.54	0.43
1:M:47:TRP:CZ2	1:M:110:LEU:HD13	2.53	0.43
8:M:502:HEM:CMC	8:M:502:HEM:HBC2	2.49	0.43
1:M:6:HIS:C	1:M:6:HIS:ND1	2.71	0.43
2:N:34:GLU:OE1	2:N:194:VAL:HG22	2.19	0.43
3:R:59:PRO:HD3	3:R:76:ARG:HH11	1.83	0.43
1:D:428:PHE:CZ	2:E:256:LYS:HB2	2.53	0.42
8:D:501:HEM:HBC2	8:D:501:HEM:HMC2	2.01	0.42
2:E:155:TYR:N	2:E:155:TYR:CD1	2.86	0.42
2:K:107:ARG:HH21	8:K:301:HEM:CGA	2.32	0.42
3:L:59:PRO:HD3	3:L:76:ARG:HH11	1.84	0.42
1:M:10:GLU:OE2	1:M:11:PRO:HD2	2.19	0.42
1:M:350:ASP:HB2	1:M:408:LEU:HD13	2.01	0.42
2:N:103:MET:C	2:N:105:LYS:H	2.21	0.42
2:B:48:ARG:HB3	2:B:85:PRO:O	2.19	0.42
3:C:138:GLY:O	3:C:141:SER:OG	2.32	0.42
3:C:59:PRO:HD3	3:C:76:ARG:HH11	1.84	0.42
1:D:79:SER:O	1:D:83:ILE:HG13	2.20	0.42
2:H:34:GLU:OE1	2:H:194:VAL:HG22	2.19	0.42
2:Q:34:GLU:OE1	2:Q:194:VAL:HG22	2.19	0.42
2:Q:42:MET:CE	2:Q:218:ALA:CB	2.97	0.42
1:A:79:SER:O	1:A:83:ILE:HG13	2.19	0.42
1:D:133:MET:SD	8:D:501:HEM:HBC1	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:PHE:CD1	2:H:222:LYS:HG2	2.54	0.42
1:M:123:ALA:O	1:M:355:ARG:NH1	2.53	0.42
3:R:124:VAL:O	3:R:173:ILE:HG23	2.19	0.42
2:B:185:MET:HB2	8:B:301:HEM:C1D	2.54	0.42
1:J:112:ILE:HG12	8:J:501:HEM:HAC	2.00	0.42
2:K:197:ALA:C	2:K:199:GLY:H	2.23	0.42
2:K:34:GLU:OE1	2:K:194:VAL:HG22	2.19	0.42
1:M:394:LEU:HA	1:M:394:LEU:HD23	1.89	0.42
3:R:179:ILE:HD13	3:R:179:ILE:HA	1.74	0.42
1:D:236:GLU:HA	1:D:239:LYS:HD2	2.02	0.42
2:H:113:PRO:HD2	2:H:118:ILE:HB	2.00	0.42
3:L:124:VAL:O	3:L:173:ILE:HG23	2.20	0.42
3:O:47:LEU:C	3:O:47:LEU:HD23	2.39	0.42
1:M:121:TYR:HB3	1:M:129:TRP:CE3	2.54	0.42
3:C:179:ILE:CG1	3:C:185:GLN:HE21	2.33	0.42
1:D:45:TRP:CZ3	1:D:224:PRO:HG3	2.54	0.42
2:E:236:PHE:CE2	3:F:25:VAL:CG1	2.95	0.42
1:G:394:LEU:HD23	1:G:394:LEU:HA	1.89	0.42
1:J:418:VAL:CG1	1:J:419:ALA:N	2.83	0.42
2:Q:183:ILE:HG12	2:Q:185:MET:H	1.85	0.42
1:D:39:ARG:NH1	2:E:255:VAL:HG12	2.34	0.42
3:I:59:PRO:HD3	3:I:76:ARG:HH11	1.84	0.42
1:J:4:ILE:HA	1:J:5:PRO:HD3	1.88	0.42
2:N:155:TYR:N	2:N:155:TYR:CD1	2.87	0.42
2:N:250:ARG:NH1	3:O:12:ARG:HA	2.33	0.42
2:N:68:THR:HG23	2:N:82:GLU:HB3	2.01	0.42
1:P:121:TYR:HB3	1:P:129:TRP:CE3	2.54	0.42
2:Q:155:TYR:N	2:Q:155:TYR:CD1	2.87	0.42
3:R:179:ILE:CG1	3:R:185:GLN:HE21	2.33	0.42
1:G:359:TYR:CD2	1:G:420:PRO:HB3	2.55	0.42
1:G:92:MET:CE	2:H:226:ARG:HG3	2.50	0.42
3:L:58:GLU:N	3:L:58:GLU:CD	2.73	0.42
1:M:105:PHE:O	1:M:108:VAL:HG23	2.20	0.42
1:M:239:LYS:HE2	1:M:425:GLU:OE2	2.20	0.42
2:N:94:LEU:HD22	8:N:301:HEM:HAC	2.01	0.42
1:P:234:LYS:O	1:P:238:GLN:HG3	2.19	0.42
1:M:215:ALA:HA	1:P:23:LEU:HD13	2.01	0.42
2:Q:165:VAL:CG1	2:Q:169:CYS:HB2	2.50	0.42
1:A:291:HIS:CE1	2:B:2:GLY:HA2	2.54	0.42
1:D:364:LYS:O	1:D:368:TRP:HD1	2.02	0.42
1:D:406:VAL:C	1:D:409:PRO:HD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:250:ARG:NH1	2:E:250:ARG:CG	2.82	0.42
2:E:30:GLN:HG2	2:E:34:GLU:OE2	2.20	0.42
2:E:76:GLU:O	2:E:77:THR:C	2.57	0.42
3:F:13:ASP:O	3:F:17:TYR:HD2	2.02	0.42
3:F:77:ARG:HB3	3:F:81:ASP:HB2	2.01	0.42
1:G:102:SER:O	1:G:106:ILE:HG13	2.20	0.42
2:H:145:CYS:O	2:H:168:THR:OG1	2.28	0.42
3:I:77:ARG:HB3	3:I:81:ASP:HB2	2.01	0.42
2:K:72:VAL:CG1	2:K:73:THR:N	2.83	0.42
3:L:179:ILE:HA	3:L:179:ILE:HD13	1.74	0.42
1:M:262:VAL:O	1:M:266:ILE:HG12	2.20	0.42
1:M:362:MET:HB3	1:M:411:LEU:HD21	2.02	0.42
1:M:45:TRP:CZ3	1:M:224:PRO:HG3	2.54	0.42
2:N:143:PRO:HG3	2:N:178:THR:HG21	2.02	0.42
3:L:179:ILE:CG1	3:L:185:GLN:HE21	2.33	0.41
1:M:239:LYS:HB3	1:M:425:GLU:OE2	2.20	0.41
1:M:314:VAL:HG23	1:M:314:VAL:H	1.63	0.41
2:N:20:PHE:CB	2:N:25:LEU:HD11	2.48	0.41
1:P:122:LYS:O	1:P:123:ALA:C	2.58	0.41
1:A:355:ARG:HD3	13:A:1122:HOH:O	2.19	0.41
2:B:40:HIS:HB3	2:B:100:LEU:HG	2.02	0.41
3:C:77:ARG:HB3	3:C:81:ASP:HB2	2.02	0.41
2:E:154:PHE:HB3	2:E:182:TRP:HB3	2.01	0.41
2:E:48:ARG:HB3	2:E:85:PRO:O	2.19	0.41
3:F:124:VAL:O	3:F:173:ILE:HG23	2.20	0.41
1:G:39:ARG:HH12	2:H:255:VAL:HG12	1.82	0.41
2:H:141:GLU:HA	2:H:142:PRO:HD3	1.87	0.41
3:I:58:GLU:N	3:I:58:GLU:CD	2.73	0.41
2:N:160:PHE:CG	2:N:183:ILE:HD12	2.55	0.41
3:O:44:VAL:O	3:O:46:ALA:N	2.53	0.41
1:P:394:LEU:HA	1:P:394:LEU:HD23	1.89	0.41
1:D:135:ILE:CG2	8:D:501:HEM:HAB	2.42	0.41
1:D:261:LEU:CD1	2:E:234:VAL:HG13	2.46	0.41
3:I:124:VAL:O	3:I:173:ILE:HG23	2.19	0.41
2:K:48:ARG:HG3	2:K:48:ARG:HH11	1.86	0.41
2:N:94:LEU:CD2	8:N:301:HEM:HAC	2.49	0.41
3:O:58:GLU:N	3:O:58:GLU:CD	2.74	0.41
1:A:111:HIS:CD2	8:A:501:HEM:NC	2.89	0.41
1:A:122:LYS:O	1:A:123:ALA:C	2.59	0.41
1:D:394:LEU:HD23	1:D:394:LEU:HA	1.90	0.41
1:D:408:LEU:HD23	1:D:408:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:162:ILE:HD11	3:I:164:LYS:O	2.21	0.41
1:M:322:SER:O	1:M:325:ILE:HD12	2.21	0.41
2:N:113:PRO:HD2	2:N:118:ILE:HB	2.02	0.41
3:O:124:VAL:O	3:O:173:ILE:HG23	2.20	0.41
1:P:408:LEU:HA	1:P:408:LEU:HD23	1.91	0.41
2:Q:20:PHE:CB	2:Q:25:LEU:HD11	2.48	0.41
3:C:47:LEU:CD2	3:C:47:LEU:O	2.63	0.41
2:E:189:LEU:O	2:E:190:MET:CB	2.68	0.41
2:H:30:GLN:HG2	2:H:34:GLU:OE2	2.20	0.41
2:N:176:LYS:HG2	2:N:178:THR:O	2.19	0.41
3:O:77:ARG:HB3	3:O:81:ASP:HB2	2.01	0.41
1:P:132:GLY:HA3	8:P:501:HEM:HBC2	2.02	0.41
2:Q:149:HIS:CG	2:Q:168:THR:HG21	2.53	0.41
1:D:306:ARG:HG3	13:D:1150:HOH:O	2.19	0.41
1:J:10:GLU:HA	1:J:11:PRO:HD3	1.87	0.41
1:J:262:VAL:O	1:J:266:ILE:HG12	2.21	0.41
2:K:30:GLN:HG2	2:K:34:GLU:OE2	2.21	0.41
2:N:143:PRO:HG3	2:N:178:THR:HG22	2.03	0.41
2:Q:154:PHE:C	2:Q:155:TYR:CD1	2.94	0.41
2:Q:48:ARG:HH11	2:Q:48:ARG:HG3	1.86	0.41
3:R:58:GLU:N	3:R:58:GLU:CD	2.73	0.41
2:H:197:ALA:C	2:H:199:GLY:H	2.23	0.41
1:J:250:ILE:HD12	2:K:251:LEU:CD2	2.51	0.41
1:J:199:TYR:CG	8:J:502:HEM:HBC1	2.56	0.41
2:N:42:MET:HE2	2:N:218:ALA:CB	2.51	0.41
3:O:162:ILE:HD11	3:O:164:LYS:O	2.20	0.41
1:P:354:VAL:HG21	1:P:417:PRO:HB2	2.03	0.41
2:Q:242:VAL:O	2:Q:246:LEU:HG	2.21	0.41
2:Q:30:GLN:HG2	2:Q:34:GLU:OE2	2.21	0.41
1:A:239:LYS:HE2	1:A:425:GLU:OE1	2.21	0.41
3:F:58:GLU:CD	3:F:58:GLU:N	2.74	0.41
1:G:51:LEU:HB3	8:G:501:HEM:HMB1	2.03	0.41
1:J:122:LYS:O	1:J:123:ALA:C	2.59	0.41
1:J:133:MET:N	8:J:501:HEM:HBC2	2.36	0.41
1:J:43:TRP:CZ3	1:J:251:LYS:HD3	2.55	0.41
1:J:64:VAL:HG11	1:J:93:LEU:HD13	2.02	0.41
2:N:48:ARG:HH11	2:N:48:ARG:HG3	1.86	0.41
3:O:54:VAL:O	3:O:54:VAL:HG13	2.20	0.41
2:B:30:GLN:HG2	2:B:34:GLU:OE2	2.20	0.41
2:B:77:THR:HG22	2:B:79:GLU:HG3	2.02	0.41
1:D:250:ILE:HD12	2:E:251:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:GLU:OE1	2:H:129:GLU:N	2.42	0.41
1:J:51:LEU:HD13	8:J:501:HEM:C3B	2.55	0.41
2:K:189:LEU:O	2:K:190:MET:CB	2.69	0.41
3:L:171:LEU:HA	3:L:172:PRO:HD3	1.95	0.41
1:M:64:VAL:HG11	1:M:93:LEU:HD13	2.03	0.41
1:P:130:ILE:HD11	1:P:348:TRP:CH2	2.47	0.41
1:A:130:ILE:HD11	1:A:348:TRP:CH2	2.46	0.41
3:C:124:VAL:O	3:C:173:ILE:HG23	2.21	0.41
3:C:58:GLU:CD	3:C:58:GLU:N	2.73	0.41
2:H:223:LEU:HD21	2:H:227:LYS:HE3	2.03	0.41
1:M:75:LEU:O	1:M:79:SER:HB3	2.21	0.41
2:N:40:HIS:HB3	2:N:100:LEU:HG	2.02	0.41
2:Q:77:THR:C	2:Q:79:GLU:N	2.73	0.41
1:A:193:ARG:NH1	3:F:38:MET:HG2	2.36	0.41
2:B:154:PHE:C	2:B:155:TYR:CD1	2.94	0.41
2:B:77:THR:HG22	2:B:79:GLU:CB	2.51	0.41
2:E:61:ASP:N	2:E:61:ASP:OD1	2.53	0.41
3:F:54:VAL:O	3:F:54:VAL:HG13	2.20	0.41
1:G:75:LEU:O	1:G:79:SER:HB3	2.21	0.41
2:H:74:ASP:CB	2:H:77:THR:HB	2.51	0.41
3:I:179:ILE:CG1	3:I:185:GLN:HE21	2.33	0.41
1:J:425:GLU:HG3	1:J:429:ASN:ND2	2.33	0.41
2:N:154:PHE:C	2:N:155:TYR:CD1	2.94	0.41
2:N:242:VAL:O	2:N:246:LEU:HG	2.21	0.41
1:P:287:ARG:NH1	1:P:287:ARG:CG	2.83	0.41
1:P:43:TRP:O	1:P:46:ILE:HG12	2.20	0.41
2:Q:113:PRO:HD2	2:Q:118:ILE:HB	2.03	0.41
1:A:64:VAL:HG11	1:A:93:LEU:HD13	2.02	0.40
2:B:154:PHE:HB3	2:B:182:TRP:HB3	2.03	0.40
1:D:236:GLU:O	1:D:239:LYS:HB2	2.20	0.40
1:G:125:ARG:HH21	1:G:221:ASN:C	2.23	0.40
1:G:43:TRP:O	1:G:46:ILE:HG12	2.22	0.40
1:G:92:MET:HE1	2:H:226:ARG:HG3	2.03	0.40
2:H:40:HIS:HB3	2:H:100:LEU:HG	2.03	0.40
2:H:250:ARG:NH2	3:I:12:ARG:HB2	2.35	0.40
1:M:106:ILE:HG13	1:M:296:TRP:CZ2	2.56	0.40
2:N:152:ASP:OD1	2:N:152:ASP:C	2.59	0.40
3:O:179:ILE:CG1	3:O:185:GLN:HE21	2.33	0.40
3:O:59:PRO:HD3	3:O:76:ARG:HH11	1.85	0.40
3:O:93:LEU:HB3	13:O:574:HOH:O	2.20	0.40
2:Q:108:ALA:HA	2:Q:125:ILE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:156:TYR:HA	3:R:161:ARG:O	2.21	0.40
2:B:197:ALA:C	2:B:199:GLY:H	2.24	0.40
1:D:64:VAL:HG11	1:D:93:LEU:HD13	2.02	0.40
2:E:154:PHE:C	2:E:155:TYR:CD1	2.94	0.40
3:F:59:PRO:HD3	3:F:76:ARG:HH11	1.86	0.40
1:M:286:LEU:HD21	3:R:66:LYS:HB2	2.04	0.40
2:Q:143:PRO:HG3	2:Q:178:THR:CG2	2.52	0.40
1:D:75:LEU:O	1:D:79:SER:HB3	2.21	0.40
2:E:146:ALA:O	2:E:147:GLU:C	2.59	0.40
3:F:155:HIS:CD2	3:F:164:LYS:HD3	2.56	0.40
3:F:179:ILE:CG1	3:F:185:GLN:HE21	2.33	0.40
1:G:130:ILE:HD11	1:G:348:TRP:CH2	2.46	0.40
1:G:79:SER:O	1:G:83:ILE:HG13	2.21	0.40
2:H:203:SER:O	2:H:204:VAL:C	2.60	0.40
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.44	0.40
1:J:43:TRP:HH2	1:J:251:LYS:HG2	1.86	0.40
2:K:154:PHE:C	2:K:155:TYR:CD1	2.94	0.40
1:M:122:LYS:HZ1	1:M:360:ARG:NH1	2.19	0.40
2:N:30:GLN:HG2	2:N:34:GLU:OE2	2.21	0.40
3:O:70:LYS:HB3	3:O:71:PRO:HD2	2.02	0.40
1:A:394:LEU:HA	1:A:394:LEU:HD23	1.90	0.40
2:B:113:PRO:O	2:B:114:MET:HB2	2.21	0.40
2:E:203:SER:O	2:E:204:VAL:C	2.60	0.40
1:J:6:HIS:ND1	1:J:6:HIS:C	2.75	0.40
3:L:118:GLU:CD	3:L:118:GLU:N	2.75	0.40
2:Q:65:ALA:O	2:Q:68:THR:HB	2.22	0.40
1:D:414:ILE:HG23	1:D:414:ILE:O	2.22	0.40
2:E:141:GLU:HA	2:E:142:PRO:HD3	1.77	0.40
2:E:197:ALA:C	2:E:199:GLY:H	2.23	0.40
2:E:250:ARG:HD3	3:F:12:ARG:CG	2.51	0.40
2:H:154:PHE:C	2:H:155:TYR:CD1	2.95	0.40
1:J:394:LEU:HA	1:J:394:LEU:HD23	1.90	0.40
1:J:423:THR:OG1	1:J:426:GLU:HB2	2.22	0.40
2:K:113:PRO:O	2:K:114:MET:HB3	2.21	0.40
2:K:137:GLY:O	2:K:139:PRO:HD3	2.20	0.40
3:L:100:ASN:HA	3:L:173:ILE:HB	2.03	0.40
2:N:65:ALA:O	2:N:68:THR:HB	2.22	0.40
2:N:40:HIS:HD1	2:N:97:ALA:HB1	1.83	0.40
1:P:75:LEU:O	1:P:79:SER:HB3	2.21	0.40
2:Q:141:GLU:HA	2:Q:142:PRO:HD3	1.88	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	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	D	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
1	G	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	J	426/445 (96%)	407 (96%)	18 (4%)	1 (0%)	51	67
1	M	426/445 (96%)	407 (96%)	19 (4%)	0	100	100
1	P	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
2	B	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	15	21
2	E	254/269 (94%)	231 (91%)	20 (8%)	3 (1%)	15	21
2	H	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	15	21
2	K	254/269 (94%)	231 (91%)	18 (7%)	5 (2%)	9	10
2	N	254/269 (94%)	229 (90%)	20 (8%)	5 (2%)	9	10
2	Q	254/269 (94%)	231 (91%)	21 (8%)	2 (1%)	22	33
3	C	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	28	41
3	F	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	28	41
3	I	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	11	13
3	L	177/187 (95%)	161 (91%)	14 (8%)	2 (1%)	17	23
3	O	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	11	13
3	R	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	28	41
All	All	5142/5406 (95%)	4817 (94%)	292 (6%)	33 (1%)	28	41

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	GLU
2	E	147	GLU
2	E	190	MET
2	H	77	THR

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Mol	Chain	Res	Type
2	H	147	GLU
2	K	147	GLU
2	K	190	MET
2	N	147	GLU
2	Q	147	GLU
2	B	198	ASP
2	E	198	ASP
2	H	198	ASP
2	K	198	ASP
2	N	198	ASP
2	Q	198	ASP
2	B	190	MET
3	C	109	ALA
3	F	109	ALA
3	I	109	ALA
1	J	43	TRP
3	L	109	ALA
2	N	75	GLU
3	O	109	ALA
3	R	109	ALA
3	I	45	GLN
2	K	145	CYS
3	O	45	GLN
2	N	104	ALA
3	O	90	LEU
3	I	140	VAL
2	K	255	VAL
2	N	255	VAL
3	L	140	VAL

### 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	353/366 (96%)	338 (96%)	15 (4%)	34	53
1	D	353/366 (96%)	345 (98%)	8 (2%)	56	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	353/366 (96%)	343 (97%)	10 (3%)	49	70
1	J	353/366 (96%)	342 (97%)	11 (3%)	45	66
1	M	353/366 (96%)	340 (96%)	13 (4%)	39	59
1	P	353/366 (96%)	341 (97%)	12 (3%)	42	63
2	B	203/215 (94%)	191 (94%)	12 (6%)	23	36
2	E	203/215 (94%)	193 (95%)	10 (5%)	29	46
2	H	203/215 (94%)	197 (97%)	6 (3%)	46	67
2	K	203/215 (94%)	192 (95%)	11 (5%)	26	41
2	N	203/215 (94%)	194 (96%)	9 (4%)	33	51
2	Q	203/215 (94%)	193 (95%)	10 (5%)	29	46
3	C	138/144 (96%)	133 (96%)	5 (4%)	40	60
3	F	138/144 (96%)	131 (95%)	7 (5%)	28	44
3	I	138/144 (96%)	132 (96%)	6 (4%)	33	52
3	L	138/144 (96%)	133 (96%)	5 (4%)	40	60
3	O	138/144 (96%)	131 (95%)	7 (5%)	28	44
3	R	138/144 (96%)	133 (96%)	5 (4%)	40	60
All	All	4164/4350 (96%)	4002 (96%)	162 (4%)	37	56

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	HIS
1	A	79	SER
1	A	92	MET
1	A	94	ARG
1	A	104	PHE
1	A	108	VAL
1	A	137	LEU
1	A	192	ASN
1	A	199	TYR
1	A	217	HIS
1	A	246	PRO
1	A	314	VAL
1	A	380	VAL
1	A	414	ILE

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Mol	Chain	Res	Type
2	B	61	ASP
2	B	80	ASP
2	B	95	GLU
2	B	136	THR
2	B	147	GLU
2	B	149	HIS
2	B	167	ASP
2	B	168	THR
2	B	177	THR
2	B	188	PRO
2	B	191	ASP
2	B	201	ASP
3	C	47	LEU
3	C	72	ILE
3	C	112	GLN
3	C	174	PRO
3	C	179	ILE
1	D	79	SER
1	D	94	ARG
1	D	104	PHE
1	D	192	ASN
1	D	199	TYR
1	D	246	PRO
1	D	380	VAL
1	D	414	ILE
2	E	43	LYS
2	E	61	ASP
2	E	76	GLU
2	E	82	GLU
2	E	136	THR
2	E	152	ASP
2	E	168	THR
2	E	177	THR
2	E	191	ASP
2	E	201	ASP
3	F	47	LEU
3	F	72	ILE
3	F	112	GLN
3	F	118	GLU
3	F	174	PRO
3	F	177	LYS
3	F	179	ILE

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Mol	Chain	Res	Type
1	G	79	SER
1	G	92	MET
1	G	94	ARG
1	G	104	PHE
1	G	108	VAL
1	G	192	ASN
1	G	199	TYR
1	G	246	PRO
1	G	380	VAL
1	G	421	PRO
2	H	136	THR
2	H	147	GLU
2	H	168	THR
2	H	177	THR
2	H	191	ASP
2	H	201	ASP
3	I	47	LEU
3	I	72	ILE
3	I	83	GLU
3	I	112	GLN
3	I	174	PRO
3	I	179	ILE
1	J	43	TRP
1	J	79	SER
1	J	94	ARG
1	J	104	PHE
1	J	108	VAL
1	J	192	ASN
1	J	199	TYR
1	J	217	HIS
1	J	246	PRO
1	J	380	VAL
1	J	425	GLU
2	K	52	GLU
2	K	61	ASP
2	K	80	ASP
2	K	136	THR
2	K	168	THR
2	K	171	ASP
2	K	177	THR
2	K	181	SER
2	K	191	ASP

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Mol	Chain	Res	Type
2	K	195	GLU
2	K	201	ASP
3	L	14	PHE
3	L	72	ILE
3	L	112	GLN
3	L	174	PRO
3	L	179	ILE
1	M	6	HIS
1	M	8	HIS
1	M	79	SER
1	M	92	MET
1	M	94	ARG
1	M	104	PHE
1	M	108	VAL
1	M	162	ILE
1	M	192	ASN
1	M	199	TYR
1	M	246	PRO
1	M	287	ARG
1	M	380	VAL
2	N	72	VAL
2	N	77	THR
2	N	136	THR
2	N	149	HIS
2	N	167	ASP
2	N	168	THR
2	N	176	LYS
2	N	177	THR
2	N	191	ASP
3	O	14	PHE
3	O	17	TYR
3	O	70	LYS
3	O	72	ILE
3	O	112	GLN
3	O	174	PRO
3	O	179	ILE
1	P	8	HIS
1	P	10	GLU
1	P	79	SER
1	P	92	MET
1	P	94	ARG
1	P	104	PHE

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Mol	Chain	Res	Type
1	P	108	VAL
1	P	192	ASN
1	P	199	TYR
1	P	246	PRO
1	P	380	VAL
1	P	421	PRO
2	Q	14	GLU
2	Q	71	THR
2	Q	73	THR
2	Q	80	ASP
2	Q	136	THR
2	Q	144	LYS
2	Q	158	ARG
2	Q	168	THR
2	Q	177	THR
2	Q	191	ASP
3	R	47	LEU
3	R	72	ILE
3	R	112	GLN
3	R	174	PRO
3	R	179	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	192	ASN
1	A	383	GLN
1	A	429	ASN
2	B	22	GLN
2	B	62	GLN
2	B	149	HIS
2	B	228	GLN
3	C	36	ASN
3	C	39	ASN
3	C	112	GLN
3	C	185	GLN
1	D	6	HIS
1	D	192	ASN
1	D	383	GLN
2	E	5	HIS
2	E	22	GLN

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Mol	Chain	Res	Type
2	E	62	GLN
2	E	149	HIS
2	E	228	GLN
3	F	36	ASN
3	F	39	ASN
3	F	45	GLN
3	F	89	GLN
3	F	112	GLN
3	F	185	GLN
1	G	192	ASN
1	G	383	GLN
2	H	22	GLN
2	H	62	GLN
2	H	149	HIS
3	I	36	ASN
3	I	39	ASN
3	I	112	GLN
3	I	185	GLN
1	J	177	GLN
1	J	192	ASN
1	J	221	ASN
1	J	429	ASN
2	K	22	GLN
2	K	62	GLN
2	K	149	HIS
2	K	228	GLN
3	L	36	ASN
3	L	39	ASN
3	L	112	GLN
3	L	185	GLN
1	M	8	HIS
1	M	177	GLN
1	M	192	ASN
1	M	221	ASN
1	M	383	GLN
1	M	429	ASN
2	N	22	GLN
2	N	62	GLN
2	N	149	HIS
2	N	228	GLN
3	O	36	ASN
3	O	39	ASN

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Mol	Chain	Res	Type
3	O	112	GLN
3	O	185	GLN
1	P	8	HIS
1	P	192	ASN
1	P	221	ASN
1	P	383	GLN
2	Q	22	GLN
2	Q	62	GLN
2	Q	149	HIS
2	Q	228	GLN
3	R	36	ASN
3	R	39	ASN
3	R	112	GLN
3	R	185	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 12 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SMA	A	1001	-	36,38,38	1.92	5 (13%)	44,52,52	2.02	8 (18%)
10	LOP	A	1021	-	44,44,44	0.61	0	46,49,49	1.16	6 (13%)
11	UQ2	A	1101	-	23,23,23	1.49	4 (17%)	28,31,31	1.09	2 (7%)
8	HEM	A	501	1	28,50,50	1.59	6 (21%)	17,82,82	1.12	0
8	HEM	A	502	1	28,50,50	1.88	8 (28%)	17,82,82	1.04	0
4	BGL	B	1041	-	20,20,20	1.08	1 (5%)	23,25,25	0.87	1 (4%)
8	HEM	B	301	2	28,50,50	1.81	6 (21%)	17,82,82	1.02	0
12	FES	C	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	D	1002	-	36,38,38	1.85	6 (16%)	44,52,52	2.00	10 (22%)
10	LOP	D	1022	-	44,44,44	0.70	0	46,49,49	1.17	4 (8%)
11	UQ2	D	1102	-	23,23,23	1.35	5 (21%)	28,31,31	1.11	2 (7%)
8	HEM	D	501	1	28,50,50	1.50	5 (17%)	17,82,82	1.10	1 (5%)
8	HEM	D	502	1	28,50,50	1.72	6 (21%)	17,82,82	1.06	0
4	BGL	E	1042	-	20,20,20	1.05	1 (5%)	23,25,25	0.94	1 (4%)
8	HEM	E	301	2	28,50,50	1.72	7 (25%)	17,82,82	1.00	0
12	FES	F	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	G	1003	-	36,38,38	1.88	6 (16%)	44,52,52	1.97	10 (22%)
10	LOP	G	1023	-	44,44,44	0.70	0	46,49,49	1.16	4 (8%)
4	BGL	G	1043	-	20,20,20	1.36	2 (10%)	23,25,25	0.76	0
11	UQ2	G	1103	-	23,23,23	1.43	5 (21%)	28,31,31	1.01	1 (3%)
8	HEM	G	501	1	28,50,50	1.67	6 (21%)	17,82,82	0.90	0
8	HEM	G	502	1	28,50,50	1.89	6 (21%)	17,82,82	1.07	0
8	HEM	H	301	2	28,50,50	1.75	9 (32%)	17,82,82	1.19	1 (5%)
12	FES	I	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	J	1004	-	36,38,38	1.82	5 (13%)	44,52,52	1.90	8 (18%)
10	LOP	J	1024	-	44,44,44	0.63	0	46,49,49	1.25	6 (13%)
11	UQ2	J	1104	-	23,23,23	1.24	3 (13%)	28,31,31	1.07	1 (3%)
8	HEM	J	501	1	28,50,50	1.83	9 (32%)	17,82,82	0.91	0
8	HEM	J	502	1	28,50,50	1.92	7 (25%)	17,82,82	1.01	0
4	BGL	K	1044	-	20,20,20	1.04	2 (10%)	23,25,25	1.08	2 (8%)
8	HEM	K	301	2	28,50,50	1.78	9 (32%)	17,82,82	1.06	0
12	FES	L	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	M	1005	-	36,38,38	1.94	5 (13%)	44,52,52	2.01	10 (22%)
10	LOP	M	1025	-	44,44,44	0.66	0	46,49,49	1.14	4 (8%)
11	UQ2	M	1105	-	23,23,23	1.46	4 (17%)	28,31,31	1.08	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	HEM	M	501	1	28,50,50	1.71	8 (28%)	17,82,82	0.97	0
8	HEM	M	502	1	28,50,50	1.75	7 (25%)	17,82,82	1.02	0
4	BGL	N	1045	-	20,20,20	1.37	2 (10%)	23,25,25	0.74	0
8	HEM	N	301	2	28,50,50	1.80	7 (25%)	17,82,82	1.01	0
12	FES	O	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	P	1006	-	36,38,38	1.87	8 (22%)	44,52,52	2.25	15 (34%)
10	LOP	P	1026	-	44,44,44	0.60	0	46,49,49	1.18	5 (10%)
4	BGL	P	1046	-	20,20,20	1.21	1 (5%)	23,25,25	0.92	1 (4%)
11	UQ2	P	1106	-	23,23,23	1.55	5 (21%)	28,31,31	1.13	3 (10%)
8	HEM	P	501	1	28,50,50	1.78	8 (28%)	17,82,82	0.90	0
8	HEM	P	502	1	28,50,50	1.83	6 (21%)	17,82,82	1.16	0
8	HEM	Q	301	2	28,50,50	1.67	5 (17%)	17,82,82	1.05	0
12	FES	R	200	3	0,4,4	0.00	-	0,4,4	0.00	-

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
9	SMA	A	1001	-	-	0/33/34/34	0/2/2/2
10	LOP	A	1021	-	-	0/48/48/48	0/0/0/0
11	UQ2	A	1101	-	-	0/15/39/39	0/1/1/1
8	HEM	A	501	1	-	0/6/54/54	0/0/8/8
8	HEM	A	502	1	-	0/6/54/54	0/0/8/8
4	BGL	B	1041	-	-	0/11/31/31	0/1/1/1
8	HEM	B	301	2	-	0/6/54/54	0/0/8/8
12	FES	C	200	3	-	0/0/4/4	0/1/1/1
9	SMA	D	1002	-	-	0/33/34/34	0/2/2/2
10	LOP	D	1022	-	-	0/48/48/48	0/0/0/0
11	UQ2	D	1102	-	-	0/15/39/39	0/1/1/1
8	HEM	D	501	1	-	0/6/54/54	0/0/8/8
8	HEM	D	502	1	-	0/6/54/54	0/0/8/8
4	BGL	E	1042	-	-	0/11/31/31	0/1/1/1
8	HEM	E	301	2	-	0/6/54/54	0/0/8/8
12	FES	F	200	3	-	0/0/4/4	0/1/1/1
9	SMA	G	1003	-	-	0/33/34/34	0/2/2/2
10	LOP	G	1023	-	-	0/48/48/48	0/0/0/0
4	BGL	G	1043	-	-	0/11/31/31	0/1/1/1
11	UQ2	G	1103	-	-	0/15/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	G	501	1	-	0/6/54/54	0/0/8/8
8	HEM	G	502	1	-	0/6/54/54	0/0/8/8
8	HEM	H	301	2	-	0/6/54/54	0/0/8/8
12	FES	I	200	3	-	0/0/4/4	0/1/1/1
9	SMA	J	1004	-	-	0/33/34/34	0/2/2/2
10	LOP	J	1024	-	-	0/48/48/48	0/0/0/0
11	UQ2	J	1104	-	-	0/15/39/39	0/1/1/1
8	HEM	J	501	1	-	0/6/54/54	0/0/8/8
8	HEM	J	502	1	-	0/6/54/54	0/0/8/8
4	BGL	K	1044	-	-	0/11/31/31	0/1/1/1
8	HEM	K	301	2	-	0/6/54/54	0/0/8/8
12	FES	L	200	3	-	0/0/4/4	0/1/1/1
9	SMA	M	1005	-	-	0/33/34/34	0/2/2/2
10	LOP	M	1025	-	-	0/48/48/48	0/0/0/0
11	UQ2	M	1105	-	-	0/15/39/39	0/1/1/1
8	HEM	M	501	1	-	0/6/54/54	0/0/8/8
8	HEM	M	502	1	-	0/6/54/54	0/0/8/8
4	BGL	N	1045	-	-	0/11/31/31	0/1/1/1
8	HEM	N	301	2	-	0/6/54/54	0/0/8/8
12	FES	O	200	3	-	0/0/4/4	0/1/1/1
9	SMA	P	1006	-	-	0/33/34/34	0/2/2/2
10	LOP	P	1026	-	-	0/48/48/48	0/0/0/0
4	BGL	P	1046	-	-	0/11/31/31	0/1/1/1
11	UQ2	P	1106	-	-	0/15/39/39	0/1/1/1
8	HEM	P	501	1	-	0/6/54/54	0/0/8/8
8	HEM	P	502	1	-	0/6/54/54	0/0/8/8
8	HEM	Q	301	2	-	0/6/54/54	0/0/8/8
12	FES	R	200	3	-	0/0/4/4	0/1/1/1

All (195) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	502	HEM	C3C-CAC	-5.64	1.36	1.47
8	G	502	HEM	C3C-CAC	-4.41	1.38	1.47
8	N	301	HEM	C3C-CAC	-4.40	1.39	1.47
8	P	502	HEM	C3C-C2C	-4.12	1.34	1.40
8	G	502	HEM	C3C-C2C	-4.11	1.34	1.40
8	A	502	HEM	C3B-CAB	-4.06	1.39	1.47
8	J	501	HEM	C3B-CAB	-4.03	1.39	1.47
8	M	502	HEM	C3B-CAB	-4.00	1.39	1.47
8	B	301	HEM	C3C-CAC	-3.88	1.40	1.47
8	G	502	HEM	C3B-C2B	-3.76	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	502	HEM	C3C-CAC	-3.60	1.40	1.47
8	Q	301	HEM	C3B-CAB	-3.59	1.40	1.47
8	A	501	HEM	C3B-CAB	-3.56	1.40	1.47
8	B	301	HEM	C3B-CAB	-3.52	1.40	1.47
8	M	502	HEM	C3B-C2B	-3.51	1.35	1.40
8	A	502	HEM	C3C-C2C	-3.49	1.35	1.40
8	J	502	HEM	C3B-CAB	-3.47	1.41	1.47
8	M	501	HEM	C3B-CAB	-3.41	1.41	1.47
8	D	502	HEM	C3B-C2B	-3.41	1.35	1.40
8	D	502	HEM	C3C-CAC	-3.41	1.40	1.47
9	D	1002	SMA	C7-C8	-3.39	1.35	1.40
8	M	501	HEM	C3C-CAC	-3.37	1.41	1.47
8	E	301	HEM	C3C-CAC	-3.35	1.41	1.47
8	A	502	HEM	C3B-C2B	-3.28	1.36	1.40
8	G	502	HEM	C3B-CAB	-3.21	1.41	1.47
8	D	502	HEM	C3B-CAB	-3.20	1.41	1.47
8	P	501	HEM	C3C-CAC	-3.20	1.41	1.47
8	M	502	HEM	C3C-CAC	-3.17	1.41	1.47
8	J	502	HEM	C3C-C2C	-3.17	1.36	1.40
8	P	501	HEM	C3B-CAB	-3.16	1.41	1.47
8	H	301	HEM	C3C-CAC	-3.15	1.41	1.47
8	J	501	HEM	C3B-C2B	-3.07	1.36	1.40
8	P	501	HEM	C3C-C2C	-3.06	1.36	1.40
8	G	501	HEM	C3B-CAB	-3.04	1.41	1.47
8	K	301	HEM	C3C-CAC	-3.03	1.41	1.47
8	E	301	HEM	C3B-CAB	-3.03	1.41	1.47
9	P	1006	SMA	C7-C8	-3.01	1.36	1.40
8	B	301	HEM	C3B-C2B	-2.99	1.36	1.40
8	J	501	HEM	C3C-CAC	-2.98	1.41	1.47
8	G	501	HEM	C3C-CAC	-2.93	1.41	1.47
8	H	301	HEM	C3B-CAB	-2.92	1.42	1.47
8	H	301	HEM	C3B-C2B	-2.92	1.36	1.40
8	P	502	HEM	C3B-CAB	-2.82	1.42	1.47
8	D	501	HEM	C3B-CAB	-2.82	1.42	1.47
8	K	301	HEM	C3B-C2B	-2.80	1.36	1.40
8	G	501	HEM	C3B-C2B	-2.76	1.36	1.40
8	Q	301	HEM	C3C-CAC	-2.71	1.42	1.47
8	N	301	HEM	C3B-CAB	-2.68	1.42	1.47
8	A	502	HEM	C3C-CAC	-2.65	1.42	1.47
8	J	501	HEM	C3C-C2C	-2.64	1.36	1.40
8	M	501	HEM	C3B-C2B	-2.61	1.36	1.40
9	J	1004	SMA	C7-C8	-2.59	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	502	HEM	C3B-C2B	-2.58	1.36	1.40
9	G	1003	SMA	C7-C8	-2.57	1.37	1.40
8	N	301	HEM	C3B-C2B	-2.56	1.37	1.40
8	E	301	HEM	C3B-C2B	-2.54	1.37	1.40
8	D	501	HEM	C3C-CAC	-2.52	1.42	1.47
8	K	301	HEM	C3B-CAB	-2.50	1.42	1.47
8	M	501	HEM	C3C-C2C	-2.47	1.37	1.40
8	E	301	HEM	C3C-C2C	-2.43	1.37	1.40
8	N	301	HEM	C3C-C2C	-2.40	1.37	1.40
9	M	1005	SMA	C7-C8	-2.39	1.37	1.40
8	B	301	HEM	C3C-C2C	-2.36	1.37	1.40
9	A	1001	SMA	C7-C8	-2.35	1.37	1.40
8	A	501	HEM	C3C-CAC	-2.28	1.43	1.47
8	H	301	HEM	C3C-C2C	-2.22	1.37	1.40
8	Q	301	HEM	C3B-C2B	-2.07	1.37	1.40
8	K	301	HEM	C3C-C2C	-2.03	1.37	1.40
8	K	301	HEM	C4C-NC	2.01	1.39	1.36
4	G	1043	BGL	O5-C1	2.03	1.46	1.43
9	G	1003	SMA	O12-C12	2.04	1.48	1.42
8	A	501	HEM	C4D-ND	2.05	1.39	1.36
9	P	1006	SMA	O5-C5M	2.05	1.48	1.42
9	P	1006	SMA	O1-C8A	2.08	1.40	1.36
9	A	1001	SMA	O1-C2	2.08	1.38	1.35
11	J	1104	UQ2	O3-C3	2.10	1.42	1.36
8	J	501	HEM	C1C-NC	2.12	1.39	1.36
8	H	301	HEM	C1B-NB	2.12	1.39	1.36
8	H	301	HEM	C1C-NC	2.13	1.39	1.36
4	K	1044	BGL	O5-C1	2.14	1.47	1.43
9	J	1004	SMA	O1-C2	2.14	1.38	1.35
8	M	501	HEM	C1C-NC	2.14	1.39	1.36
8	P	501	HEM	C1C-NC	2.14	1.39	1.36
11	D	1102	UQ2	C7-C6	2.16	1.55	1.51
9	P	1006	SMA	O12-C12	2.17	1.48	1.42
11	P	1106	UQ2	O2-C2	2.18	1.42	1.36
8	J	501	HEM	C4D-ND	2.18	1.39	1.36
8	J	501	HEM	C4C-NC	2.19	1.39	1.36
8	M	502	HEM	C1B-NB	2.20	1.39	1.36
9	D	1002	SMA	O12-C12	2.20	1.48	1.42
8	D	501	HEM	C1B-NB	2.21	1.39	1.36
8	M	501	HEM	C4C-NC	2.22	1.39	1.36
11	M	1105	UQ2	O3-C3	2.22	1.42	1.36
8	J	502	HEM	C1A-NA	2.22	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	502	HEM	C1C-NC	2.22	1.39	1.36
4	N	1045	BGL	O5-C1	2.23	1.47	1.43
8	H	301	HEM	C4C-NC	2.26	1.39	1.36
11	D	1102	UQ2	O2-C2	2.26	1.42	1.36
8	G	501	HEM	C1C-NC	2.29	1.39	1.36
11	J	1104	UQ2	C6-C5	2.30	1.40	1.35
8	A	501	HEM	C1B-NB	2.35	1.39	1.36
11	P	1106	UQ2	O3-C3	2.35	1.42	1.36
8	P	501	HEM	C4D-ND	2.38	1.39	1.36
9	D	1002	SMA	O5-C5M	2.39	1.49	1.42
8	D	502	HEM	C1B-NB	2.41	1.39	1.36
11	G	1103	UQ2	O2-C2	2.43	1.42	1.36
11	A	1101	UQ2	O2-C2	2.44	1.42	1.36
9	G	1003	SMA	O8-C8	2.45	1.44	1.35
11	G	1103	UQ2	O3-C3	2.46	1.43	1.36
9	J	1004	SMA	O8-C8	2.48	1.44	1.35
8	A	502	HEM	C4D-ND	2.48	1.39	1.36
11	D	1102	UQ2	O3-C3	2.49	1.43	1.36
9	P	1006	SMA	O8-C8	2.51	1.44	1.35
11	A	1101	UQ2	C7-C6	2.52	1.55	1.51
9	D	1002	SMA	O8-C8	2.53	1.44	1.35
8	K	301	HEM	C4D-ND	2.56	1.39	1.36
9	M	1005	SMA	O8-C8	2.57	1.44	1.35
11	G	1103	UQ2	C7-C6	2.58	1.55	1.51
11	A	1101	UQ2	C6-C5	2.60	1.41	1.35
11	D	1102	UQ2	C6-C5	2.63	1.41	1.35
8	P	501	HEM	C1B-NB	2.63	1.39	1.36
11	M	1105	UQ2	C7-C6	2.73	1.56	1.51
8	E	301	HEM	C1C-NC	2.73	1.40	1.36
11	J	1104	UQ2	C7-C8	2.74	1.55	1.50
4	K	1044	BGL	C1-C2	2.77	1.55	1.52
8	J	502	HEM	CBC-CAC	2.79	1.48	1.28
11	D	1102	UQ2	C7-C8	2.83	1.55	1.50
11	M	1105	UQ2	C6-C5	2.84	1.41	1.35
9	G	1003	SMA	O1-C2	2.86	1.39	1.35
9	A	1001	SMA	O8-C8	2.87	1.45	1.35
9	P	1006	SMA	O1-C2	2.90	1.39	1.35
8	A	502	HEM	C1B-NB	2.95	1.40	1.36
8	G	502	HEM	CBC-CAC	3.04	1.50	1.28
11	G	1103	UQ2	C7-C8	3.08	1.55	1.50
8	N	301	HEM	C1C-NC	3.14	1.40	1.36
8	P	502	HEM	CBC-CAC	3.15	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	1106	UQ2	C6-C5	3.15	1.42	1.35
11	G	1103	UQ2	C6-C5	3.17	1.42	1.35
11	P	1106	UQ2	C7-C8	3.17	1.55	1.50
8	D	502	HEM	CBC-CAC	3.19	1.51	1.28
8	M	502	HEM	CBB-CAB	3.24	1.51	1.28
8	D	502	HEM	CBB-CAB	3.26	1.51	1.28
8	G	502	HEM	CBB-CAB	3.28	1.51	1.28
8	P	501	HEM	CBC-CAC	3.28	1.52	1.28
9	M	1005	SMA	O1-C2	3.28	1.39	1.35
8	M	501	HEM	CBB-CAB	3.28	1.52	1.28
8	M	501	HEM	CBC-CAC	3.30	1.52	1.28
8	D	501	HEM	CBB-CAB	3.31	1.52	1.28
8	A	502	HEM	CBC-CAC	3.31	1.52	1.28
8	G	501	HEM	CBB-CAB	3.32	1.52	1.28
8	A	502	HEM	CBB-CAB	3.32	1.52	1.28
8	M	502	HEM	CBC-CAC	3.32	1.52	1.28
8	P	501	HEM	CBB-CAB	3.33	1.52	1.28
8	J	501	HEM	CBB-CAB	3.34	1.52	1.28
8	A	501	HEM	CBC-CAC	3.35	1.52	1.28
11	A	1101	UQ2	C7-C8	3.38	1.56	1.50
8	J	501	HEM	CBC-CAC	3.39	1.52	1.28
8	J	502	HEM	CBB-CAB	3.40	1.52	1.28
8	A	501	HEM	CBB-CAB	3.42	1.52	1.28
8	K	301	HEM	C1C-NC	3.42	1.40	1.36
11	M	1105	UQ2	C7-C8	3.43	1.56	1.50
8	D	501	HEM	CBC-CAC	3.43	1.53	1.28
8	P	502	HEM	CBB-CAB	3.46	1.53	1.28
8	G	501	HEM	CBC-CAC	3.46	1.53	1.28
8	E	301	HEM	CBC-CAC	3.48	1.53	1.28
11	P	1106	UQ2	C7-C6	3.50	1.57	1.51
4	E	1042	BGL	C1-C2	3.53	1.55	1.52
8	N	301	HEM	CBC-CAC	3.54	1.53	1.28
8	K	301	HEM	CBC-CAC	3.54	1.53	1.28
8	Q	301	HEM	CBC-CAC	3.54	1.53	1.28
8	B	301	HEM	CBB-CAB	3.55	1.53	1.28
8	E	301	HEM	CBB-CAB	3.55	1.53	1.28
8	N	301	HEM	CBB-CAB	3.55	1.53	1.28
8	H	301	HEM	CBC-CAC	3.59	1.54	1.28
8	Q	301	HEM	CBB-CAB	3.59	1.54	1.28
8	P	502	HEM	C1B-NB	3.61	1.41	1.36
8	B	301	HEM	CBC-CAC	3.62	1.54	1.28
8	H	301	HEM	CBB-CAB	3.63	1.54	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1041	BGL	C1-C2	3.68	1.55	1.52
8	K	301	HEM	CBB-CAB	3.72	1.55	1.28
4	P	1046	BGL	C1-C2	3.79	1.55	1.52
4	N	1045	BGL	C1-C2	4.48	1.56	1.52
4	G	1043	BGL	C1-C2	4.63	1.56	1.52
9	D	1002	SMA	O7-C7	5.27	1.45	1.37
9	P	1006	SMA	O7-C7	5.45	1.45	1.37
9	P	1006	SMA	O5-C5	5.60	1.47	1.36
9	G	1003	SMA	O7-C7	5.66	1.46	1.37
9	M	1005	SMA	O5-C5	5.70	1.47	1.36
9	J	1004	SMA	O7-C7	6.01	1.46	1.37
9	D	1002	SMA	O5-C5	6.04	1.47	1.36
9	J	1004	SMA	O5-C5	6.12	1.47	1.36
9	A	1001	SMA	O5-C5	6.40	1.48	1.36
9	G	1003	SMA	O5-C5	6.64	1.48	1.36
9	A	1001	SMA	O7-C7	6.66	1.47	1.37
9	M	1005	SMA	O7-C7	6.80	1.47	1.37

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1004	SMA	C9-C10-C11	-5.55	107.25	114.72
9	M	1005	SMA	C5M-O5-C5	-5.27	110.27	117.77
9	D	1002	SMA	C9-C10-C11	-4.64	108.47	114.72
9	A	1001	SMA	C9-C10-C11	-4.53	108.61	114.72
9	D	1002	SMA	C5M-O5-C5	-4.33	111.61	117.77
9	P	1006	SMA	C9-C10-C11	-4.31	108.92	114.72
9	G	1003	SMA	C9-C10-C11	-4.27	108.97	114.72
9	P	1006	SMA	C5M-O5-C5	-4.21	111.78	117.77
9	J	1004	SMA	C5M-O5-C5	-4.20	111.79	117.77
9	A	1001	SMA	C5M-O5-C5	-3.94	112.16	117.77
9	G	1003	SMA	C5M-O5-C5	-3.83	112.31	117.77
9	A	1001	SMA	O5-C5-C6	-3.49	117.72	123.49
9	M	1005	SMA	C9-C10-C11	-3.32	110.24	114.72
9	D	1002	SMA	C17-C18-C19	-3.29	117.17	126.42
4	K	1044	BGL	C1'-O2-C2	-3.20	106.31	114.32
9	P	1006	SMA	C7M-O7-C7	-3.06	113.14	117.54
9	M	1005	SMA	C7M-O7-C7	-2.92	113.33	117.54
10	G	1023	LOP	C19-C18-C17	-2.90	99.52	114.45
10	D	1022	LOP	C27-C26-C25	-2.88	102.69	113.24
9	M	1005	SMA	C17-C18-C19	-2.85	118.41	126.42
10	A	1021	LOP	C19-C18-C17	-2.79	100.09	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1046	BGL	C1'-O2-C2	-2.79	107.34	114.32
9	D	1002	SMA	C7M-O7-C7	-2.77	113.55	117.54
9	D	1002	SMA	O5-C5-C6	-2.75	118.94	123.49
10	P	1026	LOP	C9-C8-C7	-2.73	103.22	113.24
9	J	1004	SMA	C7M-O7-C7	-2.70	113.65	117.54
9	M	1005	SMA	O5-C5-C6	-2.70	119.02	123.49
10	P	1026	LOP	C27-C26-C25	-2.69	103.37	113.24
9	G	1003	SMA	C7M-O7-C7	-2.69	113.67	117.54
4	E	1042	BGL	C1'-O2-C2	-2.66	107.65	114.32
10	G	1023	LOP	C21-C20-C19	-2.64	100.87	114.45
9	A	1001	SMA	C7M-O7-C7	-2.63	113.75	117.54
11	A	1101	UQ2	C7-C8-C9	-2.54	122.46	126.71
10	M	1025	LOP	C21-C20-C19	-2.49	101.60	114.45
9	J	1004	SMA	C17-C18-C19	-2.48	119.44	126.42
10	M	1025	LOP	C19-C18-C17	-2.48	101.67	114.45
9	P	1006	SMA	O7-C7-C6	-2.47	120.01	124.17
10	D	1022	LOP	C19-C18-C17	-2.45	101.81	114.45
4	B	1041	BGL	C1'-O2-C2	-2.39	108.33	114.32
10	A	1021	LOP	C21-C20-C19	-2.39	102.16	114.45
10	J	1024	LOP	C19-C18-C17	-2.35	102.34	114.45
11	M	1105	UQ2	C7-C8-C9	-2.31	122.84	126.71
9	P	1006	SMA	O5-C5-C6	-2.29	119.69	123.49
9	G	1003	SMA	O5-C5-C6	-2.28	119.72	123.49
9	P	1006	SMA	C17-C18-C19	-2.24	120.11	126.42
4	K	1044	BGL	C3'-C2'-C1'	-2.24	103.43	113.48
9	P	1006	SMA	O1-C8A-C4A	-2.21	119.12	121.11
11	D	1102	UQ2	C7-C8-C9	-2.21	123.02	126.71
10	A	1021	LOP	C31-C30-C29	-2.20	103.10	114.45
10	A	1021	LOP	C29-C28-C27	-2.18	103.21	114.45
10	J	1024	LOP	C21-C20-C19	-2.17	103.25	114.45
9	G	1003	SMA	C17-C18-C19	-2.16	120.34	126.42
10	J	1024	LOP	C29-C28-C27	-2.16	103.35	114.45
9	A	1001	SMA	C17-C18-C19	-2.12	120.46	126.42
9	J	1004	SMA	O5-C5-C6	-2.11	119.99	123.49
10	J	1024	LOP	C27-C26-C25	-2.10	105.55	113.24
10	P	1026	LOP	C19-C18-C17	-2.09	103.67	114.45
11	G	1103	UQ2	C7-C8-C9	-2.09	123.22	126.71
11	P	1106	UQ2	C7-C8-C9	-2.07	123.25	126.71
9	P	1006	SMA	C17-C16-C15	-2.03	110.32	125.26
10	M	1025	LOP	O6-C24-C25	2.03	117.80	111.90
8	D	501	HEM	CMB-C2B-C3B	2.06	128.71	124.89
9	D	1002	SMA	C26-C19-C18	2.11	121.46	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1021	LOP	O6-C24-C25	2.14	118.12	111.90
8	H	301	HEM	C3B-C4B-NB	2.15	111.99	109.21
11	P	1106	UQ2	C10-C9-C11	2.20	119.10	115.29
9	M	1005	SMA	O1-C8A-C8	2.28	118.73	116.03
11	P	1106	UQ2	C8-C7-C6	2.31	118.35	111.85
9	P	1006	SMA	C26-C19-C18	2.36	121.86	118.10
11	D	1102	UQ2	C10-C9-C11	2.39	119.43	115.29
9	G	1003	SMA	C26-C19-C18	2.42	121.96	118.10
11	M	1105	UQ2	C10-C9-C11	2.42	119.49	115.29
9	P	1006	SMA	C13-C14-C15	2.46	118.13	112.10
10	P	1026	LOP	O6-C24-C25	2.50	119.17	111.90
11	J	1104	UQ2	C10-C9-C11	2.51	119.64	115.29
10	P	1026	LOP	O5-C6-C7	2.54	116.82	111.55
10	D	1022	LOP	O6-C24-C25	2.60	119.46	111.90
10	G	1023	LOP	O6-C24-C25	2.71	119.79	111.90
11	A	1101	UQ2	C10-C9-C11	2.80	120.15	115.29
9	M	1005	SMA	C14-C15-C16	2.88	131.62	125.61
10	J	1024	LOP	O6-C24-C25	2.88	120.29	111.90
9	D	1002	SMA	C14-C15-C16	2.91	131.68	125.61
10	D	1022	LOP	O5-C6-C7	2.96	117.69	111.55
10	M	1025	LOP	O5-C6-C7	2.99	117.77	111.55
9	P	1006	SMA	O1-C8A-C8	3.00	119.59	116.03
10	G	1023	LOP	O5-C6-C7	3.07	117.93	111.55
10	A	1021	LOP	O5-C6-C7	3.12	118.03	111.55
9	G	1003	SMA	C14-C15-C16	3.57	133.06	125.61
9	P	1006	SMA	O5-C5-C4A	3.65	121.43	115.91
9	J	1004	SMA	O5-C5-C4A	3.72	121.53	115.91
10	J	1024	LOP	O5-C6-C7	3.82	119.49	111.55
9	G	1003	SMA	O5-C5-C4A	3.93	121.85	115.91
9	D	1002	SMA	O7-C7-C8	3.98	118.43	114.49
9	M	1005	SMA	O5-C5-C4A	4.04	122.01	115.91
9	G	1003	SMA	O7-C7-C8	4.04	118.49	114.49
9	D	1002	SMA	O5-C5-C4A	4.11	122.12	115.91
9	J	1004	SMA	O7-C7-C8	4.15	118.60	114.49
9	M	1005	SMA	O7-C7-C8	4.41	118.86	114.49
9	A	1001	SMA	O5-C5-C4A	4.45	122.63	115.91
9	A	1001	SMA	O7-C7-C8	4.85	119.29	114.49
9	J	1004	SMA	O1-C2-C9	5.02	118.12	111.94
9	D	1002	SMA	O1-C2-C9	5.14	118.27	111.94
9	M	1005	SMA	O1-C2-C9	5.27	118.43	111.94
9	P	1006	SMA	O7-C7-C8	5.28	119.71	114.49
9	A	1001	SMA	O1-C2-C9	5.48	118.69	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	1006	SMA	O1-C2-C9	5.55	118.78	111.94
9	G	1003	SMA	O1-C2-C9	5.66	118.91	111.94
9	P	1006	SMA	C14-C15-C16	6.06	138.23	125.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1021	LOP	6	0
11	A	1101	UQ2	2	0
8	A	501	HEM	3	0
8	A	502	HEM	4	0
4	B	1041	BGL	1	0
8	B	301	HEM	1	0
10	D	1022	LOP	1	0
11	D	1102	UQ2	2	0
8	D	501	HEM	5	0
8	D	502	HEM	3	0
4	E	1042	BGL	3	0
8	E	301	HEM	1	0
10	G	1023	LOP	3	0
4	G	1043	BGL	2	0
11	G	1103	UQ2	3	0
8	G	501	HEM	4	0
8	G	502	HEM	5	0
8	H	301	HEM	1	0
9	J	1004	SMA	1	0
10	J	1024	LOP	1	0
11	J	1104	UQ2	1	0
8	J	501	HEM	9	0
8	J	502	HEM	6	0
4	K	1044	BGL	2	0
8	K	301	HEM	2	0
10	M	1025	LOP	3	0
11	M	1105	UQ2	2	0
8	M	501	HEM	3	0
8	M	502	HEM	5	0
4	N	1045	BGL	1	0
8	N	301	HEM	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	1006	SMA	1	0
10	P	1026	LOP	2	0
4	P	1046	BGL	2	0
11	P	1106	UQ2	4	0
8	P	501	HEM	4	0
8	P	502	HEM	3	0
8	Q	301	HEM	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	428/445 (96%)	0.41	9 (2%) 64 61	35, 53, 90, 117	0
1	D	428/445 (96%)	0.34	11 (2%) 56 54	35, 53, 93, 124	0
1	G	428/445 (96%)	0.57	27 (6%) 21 19	35, 56, 100, 124	0
1	J	428/445 (96%)	0.63	30 (7%) 17 15	36, 62, 101, 125	0
1	M	428/445 (96%)	0.69	42 (9%) 8 7	38, 67, 107, 130	0
1	P	428/445 (96%)	0.49	21 (4%) 30 29	35, 56, 100, 127	0
2	B	256/269 (95%)	0.77	30 (11%) 5 5	47, 78, 112, 134	0
2	E	256/269 (95%)	0.91	40 (15%) 2 2	50, 80, 117, 133	0
2	H	256/269 (95%)	0.57	21 (8%) 12 11	40, 72, 113, 135	0
2	K	256/269 (95%)	1.29	63 (24%) 1 1	49, 87, 120, 136	0
2	N	256/269 (95%)	1.70	88 (34%) 0 0	59, 95, 121, 135	0
2	Q	256/269 (95%)	1.13	59 (23%) 1 1	51, 87, 119, 134	0
3	C	179/187 (95%)	0.68	19 (10%) 7 6	37, 59, 101, 139	0
3	F	179/187 (95%)	0.69	29 (16%) 2 2	38, 63, 102, 140	0
3	I	179/187 (95%)	0.53	15 (8%) 12 10	41, 58, 105, 139	0
3	L	179/187 (95%)	0.54	16 (8%) 10 9	37, 59, 104, 139	0
3	O	179/187 (95%)	0.74	21 (11%) 5 5	34, 64, 108, 138	0
3	R	179/187 (95%)	1.08	39 (21%) 1 1	46, 70, 108, 138	0
All	All	5178/5406 (95%)	0.72	580 (11%) 6 5	34, 66, 112, 140	0

All (580) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	9	GLY	18.0
2	Q	2	GLY	17.9
2	E	3	GLY	17.4

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Mol	Chain	Res	Type	RSRZ
3	I	9	GLY	17.3
2	K	3	GLY	15.6
2	E	2	GLY	13.9
2	N	2	GLY	12.0
2	N	3	GLY	11.9
2	K	2	GLY	11.4
3	I	46	ALA	11.0
3	R	9	GLY	10.8
3	F	12	ARG	10.7
2	K	172	ALA	10.2
2	N	1	ALA	10.1
3	O	10	THR	9.9
3	O	12	ARG	9.7
3	O	9	GLY	9.7
3	R	11	ARG	9.6
3	C	10	THR	9.5
3	C	11	ARG	9.4
3	L	12	ARG	9.4
3	O	11	ARG	9.2
3	I	10	THR	8.9
2	N	4	GLY	8.9
3	O	16	TYR	8.9
2	E	1	ALA	8.6
3	C	12	ARG	8.2
2	N	199	GLY	8.1
2	N	109	GLY	7.9
3	O	179	ILE	7.7
2	K	4	GLY	7.6
2	H	1	ALA	7.4
3	L	10	THR	7.4
2	K	169	CYS	7.2
2	K	114	MET	7.1
3	R	10	THR	7.0
3	R	179	ILE	7.0
2	H	3	GLY	6.9
3	L	11	ARG	6.8
2	N	174	GLY	6.7
1	D	12	ARG	6.7
3	F	179	ILE	6.7
1	M	354	VAL	6.7
1	J	8	HIS	6.6
2	K	145	CYS	6.6

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Mol	Chain	Res	Type	RSRZ
2	B	1	ALA	6.5
2	N	122	PHE	6.3
2	Q	1	ALA	6.3
3	F	9	GLY	6.2
2	K	256	LYS	6.2
2	E	4	GLY	6.1
2	N	6	VAL	6.1
2	B	256	LYS	6.1
1	P	12	ARG	6.1
2	K	138	PHE	6.0
2	K	5	HIS	6.0
1	J	5	PRO	5.9
1	M	232	THR	5.9
2	H	2	GLY	5.9
3	F	187	GLY	5.9
3	I	47	LEU	5.8
3	F	10	THR	5.8
3	L	14	PHE	5.7
3	R	184	ILE	5.7
2	B	121	LEU	5.6
2	B	199	GLY	5.6
2	N	178	THR	5.6
2	K	173	ASN	5.6
3	R	12	ARG	5.5
1	J	7	ASP	5.5
2	K	143	PRO	5.5
2	N	173	ASN	5.5
2	Q	255	VAL	5.4
1	M	5	PRO	5.3
3	L	19	THR	5.3
2	K	6	VAL	5.3
2	N	172	ALA	5.3
2	B	4	GLY	5.3
2	N	110	PHE	5.3
1	M	416	LYS	5.2
3	C	179	ILE	5.2
2	N	200	HIS	5.2
2	E	199	GLY	5.2
1	M	359	TYR	5.2
2	Q	58	LEU	5.2
1	M	417	PRO	5.1
2	N	196	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	J	11	PRO	5.1
1	J	12	ARG	5.1
2	N	198	ASP	5.0
2	B	2	GLY	5.0
1	G	12	ARG	5.0
3	R	13	ASP	5.0
3	I	12	ARG	5.0
3	F	47	LEU	5.0
1	J	9	TYR	5.0
3	R	52	VAL	4.9
2	N	175	VAL	4.9
1	J	10	GLU	4.9
2	N	121	LEU	4.8
1	J	348	TRP	4.8
2	K	253	ALA	4.8
2	Q	7	GLU	4.8
2	K	144	LYS	4.8
1	M	12	ARG	4.8
1	M	15	ILE	4.7
3	R	47	LEU	4.7
1	M	418	VAL	4.7
2	N	77	THR	4.7
2	N	201	ASP	4.7
2	N	10	PRO	4.7
2	K	122	PHE	4.7
2	Q	5	HIS	4.7
3	R	14	PHE	4.6
3	I	179	ILE	4.6
2	N	169	CYS	4.6
3	L	116	LEU	4.6
2	N	78	GLY	4.6
3	R	17	TYR	4.5
2	K	150	GLU	4.5
2	B	146	ALA	4.5
1	J	362	MET	4.5
3	L	13	ASP	4.5
2	E	200	HIS	4.5
3	C	48	ALA	4.5
3	I	17	TYR	4.5
1	P	8	HIS	4.5
2	K	124	GLY	4.5
1	J	6	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
2	Q	147	GLU	4.5
3	O	15	LEU	4.4
2	K	9	VAL	4.4
1	J	416	LYS	4.4
1	G	18	TRP	4.4
2	N	256	LYS	4.4
2	Q	79	GLU	4.4
2	Q	193	LEU	4.4
2	Q	204	VAL	4.4
3	R	187	GLY	4.4
2	K	110	PHE	4.3
1	G	15	ILE	4.3
1	A	416	LYS	4.3
3	O	187	GLY	4.3
3	O	47	LEU	4.3
2	N	152	ASP	4.3
2	N	171	ASP	4.3
2	K	11	PHE	4.3
3	F	54	VAL	4.3
2	Q	190	MET	4.3
2	Q	110	PHE	4.3
3	C	47	LEU	4.2
3	O	13	ASP	4.2
2	N	197	ALA	4.2
2	N	149	HIS	4.2
2	Q	9	VAL	4.2
2	Q	152	ASP	4.2
1	P	6	HIS	4.1
2	K	171	ASP	4.1
3	I	11	ARG	4.1
2	Q	194	VAL	4.1
3	F	48	ALA	4.1
2	B	200	HIS	4.1
2	Q	196	TYR	4.1
2	H	109	GLY	4.1
2	N	7	GLU	4.1
3	F	53	ASP	4.1
3	L	9	GLY	4.1
2	N	123	ASN	4.1
2	Q	3	GLY	4.0
2	K	118	ILE	4.0
2	B	5	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
3	F	11	ARG	4.0
1	G	416	LYS	4.0
3	F	17	TYR	4.0
2	K	149	HIS	4.0
1	P	4	ILE	3.9
2	N	202	ALA	3.9
1	P	5	PRO	3.9
2	E	251	LEU	3.9
2	N	111	HIS	3.9
2	E	7	GLU	3.9
1	M	323	PHE	3.9
2	Q	35	VAL	3.9
1	G	414	ILE	3.9
2	N	192	ASP	3.8
2	Q	80	ASP	3.8
2	E	140	GLU	3.8
3	F	186	LEU	3.8
2	B	151	PRO	3.8
3	L	181	GLU	3.8
2	Q	59	PRO	3.8
2	N	153	GLY	3.8
2	B	143	PRO	3.8
3	R	186	LEU	3.7
2	N	138	PHE	3.7
1	G	17	LYS	3.7
1	A	12	ARG	3.7
1	P	11	PRO	3.7
3	R	181	GLU	3.7
3	R	50	ILE	3.7
3	R	51	PHE	3.7
1	J	311	ASP	3.7
3	L	17	TYR	3.7
1	D	13	THR	3.7
2	B	149	HIS	3.7
2	E	58	LEU	3.7
3	R	183	THR	3.7
3	O	17	TYR	3.7
3	L	15	LEU	3.7
3	O	51	PHE	3.6
1	M	8	HIS	3.6
2	K	139	PRO	3.6
1	G	19	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	149	HIS	3.6
1	P	13	THR	3.6
2	E	5	HIS	3.6
1	M	365	ILE	3.5
2	K	10	PRO	3.5
2	K	17	PHE	3.5
2	B	197	ALA	3.5
3	R	116	LEU	3.5
2	E	114	MET	3.5
3	O	14	PHE	3.5
1	D	5	PRO	3.5
2	K	113	PRO	3.5
2	N	82	GLU	3.5
1	M	11	PRO	3.5
2	N	255	VAL	3.5
3	F	183	THR	3.4
2	K	112	GLY	3.4
2	K	141	GLU	3.4
3	R	178	PHE	3.4
3	I	48	ALA	3.4
2	B	75	GLU	3.4
1	P	7	ASP	3.4
3	R	18	ALA	3.4
1	M	428	PHE	3.4
3	I	45	GLN	3.4
3	I	14	PHE	3.4
2	N	179	ALA	3.4
2	K	59	PRO	3.4
2	H	79	GLU	3.4
3	C	180	ASP	3.4
1	D	8	HIS	3.4
1	M	234	LYS	3.4
2	B	79	GLU	3.3
2	B	150	GLU	3.3
1	J	4	ILE	3.3
2	Q	192	ASP	3.3
2	Q	78	GLY	3.3
2	Q	191	ASP	3.3
2	N	125	ILE	3.3
2	Q	145	CYS	3.3
2	B	122	PHE	3.3
2	Q	57	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	58	LEU	3.3
1	G	13	THR	3.3
1	M	233	SER	3.3
2	Q	146	ALA	3.3
2	E	201	ASP	3.3
1	P	30	TYR	3.3
2	N	151	PRO	3.2
1	G	14	GLY	3.2
1	M	414	ILE	3.2
2	H	114	MET	3.2
2	Q	256	LYS	3.2
2	N	177	THR	3.2
2	N	66	TYR	3.2
2	B	198	ASP	3.2
2	E	205	HIS	3.2
2	Q	149	HIS	3.2
2	N	68	THR	3.2
1	J	365	ILE	3.2
1	M	248	PHE	3.2
2	Q	182	TRP	3.2
2	K	197	ALA	3.2
1	M	362	MET	3.2
2	E	256	LYS	3.2
2	N	39	CYS	3.2
3	C	181	GLU	3.2
2	E	182	TRP	3.2
3	O	24	ALA	3.1
1	A	414	ILE	3.1
2	E	10	PRO	3.1
2	K	7	GLU	3.1
2	H	256	LYS	3.1
3	R	61	VAL	3.1
2	Q	11	PHE	3.1
2	N	79	GLU	3.1
1	M	13	THR	3.1
3	F	52	VAL	3.1
3	O	183	THR	3.1
2	H	199	GLY	3.1
3	F	181	GLU	3.1
2	E	190	MET	3.1
2	Q	8	ASP	3.1
3	C	187	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	292	ILE	3.1
1	G	9	TYR	3.1
2	K	146	ALA	3.1
2	K	175	VAL	3.1
1	M	249	ILE	3.1
3	F	51	PHE	3.1
2	E	141	GLU	3.1
2	N	139	PRO	3.0
1	M	358	ARG	3.0
2	B	3	GLY	3.0
2	K	199	GLY	3.0
2	K	120	GLN	3.0
2	E	193	LEU	3.0
2	K	148	GLY	3.0
2	N	72	VAL	3.0
3	I	187	GLY	3.0
2	N	246	LEU	3.0
2	K	142	PRO	3.0
2	Q	4	GLY	3.0
2	K	190	MET	3.0
1	J	428	PHE	3.0
2	K	147	GLU	2.9
2	Q	200	HIS	2.9
1	J	414	ILE	2.9
2	N	155	TYR	2.9
3	R	19	THR	2.9
2	Q	189	LEU	2.9
1	G	10	GLU	2.9
2	H	75	GLU	2.9
1	D	7	ASP	2.9
2	E	8	ASP	2.9
2	H	251	LEU	2.9
3	C	183	THR	2.9
1	M	242	VAL	2.9
3	R	15	LEU	2.9
2	N	245	TYR	2.9
2	Q	6	VAL	2.9
2	N	195	GLU	2.9
1	G	417	PRO	2.9
2	E	206	ALA	2.9
1	G	247	TYR	2.9
1	M	415	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	13	ASP	2.8
2	Q	143	PRO	2.8
1	M	411	LEU	2.8
2	Q	94	LEU	2.8
3	I	13	ASP	2.8
1	G	30	TYR	2.8
2	N	9	VAL	2.8
2	N	150	GLU	2.8
2	N	166	PRO	2.8
1	D	290	ALA	2.8
2	N	249	LYS	2.8
2	E	255	VAL	2.8
2	Q	56	PRO	2.8
1	G	413	ALA	2.8
2	N	80	ASP	2.8
1	P	239	LYS	2.8
2	N	75	GLU	2.7
2	Q	153	GLY	2.7
1	M	419	ALA	2.7
2	H	72	VAL	2.7
2	E	110	PHE	2.7
3	C	104	ASP	2.7
1	G	11	PRO	2.7
2	K	231	PHE	2.7
2	E	252	TRP	2.7
1	P	14	GLY	2.7
2	E	122	PHE	2.7
1	M	6	HIS	2.7
2	E	151	PRO	2.7
1	M	348	TRP	2.7
1	D	413	ALA	2.7
3	R	58	GLU	2.7
2	N	100	LEU	2.7
1	J	30	TYR	2.7
2	Q	96	ASN	2.7
3	C	16	TYR	2.7
2	Q	188	PRO	2.7
2	K	119	SER	2.6
2	K	182	TRP	2.6
3	L	187	GLY	2.6
1	M	14	GLY	2.6
2	H	82	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	119	SER	2.6
1	M	412	GLY	2.6
3	F	182	THR	2.6
2	Q	199	GLY	2.6
1	A	13	THR	2.6
1	G	7	ASP	2.6
3	O	180	ASP	2.6
3	L	47	LEU	2.6
3	F	184	ILE	2.6
2	N	124	GLY	2.6
2	B	110	PHE	2.6
2	N	11	PHE	2.6
3	F	14	PHE	2.6
2	B	76	GLU	2.6
3	C	103	ILE	2.5
2	E	18	GLY	2.5
1	P	10	GLU	2.5
1	A	76	ALA	2.5
1	J	123	ALA	2.5
3	O	181	GLU	2.5
1	J	27	ALA	2.5
1	M	413	ALA	2.5
2	Q	202	ALA	2.5
2	Q	12	SER	2.5
2	N	114	MET	2.5
2	Q	140	GLU	2.5
3	R	180	ASP	2.5
3	R	82	ILE	2.5
3	F	55	SER	2.5
1	J	237	ALA	2.5
2	K	1	ALA	2.5
3	O	48	ALA	2.5
3	F	13	ASP	2.5
1	G	412	GLY	2.5
1	P	9	TYR	2.5
2	N	5	HIS	2.5
1	J	361	PRO	2.5
2	E	16	PRO	2.5
3	I	57	VAL	2.5
3	R	65	VAL	2.5
2	E	147	GLU	2.5
1	M	19	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	R	57	VAL	2.4
3	R	56	SER	2.4
3	R	103	ILE	2.4
2	K	58	LEU	2.4
2	N	61	ASP	2.4
1	J	323	PHE	2.4
1	M	387	PHE	2.4
2	K	20	PHE	2.4
1	J	124	PRO	2.4
2	N	251	LEU	2.4
3	R	177	LYS	2.4
3	C	178	PHE	2.4
2	Q	18	GLY	2.4
2	K	255	VAL	2.4
2	H	250	ARG	2.4
2	Q	158	ARG	2.4
1	J	244	PHE	2.4
1	P	428	PHE	2.4
2	Q	61	ASP	2.4
2	K	251	LEU	2.4
2	N	94	LEU	2.4
1	P	22	ARG	2.4
2	E	9	VAL	2.4
3	F	57	VAL	2.4
1	J	172	ILE	2.4
2	Q	141	GLU	2.4
2	N	113	PRO	2.4
1	M	18	TRP	2.4
2	Q	243	LEU	2.4
1	M	9	TYR	2.4
1	G	232	THR	2.4
2	N	35	VAL	2.3
2	K	183	ILE	2.3
3	F	50	ILE	2.3
2	Q	75	GLU	2.3
3	R	79	GLU	2.3
2	K	252	TRP	2.3
2	B	139	PRO	2.3
2	K	236	PHE	2.3
2	N	20	PHE	2.3
2	K	117	GLY	2.3
2	B	64	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	348	TRP	2.3
1	P	293	VAL	2.3
3	L	186	LEU	2.3
2	N	207	MET	2.3
2	E	253	ALA	2.3
2	K	168	THR	2.3
2	Q	150	GLU	2.3
3	O	57	VAL	2.3
2	E	145	CYS	2.3
2	H	145	CYS	2.3
2	N	62	GLN	2.3
3	F	180	ASP	2.3
2	K	245	TYR	2.3
3	O	54	VAL	2.3
1	M	237	ALA	2.3
2	K	8	ASP	2.3
3	C	14	PHE	2.3
2	K	177	THR	2.3
1	M	197	LEU	2.3
1	G	294	PRO	2.2
2	H	231	PHE	2.2
2	N	65	ALA	2.2
3	F	176	ALA	2.2
1	G	22	ARG	2.2
2	K	123	ASN	2.2
1	M	325	ILE	2.2
1	P	15	ILE	2.2
2	B	178	THR	2.2
2	N	168	THR	2.2
2	Q	132	TYR	2.2
2	E	146	ALA	2.2
2	E	208	ALA	2.2
2	H	205	HIS	2.2
2	N	73	THR	2.2
3	L	51	PHE	2.2
2	N	135	LEU	2.2
2	N	76	GLU	2.2
2	N	143	PRO	2.2
3	R	122	TRP	2.2
1	A	15	ILE	2.2
1	P	16	GLU	2.2
2	B	174	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	112	GLY	2.2
3	R	120	GLY	2.2
3	I	181	GLU	2.2
3	R	105	ALA	2.2
2	H	71	THR	2.2
2	N	183	ILE	2.2
1	A	5	PRO	2.2
1	G	3	GLY	2.2
3	F	116	LEU	2.2
2	K	155	TYR	2.2
3	L	16	TYR	2.2
2	B	69	GLN	2.2
2	K	200	HIS	2.2
2	Q	206	ALA	2.2
1	M	7	ASP	2.2
1	G	428	PHE	2.2
1	A	150	PRO	2.2
2	Q	22	GLN	2.1
2	B	78	GLY	2.1
2	Q	77	THR	2.1
1	M	251	LYS	2.1
2	H	80	ASP	2.1
2	E	254	GLY	2.1
1	J	170	PRO	2.1
1	M	292	ILE	2.1
3	F	56	SER	2.1
2	N	191	ASP	2.1
2	E	150	GLU	2.1
1	A	141	ALA	2.1
1	D	293	VAL	2.1
2	K	196	TYR	2.1
3	R	139	GLY	2.1
2	N	93	ALA	2.1
1	P	18	TRP	2.1
2	N	187	PRO	2.1
2	H	111	HIS	2.1
2	K	109	GLY	2.1
2	N	137	GLY	2.1
3	C	176	ALA	2.1
3	R	137	ILE	2.1
1	M	43	TRP	2.1
1	P	43	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	201	ASP	2.1
3	C	186	LEU	2.1
2	Q	203	SER	2.1
3	O	177	LYS	2.1
1	G	146	GLY	2.1
2	N	117	GLY	2.1
3	F	119	ALA	2.1
2	Q	19	THR	2.1
3	R	16	TYR	2.1
1	J	427	ASP	2.1
1	J	100	GLY	2.1
2	Q	26	GLN	2.1
1	J	18	TRP	2.1
1	D	150	PRO	2.0
2	E	192	ASP	2.0
2	K	198	ASP	2.0
1	G	233	SER	2.0
2	N	8	ASP	2.0
2	B	166	PRO	2.0
1	D	6	HIS	2.0
2	H	77	THR	2.0
3	R	185	GLN	2.0
2	N	254	GLY	2.0
2	E	209	GLU	2.0
1	G	235	ALA	2.0
1	G	70	THR	2.0
2	N	157	ASN	2.0
2	H	4	GLY	2.0
1	J	15	ILE	2.0
3	F	178	PHE	2.0
2	B	224	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	UQ2	A	1101	23/23	0.66	0.42	11.63	102,105,108,109	0
11	UQ2	D	1102	23/23	0.64	0.37	7.62	92,98,107,107	0
11	UQ2	G	1103	23/23	0.69	0.38	6.84	109,116,117,118	0
11	UQ2	M	1105	23/23	0.64	0.44	6.23	112,123,125,125	0
11	UQ2	J	1104	23/23	0.53	0.49	5.86	107,115,116,117	0
10	LOP	J	1024	45/45	0.82	0.36	5.73	93,113,125,126	0
11	UQ2	P	1106	23/23	0.70	0.32	3.73	101,104,107,108	0
10	LOP	P	1026	45/45	0.83	0.28	2.87	69,95,99,100	0
10	LOP	G	1023	45/45	0.77	0.27	2.84	88,102,112,113	0
10	LOP	D	1022	45/45	0.87	0.25	2.34	63,88,98,102	0
4	BGL	G	1043	20/20	0.78	0.27	1.75	89,91,101,101	0
10	LOP	M	1025	45/45	0.80	0.28	1.55	89,114,123,123	0
10	LOP	A	1021	45/45	0.89	0.22	1.50	72,86,94,99	0
12	FES	L	200	4/4	0.99	0.20	1.32	40,41,41,42	0
4	BGL	P	1046	20/20	0.88	0.26	1.29	87,93,95,95	0
9	SMA	J	1004	37/37	0.95	0.24	1.12	40,49,79,85	0
8	HEM	A	502	43/43	0.98	0.25	1.11	32,37,49,49	0
8	HEM	B	301	43/43	0.95	0.20	0.79	51,56,70,73	0
9	SMA	P	1006	37/37	0.95	0.21	0.76	34,45,76,77	0
9	SMA	D	1002	37/37	0.94	0.22	0.73	39,44,76,78	0
8	HEM	P	502	43/43	0.98	0.24	0.73	35,40,49,53	0
8	HEM	G	502	43/43	0.98	0.23	0.68	32,36,45,49	0
4	BGL	B	1041	20/20	0.80	0.23	0.50	87,97,101,102	0
9	SMA	G	1003	37/37	0.96	0.22	0.48	35,43,60,65	0
8	HEM	J	502	43/43	0.98	0.22	0.48	37,41,54,57	0
8	HEM	H	301	43/43	0.96	0.17	0.41	33,42,47,50	0
4	BGL	N	1045	20/20	0.71	0.31	0.40	107,111,113,114	0
8	HEM	D	502	43/43	0.97	0.22	0.38	32,37,49,58	0
4	BGL	E	1042	20/20	0.90	0.20	0.37	80,85,102,102	0
12	FES	F	200	4/4	0.99	0.18	0.36	43,43,44,45	0
9	SMA	M	1005	37/37	0.96	0.20	0.36	56,66,73,73	0
8	HEM	M	502	43/43	0.98	0.21	0.29	47,49,59,63	0
8	HEM	J	501	43/43	0.95	0.18	0.26	67,75,79,81	0
8	HEM	M	501	43/43	0.97	0.17	0.23	63,69,75,78	0
12	FES	O	200	4/4	0.98	0.18	0.16	42,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	FES	C	200	4/4	0.99	0.18	0.12	41,42,42,43	0
9	SMA	A	1001	37/37	0.95	0.21	0.11	38,47,54,56	0
6	CL	I	2004	1/1	0.93	0.16	0.10	67,67,67,67	0
8	HEM	A	501	43/43	0.98	0.18	0.00	43,47,51,53	0
8	HEM	G	501	43/43	0.97	0.17	-0.03	50,59,62,62	0
8	HEM	E	301	43/43	0.96	0.17	-0.07	53,62,73,76	0
8	HEM	D	501	43/43	0.97	0.15	-0.09	40,48,53,55	0
8	HEM	K	301	43/43	0.96	0.17	-0.20	49,55,67,69	0
4	BGL	K	1044	20/20	0.86	0.20	-0.25	95,99,101,101	0
8	HEM	N	301	43/43	0.94	0.20	-0.26	65,72,79,84	0
8	HEM	P	501	43/43	0.98	0.16	-0.42	48,54,57,57	0
12	FES	I	200	4/4	0.97	0.17	-0.49	47,48,48,48	0
12	FES	R	200	4/4	0.98	0.15	-0.60	55,57,58,58	0
8	HEM	Q	301	43/43	0.96	0.15	-0.83	56,65,73,78	0
6	CL	R	2005	1/1	0.94	0.09	-1.46	67,67,67,67	0
7	NA	R	2001	1/1	0.95	0.10	-1.46	62,62,62,62	0
5	SR	H	1013	1/1	0.89	0.08	-2.18	113,113,113,113	0
5	SR	Q	1016	1/1	0.70	0.08	-2.60	137,137,137,137	0
5	SR	E	1012	1/1	0.79	0.04	-2.65	138,138,138,138	0
5	SR	B	1011	1/1	0.79	0.04	-2.66	132,132,132,132	0
5	SR	K	1014	1/1	0.77	0.11	-2.92	145,145,145,145	0
5	SR	N	1015	1/1	0.94	0.06	-4.08	153,153,153,153	0
5	SR	G	1018	1/1	0.80	0.19	-	98,98,98,98	0
5	SR	M	1019	1/1	0.85	0.08	-	154,154,154,154	0
5	SR	A	1017	1/1	0.94	0.17	-	114,114,114,114	0

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

There are no such residues in this entry.