



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:57 am GMT

PDB ID : 2QJK  
Title : Crystal Structure Analysis of mutant rhodobacter sphaeroides bc1 with stigmatellin and antimycin  
Authors : Esser, L.  
Deposited on : 2007-07-07  
Resolution : 3.10 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	:	trunk28620
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

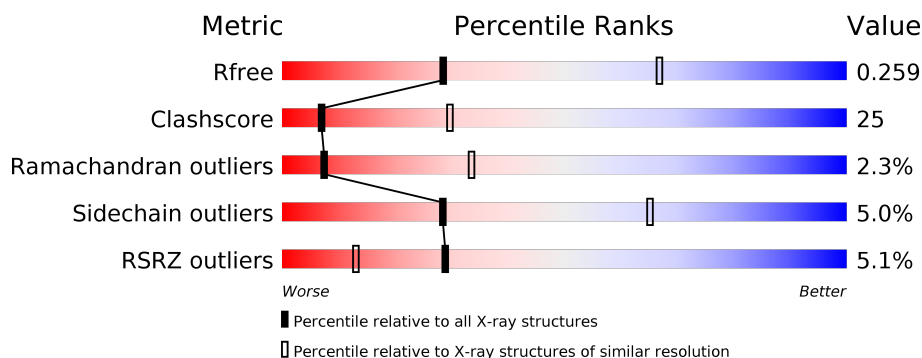
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	428	<div> <div> <div></div> <div>54%</div> <div>42%</div> <div></div> </div> <div>•</div> </div>
1	D	428	<div> <div> <div></div> <div>54%</div> <div>44%</div> <div></div> </div> <div>•</div> </div>
1	G	428	<div> <div> <div></div> <div>52%</div> <div>44%</div> <div></div> </div> <div>•</div> </div>
1	J	428	<div> <div> <div></div> <div>50%</div> <div>47%</div> <div></div> </div> <div>•</div> </div>
1	M	428	<div> <div> <div></div> <div>49%</div> <div>47%</div> <div></div> </div> <div>•</div> </div>
1	P	428	<div> <div> <div></div> <div>50%</div> <div>47%</div> <div></div> </div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	256	
2	E	256	
2	H	256	
2	K	256	
2	N	256	
2	Q	256	
3	C	179	
3	F	179	
3	I	179	
3	L	179	
3	O	179	
3	R	179	

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	ANJ	M	505	-	-	-	X
4	BGL	G	431	-	-	-	X
4	BGL	M	431	-	-	-	X
7	FES	C	200	-	-	X	-
7	FES	F	200	-	-	X	-
7	FES	I	200	-	-	X	-
7	FES	L	200	-	-	X	-
7	FES	O	200	-	-	X	-
7	FES	R	200	-	-	X	-
9	LOP	G	504	-	-	-	X
9	LOP	J	504	-	-	-	X
9	LOP	M	504	-	-	-	X
9	LOP	P	504	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 42048 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	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	N	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	Q	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

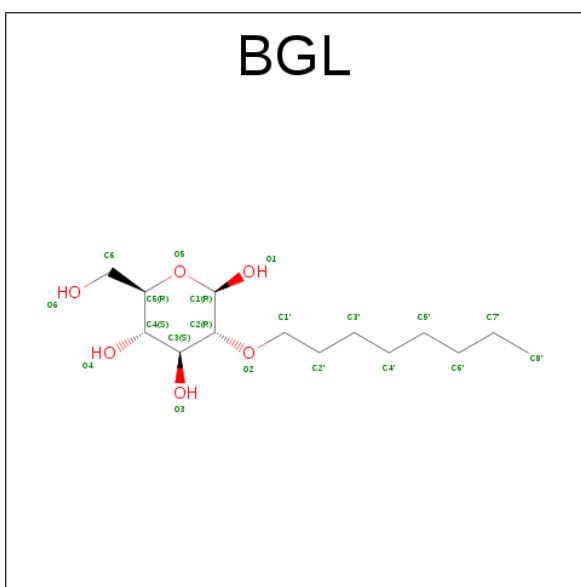
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

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>).

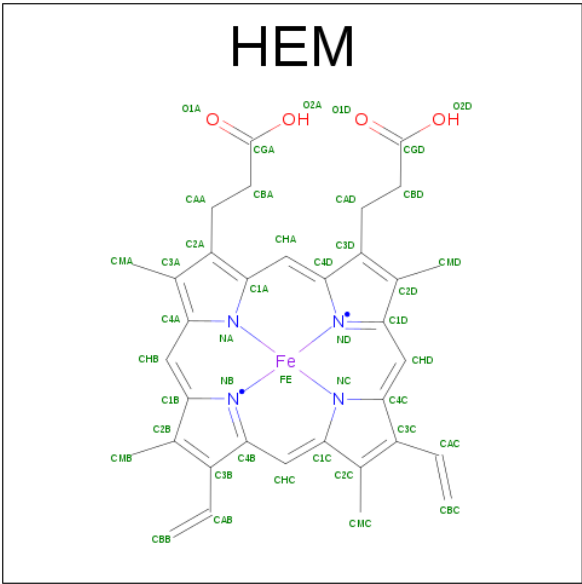


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		
4	G	1	Total	C	O	0	0
			20	14	6		
4	J	1	Total	C	O	0	0
			20	14	6		
4	M	1	Total	C	O	0	0
			20	14	6		
4	Q	1	Total	C	O	0	0
			20	14	6		

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

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

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



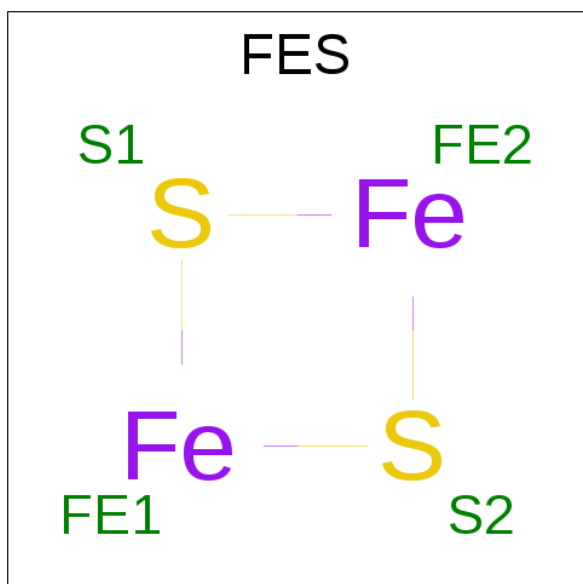
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	N	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

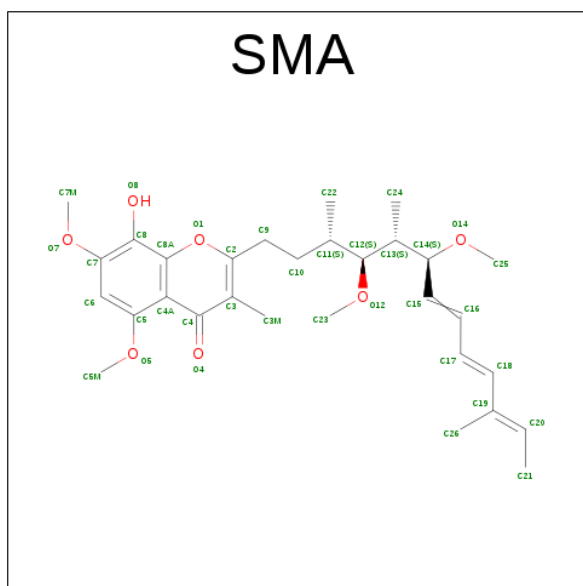
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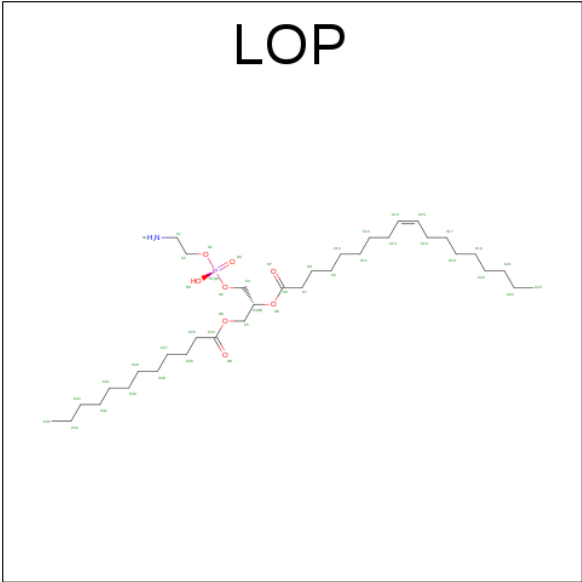
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is STIGMATELLIN A (three-letter code: SMA) (formula:  $C_{30}H_{42}O_7$ ).



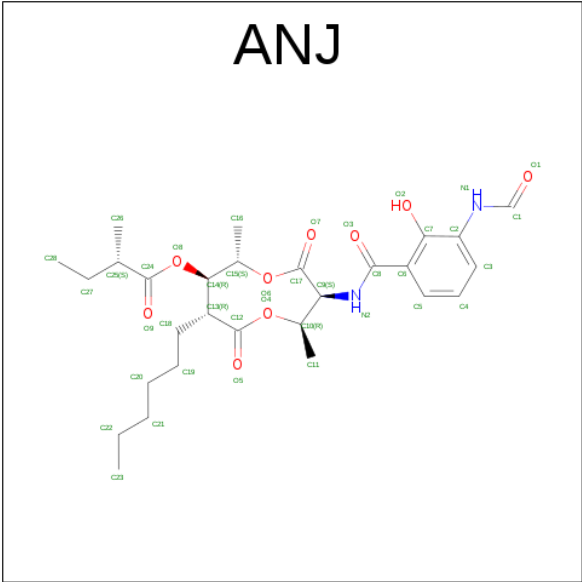
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			37	30	7		
8	D	1	Total	C	O	0	0
			37	30	7		
8	G	1	Total	C	O	0	0
			37	30	7		
8	J	1	Total	C	O	0	0
			37	30	7		
8	M	1	Total	C	O	0	0
			37	30	7		
8	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 9 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula:  $C_{35}H_{68}NO_8P$ ).



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

- Molecule 10 is (2R,3S,6S,7R,8R)-3-{[3-(FORMYLAMINO)-2-HYDROXYBENZOYL]AMINO}-8-HEXYL-2,6-DIMETHYL-4,9-DIOXO-1,5-DIOXONAN-7-YL (2S)-2-METHYLBUTANOATE (three-letter code: ANJ) (formula: C<sub>28</sub>H<sub>40</sub>N<sub>2</sub>O<sub>9</sub>).

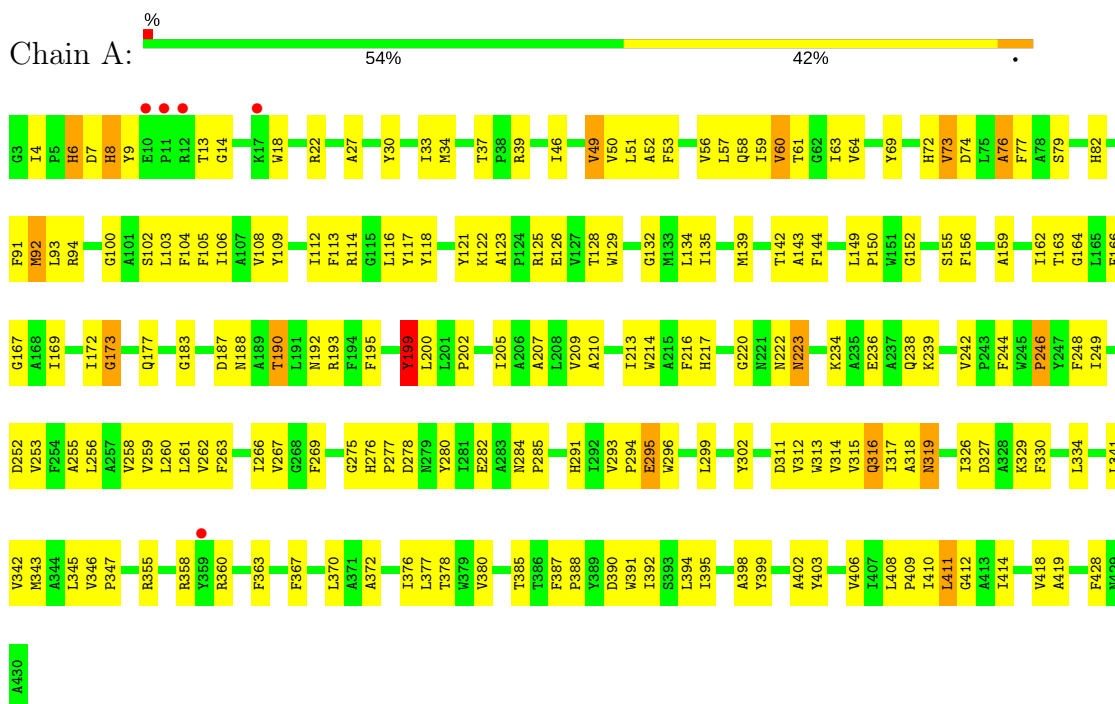


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			39	28	2	9		
10	D	1	Total	C	N	O	0	0
			39	28	2	9		
10	G	1	Total	C	N	O	0	0
			39	28	2	9		
10	J	1	Total	C	N	O	0	0
			39	28	2	9		
10	M	1	Total	C	N	O	0	0
			39	28	2	9		
10	P	1	Total	C	N	O	0	0
			39	28	2	9		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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

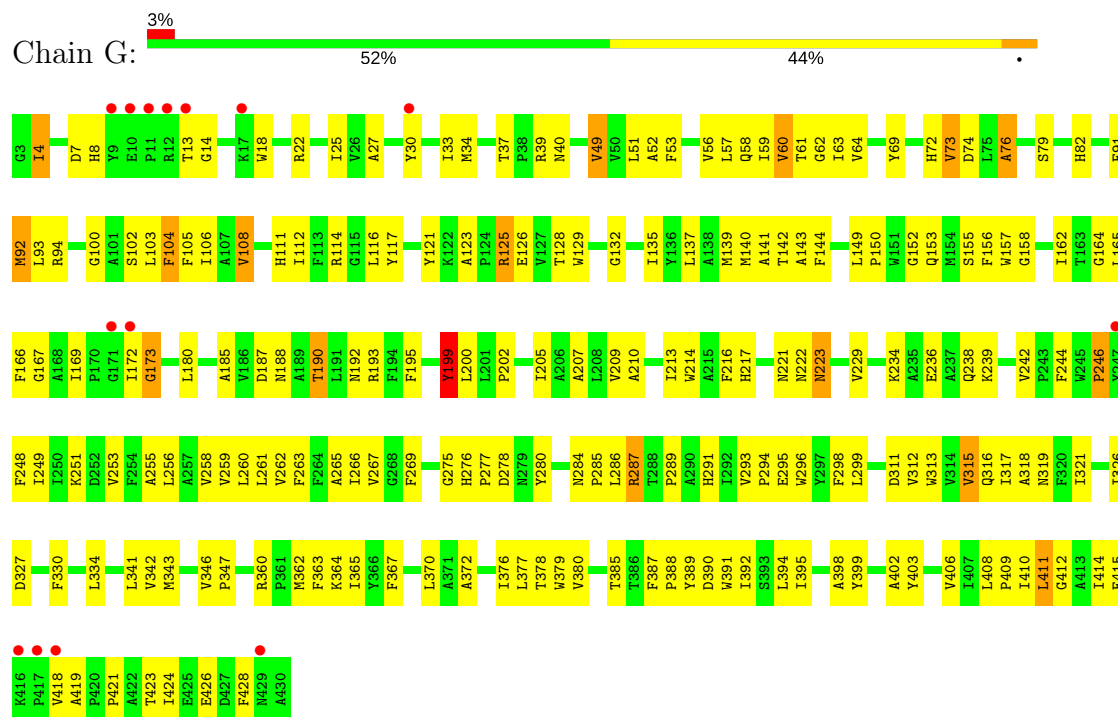


- Molecule 1: Cytochrome b

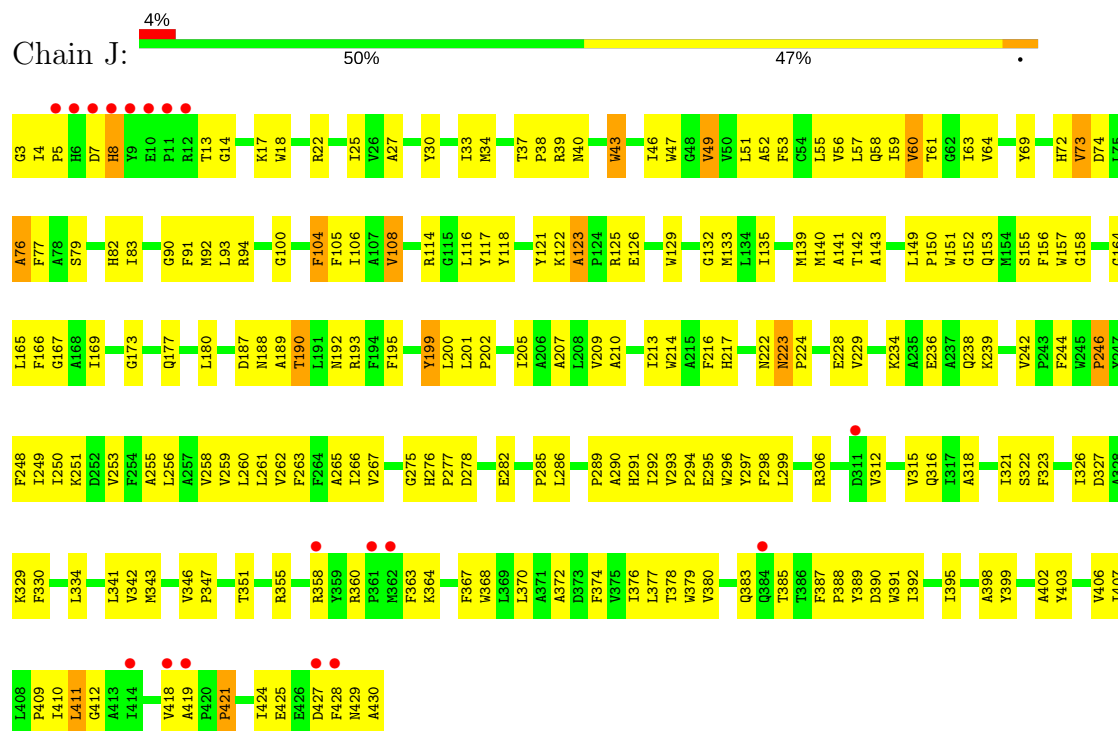




- Molecule 1: Cytochrome b



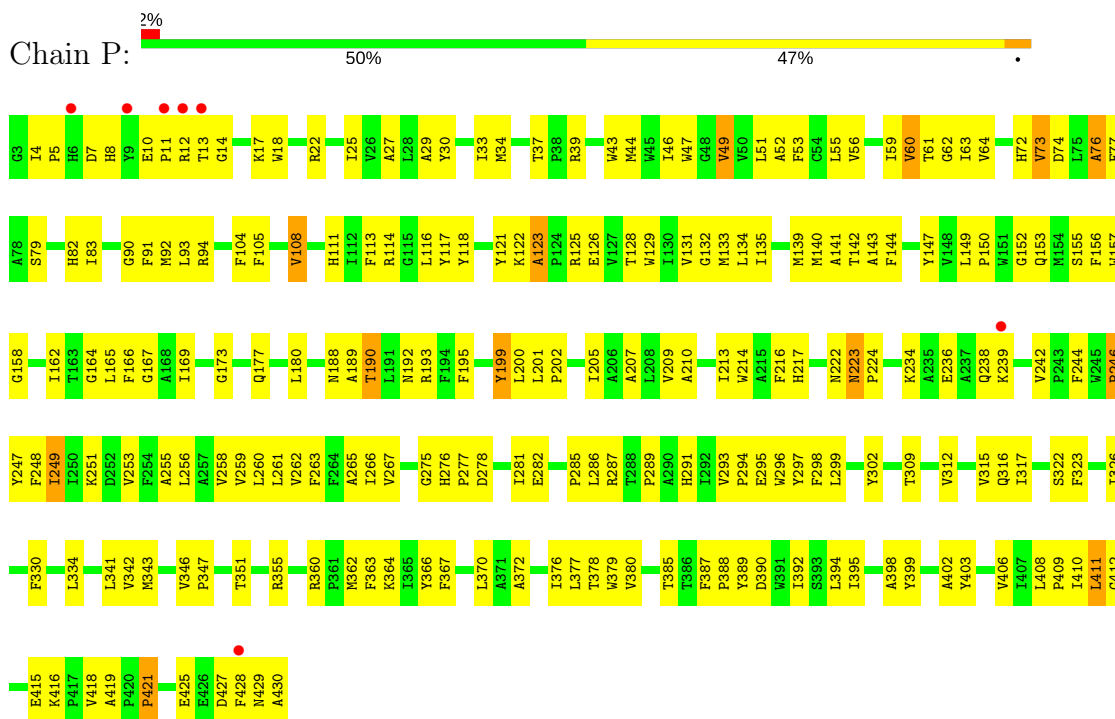
- Molecule 1: Cytochrome b



- Molecule 1: Cytochrome b

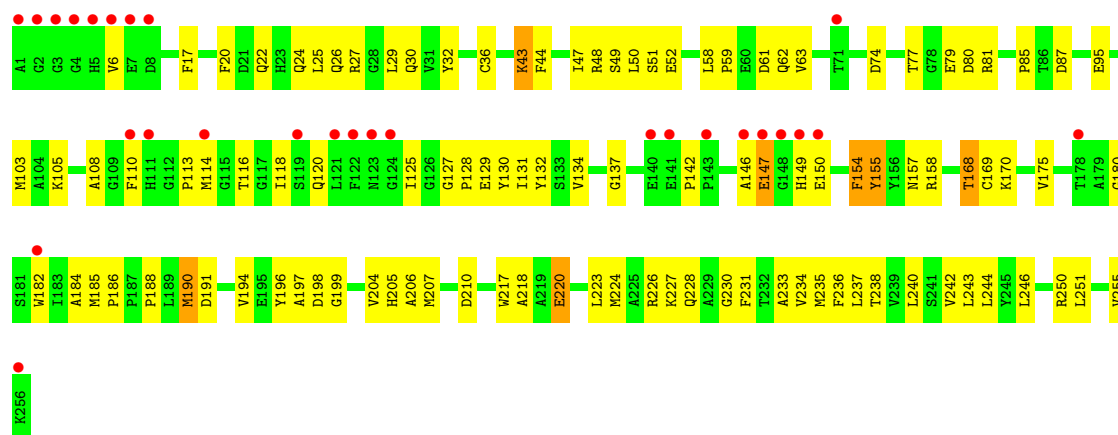


- Molecule 1: Cytochrome b

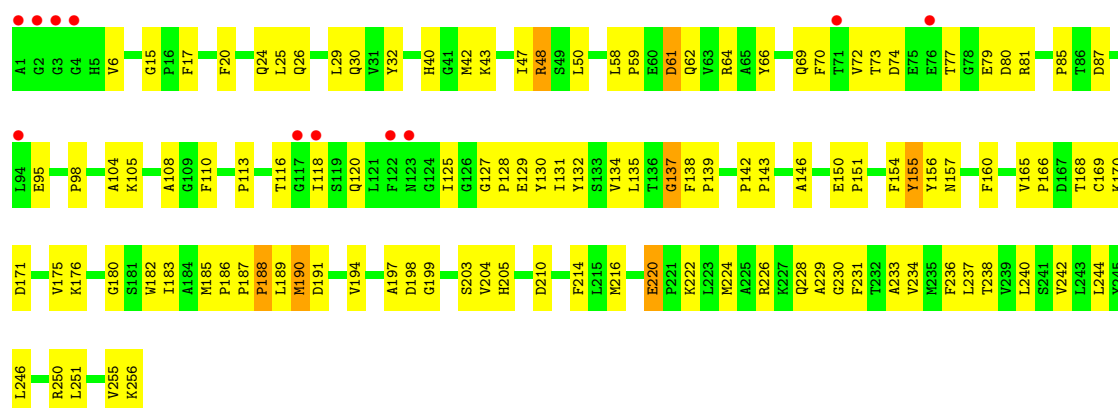


- Molecule 2: Cytochrome c1

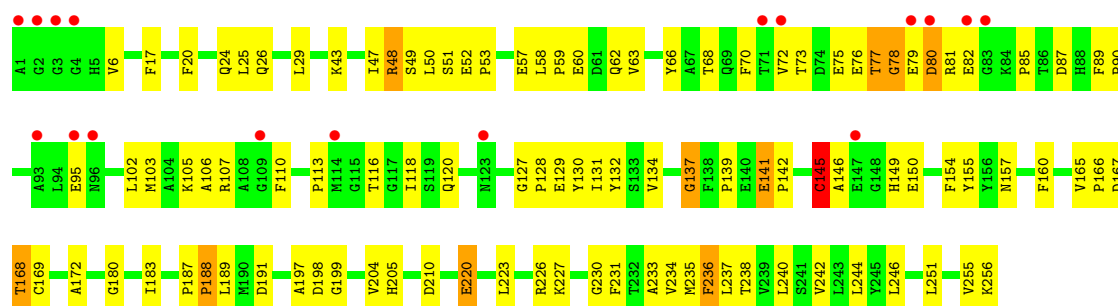




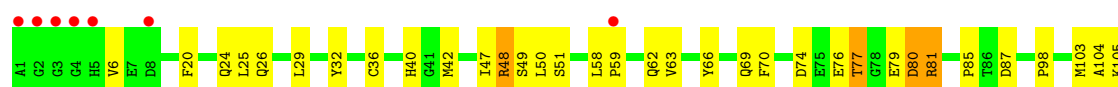
• Molecule 2: Cytochrome c1

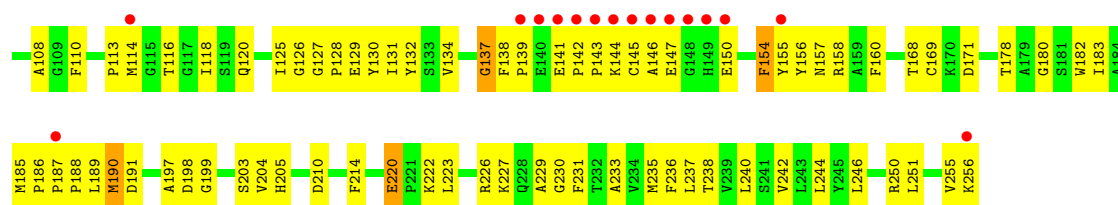


• Molecule 2: Cytochrome c1

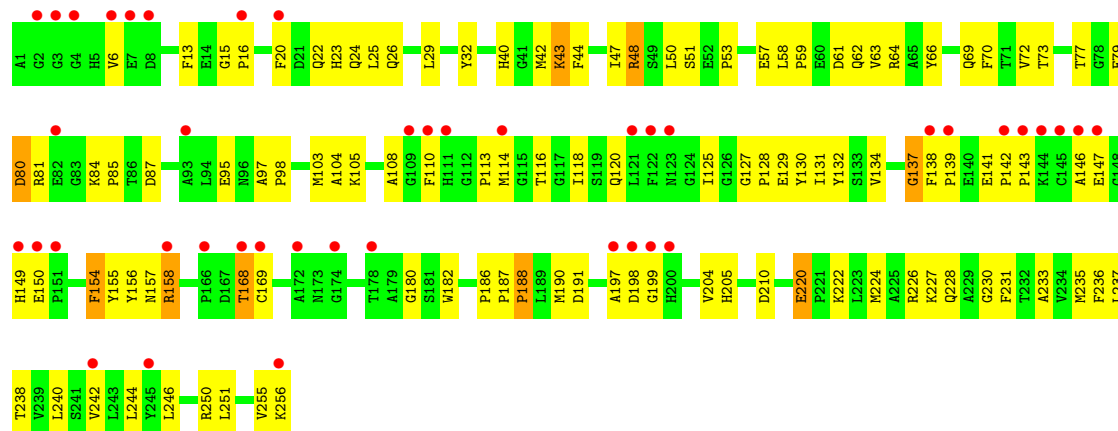


• Molecule 2: Cytochrome c1

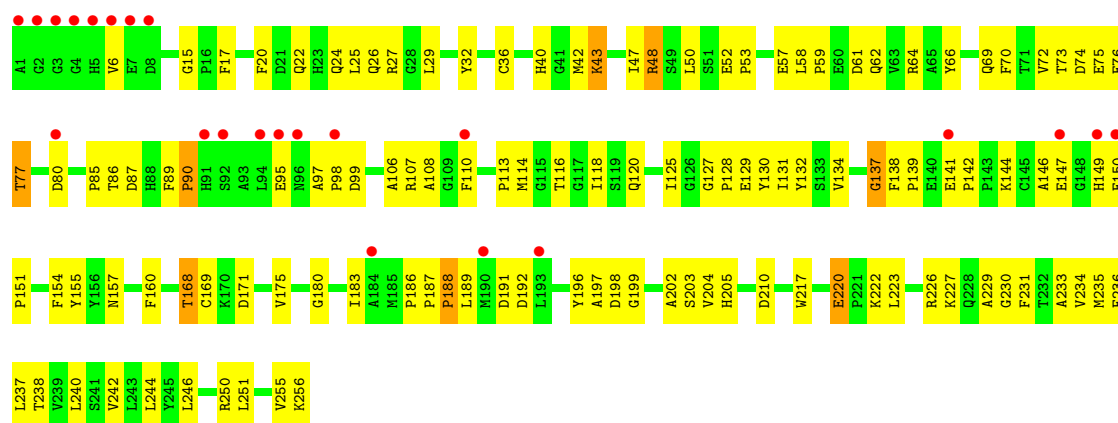




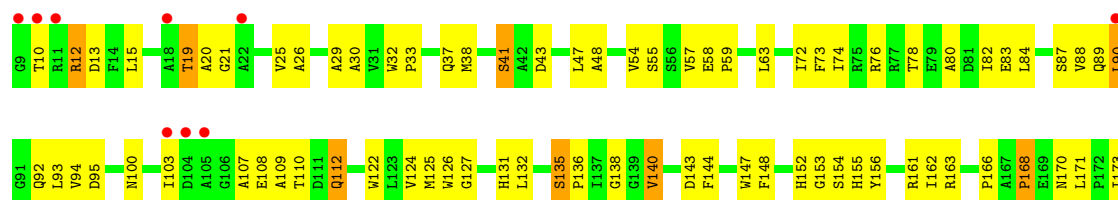
• Molecule 2: Cytochrome c1



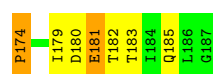
• Molecule 2: Cytochrome c1



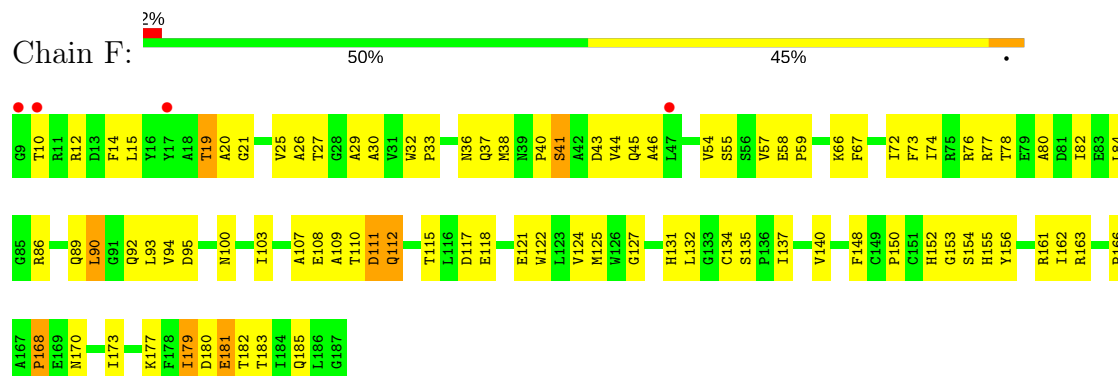
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



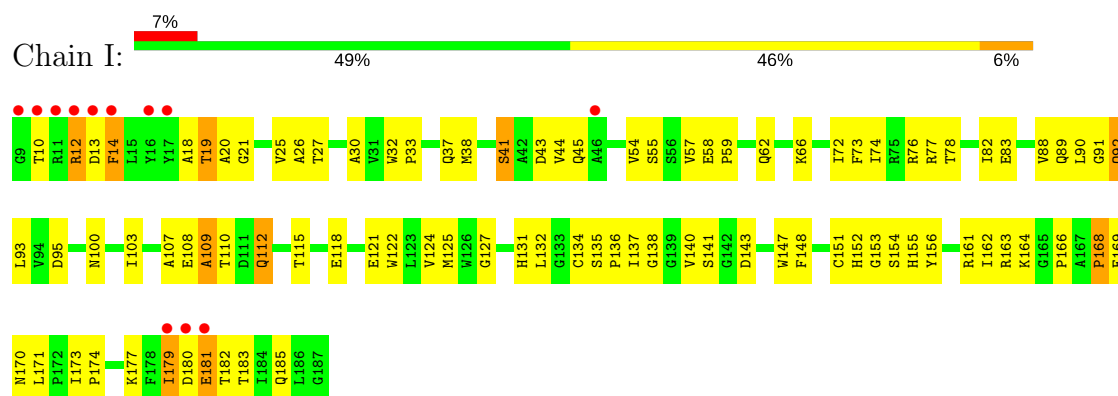




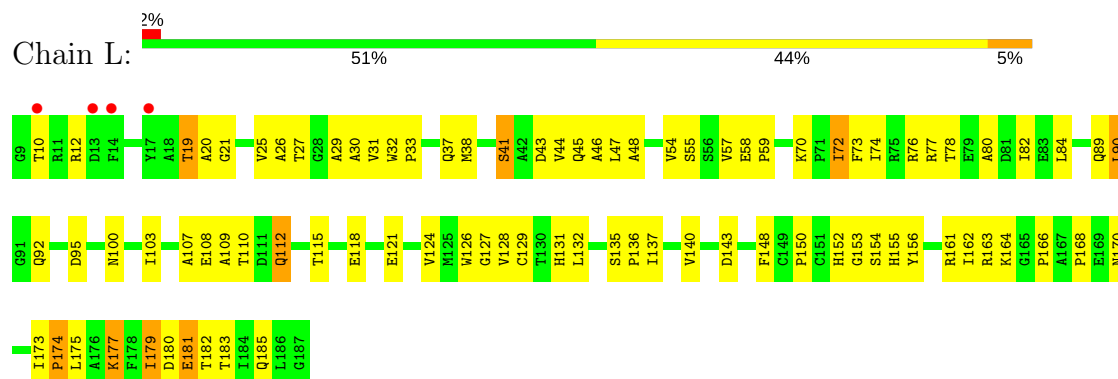
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



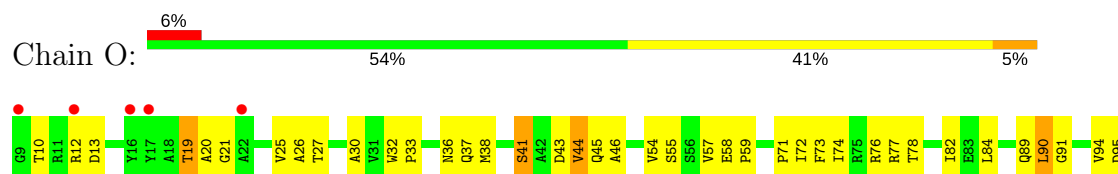
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

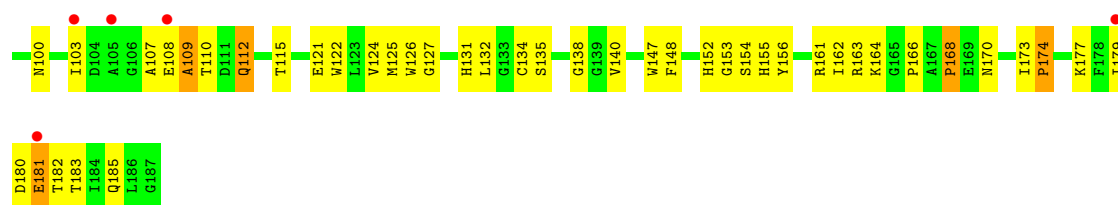


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

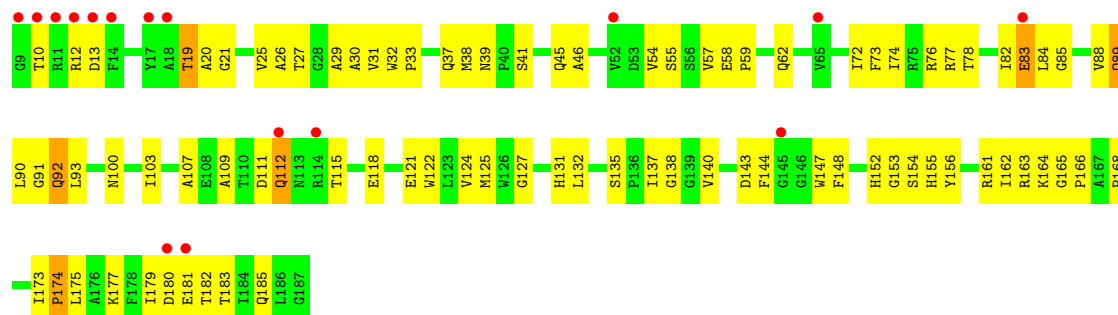


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit





● 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, $\alpha$ , $\beta$ , $\gamma$	352.29Å 147.40Å 160.76Å 90.00° 104.13° 90.00°	Depositor
Resolution (Å)	18.00 – 3.10 44.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (18.00-3.10) 96.1 (44.00-3.05)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.266 0.237 , 0.259	Depositor DCC
$R_{free}$ test set	2706 reflections (1.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 66.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	42048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SR, BGL, ANJ, LOP, FES, HEM, 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	0.59	0/3570	0.73	0/4897
1	D	0.59	0/3570	0.73	1/4897 (0.0%)
1	G	0.57	0/3570	0.72	0/4897
1	J	0.58	0/3570	0.73	0/4897
1	M	0.56	0/3570	0.73	0/4897
1	P	0.57	0/3570	0.72	0/4897
2	B	0.50	0/2010	0.71	1/2733 (0.0%)
2	E	0.50	0/2010	0.70	0/2733
2	H	0.52	0/2010	0.72	1/2733 (0.0%)
2	K	0.48	0/2010	0.69	1/2733 (0.0%)
2	N	0.49	0/2010	0.71	0/2733
2	Q	0.47	0/2010	0.70	0/2733
3	C	0.66	1/1370 (0.1%)	0.86	4/1866 (0.2%)
3	F	0.70	1/1370 (0.1%)	0.83	1/1866 (0.1%)
3	I	0.66	1/1370 (0.1%)	0.86	4/1866 (0.2%)
3	L	0.70	2/1370 (0.1%)	0.82	2/1866 (0.1%)
3	O	0.67	2/1370 (0.1%)	0.83	4/1866 (0.2%)
3	R	0.63	2/1370 (0.1%)	0.83	2/1866 (0.1%)
All	All	0.58	9/41700 (0.0%)	0.74	21/56976 (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
1	A	0	1
1	G	0	1
1	J	0	1
1	P	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	181	GLU	CB-CG	-13.28	1.26	1.52
3	F	181	GLU	CB-CG	-12.17	1.29	1.52
3	L	181	GLU	CB-CG	-11.99	1.29	1.52
3	C	181	GLU	CB-CG	-10.97	1.31	1.52
3	I	181	GLU	CB-CG	-10.23	1.32	1.52
3	L	181	GLU	CG-CD	-7.49	1.40	1.51
3	R	181	GLU	CD-OE2	5.94	1.32	1.25
3	O	181	GLU	CG-CD	-5.65	1.43	1.51
3	R	181	GLU	CG-CD	-5.10	1.44	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	181	GLU	OE1-CD-OE2	9.52	134.72	123.30
3	C	181	GLU	CG-CD-OE2	-8.83	100.64	118.30
3	R	181	GLU	OE1-CD-OE2	7.79	132.65	123.30
3	L	181	GLU	OE1-CD-OE2	7.71	132.55	123.30
2	H	145	CYS	CA-CB-SG	-7.66	100.22	114.00
3	I	181	GLU	OE1-CD-OE2	7.26	132.01	123.30
3	O	181	GLU	CA-CB-CG	-7.03	97.94	113.40
3	O	181	GLU	CG-CD-OE2	-6.23	105.84	118.30
3	O	181	GLU	OE1-CD-OE2	6.13	130.66	123.30
3	F	181	GLU	OE1-CD-OE2	6.07	130.59	123.30
3	I	181	GLU	CA-CB-CG	-6.02	100.17	113.40
3	L	181	GLU	CG-CD-OE2	-5.85	106.61	118.30
3	C	181	GLU	CA-CB-CG	-5.61	101.06	113.40
3	I	181	GLU	CG-CD-OE2	-5.35	107.59	118.30
3	C	181	GLU	N-CA-C	5.31	125.35	111.00
3	O	181	GLU	N-CA-C	5.28	125.25	111.00
3	R	181	GLU	N-CA-C	5.21	125.06	111.00
2	K	137	GLY	N-CA-C	5.12	125.89	113.10
2	B	190	MET	CA-CB-CG	5.07	121.92	113.30
3	I	181	GLU	N-CA-C	5.03	124.59	111.00
1	D	306	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
1	G	199	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	J	199	TYR	Sidechain
1	P	199	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	190	0
1	D	3440	0	3428	199	0
1	G	3440	0	3428	209	0
1	J	3440	0	3428	215	0
1	M	3440	0	3428	217	0
1	P	3440	0	3428	203	0
2	B	1953	0	1848	89	0
2	E	1953	0	1848	94	0
2	H	1953	0	1848	83	0
2	K	1953	0	1848	92	0
2	N	1953	0	1848	95	0
2	Q	1953	0	1848	105	0
3	C	1340	0	1303	82	0
3	F	1340	0	1303	77	0
3	I	1340	0	1303	79	0
3	L	1340	0	1303	71	0
3	O	1340	0	1303	65	0
3	R	1340	0	1303	71	0
4	A	20	0	28	1	0
4	D	20	0	28	2	0
4	G	20	0	28	2	0
4	J	20	0	28	0	0
4	M	20	0	28	2	0
4	Q	20	0	28	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0
5	Q	1	0	0	0	0
6	A	86	0	60	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	43	0	30	6	0
6	D	86	0	60	14	0
6	E	43	0	30	2	0
6	G	86	0	60	12	0
6	H	43	0	30	1	0
6	J	86	0	60	12	0
6	K	43	0	30	2	0
6	M	86	0	60	6	0
6	N	43	0	30	0	0
6	P	86	0	60	17	0
6	Q	43	0	30	1	0
7	C	4	0	0	2	0
7	F	4	0	0	2	0
7	I	4	0	0	2	0
7	L	4	0	0	2	0
7	O	4	0	0	2	0
7	R	4	0	0	3	0
8	A	37	0	42	6	0
8	D	37	0	42	3	0
8	G	37	0	42	6	0
8	J	37	0	42	4	0
8	M	37	0	42	3	0
8	P	37	0	42	4	0
9	A	45	0	67	5	0
9	D	45	0	67	3	0
9	G	45	0	67	4	0
9	J	45	0	67	3	0
9	M	45	0	67	7	0
9	P	45	0	67	4	0
10	A	39	0	40	7	0
10	D	39	0	39	7	0
10	G	39	0	39	7	0
10	J	39	0	40	7	0
10	M	39	0	39	6	0
10	P	39	0	39	7	0
All	All	42048	0	41072	2117	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 25.

All (2117) 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:B:103:MET:HE3	6:B:301:HEM:HAA2	1.33	1.09
2:K:250:ARG:CZ	3:L:12:ARG:HB3	1.85	1.04
1:J:236:GLU:HA	1:J:239:LYS:HD3	1.37	1.03
3:C:143:ASP:HA	3:L:89:GLN:HE21	1.24	1.01
1:M:200:LEU:HD22	1:P:63:ILE:HD13	1.41	1.01
2:E:138:PHE:CD2	2:E:187:PRO:HG3	1.95	1.01
1:A:200:LEU:HD22	1:D:63:ILE:HD13	1.40	0.99
1:G:63:ILE:HD13	1:J:200:LEU:HD22	1.46	0.97
1:P:33:ILE:HD11	1:P:249:ILE:HD11	1.48	0.96
1:G:195:PHE:HE2	1:J:195:PHE:HE2	1.11	0.94
1:M:63:ILE:HD13	1:P:200:LEU:HD22	1.47	0.94
1:A:195:PHE:HE2	1:D:195:PHE:HE2	1.01	0.94
1:J:33:ILE:HD11	1:J:249:ILE:HD11	1.46	0.94
1:M:33:ILE:HD11	1:M:249:ILE:HD11	1.48	0.93
1:G:33:ILE:HD11	1:G:249:ILE:HD11	1.47	0.93
1:A:63:ILE:HD13	1:D:200:LEU:HD22	1.48	0.93
1:M:195:PHE:HE2	1:P:195:PHE:HE2	1.06	0.92
1:G:294:PRO:HA	8:G:503:SMA:H10	1.52	0.91
1:M:329:LYS:HE3	3:R:131:HIS:O	1.71	0.91
1:D:294:PRO:HA	8:D:2:SMA:H10	1.53	0.91
2:B:223:LEU:HD21	2:B:227:LYS:HE3	1.54	0.90
1:G:248:PHE:HD1	1:G:251:LYS:HD3	1.36	0.90
2:N:138:PHE:CD2	2:N:187:PRO:HG3	2.06	0.90
1:A:33:ILE:HD11	1:A:249:ILE:HD11	1.52	0.89
1:D:33:ILE:HD11	1:D:249:ILE:HD11	1.52	0.89
1:G:200:LEU:HD22	1:J:63:ILE:HD13	1.56	0.87
3:R:89:GLN:HB2	3:R:92:GLN:HG2	1.58	0.86
2:E:250:ARG:HD3	3:F:12:ARG:CD	2.06	0.85
1:D:39:ARG:HH12	2:E:255:VAL:HG12	1.41	0.85
2:K:250:ARG:NE	3:L:12:ARG:HB3	1.90	0.84
2:K:77:THR:HG22	2:K:79:GLU:H	1.42	0.84
1:A:195:PHE:CE2	1:D:195:PHE:HE2	1.93	0.84
1:J:125:ARG:CZ	1:J:222:ASN:HB2	2.07	0.84
2:Q:138:PHE:CD2	2:Q:187:PRO:HG3	2.12	0.84
1:G:236:GLU:HA	1:G:239:LYS:HD3	1.58	0.83
1:J:294:PRO:HA	8:J:503:SMA:H10	1.58	0.83
1:P:39:ARG:HH12	2:Q:255:VAL:HG12	1.44	0.83
2:Q:142:PRO:HG2	2:Q:150:GLU:OE2	1.77	0.83
1:J:142:THR:HG21	6:J:502:HEM:HBB2	1.59	0.82
2:K:128:PRO:HG2	2:K:129:GLU:OE1	1.80	0.82
1:A:195:PHE:HE2	1:D:195:PHE:CE2	1.94	0.81
1:P:418:VAL:HG12	1:P:419:ALA:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:LEU:HD13	9:G:504:LOP:H212	1.61	0.81
2:K:250:ARG:NH2	3:L:12:ARG:HB3	1.95	0.81
3:R:74:ILE:HG12	3:R:124:VAL:HG22	1.63	0.81
2:H:128:PRO:HG2	2:H:129:GLU:OE1	1.80	0.80
1:G:39:ARG:HD3	1:G:428:PHE:CD2	2.16	0.80
2:K:74:ASP:HB3	2:K:77:THR:HB	1.62	0.80
1:D:246:PRO:HG2	2:E:251:LEU:HD21	1.62	0.80
1:G:410:ILE:HG23	1:G:414:ILE:HD12	1.63	0.80
1:G:125:ARG:CZ	1:G:222:ASN:HB2	2.12	0.79
2:N:149:HIS:CE1	2:N:168:THR:HG21	2.17	0.79
2:E:74:ASP:HB3	2:E:77:THR:HB	1.64	0.79
3:F:74:ILE:HG12	3:F:124:VAL:HG22	1.64	0.79
1:M:195:PHE:HE2	1:P:195:PHE:CE2	1.97	0.79
1:M:195:PHE:CE2	1:P:195:PHE:HE2	1.96	0.79
1:D:406:VAL:O	1:D:409:PRO:HD2	1.83	0.79
1:P:294:PRO:HA	8:P:503:SMA:H10	1.64	0.78
1:G:76:ALA:O	1:G:79:SER:HB3	1.84	0.78
1:J:105:PHE:O	1:J:108:VAL:HG23	1.82	0.78
2:N:128:PRO:HG2	2:N:129:GLU:OE1	1.82	0.78
1:D:236:GLU:HA	1:D:239:LYS:HD3	1.63	0.78
2:E:250:ARG:HD3	3:F:12:ARG:NE	1.99	0.78
3:I:89:GLN:H	3:I:92:GLN:HE21	1.31	0.78
3:L:89:GLN:HB2	3:L:92:GLN:HG3	1.65	0.78
1:P:418:VAL:HG12	1:P:419:ALA:N	1.98	0.77
1:G:213:ILE:HA	1:G:216:PHE:CE2	2.20	0.77
3:I:90:LEU:HD11	3:I:108:GLU:HB3	1.65	0.77
3:O:74:ILE:HG12	3:O:124:VAL:HG22	1.67	0.77
1:D:418:VAL:HG12	1:D:419:ALA:N	2.00	0.77
1:G:39:ARG:HH12	2:H:255:VAL:HG12	1.49	0.77
1:G:248:PHE:CD1	1:G:251:LYS:HD3	2.18	0.77
2:B:147:GLU:O	2:B:147:GLU:HG3	1.85	0.77
1:D:30:TYR:CE1	1:D:34:MET:HG3	2.21	0.76
10:P:505:ANJ:O6	10:P:505:ANJ:C12	2.33	0.76
1:G:410:ILE:CG2	1:G:414:ILE:HD12	2.16	0.76
2:Q:61:ASP:HA	2:Q:64:ARG:NH1	2.00	0.76
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.20	0.76
1:P:199:TYR:CE2	6:P:502:HEM:HBC1	2.21	0.76
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.21	0.76
1:A:91:PHE:CE1	1:A:92:MET:HG2	2.20	0.76
2:E:142:PRO:HG2	2:E:150:GLU:OE2	1.86	0.75
3:L:74:ILE:HG12	3:L:124:VAL:HG22	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:213:ILE:HA	1:J:216:PHE:CE2	2.21	0.75
3:I:74:ILE:HG12	3:I:124:VAL:HG22	1.68	0.75
1:M:213:ILE:HA	1:M:216:PHE:CE2	2.22	0.75
1:M:406:VAL:O	1:M:409:PRO:HD2	1.86	0.75
2:E:108:ALA:HA	2:E:125:ILE:HG22	1.69	0.75
1:M:236:GLU:HA	1:M:239:LYS:HD3	1.67	0.75
2:E:77:THR:HG22	2:E:79:GLU:H	1.52	0.74
2:Q:61:ASP:HA	2:Q:64:ARG:HH12	1.49	0.74
3:C:74:ILE:HG12	3:C:124:VAL:HG22	1.68	0.74
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.02	0.74
2:Q:128:PRO:HG2	2:Q:129:GLU:OE1	1.86	0.74
3:O:95:ASP:HB3	3:O:170:ASN:ND2	2.00	0.74
1:J:199:TYR:HA	6:J:502:HEM:HBC2	1.69	0.74
1:P:55:LEU:HD23	10:P:505:ANJ:H281	1.67	0.74
8:A:1:SMA:H33	8:A:1:SMA:H39	1.68	0.73
1:J:406:VAL:O	1:J:409:PRO:HD2	1.87	0.73
1:J:59:ILE:O	1:J:63:ILE:HG13	1.88	0.73
10:M:505:ANJ:C12	10:M:505:ANJ:O6	2.37	0.73
2:B:184:ALA:HB3	6:B:301:HEM:HBD2	1.71	0.73
2:B:250:ARG:NE	3:C:12:ARG:HB2	2.03	0.73
1:M:76:ALA:O	1:M:79:SER:HB3	1.88	0.73
1:J:76:ALA:O	1:J:79:SER:HB3	1.88	0.73
1:P:213:ILE:HA	1:P:216:PHE:CE2	2.23	0.73
10:D:504:ANJ:C12	10:D:504:ANJ:O6	2.37	0.73
2:N:220:GLU:OE2	2:N:226:ARG:NH1	2.22	0.72
2:B:250:ARG:HE	3:C:12:ARG:HB2	1.54	0.72
2:N:250:ARG:NE	3:O:12:ARG:HB2	2.04	0.72
1:G:195:PHE:HE2	1:J:195:PHE:CE2	2.03	0.72
2:Q:48:ARG:HH11	2:Q:48:ARG:HG3	1.53	0.72
1:J:91:PHE:HE1	1:J:92:MET:HE3	1.54	0.72
1:P:59:ILE:O	1:P:63:ILE:HG13	1.90	0.72
10:A:504:ANJ:C12	10:A:504:ANJ:O6	2.36	0.72
1:G:387:PHE:CD1	1:G:388:PRO:HA	2.25	0.72
1:D:76:ALA:O	1:D:79:SER:HB3	1.89	0.72
1:G:317:ILE:O	1:G:321:ILE:HG13	1.90	0.71
10:J:505:ANJ:O6	10:J:505:ANJ:C12	2.37	0.71
8:P:503:SMA:H33	8:P:503:SMA:H39	1.71	0.71
2:E:66:TYR:O	2:E:69:GLN:HG2	1.91	0.71
1:A:76:ALA:O	1:A:79:SER:HB3	1.90	0.71
1:A:294:PRO:HA	8:A:1:SMA:H10	1.72	0.71
2:H:48:ARG:HH11	2:H:48:ARG:HG3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:66:TYR:O	2:K:69:GLN:HG2	1.90	0.71
1:P:236:GLU:HA	1:P:239:LYS:HD3	1.71	0.71
10:G:505:ANJ:O6	10:G:505:ANJ:C12	2.37	0.71
1:G:92:MET:HE2	1:G:92:MET:HA	1.72	0.71
1:J:4:ILE:N	1:J:4:ILE:HD12	2.06	0.71
6:D:502:HEM:HBB2	6:D:502:HEM:CMB	2.20	0.71
1:J:358:ARG:HH21	9:J:504:LOP:H21	1.56	0.71
1:M:105:PHE:O	1:M:108:VAL:HG23	1.91	0.71
1:J:105:PHE:HA	1:J:108:VAL:CG2	2.20	0.70
1:J:312:VAL:O	1:J:316:GLN:HG3	1.89	0.70
2:N:48:ARG:HH11	2:N:48:ARG:HG3	1.53	0.70
1:M:317:ILE:HG22	1:M:321:ILE:HD11	1.72	0.70
1:M:59:ILE:O	1:M:63:ILE:HG13	1.91	0.70
2:B:103:MET:CE	6:B:301:HEM:HAA2	2.18	0.70
1:P:326:ILE:HG22	1:P:326:ILE:O	1.91	0.70
1:P:76:ALA:O	1:P:79:SER:HB3	1.91	0.70
1:D:360:ARG:O	1:D:364:LYS:HG3	1.92	0.70
1:A:263:PHE:O	1:A:267:VAL:HG23	1.92	0.70
2:B:250:ARG:NH2	3:C:12:ARG:HB3	2.07	0.70
1:G:213:ILE:CD1	10:G:505:ANJ:H14	2.22	0.70
1:A:39:ARG:HH12	2:B:255:VAL:HG12	1.57	0.69
3:O:55:SER:HB3	3:O:182:THR:OG1	1.91	0.69
1:A:408:LEU:HB2	1:A:409:PRO:HD3	1.73	0.69
1:D:263:PHE:O	1:D:267:VAL:HG23	1.92	0.69
2:H:146:ALA:HB2	2:H:169:CYS:SG	2.32	0.69
1:A:213:ILE:CD1	10:A:504:ANJ:H14	2.22	0.69
3:R:124:VAL:O	3:R:173:ILE:HG23	1.91	0.69
2:H:141:GLU:HG3	2:H:141:GLU:O	1.93	0.69
1:A:372:ALA:O	1:A:376:ILE:HG13	1.93	0.69
1:D:43:TRP:CZ3	1:D:251:LYS:HE3	2.27	0.69
2:E:138:PHE:HD2	2:E:187:PRO:HG3	1.51	0.69
1:J:39:ARG:HG2	1:J:242:VAL:HG13	1.75	0.69
3:O:138:GLY:CA	3:O:147:TRP:CD1	2.75	0.69
3:F:55:SER:HB3	3:F:182:THR:OG1	1.93	0.69
1:M:326:ILE:HG22	1:M:326:ILE:O	1.91	0.69
3:F:124:VAL:O	3:F:173:ILE:HG23	1.92	0.69
2:K:77:THR:HG22	2:K:79:GLU:N	2.07	0.69
1:M:105:PHE:HA	1:M:108:VAL:CG2	2.23	0.69
1:M:108:VAL:O	1:M:112:ILE:HG13	1.92	0.69
1:A:291:HIS:O	1:A:293:VAL:HG23	1.93	0.69
1:G:52:ALA:HB2	10:G:505:ANJ:H163	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:66:TYR:HE1	2:N:70:PHE:HE2	1.41	0.68
1:A:73:VAL:HG22	1:A:188:ASN:OD1	1.93	0.68
1:D:132:GLY:C	6:D:501:HEM:HBC2	2.14	0.68
3:F:84:LEU:H	3:F:84:LEU:HD12	1.57	0.68
3:F:93:LEU:HD13	3:F:161:ARG:HD2	1.74	0.68
1:M:156:PHE:CE2	1:M:285:PRO:HA	2.29	0.68
3:R:89:GLN:O	3:R:91:GLY:N	2.25	0.68
2:N:156:TYR:HB2	2:N:182:TRP:CZ2	2.28	0.68
2:Q:223:LEU:HD21	2:Q:227:LYS:HE3	1.76	0.68
3:R:55:SER:HB3	3:R:182:THR:OG1	1.93	0.68
4:D:431:BGL:H5	2:E:15:GLY:H	1.56	0.68
1:G:39:ARG:HG2	1:G:242:VAL:HG13	1.76	0.68
1:A:280:TYR:CZ	2:B:105:LYS:HD2	2.29	0.68
1:G:59:ILE:O	1:G:63:ILE:HG13	1.93	0.68
1:P:39:ARG:HH12	2:Q:255:VAL:CG1	2.05	0.68
3:R:84:LEU:O	3:R:88:VAL:HG23	1.93	0.68
2:H:145:CYS:SG	2:H:145:CYS:O	2.49	0.68
2:B:48:ARG:HG3	2:B:48:ARG:HH11	1.59	0.67
1:P:105:PHE:HA	1:P:108:VAL:HG22	1.74	0.67
1:J:105:PHE:HA	1:J:108:VAL:HG23	1.75	0.67
1:J:91:PHE:CE1	1:J:92:MET:HE3	2.28	0.67
1:P:30:TYR:CE1	1:P:34:MET:HG3	2.29	0.67
2:N:138:PHE:HD2	2:N:187:PRO:HG3	1.58	0.67
1:G:209:VAL:HG22	6:G:501:HEM:HBB2	1.76	0.67
3:L:55:SER:HB3	3:L:182:THR:OG1	1.95	0.67
2:Q:89:PHE:HB3	2:Q:90:PRO:HD2	1.75	0.67
1:M:164:GLY:HA2	1:M:177:GLN:NE2	2.09	0.67
2:E:72:VAL:HG12	2:E:73:THR:N	2.10	0.67
1:G:4:ILE:N	1:G:4:ILE:HD12	2.09	0.67
1:P:291:HIS:O	1:P:293:VAL:HG23	1.94	0.67
1:A:166:PHE:O	1:A:169:ILE:HD12	1.94	0.67
1:A:330:PHE:CE2	1:A:334:LEU:HD11	2.30	0.67
1:A:406:VAL:O	1:A:409:PRO:HD2	1.95	0.67
1:D:39:ARG:HG2	1:D:242:VAL:HG13	1.76	0.67
3:I:55:SER:HB3	3:I:182:THR:OG1	1.93	0.67
2:K:48:ARG:HG3	2:K:48:ARG:HH11	1.58	0.67
2:Q:242:VAL:O	2:Q:246:LEU:HG	1.95	0.67
3:I:124:VAL:O	3:I:173:ILE:HG23	1.95	0.67
2:N:242:VAL:O	2:N:246:LEU:HG	1.94	0.67
1:A:236:GLU:HA	1:A:239:LYS:HG3	1.75	0.67
2:E:48:ARG:HH11	2:E:48:ARG:HG3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:124:VAL:O	3:L:173:ILE:HG23	1.94	0.67
1:P:128:THR:HG21	6:P:501:HEM:HBD1	1.77	0.67
1:D:59:ILE:O	1:D:63:ILE:HG13	1.94	0.66
1:A:39:ARG:HG2	1:A:242:VAL:HG13	1.78	0.66
1:A:418:VAL:HG12	1:A:419:ALA:N	2.09	0.66
1:J:263:PHE:O	1:J:267:VAL:HG23	1.95	0.66
1:J:30:TYR:CE1	1:J:34:MET:HG3	2.31	0.66
1:M:418:VAL:HG12	1:M:419:ALA:H	1.59	0.66
3:O:124:VAL:O	3:O:173:ILE:HG23	1.95	0.66
2:K:139:PRO:HB3	2:K:158:ARG:NH1	2.10	0.66
1:G:286:LEU:O	1:G:287:ARG:HG3	1.96	0.66
3:C:55:SER:HB3	3:C:182:THR:OG1	1.95	0.66
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.29	0.66
1:M:39:ARG:HG2	1:M:242:VAL:HG13	1.77	0.66
1:P:39:ARG:HG2	1:P:242:VAL:HG13	1.78	0.66
1:J:418:VAL:HG12	1:J:419:ALA:N	2.10	0.66
2:K:138:PHE:CD1	2:K:187:PRO:HG3	2.31	0.66
1:M:117:TYR:HB2	1:M:367:PHE:CZ	2.31	0.66
1:D:105:PHE:HA	1:D:108:VAL:HG22	1.77	0.66
1:D:128:THR:HG21	6:D:501:HEM:HBD1	1.78	0.65
1:G:105:PHE:HA	1:G:108:VAL:CG2	2.26	0.65
1:M:418:VAL:HG12	1:M:419:ALA:N	2.10	0.65
1:P:117:TYR:HB2	1:P:367:PHE:CZ	2.31	0.65
1:P:406:VAL:O	1:P:409:PRO:HD2	1.95	0.65
3:R:89:GLN:C	3:R:91:GLY:H	1.97	0.65
1:J:166:PHE:O	1:J:169:ILE:HD12	1.96	0.65
1:J:39:ARG:HH12	2:K:255:VAL:HG12	1.60	0.65
3:R:155:HIS:O	3:R:162:ILE:HD12	1.96	0.65
3:C:19:THR:HG22	3:C:20:ALA:N	2.11	0.65
1:G:263:PHE:O	1:G:267:VAL:HG23	1.96	0.65
1:D:418:VAL:HG12	1:D:419:ALA:H	1.61	0.65
1:G:330:PHE:CE2	1:G:334:LEU:HD11	2.32	0.65
1:G:39:ARG:HH12	2:H:255:VAL:CG1	2.09	0.65
3:F:54:VAL:O	3:F:54:VAL:HG22	1.97	0.65
1:M:123:ALA:O	1:M:355:ARG:NH1	2.30	0.65
1:M:425:GLU:HG2	1:M:429:ASN:HD21	1.60	0.65
1:P:406:VAL:C	1:P:409:PRO:HD2	2.17	0.65
3:R:138:GLY:HA2	3:R:147:TRP:CD1	2.31	0.65
1:A:312:VAL:O	1:A:315:VAL:HB	1.97	0.65
1:J:418:VAL:CG1	1:J:419:ALA:N	2.58	0.65
2:K:108:ALA:HA	2:K:125:ILE:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:263:PHE:O	1:P:267:VAL:HG23	1.95	0.65
1:D:73:VAL:HG22	1:D:188:ASN:OD1	1.96	0.65
1:G:4:ILE:H	1:G:4:ILE:HD12	1.60	0.65
3:I:131:HIS:O	1:J:329:LYS:HE3	1.97	0.65
1:M:294:PRO:HA	8:M:503:SMA:H10	1.78	0.65
2:Q:47:ILE:HG13	2:Q:87:ASP:O	1.96	0.65
2:B:74:ASP:HB2	2:B:81:ARG:HE	1.62	0.65
2:E:17:PHE:CE1	2:E:231:PHE:HE1	2.14	0.65
1:M:236:GLU:HA	1:M:239:LYS:CD	2.26	0.65
1:A:59:ILE:O	1:A:63:ILE:HG13	1.97	0.65
1:D:4:ILE:HD12	1:D:4:ILE:N	2.12	0.65
3:F:37:GLN:NE2	3:F:38:MET:HG3	2.12	0.65
2:N:47:ILE:HG13	2:N:87:ASP:O	1.97	0.65
1:D:164:GLY:HA2	1:D:177:GLN:NE2	2.12	0.64
1:D:326:ILE:O	1:D:326:ILE:HG22	1.97	0.64
1:G:166:PHE:O	1:G:169:ILE:HD12	1.97	0.64
1:J:330:PHE:CE2	1:J:334:LEU:HD11	2.32	0.64
1:A:193:ARG:HH11	3:F:38:MET:HE2	1.61	0.64
1:D:166:PHE:O	1:D:169:ILE:HD12	1.97	0.64
1:D:372:ALA:O	1:D:376:ILE:HG13	1.97	0.64
2:E:146:ALA:HB2	2:E:169:CYS:SG	2.37	0.64
1:A:193:ARG:HD3	3:F:38:MET:HE3	1.79	0.64
1:A:105:PHE:HA	1:A:108:VAL:HG12	1.79	0.64
1:D:291:HIS:O	1:D:293:VAL:HG23	1.97	0.64
1:A:30:TYR:CE1	1:A:34:MET:HG3	2.32	0.64
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.31	0.64
2:N:149:HIS:ND1	2:N:168:THR:HG21	2.13	0.64
2:E:250:ARG:HD3	3:F:12:ARG:HD2	1.79	0.64
1:M:234:LYS:O	1:M:238:GLN:HG3	1.97	0.64
1:G:291:HIS:O	1:G:293:VAL:HG23	1.97	0.64
1:J:117:TYR:HB2	1:J:367:PHE:CZ	2.33	0.64
2:K:48:ARG:HB3	2:K:85:PRO:O	1.98	0.64
1:M:263:PHE:O	1:M:267:VAL:HG23	1.97	0.64
1:P:418:VAL:CG1	1:P:419:ALA:H	2.11	0.64
2:Q:220:GLU:OE2	2:Q:226:ARG:NH1	2.30	0.64
1:A:319:ASN:HD22	1:A:319:ASN:C	2.00	0.64
1:G:418:VAL:HG12	1:G:419:ALA:N	2.13	0.64
2:N:51:SER:OG	2:N:63:VAL:HG21	1.98	0.64
1:G:117:TYR:HB2	1:G:367:PHE:CZ	2.32	0.64
1:G:326:ILE:O	1:G:326:ILE:HG22	1.97	0.64
1:J:104:PHE:O	1:J:108:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:155:HIS:O	3:L:162:ILE:HD12	1.98	0.64
3:O:138:GLY:HA2	3:O:147:TRP:CD1	2.33	0.64
1:A:144:PHE:HE2	8:A:1:SMA:H43	1.63	0.63
1:J:291:HIS:O	1:J:293:VAL:HG23	1.98	0.63
1:M:291:HIS:O	1:M:293:VAL:HG23	1.98	0.63
1:A:326:ILE:HG22	1:A:326:ILE:O	1.97	0.63
3:L:54:VAL:HG22	3:L:54:VAL:O	1.97	0.63
1:J:306:ARG:NH2	1:J:383:GLN:O	2.27	0.63
1:D:51:LEU:HD21	1:D:108:VAL:HG13	1.79	0.63
1:M:408:LEU:HB2	1:M:409:PRO:HD3	1.81	0.63
10:A:504:ANJ:O6	10:A:504:ANJ:O4	2.16	0.63
3:I:155:HIS:O	3:I:162:ILE:HD12	1.99	0.63
3:C:131:HIS:O	1:D:329:LYS:HE3	1.98	0.63
1:M:64:VAL:HG11	1:M:93:LEU:HD13	1.81	0.63
1:A:108:VAL:HG22	1:A:112:ILE:HD11	1.80	0.63
1:P:156:PHE:CE2	1:P:285:PRO:HA	2.33	0.63
1:A:105:PHE:O	1:A:108:VAL:HG12	1.98	0.63
1:G:39:ARG:HH11	1:G:428:PHE:HE2	1.45	0.63
1:P:376:ILE:O	1:P:380:VAL:HG22	1.99	0.63
2:Q:171:ASP:OD2	2:Q:175:VAL:HB	1.99	0.63
1:D:91:PHE:HE1	1:D:92:MET:HE3	1.64	0.62
2:E:128:PRO:HG2	2:E:129:GLU:OE1	1.99	0.62
3:O:90:LEU:HD11	3:O:108:GLU:HB3	1.81	0.62
1:P:158:GLY:O	1:P:162:ILE:HG13	1.98	0.62
1:P:44:MET:CE	9:P:504:LOP:H92	2.29	0.62
2:Q:114:MET:HG2	2:Q:114:MET:O	1.98	0.62
3:L:148:PHE:CE1	3:L:153:GLY:HA2	2.34	0.62
3:I:162:ILE:HD11	3:I:164:LYS:O	1.99	0.62
1:M:370:LEU:HD22	1:M:403:TYR:CE2	2.35	0.62
1:M:372:ALA:O	1:M:376:ILE:HG13	1.99	0.62
2:N:77:THR:HG22	2:N:79:GLU:H	1.65	0.62
1:A:108:VAL:O	1:A:112:ILE:HG13	1.99	0.62
2:K:42:MET:HE1	2:K:214:PHE:CZ	2.34	0.62
1:M:330:PHE:CE2	1:M:334:LEU:HD11	2.34	0.62
1:A:199:TYR:O	1:A:202:PRO:HD2	2.00	0.62
1:A:246:PRO:HG2	2:B:251:LEU:HD21	1.81	0.62
1:M:103:LEU:HD13	9:M:504:LOP:H222	1.82	0.62
6:P:502:HEM:O2D	6:P:502:HEM:O1A	2.17	0.62
3:R:148:PHE:CE1	3:R:153:GLY:HA2	2.35	0.62
1:J:180:LEU:HD13	8:J:503:SMA:H25	1.81	0.62
1:M:410:ILE:CG2	1:M:414:ILE:HD12	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:505:ANJ:O4	10:M:505:ANJ:O6	2.18	0.62
1:A:117:TYR:HB2	1:A:367:PHE:CZ	2.35	0.62
1:G:313:TRP:O	1:G:317:ILE:HG13	1.98	0.62
1:J:326:ILE:O	1:J:326:ILE:HG22	2.00	0.62
1:J:213:ILE:CD1	10:J:505:ANJ:H14	2.30	0.62
2:N:66:TYR:O	2:N:69:GLN:HG2	1.99	0.62
3:R:54:VAL:HG22	3:R:54:VAL:O	1.99	0.62
2:N:66:TYR:CE1	2:N:70:PHE:HE2	2.17	0.61
3:O:54:VAL:O	3:O:54:VAL:HG22	1.99	0.61
2:E:171:ASP:OD2	2:E:175:VAL:HB	2.00	0.61
3:F:137:ILE:HD13	3:F:150:PRO:HD3	1.81	0.61
2:N:48:ARG:HB3	2:N:85:PRO:O	2.00	0.61
1:G:105:PHE:O	1:G:108:VAL:HG23	1.99	0.61
3:I:19:THR:HG22	3:I:20:ALA:N	2.15	0.61
3:C:127:GLY:O	3:C:135:SER:HA	2.00	0.61
3:C:54:VAL:O	3:C:54:VAL:HG22	1.99	0.61
1:D:39:ARG:HH12	2:E:255:VAL:CG1	2.11	0.61
1:G:64:VAL:HG11	1:G:93:LEU:HD13	1.81	0.61
2:K:160:PHE:CD2	2:K:183:ILE:HB	2.35	0.61
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.35	0.61
1:G:372:ALA:O	1:G:376:ILE:HG13	1.99	0.61
1:J:199:TYR:CE2	6:J:502:HEM:HBC1	2.36	0.61
1:J:64:VAL:HG11	1:J:93:LEU:HD13	1.82	0.61
2:K:242:VAL:O	2:K:246:LEU:HG	2.01	0.61
1:P:213:ILE:CD1	10:P:505:ANJ:H14	2.31	0.61
1:A:418:VAL:CG1	1:A:419:ALA:N	2.63	0.61
1:A:8:HIS:CD2	1:A:8:HIS:H	2.18	0.61
1:D:376:ILE:O	1:D:380:VAL:HG22	2.01	0.61
2:E:61:ASP:HA	2:E:64:ARG:NH1	2.14	0.61
2:K:32:TYR:CE2	2:K:42:MET:HE3	2.35	0.61
3:C:80:ALA:O	3:C:84:LEU:HD13	2.00	0.61
1:J:132:GLY:C	6:J:501:HEM:HBC2	2.21	0.61
3:I:62:GLN:NE2	3:I:73:PHE:CG	2.68	0.61
1:A:118:TYR:OH	9:A:503:LOP:H32	2.01	0.61
1:A:4:ILE:HD12	1:A:4:ILE:H	1.66	0.61
1:P:199:TYR:CD2	6:P:502:HEM:HBC1	2.36	0.61
3:R:19:THR:HG22	3:R:20:ALA:N	2.15	0.61
2:B:146:ALA:HB2	2:B:169:CYS:SG	2.41	0.61
10:D:504:ANJ:O4	10:D:504:ANJ:O6	2.19	0.61
1:A:193:ARG:HH11	3:F:38:MET:CE	2.14	0.61
1:J:234:LYS:O	1:J:238:GLN:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:64:VAL:HG11	1:P:93:LEU:HD13	1.82	0.61
3:I:95:ASP:HB3	3:I:170:ASN:ND2	2.16	0.60
2:E:48:ARG:HB3	2:E:85:PRO:O	2.00	0.60
3:L:19:THR:HG22	3:L:20:ALA:N	2.14	0.60
1:A:73:VAL:HG23	1:A:74:ASP:H	1.65	0.60
2:K:139:PRO:HB3	2:K:158:ARG:HH12	1.64	0.60
3:C:155:HIS:O	3:C:162:ILE:HD12	2.02	0.60
3:C:124:VAL:O	3:C:173:ILE:HG23	2.01	0.60
1:D:91:PHE:CD2	2:E:222:LYS:HG2	2.36	0.60
1:G:92:MET:HE2	1:G:92:MET:CA	2.28	0.60
2:H:77:THR:C	2:H:79:GLU:H	2.04	0.60
1:J:322:SER:O	1:J:323:PHE:HB2	2.02	0.60
1:M:199:TYR:O	1:M:202:PRO:HD2	2.02	0.60
1:M:60:VAL:CG2	1:M:61:THR:N	2.65	0.60
2:N:66:TYR:CE1	2:N:70:PHE:CE2	2.90	0.60
2:N:66:TYR:HE1	2:N:70:PHE:CE2	2.18	0.60
3:C:148:PHE:CE1	3:C:153:GLY:HA2	2.37	0.60
1:G:411:LEU:HD22	1:G:415:GLU:HB2	1.84	0.60
1:P:166:PHE:O	1:P:169:ILE:HD12	2.01	0.60
1:D:312:VAL:O	1:D:316:GLN:HG3	2.00	0.60
1:D:213:ILE:CD1	10:D:504:ANJ:H14	2.32	0.60
1:G:418:VAL:CG1	1:G:419:ALA:N	2.64	0.60
2:H:48:ARG:HB3	2:H:85:PRO:O	2.02	0.60
1:A:4:ILE:HD12	1:A:4:ILE:N	2.16	0.60
2:B:17:PHE:CE1	2:B:231:PHE:CE1	2.90	0.60
3:I:54:VAL:HG22	3:I:54:VAL:O	2.02	0.60
1:J:51:LEU:HD13	6:J:501:HEM:C3B	2.37	0.60
1:D:29:ALA:HB2	10:D:504:ANJ:H233	1.84	0.60
1:G:156:PHE:CE2	1:G:285:PRO:HA	2.36	0.60
3:I:12:ARG:HG2	3:I:13:ASP:N	2.16	0.60
1:M:317:ILE:O	1:M:321:ILE:HG13	2.02	0.60
3:R:156:TYR:HA	3:R:161:ARG:O	2.02	0.60
2:K:77:THR:CG2	2:K:79:GLU:HB2	2.32	0.60
1:P:51:LEU:HD13	6:P:501:HEM:C3B	2.37	0.60
2:Q:48:ARG:HB3	2:Q:85:PRO:O	2.02	0.60
2:K:130:TYR:O	2:K:134:VAL:HG23	2.01	0.60
1:M:4:ILE:HD12	1:M:4:ILE:N	2.17	0.60
1:A:60:VAL:CG2	1:A:61:THR:N	2.64	0.59
2:B:184:ALA:HB3	6:B:301:HEM:CBD	2.31	0.59
2:E:17:PHE:CE1	2:E:231:PHE:CE1	2.90	0.59
1:J:213:ILE:HD11	10:J:505:ANJ:H162	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:505:ANJ:O4	10:P:505:ANJ:O6	2.20	0.59
1:D:117:TYR:HB2	1:D:367:PHE:CZ	2.36	0.59
1:D:199:TYR:O	1:D:202:PRO:HD2	2.01	0.59
1:D:418:VAL:CG1	1:D:419:ALA:N	2.65	0.59
3:I:148:PHE:CE1	3:I:153:GLY:HA2	2.36	0.59
1:M:91:PHE:CD1	1:M:92:MET:N	2.71	0.59
1:A:64:VAL:HG11	1:A:93:LEU:HD13	1.83	0.59
2:H:142:PRO:HG2	2:H:150:GLU:OE2	2.02	0.59
2:H:242:VAL:O	2:H:246:LEU:HG	2.02	0.59
1:P:199:TYR:O	1:P:202:PRO:HD2	2.01	0.59
3:R:89:GLN:C	3:R:91:GLY:N	2.56	0.59
1:A:125:ARG:NH1	1:A:220:GLY:O	2.35	0.59
1:D:330:PHE:CE2	1:D:334:LEU:HD11	2.37	0.59
2:H:130:TYR:O	2:H:134:VAL:HG23	2.02	0.59
3:R:10:THR:O	3:R:10:THR:HG22	2.02	0.59
1:A:91:PHE:CD1	1:A:92:MET:N	2.70	0.59
1:D:91:PHE:CD1	1:D:92:MET:N	2.71	0.59
1:J:73:VAL:HG22	1:J:188:ASN:OD1	2.03	0.59
1:M:213:ILE:CD1	10:M:505:ANJ:H14	2.32	0.59
1:P:370:LEU:HD22	1:P:403:TYR:CE2	2.38	0.59
3:F:148:PHE:CE1	3:F:153:GLY:HA2	2.38	0.59
2:K:40:HIS:HE1	2:K:98:PRO:HD2	1.67	0.59
1:M:39:ARG:HH12	2:N:255:VAL:HG12	1.67	0.59
3:O:37:GLN:NE2	3:O:38:MET:HG3	2.17	0.59
1:A:329:LYS:HE3	3:F:131:HIS:O	2.03	0.59
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.36	0.59
1:D:370:LEU:HD22	1:D:403:TYR:CE2	2.37	0.59
1:J:376:ILE:O	1:J:380:VAL:HG22	2.03	0.59
1:P:91:PHE:CD2	2:Q:222:LYS:HG2	2.38	0.59
1:A:52:ALA:HB2	10:A:504:ANJ:H163	1.83	0.59
3:I:89:GLN:O	3:I:92:GLN:N	2.36	0.59
1:J:199:TYR:O	1:J:202:PRO:HD2	2.03	0.59
2:K:42:MET:HE1	2:K:214:PHE:CE2	2.38	0.59
3:O:89:GLN:O	3:O:91:GLY:N	2.36	0.59
1:D:280:TYR:CE2	2:E:105:LYS:HD2	2.37	0.59
3:I:156:TYR:HA	3:I:161:ARG:O	2.03	0.59
1:J:164:GLY:HA2	1:J:177:GLN:NE2	2.18	0.59
1:M:376:ILE:O	1:M:380:VAL:HG22	2.02	0.59
3:O:148:PHE:CE1	3:O:153:GLY:HA2	2.38	0.59
3:C:152:HIS:HB2	7:C:200:FES:S1	2.43	0.58
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:54:VAL:HG23	3:F:57:VAL:HG21	1.84	0.58
1:G:102:SER:O	1:G:106:ILE:HG13	2.03	0.58
1:M:91:PHE:HE1	1:M:92:MET:HE3	1.68	0.58
1:P:114:ARG:C	1:P:114:ARG:HD2	2.23	0.58
2:B:74:ASP:HB2	2:B:81:ARG:NE	2.18	0.58
1:J:91:PHE:HE1	1:J:92:MET:CE	2.16	0.58
1:P:52:ALA:HB2	10:P:505:ANJ:H163	1.85	0.58
1:A:370:LEU:HD22	1:A:403:TYR:CE2	2.38	0.58
1:D:43:TRP:CH2	1:D:251:LYS:HE3	2.37	0.58
1:G:370:LEU:HD22	1:G:403:TYR:CE2	2.38	0.58
1:P:346:VAL:HG12	1:P:347:PRO:HD3	1.85	0.58
1:P:39:ARG:NH1	2:Q:255:VAL:HG12	2.15	0.58
2:B:48:ARG:HB3	2:B:85:PRO:O	2.03	0.58
3:F:19:THR:HG22	3:F:20:ALA:N	2.17	0.58
3:I:10:THR:O	3:I:10:THR:HG22	2.03	0.58
3:L:162:ILE:HD12	3:L:163:ARG:H	1.69	0.58
3:C:54:VAL:HG23	3:C:57:VAL:HG21	1.85	0.58
1:D:164:GLY:HA2	1:D:177:GLN:HE21	1.66	0.58
1:D:92:MET:HA	1:D:92:MET:HE2	1.83	0.58
3:F:78:THR:O	3:F:82:ILE:HG13	2.03	0.58
10:J:505:ANJ:O4	10:J:505:ANJ:O6	2.19	0.58
3:R:162:ILE:HD11	3:R:164:LYS:O	2.04	0.58
1:A:341:LEU:O	1:A:341:LEU:HD12	2.04	0.58
10:G:505:ANJ:O4	10:G:505:ANJ:O6	2.20	0.58
3:R:21:GLY:O	3:R:25:VAL:HG23	2.02	0.58
1:A:296:TRP:HA	1:A:299:LEU:HG	1.85	0.58
1:D:406:VAL:C	1:D:409:PRO:HD2	2.24	0.58
3:F:10:THR:HG22	3:F:10:THR:O	2.04	0.58
1:J:92:MET:HA	1:J:92:MET:HE2	1.86	0.58
2:K:80:ASP:O	2:K:81:ARG:HB3	2.03	0.58
3:O:155:HIS:O	3:O:162:ILE:HD12	2.04	0.58
1:P:330:PHE:CE2	1:P:334:LEU:HD11	2.38	0.58
1:P:372:ALA:O	1:P:376:ILE:HG13	2.03	0.58
1:A:51:LEU:HD13	6:A:501:HEM:C3B	2.39	0.58
1:A:91:PHE:CE1	1:A:92:MET:CG	2.86	0.58
3:C:10:THR:HG22	3:C:10:THR:O	2.03	0.58
2:E:130:TYR:O	2:E:134:VAL:HG23	2.04	0.58
1:G:30:TYR:CE1	1:G:34:MET:HG3	2.38	0.58
1:J:60:VAL:CG2	1:J:61:THR:N	2.66	0.58
2:N:250:ARG:NH2	3:O:12:ARG:HB3	2.19	0.58
1:P:346:VAL:CG1	1:P:347:PRO:HD3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:VAL:CG1	1:D:419:ALA:H	2.16	0.58
1:D:64:VAL:HG11	1:D:93:LEU:HD13	1.85	0.58
1:G:144:PHE:CE2	8:G:503:SMA:H42	2.38	0.58
1:G:199:TYR:O	1:G:202:PRO:HD2	2.04	0.58
1:G:60:VAL:CG2	1:G:61:THR:N	2.65	0.58
3:L:10:THR:O	3:L:10:THR:HG22	2.03	0.58
1:M:166:PHE:O	1:M:169:ILE:HD12	2.04	0.58
2:N:157:ASN:O	2:N:180:GLY:HA3	2.04	0.58
1:P:60:VAL:CG2	1:P:61:THR:N	2.67	0.58
2:B:242:VAL:O	2:B:246:LEU:HG	2.04	0.58
3:C:78:THR:O	3:C:82:ILE:HG13	2.04	0.58
1:D:346:VAL:HG12	1:D:347:PRO:HD3	1.86	0.58
1:M:114:ARG:HD2	1:M:114:ARG:C	2.23	0.58
1:A:125:ARG:HD3	6:A:501:HEM:O2D	2.04	0.57
2:E:142:PRO:CG	2:E:150:GLU:OE2	2.52	0.57
1:J:43:TRP:HZ3	1:J:251:LYS:HE2	1.69	0.57
3:O:78:THR:O	3:O:82:ILE:HG13	2.04	0.57
1:A:280:TYR:CE2	2:B:105:LYS:HD2	2.39	0.57
2:B:17:PHE:CE1	2:B:231:PHE:HE1	2.22	0.57
2:B:250:ARG:NE	3:C:12:ARG:CB	2.66	0.57
3:C:162:ILE:HD12	3:C:163:ARG:H	1.69	0.57
1:D:346:VAL:CG1	1:D:347:PRO:HD3	2.34	0.57
6:G:502:HEM:O1D	6:G:502:HEM:HBA2	2.04	0.57
3:I:78:THR:O	3:I:82:ILE:HG13	2.04	0.57
1:J:3:GLY:C	1:J:4:ILE:HD12	2.25	0.57
1:M:341:LEU:HD12	1:M:341:LEU:O	2.04	0.57
3:O:95:ASP:HB3	3:O:170:ASN:HD21	1.69	0.57
1:G:376:ILE:O	1:G:380:VAL:HG22	2.03	0.57
1:J:133:MET:N	6:J:501:HEM:HBC2	2.20	0.57
2:K:250:ARG:HH21	3:L:12:ARG:HD3	1.69	0.57
1:A:376:ILE:O	1:A:380:VAL:HG22	2.05	0.57
1:G:418:VAL:CG1	1:G:419:ALA:H	2.18	0.57
1:J:418:VAL:CG1	1:J:419:ALA:H	2.17	0.57
3:O:10:THR:O	3:O:10:THR:HG22	2.03	0.57
3:O:19:THR:HG22	3:O:20:ALA:N	2.18	0.57
1:P:125:ARG:NE	1:P:222:ASN:HB2	2.19	0.57
2:Q:106:ALA:O	2:Q:107:ARG:HG2	2.04	0.57
2:B:27:ARG:HB3	2:B:196:TYR:CZ	2.39	0.57
1:P:105:PHE:HA	1:P:108:VAL:CG2	2.34	0.57
2:E:242:VAL:O	2:E:246:LEU:HG	2.05	0.57
1:G:248:PHE:HA	1:G:251:LYS:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:89:GLN:H	3:I:92:GLN:NE2	2.02	0.57
3:O:131:HIS:HB3	7:O:200:FES:S2	2.45	0.57
1:P:418:VAL:CG1	1:P:419:ALA:N	2.66	0.57
1:P:91:PHE:HE1	1:P:92:MET:HE3	1.69	0.57
3:F:90:LEU:CD1	3:F:108:GLU:HB3	2.34	0.57
3:F:132:LEU:HD12	3:F:152:HIS:CE1	2.39	0.57
1:J:114:ARG:HD2	1:J:114:ARG:C	2.25	0.57
1:J:5:PRO:HB3	1:J:234:LYS:HG2	1.87	0.57
3:L:84:LEU:H	3:L:84:LEU:HD12	1.69	0.57
3:L:90:LEU:CD1	3:L:108:GLU:HB3	2.35	0.57
8:M:503:SMA:H21	8:M:503:SMA:H35	1.86	0.57
1:A:91:PHE:HE1	1:A:92:MET:HG2	1.66	0.57
2:B:113:PRO:HD2	2:B:118:ILE:HB	1.86	0.57
3:I:88:VAL:HG11	3:I:93:LEU:HD21	1.85	0.57
3:R:78:THR:O	3:R:82:ILE:HG13	2.04	0.57
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.85	0.57
2:B:149:HIS:CE1	2:B:168:THR:HG21	2.40	0.57
2:E:47:ILE:HG13	2:E:87:ASP:O	2.05	0.57
3:F:155:HIS:O	3:F:162:ILE:HD12	2.04	0.57
3:F:162:ILE:HD12	3:F:163:ARG:H	1.69	0.57
1:G:406:VAL:O	1:G:409:PRO:HD2	2.04	0.57
1:J:372:ALA:O	1:J:376:ILE:HG13	2.05	0.57
1:J:370:LEU:HD22	1:J:403:TYR:CE2	2.40	0.57
2:E:40:HIS:HE1	2:E:98:PRO:HD2	1.70	0.57
2:H:17:PHE:CE1	2:H:231:PHE:CE1	2.93	0.57
3:I:21:GLY:O	3:I:25:VAL:HG23	2.05	0.57
2:K:189:LEU:O	2:K:190:MET:HB2	2.05	0.57
1:M:190:THR:O	1:M:193:ARG:HG2	2.05	0.57
3:I:162:ILE:HD12	3:I:163:ARG:H	1.70	0.56
1:J:246:PRO:HG2	2:K:251:LEU:HD21	1.87	0.56
2:N:191:ASP:N	2:N:204:VAL:HG23	2.19	0.56
1:J:156:PHE:CE2	1:J:285:PRO:HA	2.40	0.56
1:M:249:ILE:O	1:M:253:VAL:HG23	2.05	0.56
1:P:205:ILE:O	1:P:209:VAL:HG23	2.06	0.56
1:P:296:TRP:HA	1:P:299:LEU:HG	1.87	0.56
1:A:73:VAL:HG23	1:A:74:ASP:N	2.20	0.56
2:B:157:ASN:O	2:B:180:GLY:HA3	2.05	0.56
1:G:269:PHE:HB3	4:G:431:BGL:H1'2	1.86	0.56
1:G:312:VAL:O	1:G:316:GLN:HG3	2.05	0.56
1:M:73:VAL:HG22	1:M:188:ASN:OD1	2.06	0.56
1:P:92:MET:HE2	1:P:92:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLU:O	1:D:239:LYS:HB2	2.05	0.56
1:G:91:PHE:CD1	1:G:92:MET:N	2.73	0.56
3:I:38:MET:HE3	1:J:193:ARG:HD3	1.86	0.56
1:J:27:ALA:O	1:J:30:TYR:HB3	2.05	0.56
3:L:54:VAL:HG23	3:L:57:VAL:HG21	1.86	0.56
1:A:319:ASN:ND2	1:A:319:ASN:C	2.58	0.56
1:G:312:VAL:O	1:G:315:VAL:HB	2.05	0.56
3:I:38:MET:CE	1:J:193:ARG:HH11	2.17	0.56
3:I:38:MET:HG2	1:J:193:ARG:NH1	2.21	0.56
2:K:250:ARG:NE	3:L:12:ARG:CB	2.66	0.56
3:O:54:VAL:HG23	3:O:57:VAL:HG21	1.88	0.56
3:R:138:GLY:CA	3:R:147:TRP:CD1	2.88	0.56
1:A:156:PHE:CE2	1:A:285:PRO:HA	2.40	0.56
1:G:229:VAL:HG22	1:G:424:ILE:CD1	2.36	0.56
3:L:37:GLN:NE2	3:L:38:MET:HG3	2.20	0.56
1:M:128:THR:HG21	6:M:501:HEM:HBD1	1.86	0.56
2:Q:157:ASN:O	2:Q:180:GLY:HA3	2.06	0.56
3:R:127:GLY:O	3:R:135:SER:HA	2.06	0.56
1:D:428:PHE:CE1	2:E:256:LYS:HD3	2.41	0.56
1:M:406:VAL:C	1:M:409:PRO:HD2	2.25	0.56
3:O:156:TYR:HA	3:O:161:ARG:O	2.05	0.56
1:P:295:GLU:N	1:P:295:GLU:OE1	2.37	0.56
1:A:125:ARG:CZ	1:A:222:ASN:HB2	2.36	0.56
3:I:131:HIS:O	1:J:329:LYS:CE	2.54	0.56
3:L:21:GLY:O	3:L:25:VAL:HG23	2.06	0.56
1:M:37:THR:HB	1:M:248:PHE:HE2	1.71	0.56
2:N:48:ARG:NH1	2:N:48:ARG:HG3	2.21	0.56
2:Q:191:ASP:N	2:Q:204:VAL:HG23	2.21	0.56
1:D:116:LEU:HA	1:D:121:TYR:HE2	1.71	0.56
1:G:362:MET:N	1:G:415:GLU:OE2	2.37	0.56
1:J:116:LEU:HA	1:J:121:TYR:HE2	1.71	0.56
1:J:91:PHE:CE1	1:J:92:MET:CE	2.89	0.56
1:G:193:ARG:HH11	3:L:38:MET:CE	2.19	0.56
1:P:312:VAL:O	1:P:315:VAL:HB	2.04	0.56
3:R:54:VAL:HG23	3:R:57:VAL:HG21	1.88	0.56
1:A:39:ARG:HH12	2:B:255:VAL:CG1	2.19	0.56
1:A:410:ILE:CG2	1:A:414:ILE:HD12	2.36	0.56
1:D:341:LEU:HD12	1:D:341:LEU:O	2.06	0.56
1:J:91:PHE:CD1	1:J:92:MET:N	2.75	0.56
2:N:59:PRO:HD2	2:N:62:GLN:NE2	2.21	0.56
1:G:114:ARG:C	1:G:114:ARG:HD2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:377:LEU:O	1:M:380:VAL:HG23	2.05	0.55
1:G:346:VAL:HG12	1:G:347:PRO:HD3	1.88	0.55
1:J:190:THR:O	1:J:193:ARG:HG2	2.07	0.55
1:J:205:ILE:O	1:J:209:VAL:HG23	2.06	0.55
1:J:346:VAL:CG1	1:J:347:PRO:HD3	2.36	0.55
3:L:78:THR:O	3:L:82:ILE:HG13	2.06	0.55
1:M:91:PHE:CD2	2:N:222:LYS:HG2	2.41	0.55
1:D:27:ALA:O	1:D:30:TYR:HB3	2.06	0.55
2:E:59:PRO:HD2	2:E:62:GLN:NE2	2.22	0.55
1:G:199:TYR:CE2	6:G:502:HEM:HBC1	2.41	0.55
1:G:261:LEU:HD11	2:H:234:VAL:HG13	1.88	0.55
1:G:39:ARG:NH1	1:G:428:PHE:HE2	2.03	0.55
2:H:59:PRO:HD2	2:H:62:GLN:NE2	2.21	0.55
1:J:341:LEU:HD12	1:J:341:LEU:O	2.06	0.55
1:J:199:TYR:CD2	6:J:502:HEM:HBC1	2.41	0.55
1:M:193:ARG:HH11	3:R:38:MET:CE	2.20	0.55
1:P:27:ALA:O	1:P:30:TYR:HB3	2.07	0.55
1:D:149:LEU:HB2	1:D:150:PRO:HD3	1.87	0.55
3:F:21:GLY:O	3:F:25:VAL:HG23	2.06	0.55
1:J:149:LEU:HB2	1:J:150:PRO:HD3	1.88	0.55
2:N:72:VAL:HG12	2:N:73:THR:N	2.22	0.55
3:R:132:LEU:HD12	3:R:152:HIS:CE1	2.42	0.55
2:B:129:GLU:O	2:B:132:TYR:HB3	2.06	0.55
2:E:113:PRO:HD2	2:E:118:ILE:HB	1.87	0.55
1:G:37:THR:HB	1:G:248:PHE:HE2	1.72	0.55
1:G:387:PHE:HA	1:G:390:ASP:OD1	2.06	0.55
1:J:43:TRP:CZ3	1:J:251:LYS:HE2	2.42	0.55
1:J:296:TRP:HA	1:J:299:LEU:HG	1.89	0.55
2:K:47:ILE:HG13	2:K:87:ASP:O	2.07	0.55
1:M:44:MET:CE	9:M:504:LOP:H101	2.37	0.55
1:P:62:GLY:C	6:P:502:HEM:HAC	2.27	0.55
1:P:91:PHE:CD1	1:P:92:MET:N	2.75	0.55
2:Q:66:TYR:CE1	2:Q:70:PHE:HE2	2.23	0.55
3:C:38:MET:CE	1:D:193:ARG:HH11	2.19	0.55
1:M:374:PHE:CD2	9:M:504:LOP:H321	2.42	0.55
1:P:52:ALA:HB2	10:P:505:ANJ:C16	2.37	0.55
2:Q:108:ALA:HA	2:Q:125:ILE:O	2.07	0.55
1:A:276:HIS:CE1	1:A:278:ASP:HB2	2.42	0.55
2:B:47:ILE:HG13	2:B:87:ASP:O	2.06	0.55
3:I:77:ARG:HH21	3:I:115:THR:HG21	1.72	0.55
3:O:84:LEU:HD12	3:O:84:LEU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:VAL:CG2	1:D:61:THR:N	2.69	0.55
2:H:113:PRO:HD2	2:H:118:ILE:HB	1.88	0.55
3:I:88:VAL:CG1	3:I:93:LEU:HD21	2.37	0.55
1:J:91:PHE:CD2	2:K:222:LYS:HG2	2.42	0.55
2:N:156:TYR:HB2	2:N:182:TRP:CE2	2.41	0.55
1:A:234:LYS:O	1:A:238:GLN:HG3	2.07	0.55
2:B:128:PRO:HG2	2:B:129:GLU:OE1	2.07	0.55
2:B:59:PRO:HD2	2:B:62:GLN:NE2	2.22	0.55
1:G:116:LEU:HA	1:G:121:TYR:HE2	1.72	0.55
1:G:341:LEU:HD12	1:G:341:LEU:O	2.07	0.55
1:J:346:VAL:HG12	1:J:347:PRO:HD3	1.88	0.55
1:J:425:GLU:CG	1:J:429:ASN:HD21	2.19	0.55
3:C:138:GLY:HA2	3:C:147:TRP:CD1	2.41	0.55
2:H:47:ILE:HG13	2:H:87:ASP:O	2.06	0.55
2:K:59:PRO:HD2	2:K:62:GLN:NE2	2.21	0.55
3:L:137:ILE:HD12	3:L:150:PRO:HD3	1.89	0.55
2:B:130:TYR:O	2:B:134:VAL:HG23	2.06	0.54
6:D:502:HEM:HMB1	6:D:502:HEM:HBB2	1.88	0.54
2:E:238:THR:O	2:E:242:VAL:HG23	2.07	0.54
3:F:156:TYR:HA	3:F:161:ARG:O	2.06	0.54
1:G:185:ALA:HB2	3:L:70:LYS:HG3	1.89	0.54
1:G:27:ALA:O	1:G:30:TYR:HB3	2.07	0.54
2:K:113:PRO:HD2	2:K:118:ILE:HB	1.88	0.54
2:N:77:THR:CG2	2:N:79:GLU:HB2	2.37	0.54
2:N:77:THR:HG21	2:N:79:GLU:HB2	1.89	0.54
3:C:156:TYR:HA	3:C:161:ARG:O	2.07	0.54
1:G:296:TRP:HA	1:G:299:LEU:HG	1.89	0.54
3:I:76:ARG:HG2	3:I:121:GLU:HG2	1.88	0.54
3:I:127:GLY:O	3:I:135:SER:HA	2.06	0.54
2:K:129:GLU:O	2:K:132:TYR:HB3	2.07	0.54
1:M:296:TRP:HA	1:M:299:LEU:HG	1.87	0.54
2:Q:48:ARG:HG3	2:Q:48:ARG:NH1	2.22	0.54
3:I:131:HIS:O	1:J:329:LYS:NZ	2.41	0.54
1:M:346:VAL:HG12	1:M:347:PRO:HD3	1.89	0.54
1:M:49:VAL:CG1	1:M:256:LEU:HD13	2.37	0.54
3:O:162:ILE:HD12	3:O:163:ARG:H	1.73	0.54
1:P:190:THR:O	1:P:193:ARG:HG2	2.08	0.54
1:A:9:TYR:HB2	1:A:30:TYR:CG	2.43	0.54
3:C:95:ASP:HB3	3:C:170:ASN:ND2	2.21	0.54
2:E:129:GLU:O	2:E:132:TYR:HB3	2.06	0.54
1:G:249:ILE:O	1:G:253:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:132:GLY:HA3	6:M:501:HEM:HBC2	1.89	0.54
1:M:37:THR:HB	1:M:248:PHE:CE2	2.42	0.54
2:N:103:MET:O	2:N:105:LYS:N	2.40	0.54
2:N:40:HIS:HE1	2:N:98:PRO:HD2	1.72	0.54
3:O:162:ILE:HD11	3:O:164:LYS:O	2.07	0.54
2:Q:59:PRO:HD2	2:Q:62:GLN:NE2	2.21	0.54
1:D:123:ALA:O	1:D:355:ARG:NH1	2.40	0.54
1:D:261:LEU:HD11	2:E:234:VAL:HG13	1.89	0.54
1:G:37:THR:HB	1:G:248:PHE:CE2	2.43	0.54
3:I:89:GLN:C	3:I:91:GLY:N	2.55	0.54
3:L:127:GLY:O	3:L:135:SER:HA	2.07	0.54
3:O:21:GLY:O	3:O:25:VAL:HG23	2.06	0.54
1:A:263:PHE:HA	9:A:503:LOP:H221	1.90	0.54
3:C:140:VAL:O	3:C:140:VAL:HG12	2.07	0.54
1:M:214:TRP:CH2	1:P:25:ILE:HA	2.43	0.54
1:M:360:ARG:O	1:M:364:LYS:HG3	2.08	0.54
2:N:113:PRO:HD2	2:N:118:ILE:HB	1.90	0.54
1:A:193:ARG:NH1	3:F:38:MET:HG2	2.23	0.54
1:D:276:HIS:CE1	1:D:278:ASP:HB2	2.42	0.54
1:G:125:ARG:NE	1:G:222:ASN:HB2	2.22	0.54
1:P:377:LEU:O	1:P:380:VAL:HG23	2.08	0.54
2:Q:189:LEU:HB2	2:Q:204:VAL:HG13	1.89	0.54
2:Q:53:PRO:HA	2:Q:57:GLU:CD	2.27	0.54
2:Q:74:ASP:HB3	2:Q:77:THR:HB	1.88	0.54
3:F:84:LEU:N	3:F:84:LEU:HD12	2.21	0.54
1:J:123:ALA:O	1:J:355:ARG:NH1	2.41	0.54
2:K:114:MET:HG2	2:K:114:MET:O	2.07	0.54
3:R:77:ARG:HH21	3:R:115:THR:HG21	1.72	0.54
6:D:502:HEM:O2D	6:D:502:HEM:O1A	2.26	0.54
1:G:205:ILE:O	1:G:209:VAL:HG23	2.07	0.54
1:J:13:THR:O	1:J:17:LYS:HG3	2.07	0.54
1:M:425:GLU:O	1:M:429:ASN:ND2	2.41	0.54
3:O:127:GLY:O	3:O:135:SER:HA	2.08	0.54
1:P:77:PHE:CD2	1:P:282:GLU:HG2	2.43	0.54
1:P:341:LEU:O	1:P:341:LEU:HD12	2.08	0.54
3:R:93:LEU:HD13	3:R:161:ARG:HD2	1.90	0.54
1:A:193:ARG:HH12	3:F:38:MET:CB	2.21	0.54
1:A:399:TYR:O	1:A:402:ALA:HB3	2.08	0.54
3:C:73:PHE:CE1	3:C:127:GLY:HA3	2.42	0.54
3:I:54:VAL:HG23	3:I:57:VAL:HG21	1.88	0.54
1:J:387:PHE:HA	1:J:390:ASP:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4:ILE:HD12	1:M:4:ILE:H	1.73	0.54
3:O:132:LEU:HD12	3:O:152:HIS:CE1	2.43	0.54
1:P:144:PHE:HE2	8:P:503:SMA:H43	1.72	0.54
1:A:315:VAL:O	1:A:318:ALA:HB3	2.09	0.53
1:D:39:ARG:NH1	2:E:255:VAL:HG12	2.17	0.53
1:G:315:VAL:HG12	1:G:316:GLN:N	2.23	0.53
2:H:66:TYR:CE1	2:H:70:PHE:HE2	2.26	0.53
1:G:190:THR:O	1:G:193:ARG:HG2	2.08	0.53
1:G:377:LEU:O	1:G:380:VAL:HG23	2.08	0.53
1:A:116:LEU:HA	1:A:121:TYR:HE2	1.72	0.53
1:G:213:ILE:HA	1:G:216:PHE:CD2	2.43	0.53
1:G:346:VAL:CG1	1:G:347:PRO:HD3	2.38	0.53
1:J:377:LEU:O	1:J:380:VAL:HG23	2.08	0.53
2:K:231:PHE:O	2:K:235:MET:HG2	2.08	0.53
1:M:125:ARG:NE	1:M:222:ASN:HB2	2.22	0.53
1:M:193:ARG:HH11	3:R:38:MET:HE2	1.72	0.53
2:Q:129:GLU:O	2:Q:132:TYR:HB3	2.08	0.53
1:D:377:LEU:O	1:D:380:VAL:HG23	2.09	0.53
1:G:105:PHE:HA	1:G:108:VAL:HG23	1.91	0.53
1:G:144:PHE:CD1	1:G:162:ILE:HD13	2.43	0.53
1:G:91:PHE:HE1	1:G:92:MET:HE3	1.74	0.53
3:I:131:HIS:HB3	7:I:200:FES:S2	2.49	0.53
1:M:276:HIS:CE1	1:M:278:ASP:HB2	2.43	0.53
1:P:427:ASP:O	1:P:430:ALA:HB3	2.08	0.53
2:B:250:ARG:CZ	3:C:12:ARG:HB3	2.39	0.53
3:C:138:GLY:CA	3:C:147:TRP:CD1	2.92	0.53
3:L:132:LEU:HD12	3:L:152:HIS:CE1	2.43	0.53
1:A:377:LEU:O	1:A:380:VAL:HG23	2.08	0.53
1:D:77:PHE:CD2	1:D:282:GLU:HG2	2.44	0.53
2:H:149:HIS:CD2	2:H:168:THR:HG21	2.43	0.53
3:L:156:TYR:HA	3:L:161:ARG:O	2.07	0.53
1:M:388:PRO:O	1:M:392:ILE:HG13	2.08	0.53
1:A:114:ARG:HD2	1:A:114:ARG:C	2.29	0.53
1:A:387:PHE:HA	1:A:390:ASP:OD1	2.07	0.53
2:B:74:ASP:CB	2:B:81:ARG:HE	2.21	0.53
3:C:12:ARG:CG	3:C:13:ASP:N	2.71	0.53
3:F:80:ALA:O	3:F:84:LEU:HD13	2.09	0.53
3:F:95:ASP:HB3	3:F:170:ASN:ND2	2.23	0.53
2:H:155:TYR:N	2:H:155:TYR:CD1	2.77	0.53
1:J:37:THR:HB	1:J:248:PHE:HE2	1.73	0.53
2:K:66:TYR:CE1	2:K:70:PHE:HE2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:154:SER:OG	3:L:166:PRO:HD2	2.09	0.53
2:N:77:THR:HG22	2:N:79:GLU:N	2.24	0.53
1:P:249:ILE:O	1:P:253:VAL:HG23	2.08	0.53
2:B:238:THR:O	2:B:242:VAL:HG23	2.08	0.53
2:Q:188:PRO:HG2	2:Q:189:LEU:H	1.73	0.53
1:D:387:PHE:CE1	1:D:388:PRO:HB3	2.44	0.53
1:J:399:TYR:O	1:J:402:ALA:HB3	2.09	0.53
2:K:157:ASN:O	2:K:180:GLY:HA3	2.08	0.53
1:P:123:ALA:O	1:P:355:ARG:NH1	2.42	0.53
1:A:190:THR:O	1:A:193:ARG:HG2	2.09	0.53
1:A:410:ILE:HG23	1:A:414:ILE:HD12	1.90	0.53
2:E:191:ASP:N	2:E:204:VAL:HG23	2.24	0.53
1:J:123:ALA:HB2	1:J:126:GLU:OE2	2.08	0.53
1:J:249:ILE:O	1:J:253:VAL:HG23	2.09	0.53
2:N:114:MET:HG2	2:N:114:MET:O	2.09	0.53
3:F:127:GLY:O	3:F:135:SER:HA	2.09	0.52
3:I:100:ASN:HB3	3:I:103:ILE:HG12	1.91	0.52
1:M:205:ILE:O	1:M:209:VAL:HG23	2.09	0.52
2:N:129:GLU:O	2:N:132:TYR:HB3	2.08	0.52
1:A:249:ILE:O	1:A:253:VAL:HG23	2.08	0.52
1:A:406:VAL:C	1:A:409:PRO:HD2	2.30	0.52
1:D:213:ILE:HA	1:D:216:PHE:CD2	2.44	0.52
1:G:399:TYR:O	1:G:402:ALA:HB3	2.09	0.52
2:H:49:SER:HA	2:H:52:GLU:HG3	1.89	0.52
1:J:37:THR:HB	1:J:248:PHE:CE2	2.43	0.52
2:H:236:PHE:CZ	3:I:25:VAL:HG12	2.44	0.52
1:J:406:VAL:C	1:J:409:PRO:HD2	2.29	0.52
3:L:73:PHE:CE1	3:L:127:GLY:HA3	2.44	0.52
1:M:407:ILE:HG22	1:M:411:LEU:HD12	1.92	0.52
1:P:246:PRO:HG2	2:Q:251:LEU:HD21	1.90	0.52
1:P:360:ARG:O	1:P:364:LYS:HG3	2.10	0.52
1:P:44:MET:HE3	9:P:504:LOP:H92	1.90	0.52
2:Q:66:TYR:CE1	2:Q:70:PHE:CE2	2.98	0.52
1:M:319:ASN:OD1	1:M:324:GLY:HA2	2.09	0.52
1:M:399:TYR:O	1:M:402:ALA:HB3	2.09	0.52
2:Q:113:PRO:HD2	2:Q:118:ILE:HB	1.92	0.52
1:D:256:LEU:O	1:D:260:LEU:HG	2.09	0.52
1:D:296:TRP:HA	1:D:299:LEU:HG	1.91	0.52
3:R:73:PHE:CE1	3:R:127:GLY:HA3	2.45	0.52
1:G:123:ALA:HB2	1:G:126:GLU:OE2	2.10	0.52
1:G:49:VAL:CG1	1:G:256:LEU:HD13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:PRO:HG2	2:H:251:LEU:HD21	1.91	0.52
2:H:52:GLU:HB3	2:H:53:PRO:HD2	1.92	0.52
1:J:427:ASP:O	1:J:430:ALA:HB3	2.09	0.52
1:M:116:LEU:HA	1:M:121:TYR:HE2	1.74	0.52
2:N:32:TYR:CE2	2:N:42:MET:HE3	2.45	0.52
1:A:316:GLN:O	1:A:317:ILE:C	2.48	0.52
1:G:408:LEU:HB2	1:G:409:PRO:HD3	1.91	0.52
1:J:213:ILE:HA	1:J:216:PHE:CD2	2.45	0.52
3:O:109:ALA:O	3:O:161:ARG:NH1	2.37	0.52
2:Q:250:ARG:CZ	3:R:12:ARG:HB3	2.39	0.52
3:R:162:ILE:HD12	3:R:163:ARG:H	1.75	0.52
1:A:37:THR:HB	1:A:248:PHE:HE2	1.75	0.52
1:A:27:ALA:O	1:A:30:TYR:HB3	2.10	0.52
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.90	0.52
3:C:100:ASN:HB3	3:C:103:ILE:HG12	1.92	0.52
1:D:123:ALA:HB2	1:D:126:GLU:OE2	2.09	0.52
3:F:84:LEU:H	3:F:84:LEU:CD1	2.23	0.52
1:G:193:ARG:HH11	3:L:38:MET:HE2	1.73	0.52
2:H:53:PRO:HA	2:H:57:GLU:CG	2.39	0.52
3:O:77:ARG:HH21	3:O:115:THR:HG21	1.75	0.52
1:D:190:THR:O	1:D:193:ARG:HG2	2.10	0.52
1:D:49:VAL:HG21	1:D:252:ASP:OD2	2.10	0.52
2:E:157:ASN:O	2:E:180:GLY:HA3	2.10	0.52
2:K:191:ASP:N	2:K:204:VAL:HG23	2.25	0.52
1:P:37:THR:HB	1:P:248:PHE:CE2	2.45	0.52
1:P:39:ARG:HD3	1:P:428:PHE:CD2	2.45	0.52
3:R:37:GLN:NE2	3:R:38:MET:HG3	2.25	0.52
1:A:123:ALA:HB2	1:A:126:GLU:OE2	2.09	0.52
1:D:156:PHE:CE2	1:D:285:PRO:HA	2.45	0.52
1:D:213:ILE:HD11	10:D:504:ANJ:H162	1.91	0.52
2:E:236:PHE:HE1	3:F:25:VAL:CG1	2.23	0.52
1:P:116:LEU:HA	1:P:121:TYR:HE2	1.74	0.52
1:D:269:PHE:HB3	4:D:431:BGL:O1	2.10	0.51
1:D:399:TYR:O	1:D:402:ALA:HB3	2.09	0.51
1:J:275:GLY:O	1:J:277:PRO:HD3	2.11	0.51
1:J:73:VAL:HG12	1:J:151:TRP:CE2	2.44	0.51
1:M:213:ILE:HA	1:M:216:PHE:CD2	2.44	0.51
1:M:7:ASP:HB3	1:M:234:LYS:NZ	2.25	0.51
1:P:147:TYR:HA	6:P:502:HEM:HAA2	1.92	0.51
1:P:37:THR:HB	1:P:248:PHE:HE2	1.75	0.51
1:A:152:GLY:H	1:A:155:SER:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ASP:N	2:B:204:VAL:HG23	2.26	0.51
3:C:154:SER:OG	3:C:166:PRO:HD2	2.10	0.51
3:C:38:MET:HE3	1:D:193:ARG:HD3	1.93	0.51
1:G:104:PHE:O	1:G:108:VAL:HG22	2.11	0.51
1:G:39:ARG:NH1	2:H:255:VAL:HG12	2.22	0.51
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.92	0.51
1:M:27:ALA:O	1:M:30:TYR:HB3	2.09	0.51
1:M:317:ILE:O	1:M:320:PHE:HB3	2.11	0.51
2:N:40:HIS:CE1	2:N:97:ALA:HB1	2.45	0.51
1:P:213:ILE:HA	1:P:216:PHE:CD2	2.45	0.51
3:R:152:HIS:N	7:R:200:FES:S1	2.83	0.51
1:G:234:LYS:O	1:G:238:GLN:HG3	2.10	0.51
2:H:154:PHE:N	2:H:154:PHE:CD1	2.78	0.51
1:P:234:LYS:O	1:P:238:GLN:HG3	2.10	0.51
1:A:37:THR:HB	1:A:248:PHE:CE2	2.46	0.51
2:B:154:PHE:N	2:B:154:PHE:CD1	2.76	0.51
2:B:27:ARG:HD2	2:B:196:TYR:CE2	2.45	0.51
3:F:154:SER:OG	3:F:166:PRO:HD2	2.10	0.51
1:G:62:GLY:C	6:G:502:HEM:HAC	2.31	0.51
3:O:180:ASP:OD2	3:O:183:THR:HB	2.11	0.51
1:P:123:ALA:HB2	1:P:126:GLU:OE2	2.11	0.51
1:P:73:VAL:HG22	1:P:188:ASN:OD1	2.10	0.51
1:P:316:GLN:O	1:P:317:ILE:C	2.49	0.51
1:A:162:ILE:CG2	8:A:1:SMA:H19	2.41	0.51
1:D:362:MET:HB2	1:D:415:GLU:OE2	2.10	0.51
6:D:502:HEM:O2D	6:D:502:HEM:HHA	2.11	0.51
1:M:51:LEU:HD13	6:M:501:HEM:C3B	2.46	0.51
1:A:346:VAL:CG1	1:A:347:PRO:HD3	2.41	0.51
2:B:243:LEU:HD13	3:C:19:THR:HA	1.92	0.51
2:E:61:ASP:HA	2:E:64:ARG:HH12	1.74	0.51
1:M:52:ALA:HB2	10:M:505:ANJ:H163	1.91	0.51
2:N:130:TYR:O	2:N:134:VAL:HG23	2.10	0.51
1:P:366:TYR:CD2	1:P:411:LEU:HD11	2.45	0.51
1:P:199:TYR:HA	6:P:502:HEM:HBC2	1.91	0.51
3:C:180:ASP:OD2	3:C:183:THR:HB	2.11	0.51
3:C:21:GLY:O	3:C:25:VAL:HG23	2.09	0.51
3:I:73:PHE:CE1	3:I:127:GLY:HA3	2.45	0.51
1:J:315:VAL:O	1:J:318:ALA:HB3	2.10	0.51
2:K:29:LEU:HD22	2:K:50:LEU:HD22	1.91	0.51
1:M:346:VAL:CG1	1:M:347:PRO:HD3	2.40	0.51
2:N:154:PHE:CD1	2:N:154:PHE:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:105:PHE:O	1:P:108:VAL:HG23	2.10	0.51
1:A:313:TRP:HA	1:A:316:GLN:HG3	1.93	0.51
1:D:91:PHE:CE1	1:D:92:MET:HE3	2.45	0.51
1:G:214:TRP:CH2	1:J:25:ILE:HA	2.46	0.51
1:G:103:LEU:CD1	9:G:504:LOP:H212	2.37	0.51
1:J:395:ILE:O	1:J:398:ALA:HB3	2.11	0.51
1:J:425:GLU:HG3	1:J:429:ASN:HD21	1.76	0.51
1:M:49:VAL:HG21	1:M:252:ASP:OD2	2.10	0.51
1:M:25:ILE:HA	1:P:214:TRP:CH2	2.46	0.51
1:A:213:ILE:HA	1:A:216:PHE:CD2	2.45	0.51
3:C:37:GLN:NE2	3:C:38:MET:HG3	2.25	0.51
1:D:52:ALA:HB2	10:D:504:ANJ:H163	1.92	0.51
3:F:180:ASP:OD2	3:F:183:THR:HB	2.11	0.51
1:G:360:ARG:HB3	1:G:415:GLU:OE1	2.10	0.51
2:H:191:ASP:N	2:H:204:VAL:HG23	2.25	0.51
1:P:256:LEU:O	1:P:260:LEU:HG	2.10	0.51
3:R:100:ASN:HB3	3:R:103:ILE:HG12	1.91	0.51
1:G:193:ARG:HD3	3:L:38:MET:HE3	1.93	0.51
1:M:49:VAL:HG12	1:M:256:LEU:HD13	1.92	0.51
2:Q:142:PRO:CG	2:Q:150:GLU:OE2	2.56	0.51
1:P:39:ARG:NH1	2:Q:255:VAL:CG1	2.71	0.51
1:J:43:TRP:CZ3	1:J:251:LYS:CE	2.93	0.50
1:M:73:VAL:HG23	1:M:74:ASP:H	1.77	0.50
1:A:193:ARG:HH12	3:F:38:MET:HB3	1.75	0.50
1:D:114:ARG:HD2	1:D:114:ARG:C	2.31	0.50
1:D:158:GLY:O	1:D:162:ILE:HG13	2.11	0.50
1:D:295:GLU:O	1:D:296:TRP:C	2.50	0.50
1:D:387:PHE:CD1	1:D:387:PHE:C	2.84	0.50
2:E:155:TYR:N	2:E:155:TYR:CD1	2.78	0.50
2:H:107:ARG:HH21	6:H:301:HEM:CGA	2.23	0.50
1:M:123:ALA:HB2	1:M:126:GLU:OE2	2.12	0.50
1:P:49:VAL:CG1	1:P:256:LEU:HD13	2.41	0.50
2:Q:113:PRO:O	2:Q:114:MET:HB3	2.11	0.50
3:R:62:GLN:NE2	3:R:73:PHE:CG	2.79	0.50
1:A:256:LEU:O	1:A:260:LEU:HG	2.12	0.50
1:D:239:LYS:HE2	1:D:425:GLU:OE1	2.11	0.50
2:H:53:PRO:HA	2:H:57:GLU:HG2	1.93	0.50
3:I:76:ARG:HG3	3:I:122:TRP:CH2	2.47	0.50
1:J:312:VAL:O	1:J:316:GLN:CG	2.59	0.50
1:J:209:VAL:HG22	6:J:501:HEM:HBB2	1.94	0.50
3:O:95:ASP:HB3	3:O:170:ASN:CG	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:HG22	1:D:217:HIS:CD2	2.47	0.50
1:G:73:VAL:HG23	1:G:74:ASP:N	2.27	0.50
2:H:106:ALA:O	2:H:107:ARG:HD3	2.12	0.50
2:H:129:GLU:O	2:H:132:TYR:HB3	2.10	0.50
2:H:29:LEU:HD22	2:H:50:LEU:HD22	1.92	0.50
3:I:89:GLN:O	3:I:90:LEU:C	2.49	0.50
2:K:144:LYS:O	2:K:147:GLU:N	2.44	0.50
2:K:155:TYR:CD1	2:K:155:TYR:N	2.79	0.50
2:K:77:THR:HG21	2:K:79:GLU:HB2	1.94	0.50
3:L:180:ASP:OD2	3:L:183:THR:HB	2.12	0.50
1:M:125:ARG:CZ	1:M:222:ASN:HB2	2.41	0.50
3:O:90:LEU:CD1	3:O:108:GLU:HB3	2.41	0.50
1:P:149:LEU:HB2	1:P:150:PRO:HD3	1.93	0.50
1:D:113:PHE:HB3	9:D:503:LOP:H272	1.93	0.50
2:H:165:VAL:CG1	2:H:169:CYS:HB2	2.41	0.50
1:J:364:LYS:O	1:J:368:TRP:HD1	1.94	0.50
3:O:12:ARG:HG2	3:O:13:ASP:N	2.26	0.50
1:P:113:PHE:HB3	9:P:504:LOP:H272	1.94	0.50
2:Q:233:ALA:O	2:Q:237:LEU:HD12	2.12	0.50
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.47	0.50
2:B:155:TYR:N	2:B:155:TYR:CD1	2.79	0.50
3:C:162:ILE:HD12	3:C:163:ARG:N	2.27	0.50
3:I:180:ASP:OD2	3:I:183:THR:HB	2.12	0.50
1:J:125:ARG:NE	1:J:222:ASN:HB2	2.27	0.50
1:A:418:VAL:CG1	1:A:419:ALA:H	2.23	0.50
1:D:103:LEU:HD13	9:D:503:LOP:H202	1.93	0.50
2:H:238:THR:O	2:H:242:VAL:HG23	2.11	0.50
3:I:125:MET:CE	3:I:171:LEU:HD12	2.42	0.50
3:I:37:GLN:NE2	3:I:38:MET:HG3	2.27	0.50
2:K:238:THR:O	2:K:242:VAL:HG23	2.11	0.50
3:L:100:ASN:HB3	3:L:103:ILE:HG12	1.93	0.50
2:Q:32:TYR:CD2	2:Q:42:MET:HE2	2.47	0.50
1:D:133:MET:N	6:D:501:HEM:HBC2	2.27	0.50
1:D:223:ASN:ND2	1:D:223:ASN:H	2.10	0.50
1:D:249:ILE:O	1:D:253:VAL:HG23	2.12	0.50
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.94	0.50
2:N:155:TYR:N	2:N:155:TYR:CD1	2.79	0.50
2:N:20:PHE:HB3	2:N:25:LEU:HD11	1.93	0.50
2:Q:130:TYR:O	2:Q:134:VAL:HG23	2.12	0.50
2:Q:20:PHE:HB3	2:Q:25:LEU:HD11	1.94	0.50
3:C:112:GLN:H	3:C:112:GLN:NE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:ASN:ND2	1:G:319:ASN:C	2.66	0.50
2:H:17:PHE:CE1	2:H:231:PHE:HE1	2.30	0.50
2:K:233:ALA:O	2:K:237:LEU:HD12	2.11	0.50
1:M:8:HIS:H	1:M:8:HIS:CD2	2.29	0.50
2:N:146:ALA:HB2	2:N:169:CYS:SG	2.51	0.50
1:M:193:ARG:NH1	3:R:38:MET:HG2	2.27	0.50
1:D:37:THR:HB	1:D:248:PHE:HE2	1.76	0.49
6:D:502:HEM:CBB	6:D:502:HEM:CMB	2.88	0.49
2:E:66:TYR:CE1	2:E:70:PHE:HE2	2.29	0.49
1:G:121:TYR:HB3	1:G:129:TRP:CE3	2.47	0.49
3:I:62:GLN:NE2	3:I:73:PHE:CD1	2.80	0.49
2:K:143:PRO:HG3	2:K:178:THR:HG21	1.94	0.49
3:L:44:VAL:C	3:L:46:ALA:H	2.15	0.49
1:M:39:ARG:HH12	2:N:255:VAL:CG1	2.24	0.49
2:N:103:MET:C	2:N:105:LYS:H	2.14	0.49
2:N:233:ALA:O	2:N:237:LEU:HD12	2.11	0.49
3:O:154:SER:OG	3:O:166:PRO:HD2	2.12	0.49
1:P:342:VAL:HG23	1:P:343:MET:N	2.27	0.49
2:Q:15:GLY:O	2:Q:227:LYS:NZ	2.43	0.49
2:Q:89:PHE:HB3	2:Q:90:PRO:CD	2.41	0.49
2:E:236:PHE:HE1	3:F:25:VAL:HG12	1.76	0.49
1:G:123:ALA:HA	1:G:126:GLU:OE1	2.12	0.49
2:H:48:ARG:HG3	2:H:48:ARG:NH1	2.24	0.49
3:I:132:LEU:HD12	3:I:152:HIS:CE1	2.47	0.49
2:K:142:PRO:HG2	2:K:150:GLU:OE2	2.12	0.49
1:M:121:TYR:HB3	1:M:129:TRP:CE3	2.46	0.49
1:M:73:VAL:HG23	1:M:74:ASP:N	2.28	0.49
1:D:152:GLY:H	1:D:155:SER:HB2	1.77	0.49
3:I:89:GLN:O	3:I:91:GLY:N	2.45	0.49
1:J:52:ALA:HB2	10:J:505:ANJ:H163	1.94	0.49
1:P:44:MET:HE1	9:P:504:LOP:H92	1.93	0.49
2:B:250:ARG:HE	3:C:12:ARG:CB	2.22	0.49
1:G:152:GLY:H	1:G:155:SER:HB2	1.77	0.49
2:H:157:ASN:O	2:H:180:GLY:HA3	2.11	0.49
3:C:90:LEU:HB2	2:H:172:ALA:HB1	1.93	0.49
3:I:38:MET:HE2	1:J:193:ARG:HH11	1.77	0.49
1:J:256:LEU:O	1:J:260:LEU:HG	2.12	0.49
2:K:154:PHE:N	2:K:154:PHE:CD1	2.81	0.49
2:K:156:TYR:HD1	2:K:182:TRP:CZ3	2.30	0.49
1:M:149:LEU:HB2	1:M:150:PRO:HD3	1.94	0.49
1:M:280:TYR:CE2	2:N:105:LYS:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:127:GLY:N	2:N:128:PRO:HD2	2.27	0.49
2:N:137:GLY:O	2:N:139:PRO:HD3	2.11	0.49
1:P:366:TYR:HD2	1:P:411:LEU:HD11	1.78	0.49
1:P:132:GLY:C	6:P:501:HEM:HBC2	2.32	0.49
2:Q:110:PHE:O	2:Q:120:GLN:HG2	2.12	0.49
2:B:29:LEU:HD22	2:B:50:LEU:HD22	1.93	0.49
3:C:125:MET:CE	3:C:171:LEU:HD12	2.43	0.49
1:D:37:THR:HB	1:D:248:PHE:CE2	2.47	0.49
3:F:162:ILE:HD12	3:F:163:ARG:N	2.26	0.49
1:G:276:HIS:CE1	1:G:278:ASP:HB2	2.47	0.49
1:G:49:VAL:HG12	1:G:256:LEU:HD13	1.94	0.49
1:G:63:ILE:HD13	1:J:200:LEU:CD2	2.33	0.49
1:J:4:ILE:N	1:J:4:ILE:CD1	2.74	0.49
3:L:162:ILE:HD12	3:L:163:ARG:N	2.27	0.49
1:M:125:ARG:HG3	1:M:125:ARG:HH11	1.77	0.49
1:M:428:PHE:CE1	2:N:256:LYS:HD3	2.48	0.49
1:M:91:PHE:HE1	1:M:92:MET:CE	2.25	0.49
2:N:238:THR:O	2:N:242:VAL:HG23	2.12	0.49
3:O:100:ASN:HB3	3:O:103:ILE:HG12	1.94	0.49
1:P:152:GLY:H	1:P:155:SER:HB2	1.77	0.49
3:R:180:ASP:OD2	3:R:183:THR:HB	2.12	0.49
1:D:162:ILE:HD13	8:D:2:SMA:H14	1.95	0.49
2:H:81:ARG:NH1	2:H:82:GLU:O	2.46	0.49
1:P:275:GLY:O	1:P:277:PRO:HD3	2.12	0.49
1:P:49:VAL:HG12	1:P:256:LEU:HD13	1.94	0.49
1:D:258:VAL:O	1:D:261:LEU:HB3	2.12	0.49
1:D:294:PRO:HA	8:D:2:SMA:C7M	2.34	0.49
2:E:20:PHE:HB3	2:E:25:LEU:HD11	1.95	0.49
2:E:29:LEU:HD22	2:E:50:LEU:HD22	1.95	0.49
2:E:32:TYR:CE2	2:E:42:MET:HE3	2.47	0.49
3:I:162:ILE:HD12	3:I:163:ARG:N	2.28	0.49
1:J:123:ALA:HA	1:J:126:GLU:OE1	2.12	0.49
1:M:51:LEU:HB3	6:M:501:HEM:HMB1	1.93	0.49
2:N:110:PHE:O	2:N:120:GLN:HG2	2.13	0.49
2:N:149:HIS:CG	2:N:168:THR:HG21	2.48	0.49
1:A:358:ARG:HH21	9:A:503:LOP:H21	1.78	0.49
1:A:395:ILE:O	1:A:398:ALA:HB3	2.13	0.49
1:G:60:VAL:HG23	1:G:61:THR:N	2.28	0.49
2:K:142:PRO:CG	2:K:150:GLU:OE2	2.61	0.49
1:M:275:GLY:O	1:M:277:PRO:HD3	2.12	0.49
1:M:427:ASP:O	1:M:430:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:155:TYR:N	2:Q:155:TYR:CD1	2.80	0.49
2:Q:189:LEU:CB	2:Q:204:VAL:HG13	2.42	0.49
1:D:51:LEU:HD13	6:D:501:HEM:C3B	2.48	0.49
3:I:88:VAL:HA	3:I:92:GLN:NE2	2.28	0.49
1:J:152:GLY:H	1:J:155:SER:HB2	1.77	0.49
1:J:276:HIS:CE1	1:J:278:ASP:HB2	2.47	0.49
1:P:12:ARG:O	1:P:17:LYS:HE2	2.13	0.49
1:P:390:ASP:OD1	1:P:390:ASP:N	2.46	0.49
1:D:313:TRP:O	1:D:317:ILE:HG13	2.13	0.49
2:E:233:ALA:O	2:E:237:LEU:HD12	2.13	0.49
1:M:135:ILE:O	1:M:139:MET:HG3	2.13	0.49
1:M:389:TYR:HA	1:M:392:ILE:HD12	1.95	0.49
2:N:72:VAL:O	2:N:80:ASP:HA	2.12	0.49
1:A:319:ASN:O	1:A:319:ASN:ND2	2.46	0.48
1:J:121:TYR:HB3	1:J:129:TRP:CE3	2.48	0.48
1:J:228:GLU:O	1:J:424:ILE:HD11	2.13	0.48
1:J:295:GLU:N	1:J:295:GLU:OE1	2.46	0.48
1:J:51:LEU:HB3	6:J:501:HEM:HMB1	1.95	0.48
1:J:60:VAL:HG23	1:J:61:THR:N	2.28	0.48
3:O:108:GLU:O	3:O:110:THR:N	2.40	0.48
1:P:121:TYR:HB3	1:P:129:TRP:CE3	2.48	0.48
1:P:261:LEU:HD11	2:Q:234:VAL:HG13	1.95	0.48
1:P:399:TYR:O	1:P:402:ALA:HB3	2.13	0.48
2:Q:250:ARG:HH21	3:R:12:ARG:HD3	1.77	0.48
1:M:193:ARG:HD3	3:R:38:MET:HE3	1.94	0.48
3:F:44:VAL:C	3:F:46:ALA:H	2.17	0.48
1:P:351:THR:OG1	1:P:412:GLY:HA3	2.14	0.48
1:P:389:TYR:HA	1:P:392:ILE:HD12	1.95	0.48
2:K:32:TYR:CE2	2:K:42:MET:CE	2.96	0.48
1:M:7:ASP:HB3	1:M:234:LYS:HZ1	1.78	0.48
2:N:108:ALA:HA	2:N:125:ILE:O	2.13	0.48
1:P:262:VAL:O	1:P:265:ALA:HB3	2.13	0.48
1:A:60:VAL:HG23	1:A:61:THR:N	2.27	0.48
1:J:105:PHE:CA	1:J:108:VAL:HG23	2.44	0.48
2:K:76:GLU:O	2:K:77:THR:C	2.52	0.48
3:R:62:GLN:NE2	3:R:73:PHE:CD1	2.82	0.48
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.13	0.48
1:M:156:PHE:HE2	1:M:285:PRO:HA	1.74	0.48
2:N:154:PHE:C	2:N:155:TYR:CD1	2.86	0.48
1:P:4:ILE:HG22	1:P:5:PRO:N	2.28	0.48
1:A:295:GLU:O	1:A:296:TRP:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:ARG:HG2	3:C:13:ASP:N	2.28	0.48
1:D:255:ALA:O	1:D:259:VAL:HG23	2.14	0.48
1:J:49:VAL:CG1	1:J:256:LEU:HD13	2.43	0.48
1:M:342:VAL:HG23	1:M:343:MET:N	2.29	0.48
2:N:230:GLY:O	2:N:231:PHE:C	2.51	0.48
3:F:111:ASP:C	3:F:111:ASP:OD1	2.51	0.48
1:G:149:LEU:HB2	1:G:150:PRO:HD3	1.94	0.48
2:H:160:PHE:CD2	2:H:183:ILE:HB	2.48	0.48
3:L:80:ALA:O	3:L:84:LEU:HD13	2.14	0.48
3:O:30:ALA:O	3:O:33:PRO:HG2	2.14	0.48
2:E:116:THR:O	2:E:116:THR:HG22	2.14	0.48
1:G:116:LEU:HA	1:G:121:TYR:CE2	2.49	0.48
1:G:406:VAL:C	1:G:409:PRO:HD2	2.34	0.48
2:H:89:PHE:HB3	2:H:90:PRO:HD2	1.96	0.48
3:I:138:GLY:HA2	3:I:147:TRP:CD1	2.48	0.48
2:K:144:LYS:O	2:K:146:ALA:N	2.47	0.48
1:P:132:GLY:HA3	6:P:501:HEM:HBC2	1.95	0.48
1:P:281:ILE:HD11	2:Q:107:ARG:HH12	1.78	0.48
2:Q:238:THR:O	2:Q:242:VAL:HG23	2.14	0.48
1:A:105:PHE:O	1:A:106:ILE:C	2.51	0.48
1:A:262:VAL:O	1:A:266:ILE:HG12	2.13	0.48
1:A:46:ILE:O	1:A:50:VAL:HG23	2.13	0.48
2:B:48:ARG:NH1	2:B:48:ARG:HG3	2.27	0.48
2:H:236:PHE:HZ	3:I:25:VAL:HG12	1.78	0.48
1:M:255:ALA:O	1:M:259:VAL:HG23	2.13	0.48
2:N:29:LEU:HD22	2:N:50:LEU:HD22	1.96	0.48
1:P:276:HIS:CE1	1:P:278:ASP:HB2	2.49	0.48
1:P:363:PHE:O	1:P:364:LYS:C	2.51	0.48
2:B:149:HIS:CD2	2:B:168:THR:HG21	2.49	0.48
3:C:143:ASP:HA	3:L:89:GLN:NE2	2.09	0.48
1:D:58:GLN:OE1	1:D:100:GLY:HA3	2.14	0.48
3:F:100:ASN:HB3	3:F:103:ILE:HG12	1.96	0.48
1:G:244:PHE:CD1	1:G:248:PHE:HB2	2.49	0.48
1:M:123:ALA:HA	1:M:126:GLU:OE1	2.14	0.48
1:M:223:ASN:H	1:M:223:ASN:ND2	2.12	0.48
3:R:112:GLN:H	3:R:112:GLN:NE2	2.12	0.48
1:A:255:ALA:O	1:A:259:VAL:HG23	2.14	0.47
1:A:342:VAL:HG23	1:A:343:MET:N	2.29	0.47
1:A:52:ALA:HB2	10:A:504:ANJ:C16	2.44	0.47
1:A:213:ILE:HD11	10:A:504:ANJ:H14	1.95	0.47
2:B:20:PHE:HB3	2:B:25:LEU:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:PHE:HA	1:D:390:ASP:OD1	2.14	0.47
1:G:315:VAL:O	1:G:318:ALA:HB3	2.14	0.47
3:I:180:ASP:OD1	3:I:181:GLU:N	2.47	0.47
1:M:60:VAL:HG23	1:M:61:THR:N	2.28	0.47
1:P:135:ILE:O	1:P:139:MET:HG3	2.15	0.47
1:P:388:PRO:O	1:P:392:ILE:HG13	2.14	0.47
2:Q:53:PRO:HA	2:Q:57:GLU:CG	2.44	0.47
6:D:502:HEM:HMB1	6:D:502:HEM:CBB	2.43	0.47
2:E:72:VAL:HG12	2:E:73:THR:H	1.76	0.47
3:F:89:GLN:HB2	3:F:92:GLN:HG3	1.95	0.47
2:K:110:PHE:O	2:K:120:GLN:HG2	2.14	0.47
2:K:141:GLU:HA	2:K:142:PRO:HD3	1.76	0.47
1:M:244:PHE:CD1	1:M:248:PHE:HB2	2.49	0.47
1:M:251:LYS:HA	1:M:254:PHE:HB3	1.95	0.47
1:P:164:GLY:O	1:P:167:GLY:N	2.47	0.47
1:P:223:ASN:H	1:P:223:ASN:ND2	2.12	0.47
2:Q:29:LEU:HD22	2:Q:50:LEU:HD22	1.96	0.47
2:Q:66:TYR:O	2:Q:69:GLN:HG2	2.14	0.47
1:A:116:LEU:HA	1:A:121:TYR:CE2	2.50	0.47
1:A:149:LEU:HB2	1:A:150:PRO:HD3	1.95	0.47
2:B:125:ILE:HD13	2:B:125:ILE:N	2.29	0.47
3:C:76:ARG:HG3	3:C:122:TRP:CH2	2.49	0.47
1:D:105:PHE:O	1:D:106:ILE:C	2.51	0.47
1:G:125:ARG:HH21	1:G:221:ASN:C	2.18	0.47
1:G:166:PHE:HA	1:G:169:ILE:HD12	1.96	0.47
1:J:5:PRO:HB2	1:J:234:LYS:HA	1.96	0.47
3:L:112:GLN:NE2	3:L:112:GLN:H	2.13	0.47
1:M:164:GLY:O	1:M:167:GLY:N	2.47	0.47
1:M:269:PHE:HB3	4:M:431:BGL:H1'2	1.96	0.47
1:A:109:TYR:HA	1:A:112:ILE:HD12	1.96	0.47
1:A:244:PHE:CD1	1:A:248:PHE:HB2	2.49	0.47
1:A:58:GLN:OE1	1:A:100:GLY:HA3	2.15	0.47
3:C:90:LEU:HD11	3:C:108:GLU:HB3	1.96	0.47
1:D:275:GLY:O	1:D:277:PRO:HD3	2.14	0.47
3:F:30:ALA:O	3:F:33:PRO:HG2	2.13	0.47
2:H:127:GLY:N	2:H:128:PRO:HD2	2.29	0.47
1:J:244:PHE:CD1	1:J:248:PHE:HB2	2.50	0.47
1:P:125:ARG:CZ	1:P:222:ASN:HB2	2.44	0.47
2:Q:26:GLN:HG2	2:Q:58:LEU:HD21	1.96	0.47
1:A:13:THR:HG22	1:A:14:GLY:N	2.30	0.47
1:A:199:TYR:CD2	6:A:502:HEM:HBC1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:VAL:O	1:D:318:ALA:HB3	2.13	0.47
1:D:342:VAL:HG23	1:D:343:MET:N	2.29	0.47
2:E:48:ARG:NH1	2:E:48:ARG:HG3	2.29	0.47
2:E:26:GLN:HG2	2:E:58:LEU:HD21	1.97	0.47
1:G:275:GLY:O	1:G:277:PRO:HD3	2.15	0.47
1:G:295:GLU:O	1:G:296:TRP:C	2.53	0.47
1:G:144:PHE:CD2	8:G:503:SMA:H42	2.50	0.47
1:J:140:MET:O	1:J:141:ALA:C	2.51	0.47
2:K:32:TYR:CD2	2:K:42:MET:CE	2.98	0.47
1:M:358:ARG:NE	9:M:504:LOP:H21	2.29	0.47
1:M:44:MET:HE1	9:M:504:LOP:H101	1.97	0.47
1:P:43:TRP:CZ3	1:P:251:LYS:HE3	2.49	0.47
3:R:77:ARG:NH2	3:R:115:THR:HG21	2.29	0.47
1:A:102:SER:O	1:A:106:ILE:HG13	2.15	0.47
3:C:108:GLU:O	3:C:110:THR:N	2.43	0.47
1:D:244:PHE:CD1	1:D:248:PHE:HB2	2.50	0.47
2:E:224:MET:O	2:E:228:GLN:HG3	2.14	0.47
1:D:261:LEU:CD1	2:E:234:VAL:HG13	2.44	0.47
2:E:80:ASP:O	2:E:81:ARG:HB3	2.14	0.47
1:G:117:TYR:HB2	1:G:367:PHE:CE1	2.49	0.47
1:G:236:GLU:HA	1:G:239:LYS:CD	2.36	0.47
1:J:49:VAL:HG12	1:J:256:LEU:HD13	1.95	0.47
1:M:276:HIS:ND1	1:M:278:ASP:HB2	2.30	0.47
1:P:117:TYR:HB2	1:P:367:PHE:CE1	2.49	0.47
1:A:275:GLY:O	1:A:277:PRO:HD3	2.14	0.47
2:B:127:GLY:N	2:B:128:PRO:HD2	2.29	0.47
3:F:77:ARG:HH21	3:F:115:THR:HG21	1.79	0.47
1:G:411:LEU:HD23	1:G:411:LEU:HA	1.63	0.47
2:H:154:PHE:C	2:H:155:TYR:CD1	2.88	0.47
2:H:77:THR:C	2:H:79:GLU:N	2.68	0.47
1:J:248:PHE:HD1	1:J:251:LYS:HD3	1.79	0.47
1:M:117:TYR:HB2	1:M:367:PHE:CE1	2.49	0.47
1:M:13:THR:HG22	1:M:14:GLY:N	2.30	0.47
1:M:370:LEU:HD22	1:M:403:TYR:CD2	2.49	0.47
2:N:158:ARG:HG3	2:N:158:ARG:HH11	1.80	0.47
1:P:164:GLY:HA2	1:P:177:GLN:NE2	2.29	0.47
2:Q:48:ARG:HH11	2:Q:48:ARG:CG	2.26	0.47
3:C:131:HIS:HB3	7:C:200:FES:S2	2.54	0.47
2:E:160:PHE:CG	2:E:183:ILE:HD12	2.50	0.47
3:F:73:PHE:CE1	3:F:127:GLY:HA3	2.49	0.47
1:G:342:VAL:HG23	1:G:343:MET:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:PRO:HG2	2:H:189:LEU:H	1.80	0.47
2:K:127:GLY:N	2:K:128:PRO:HD2	2.30	0.47
3:L:143:ASP:OD2	3:L:164:LYS:NZ	2.40	0.47
3:L:90:LEU:HD11	3:L:108:GLU:HB3	1.96	0.47
1:A:117:TYR:HB2	1:A:367:PHE:CE1	2.50	0.47
3:C:125:MET:HE1	3:C:171:LEU:HD12	1.97	0.47
3:C:144:PHE:CD1	3:C:144:PHE:N	2.82	0.47
1:D:370:LEU:HD22	1:D:403:TYR:CD2	2.50	0.47
2:E:170:LYS:HA	2:E:175:VAL:O	2.15	0.47
2:E:72:VAL:CG1	2:E:73:THR:N	2.78	0.47
1:J:295:GLU:O	1:J:296:TRP:C	2.52	0.47
1:M:34:MET:SD	1:M:245:TRP:HB3	2.55	0.47
1:P:18:TRP:CD1	1:P:22:ARG:NH1	2.83	0.47
1:P:295:GLU:O	1:P:296:TRP:C	2.53	0.47
2:Q:154:PHE:C	2:Q:155:TYR:CD1	2.88	0.47
1:A:223:ASN:H	1:A:223:ASN:ND2	2.13	0.47
1:A:49:VAL:CG1	1:A:256:LEU:HD13	2.45	0.47
1:D:123:ALA:HA	1:D:126:GLU:OE1	2.14	0.47
1:G:280:TYR:CE2	2:H:105:LYS:HD2	2.49	0.47
1:M:367:PHE:O	1:M:370:LEU:HB3	2.15	0.47
1:M:214:TRP:HH2	1:P:25:ILE:HA	1.80	0.47
1:D:51:LEU:CD2	1:D:108:VAL:HG13	2.45	0.47
1:D:395:ILE:O	1:D:398:ALA:HB3	2.15	0.47
2:E:185:MET:HB2	6:E:301:HEM:C1D	2.50	0.47
1:G:263:PHE:HD1	9:G:504:LOP:H232	1.80	0.47
1:G:395:ILE:O	1:G:398:ALA:HB3	2.15	0.47
2:H:110:PHE:O	2:H:120:GLN:HG2	2.15	0.47
2:H:66:TYR:HE1	2:H:70:PHE:HE2	1.63	0.47
3:I:77:ARG:NH2	3:I:115:THR:HG21	2.30	0.47
1:J:213:ILE:HD12	10:J:505:ANJ:O9	2.15	0.47
1:J:53:PHE:CE2	1:J:260:LEU:HD21	2.50	0.47
1:M:116:LEU:HA	1:M:121:TYR:CE2	2.50	0.47
1:M:72:HIS:HE1	1:M:74:ASP:OD2	1.98	0.47
3:O:73:PHE:CE1	3:O:127:GLY:HA3	2.50	0.47
1:P:60:VAL:HG23	1:P:61:THR:N	2.30	0.47
1:A:162:ILE:CD1	8:A:1:SMA:H14	2.45	0.46
1:A:79:SER:O	1:A:82:HIS:HB3	2.15	0.46
1:D:121:TYR:HB3	1:D:129:TRP:CE3	2.50	0.46
2:E:183:ILE:HG23	2:E:185:MET:H	1.80	0.46
2:H:230:GLY:O	2:H:231:PHE:C	2.53	0.46
2:K:116:THR:O	2:K:116:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:256:LEU:O	1:M:260:LEU:HG	2.14	0.46
1:M:209:VAL:HG22	6:M:501:HEM:HBB2	1.97	0.46
2:N:108:ALA:HA	2:N:125:ILE:HG22	1.97	0.46
1:P:255:ALA:O	1:P:259:VAL:HG23	2.15	0.46
1:M:329:LYS:CE	3:R:131:HIS:O	2.56	0.46
2:B:6:VAL:O	2:B:6:VAL:HG23	2.16	0.46
1:D:187:ASP:CG	1:D:188:ASN:H	2.18	0.46
1:D:205:ILE:O	1:D:209:VAL:HG23	2.16	0.46
2:E:66:TYR:CE1	2:E:70:PHE:CE2	3.03	0.46
1:G:128:THR:HG21	6:G:501:HEM:HBD1	1.97	0.46
1:J:213:ILE:HD13	10:J:505:ANJ:H14	1.98	0.46
1:J:8:HIS:H	1:J:8:HIS:CD2	2.33	0.46
3:L:108:GLU:O	3:L:110:THR:N	2.44	0.46
1:M:295:GLU:O	1:M:298:PHE:N	2.39	0.46
1:P:367:PHE:O	1:P:370:LEU:HB3	2.15	0.46
1:P:83:ILE:O	1:P:90:GLY:HA3	2.16	0.46
1:A:135:ILE:O	1:A:139:MET:HG3	2.15	0.46
1:G:299:LEU:HB2	1:G:378:THR:HG23	1.98	0.46
2:H:68:THR:HG23	2:H:82:GLU:HG2	1.96	0.46
2:H:77:THR:O	2:H:79:GLU:N	2.48	0.46
1:J:117:TYR:HB2	1:J:367:PHE:CE1	2.51	0.46
1:J:358:ARG:NH2	9:J:504:LOP:H21	2.27	0.46
1:M:39:ARG:HD3	1:M:428:PHE:CD2	2.50	0.46
1:M:79:SER:O	1:M:82:HIS:HB3	2.15	0.46
1:P:295:GLU:O	1:P:298:PHE:N	2.38	0.46
1:A:108:VAL:HG22	1:A:112:ILE:CD1	2.46	0.46
2:B:142:PRO:HG2	2:B:150:GLU:OE2	2.14	0.46
1:D:105:PHE:HA	1:D:108:VAL:CG2	2.42	0.46
1:D:223:ASN:ND2	1:D:223:ASN:N	2.63	0.46
2:E:154:PHE:CD1	2:E:154:PHE:N	2.83	0.46
3:F:108:GLU:O	3:F:110:THR:N	2.41	0.46
1:G:209:VAL:O	1:G:213:ILE:HG13	2.16	0.46
3:O:138:GLY:HA3	3:O:147:TRP:CD1	2.49	0.46
1:P:123:ALA:HA	1:P:126:GLU:OE1	2.15	0.46
1:D:223:ASN:HD22	1:D:223:ASN:N	2.13	0.46
1:D:49:VAL:HG12	1:D:256:LEU:HD13	1.98	0.46
1:G:132:GLY:HA3	6:G:501:HEM:HBC2	1.97	0.46
1:G:180:LEU:O	1:G:193:ARG:HD2	2.15	0.46
2:H:223:LEU:HD21	2:H:227:LYS:HE3	1.96	0.46
1:J:116:LEU:HA	1:J:121:TYR:CE2	2.49	0.46
1:J:258:VAL:O	1:J:261:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:418:VAL:CG1	1:M:419:ALA:H	2.28	0.46
2:Q:127:GLY:N	2:Q:128:PRO:HD2	2.30	0.46
2:B:224:MET:O	2:B:228:GLN:HG3	2.16	0.46
2:B:43:LYS:HE3	2:B:44:PHE:CZ	2.51	0.46
1:D:49:VAL:CG1	1:D:256:LEU:HD13	2.46	0.46
3:I:152:HIS:HB2	7:I:200:FES:S1	2.56	0.46
1:J:295:GLU:O	1:J:298:PHE:N	2.38	0.46
1:M:387:PHE:HA	1:M:390:ASP:OD1	2.15	0.46
2:Q:43:LYS:HG2	2:Q:99:ASP:OD1	2.16	0.46
1:D:116:LEU:HA	1:D:121:TYR:CE2	2.50	0.46
1:D:73:VAL:HG12	1:D:151:TRP:CE2	2.51	0.46
1:G:53:PHE:CE2	1:G:260:LEU:HD21	2.50	0.46
1:J:389:TYR:HA	1:J:392:ILE:HD12	1.97	0.46
1:J:43:TRP:HA	1:J:43:TRP:HE3	1.81	0.46
3:L:148:PHE:HE1	3:L:153:GLY:HA2	1.80	0.46
2:N:15:GLY:O	2:N:227:LYS:NZ	2.36	0.46
1:A:132:GLY:HA3	6:A:501:HEM:HBC2	1.98	0.46
1:A:327:ASP:C	1:A:327:ASP:OD1	2.55	0.46
1:A:53:PHE:CE2	1:A:260:LEU:HD21	2.50	0.46
3:F:117:ASP:OD2	3:F:121:GLU:N	2.45	0.46
1:G:103:LEU:HB2	9:G:504:LOP:H233	1.98	0.46
1:G:370:LEU:HD22	1:G:403:TYR:CD2	2.51	0.46
3:I:138:GLY:CA	3:I:147:TRP:CD1	2.98	0.46
2:K:26:GLN:HG2	2:K:58:LEU:HD21	1.98	0.46
1:P:79:SER:O	1:P:82:HIS:HB3	2.16	0.46
2:Q:72:VAL:HG12	2:Q:73:THR:N	2.30	0.46
2:Q:76:GLU:CD	2:Q:76:GLU:H	2.19	0.46
3:R:30:ALA:O	3:R:33:PRO:HG2	2.15	0.46
1:A:341:LEU:HD11	1:A:345:LEU:HD11	1.98	0.46
1:A:209:VAL:HG22	6:A:501:HEM:HBB2	1.97	0.46
1:D:29:ALA:CB	10:D:504:ANJ:H233	2.45	0.46
1:D:4:ILE:HD12	1:D:4:ILE:H	1.81	0.46
3:F:77:ARG:NH2	3:F:115:THR:HG21	2.31	0.46
1:G:298:PHE:CZ	8:G:503:SMA:H36	2.51	0.46
1:G:73:VAL:HG13	1:G:188:ASN:OD1	2.16	0.46
2:H:6:VAL:HG23	2:H:6:VAL:O	2.16	0.46
3:I:14:PHE:CE1	3:I:18:ALA:HB2	2.51	0.46
3:I:59:PRO:HD3	3:I:76:ARG:NH1	2.31	0.46
3:I:88:VAL:HG13	3:I:92:GLN:HG3	1.98	0.46
2:K:126:GLY:HA2	2:K:129:GLU:OE2	2.16	0.46
1:P:140:MET:O	1:P:141:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:244:PHE:CD1	1:P:248:PHE:HB2	2.50	0.46
2:Q:116:THR:HG22	2:Q:116:THR:O	2.16	0.46
3:C:47:LEU:HD23	3:C:48:ALA:O	2.16	0.46
1:D:387:PHE:CD1	1:D:388:PRO:N	2.84	0.46
1:G:312:VAL:HB	1:G:315:VAL:HB	1.96	0.46
1:G:25:ILE:HA	1:J:214:TRP:CH2	2.51	0.46
1:M:91:PHE:CE1	1:M:92:MET:HE3	2.50	0.46
1:P:144:PHE:CD1	1:P:162:ILE:HD12	2.50	0.46
1:P:53:PHE:CE2	1:P:260:LEU:HD21	2.51	0.46
2:Q:154:PHE:CD1	2:Q:154:PHE:N	2.83	0.46
1:G:164:GLY:O	1:G:165:LEU:C	2.55	0.45
1:G:256:LEU:O	1:G:260:LEU:HG	2.16	0.45
1:G:394:LEU:HA	1:G:394:LEU:HD23	1.73	0.45
2:H:233:ALA:O	2:H:237:LEU:HD12	2.15	0.45
3:I:154:SER:OG	3:I:166:PRO:HD2	2.15	0.45
3:I:93:LEU:HD12	3:I:109:ALA:HB3	1.98	0.45
1:J:164:GLY:HA2	1:J:177:GLN:HE22	1.80	0.45
1:M:10:GLU:HA	1:M:11:PRO:HD3	1.77	0.45
1:M:262:VAL:O	1:M:265:ALA:HB3	2.16	0.45
1:P:394:LEU:HA	1:P:394:LEU:HD23	1.72	0.45
1:A:205:ILE:O	1:A:209:VAL:HG23	2.17	0.45
2:E:154:PHE:C	2:E:155:TYR:CD1	2.89	0.45
1:G:388:PRO:O	1:G:392:ILE:HG13	2.15	0.45
3:I:30:ALA:O	3:I:33:PRO:HG2	2.16	0.45
1:J:164:GLY:O	1:J:167:GLY:N	2.49	0.45
1:J:39:ARG:HG2	1:J:242:VAL:CG1	2.44	0.45
1:J:229:VAL:HG22	1:J:424:ILE:HD12	1.99	0.45
1:J:39:ARG:NH1	2:K:255:VAL:HG12	2.30	0.45
1:P:133:MET:N	6:P:501:HEM:HBC2	2.31	0.45
2:Q:127:GLY:O	2:Q:131:ILE:HG13	2.17	0.45
3:R:76:ARG:HG3	3:R:122:TRP:CH2	2.51	0.45
1:A:207:ALA:O	1:A:210:ALA:HB3	2.16	0.45
1:A:258:VAL:O	1:A:261:LEU:HB3	2.16	0.45
1:A:312:VAL:HB	1:A:315:VAL:CG2	2.46	0.45
2:B:105:LYS:HE2	2:B:220:GLU:HG2	1.98	0.45
1:G:258:VAL:O	1:G:261:LEU:HB3	2.17	0.45
1:M:246:PRO:HG2	2:N:251:LEU:HD21	1.98	0.45
1:P:188:ASN:O	1:P:189:ALA:C	2.55	0.45
1:P:73:VAL:HG23	1:P:74:ASP:N	2.31	0.45
1:A:123:ALA:HA	1:A:126:GLU:OE1	2.16	0.45
2:B:51:SER:OG	2:B:63:VAL:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:MET:HE2	1:D:193:ARG:HH11	1.80	0.45
3:I:108:GLU:O	3:I:110:THR:N	2.43	0.45
1:J:105:PHE:O	1:J:106:ILE:C	2.54	0.45
1:M:125:ARG:HG3	1:M:125:ARG:NH1	2.31	0.45
1:M:91:PHE:CE1	1:M:92:MET:HB2	2.51	0.45
2:N:141:GLU:HG3	2:N:141:GLU:O	2.16	0.45
1:P:122:LYS:HZ3	1:P:360:ARG:NH1	2.13	0.45
2:Q:226:ARG:O	2:Q:229:ALA:HB3	2.17	0.45
1:A:113:PHE:CD2	9:A:503:LOP:H301	2.52	0.45
1:A:128:THR:HG21	6:A:501:HEM:HBD1	1.98	0.45
2:B:110:PHE:O	2:B:120:GLN:HG2	2.16	0.45
2:E:127:GLY:O	2:E:131:ILE:HG13	2.16	0.45
1:G:18:TRP:CD1	1:G:22:ARG:NH1	2.85	0.45
1:J:13:THR:HG22	1:J:14:GLY:N	2.32	0.45
1:J:43:TRP:HA	1:J:43:TRP:CE3	2.52	0.45
1:M:374:PHE:HD2	9:M:504:LOP:H321	1.80	0.45
3:O:76:ARG:HG3	3:O:122:TRP:CH2	2.52	0.45
1:M:25:ILE:HA	1:P:214:TRP:HH2	1.82	0.45
1:P:416:LYS:HA	1:P:416:LYS:HD3	1.80	0.45
2:Q:141:GLU:HA	2:Q:142:PRO:HD3	1.83	0.45
2:Q:189:LEU:HD23	2:Q:189:LEU:N	2.30	0.45
1:A:370:LEU:HD22	1:A:403:TYR:CD2	2.52	0.45
1:G:13:THR:HG22	1:G:14:GLY:N	2.32	0.45
1:G:52:ALA:HB2	10:G:505:ANJ:C16	2.46	0.45
2:H:116:THR:HG22	2:H:116:THR:O	2.17	0.45
1:J:296:TRP:CD2	1:J:297:TYR:N	2.85	0.45
2:K:103:MET:O	2:K:105:LYS:N	2.49	0.45
2:K:230:GLY:O	2:K:231:PHE:C	2.55	0.45
2:N:53:PRO:HA	2:N:57:GLU:CD	2.37	0.45
3:O:162:ILE:HD12	3:O:163:ARG:N	2.31	0.45
3:O:180:ASP:OD1	3:O:181:GLU:N	2.50	0.45
1:P:13:THR:HG22	1:P:14:GLY:N	2.32	0.45
1:P:209:VAL:O	1:P:213:ILE:HG13	2.16	0.45
1:P:122:LYS:NZ	1:P:360:ARG:NH1	2.65	0.45
2:Q:149:HIS:CG	2:Q:168:THR:HG21	2.52	0.45
3:R:185:GLN:O	3:R:185:GLN:HG2	2.17	0.45
2:B:154:PHE:C	2:B:155:TYR:CD1	2.90	0.45
2:E:127:GLY:N	2:E:128:PRO:HD2	2.32	0.45
1:J:58:GLN:OE1	1:J:100:GLY:HA3	2.17	0.45
3:L:47:LEU:HD23	3:L:48:ALA:O	2.16	0.45
1:M:180:LEU:O	1:M:193:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:53:PHE:CE2	1:M:260:LEU:HD21	2.51	0.45
2:N:16:PRO:O	2:N:231:PHE:CZ	2.70	0.45
1:P:395:ILE:O	1:P:398:ALA:HB3	2.17	0.45
1:A:187:ASP:CG	1:A:188:ASN:H	2.20	0.45
3:C:185:GLN:HG2	3:C:185:GLN:O	2.16	0.45
3:C:87:SER:OG	3:C:88:VAL:N	2.50	0.45
2:E:30:GLN:NE2	2:E:194:VAL:HG13	2.32	0.45
3:I:66:LYS:HB2	1:J:286:LEU:HD11	1.98	0.45
1:J:209:VAL:O	1:J:213:ILE:HG13	2.16	0.45
1:J:299:LEU:HB2	1:J:378:THR:HG23	1.99	0.45
2:K:154:PHE:C	2:K:155:TYR:CD1	2.90	0.45
2:K:48:ARG:HG3	2:K:48:ARG:NH1	2.27	0.45
2:N:240:LEU:HG	2:N:244:LEU:HD12	1.99	0.45
2:Q:189:LEU:HD21	6:Q:301:HEM:HBB1	1.97	0.45
2:Q:230:GLY:O	2:Q:231:PHE:C	2.53	0.45
1:A:213:ILE:HD11	10:A:504:ANJ:H162	1.97	0.45
1:G:135:ILE:O	1:G:139:MET:HG3	2.17	0.45
1:G:223:ASN:H	1:G:223:ASN:ND2	2.15	0.45
3:I:112:GLN:H	3:I:112:GLN:NE2	2.15	0.45
3:I:58:GLU:HB3	3:I:59:PRO:HD2	1.99	0.45
1:J:18:TRP:CD1	1:J:22:ARG:NH1	2.84	0.45
2:K:156:TYR:CD1	2:K:182:TRP:CZ3	3.05	0.45
1:M:46:ILE:HG13	1:M:47:TRP:N	2.31	0.45
2:N:250:ARG:NE	3:O:12:ARG:CB	2.75	0.45
3:O:89:GLN:C	3:O:91:GLY:H	2.21	0.45
1:A:39:ARG:HD3	1:A:428:PHE:CD2	2.51	0.45
3:C:12:ARG:HG2	3:C:13:ASP:H	1.82	0.45
3:C:19:THR:CG2	3:C:20:ALA:N	2.80	0.45
1:D:317:ILE:HG22	1:D:321:ILE:HD12	1.99	0.45
3:L:32:TRP:HB3	3:L:33:PRO:CD	2.47	0.45
1:M:209:VAL:O	1:M:213:ILE:HG13	2.17	0.45
1:M:262:VAL:O	1:M:266:ILE:HG12	2.17	0.45
1:P:379:TRP:NE1	2:Q:114:MET:HE2	2.32	0.45
1:M:329:LYS:HG3	3:R:131:HIS:HD2	1.82	0.45
3:C:59:PRO:HD3	3:C:76:ARG:NH1	2.33	0.44
1:D:234:LYS:O	1:D:238:GLN:HG3	2.17	0.44
1:D:262:VAL:O	1:D:265:ALA:HB3	2.17	0.44
2:E:6:VAL:O	2:E:6:VAL:HG23	2.17	0.44
1:G:269:PHE:HB3	4:G:431:BGL:O1	2.17	0.44
1:G:79:SER:O	1:G:82:HIS:HB3	2.17	0.44
3:I:109:ALA:O	3:I:161:ARG:NH1	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:185:GLN:O	3:I:185:GLN:HG2	2.17	0.44
1:J:342:VAL:HG23	1:J:343:MET:N	2.32	0.44
1:M:140:MET:O	1:M:141:ALA:C	2.55	0.44
1:M:73:VAL:HG12	1:M:151:TRP:CE2	2.52	0.44
1:M:299:LEU:HB2	1:M:378:THR:HG23	1.99	0.44
2:N:235:MET:CE	2:N:235:MET:HA	2.46	0.44
3:O:44:VAL:C	3:O:46:ALA:H	2.19	0.44
3:O:58:GLU:HB3	3:O:59:PRO:HD2	1.97	0.44
3:R:32:TRP:HB3	3:R:33:PRO:CD	2.46	0.44
3:C:58:GLU:HB3	3:C:59:PRO:HD2	1.99	0.44
1:J:122:LYS:O	1:J:123:ALA:C	2.55	0.44
3:L:77:ARG:HH21	3:L:115:THR:HG21	1.82	0.44
1:P:116:LEU:HA	1:P:121:TYR:CE2	2.51	0.44
1:P:10:GLU:HA	1:P:11:PRO:HD3	1.78	0.44
3:R:143:ASP:C	3:R:144:PHE:CD1	2.91	0.44
2:B:116:THR:HG22	2:B:116:THR:O	2.17	0.44
3:C:180:ASP:OD1	3:C:181:GLU:N	2.51	0.44
3:C:94:VAL:HG23	3:C:162:ILE:O	2.17	0.44
1:D:209:VAL:O	1:D:213:ILE:HG13	2.17	0.44
1:D:262:VAL:O	1:D:266:ILE:HG12	2.17	0.44
1:D:327:ASP:C	1:D:327:ASP:OD1	2.56	0.44
1:D:79:SER:O	1:D:82:HIS:HB3	2.18	0.44
3:F:32:TRP:CE2	3:F:36:ASN:HB2	2.53	0.44
3:L:58:GLU:HB3	3:L:59:PRO:HD2	1.99	0.44
1:M:30:TYR:CE1	1:M:34:MET:HG3	2.53	0.44
1:M:418:VAL:CG1	1:M:419:ALA:N	2.78	0.44
1:D:164:GLY:O	1:D:167:GLY:N	2.50	0.44
1:G:39:ARG:HG2	1:G:242:VAL:CG1	2.46	0.44
1:M:390:ASP:OD1	1:M:390:ASP:N	2.51	0.44
1:M:60:VAL:O	1:M:64:VAL:HG23	2.18	0.44
2:N:26:GLN:HG2	2:N:58:LEU:HD21	1.99	0.44
1:P:156:PHE:HE2	1:P:285:PRO:HA	1.82	0.44
1:A:163:THR:O	1:A:177:GLN:HG3	2.18	0.44
1:A:223:ASN:HD22	1:A:223:ASN:N	2.15	0.44
1:A:49:VAL:HG12	1:A:256:LEU:HD13	2.00	0.44
3:C:84:LEU:HD12	3:C:84:LEU:H	1.83	0.44
1:D:295:GLU:N	1:D:295:GLU:OE1	2.49	0.44
1:D:117:TYR:HB2	1:D:367:PHE:CE1	2.53	0.44
3:I:89:GLN:N	3:I:92:GLN:HE21	2.07	0.44
1:J:139:MET:O	1:J:142:THR:HB	2.17	0.44
1:J:157:TRP:O	1:J:158:GLY:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:367:PHE:O	1:J:370:LEU:HB3	2.17	0.44
1:M:139:MET:O	1:M:142:THR:HB	2.17	0.44
3:O:41:SER:HB2	3:O:43:ASP:OD1	2.17	0.44
1:P:13:THR:O	1:P:17:LYS:HG3	2.17	0.44
1:P:223:ASN:N	1:P:223:ASN:ND2	2.66	0.44
1:P:370:LEU:HD22	1:P:403:TYR:CD2	2.52	0.44
1:P:387:PHE:CD1	1:P:387:PHE:C	2.91	0.44
2:Q:27:ARG:HB3	2:Q:196:TYR:CE1	2.53	0.44
2:Q:40:HIS:HE1	2:Q:98:PRO:HD2	1.82	0.44
1:A:388:PRO:O	1:A:392:ILE:HG13	2.18	0.44
1:A:103:LEU:HD13	9:A:503:LOP:H222	2.00	0.44
3:C:132:LEU:HD12	3:C:152:HIS:CE1	2.52	0.44
1:D:13:THR:HG22	1:D:14:GLY:N	2.32	0.44
1:D:43:TRP:CE3	1:D:43:TRP:HA	2.52	0.44
3:F:112:GLN:NE2	3:F:112:GLN:H	2.16	0.44
1:G:410:ILE:O	1:G:412:GLY:N	2.50	0.44
1:J:418:VAL:HG13	1:J:419:ALA:H	1.82	0.44
3:L:32:TRP:HB3	3:L:33:PRO:HD3	2.00	0.44
3:L:44:VAL:O	3:L:46:ALA:N	2.51	0.44
1:M:18:TRP:CD1	1:M:22:ARG:NH1	2.85	0.44
1:M:9:TYR:CD2	1:M:27:ALA:HA	2.53	0.44
2:N:127:GLY:O	2:N:131:ILE:HG13	2.18	0.44
2:Q:53:PRO:HA	2:Q:57:GLU:HG2	2.00	0.44
3:R:132:LEU:HB2	7:R:200:FES:S2	2.58	0.44
2:B:26:GLN:HG2	2:B:58:LEU:HD21	1.98	0.44
3:F:110:THR:HB	3:F:112:GLN:NE2	2.33	0.44
1:G:262:VAL:O	1:G:265:ALA:HB3	2.18	0.44
8:G:503:SMA:H11	8:G:503:SMA:H30	1.73	0.44
2:H:205:HIS:C	2:H:205:HIS:ND1	2.71	0.44
1:J:43:TRP:HZ3	1:J:251:LYS:CE	2.29	0.44
2:K:24:GLN:HG3	2:K:210:ASP:OD1	2.18	0.44
1:M:104:PHE:O	1:M:108:VAL:HG22	2.18	0.44
1:M:223:ASN:ND2	1:M:223:ASN:N	2.66	0.44
1:M:44:MET:HE3	9:M:504:LOP:H101	1.99	0.44
2:N:205:HIS:C	2:N:205:HIS:ND1	2.71	0.44
2:N:235:MET:O	2:N:236:PHE:C	2.56	0.44
3:O:89:GLN:C	3:O:91:GLY:N	2.70	0.44
2:Q:240:LEU:HG	2:Q:244:LEU:HD12	1.99	0.44
1:P:247:TYR:CE1	2:Q:251:LEU:HD11	2.53	0.44
1:A:122:LYS:HD2	1:A:355:ARG:HA	1.99	0.44
1:A:223:ASN:ND2	1:A:223:ASN:N	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ALA:O	2:B:237:LEU:HD12	2.18	0.44
1:G:389:TYR:HA	1:G:392:ILE:HD12	2.00	0.44
1:G:423:THR:O	1:G:426:GLU:HB3	2.18	0.44
1:J:180:LEU:O	1:J:193:ARG:HD2	2.18	0.44
1:P:105:PHE:O	1:P:108:VAL:CG2	2.66	0.44
3:O:71:PRO:HB3	1:P:286:LEU:HD22	2.00	0.44
1:P:56:VAL:O	1:P:60:VAL:HG13	2.18	0.44
2:Q:24:GLN:HG3	2:Q:210:ASP:OD1	2.16	0.44
2:B:250:ARG:HH21	3:C:12:ARG:HB3	1.76	0.44
1:D:252:ASP:O	1:D:256:LEU:HB2	2.18	0.44
1:G:140:MET:HB3	8:G:503:SMA:H37	1.99	0.44
2:K:251:LEU:HD12	2:K:251:LEU:O	2.17	0.44
2:K:77:THR:HG22	2:K:79:GLU:CB	2.48	0.44
2:K:77:THR:CG2	2:K:79:GLU:H	2.24	0.44
3:L:128:VAL:O	3:L:129:CYS:C	2.57	0.44
1:M:153:GLN:HB3	1:M:289:PRO:HG2	2.00	0.44
1:M:295:GLU:O	1:M:296:TRP:C	2.56	0.44
2:N:142:PRO:HG2	2:N:150:GLU:OE2	2.18	0.44
3:O:76:ARG:HA	3:O:121:GLU:O	2.18	0.44
3:O:185:GLN:O	3:O:185:GLN:HG2	2.17	0.44
1:P:180:LEU:O	1:P:193:ARG:HD2	2.18	0.44
1:P:111:HIS:HE1	6:P:501:HEM:C1A	2.36	0.44
1:P:209:VAL:HG22	6:P:501:HEM:HBB2	2.00	0.44
2:Q:6:VAL:O	2:Q:6:VAL:HG23	2.18	0.44
1:A:302:TYR:CE1	8:A:1:SMA:H5	2.52	0.43
2:B:205:HIS:ND1	2:B:205:HIS:C	2.71	0.43
1:D:316:GLN:O	1:D:317:ILE:C	2.56	0.43
8:J:503:SMA:H11	8:J:503:SMA:H30	1.66	0.43
1:M:223:ASN:HD22	1:M:223:ASN:N	2.16	0.43
2:N:224:MET:O	2:N:228:GLN:HG3	2.18	0.43
3:R:125:MET:HE2	3:R:147:TRP:CZ2	2.53	0.43
1:A:164:GLY:O	1:A:167:GLY:N	2.51	0.43
1:D:213:ILE:CG2	1:D:217:HIS:HD2	2.31	0.43
2:E:230:GLY:O	2:E:231:PHE:C	2.56	0.43
3:F:132:LEU:HA	3:F:132:LEU:HD23	1.84	0.43
3:F:185:GLN:O	3:F:185:GLN:HG2	2.18	0.43
2:E:236:PHE:CE1	3:F:25:VAL:HG12	2.54	0.43
1:G:255:ALA:O	1:G:259:VAL:HG23	2.18	0.43
2:H:26:GLN:HG2	2:H:58:LEU:HD21	1.99	0.43
1:J:73:VAL:HG23	1:J:74:ASP:N	2.33	0.43
1:M:379:TRP:CE3	1:M:380:VAL:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:HIS:HE1	1:P:74:ASP:OD2	2.01	0.43
1:A:39:ARG:HG2	1:A:242:VAL:CG1	2.47	0.43
2:B:170:LYS:HA	2:B:175:VAL:O	2.18	0.43
3:C:38:MET:HG2	1:D:193:ARG:NH1	2.33	0.43
1:D:39:ARG:HD3	1:D:428:PHE:CD2	2.53	0.43
1:D:132:GLY:CA	6:D:501:HEM:HBC2	2.49	0.43
2:E:160:PHE:CE2	2:E:183:ILE:HG13	2.54	0.43
2:H:24:GLN:HG3	2:H:210:ASP:OD1	2.18	0.43
3:I:32:TRP:HB3	3:I:33:PRO:CD	2.48	0.43
1:J:77:PHE:CD2	1:J:282:GLU:HG2	2.53	0.43
2:Q:22:GLN:HE21	2:Q:22:GLN:HB2	1.70	0.43
2:B:185:MET:HB2	6:B:301:HEM:C1D	2.54	0.43
3:C:95:ASP:HB3	3:C:170:ASN:HD21	1.83	0.43
1:D:103:LEU:CD1	9:D:503:LOP:H202	2.48	0.43
1:G:4:ILE:N	1:G:4:ILE:CD1	2.77	0.43
1:J:164:GLY:O	1:J:165:LEU:C	2.56	0.43
1:J:180:LEU:CD1	8:J:503:SMA:H25	2.47	0.43
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.29	0.43
2:K:6:VAL:HG23	2:K:6:VAL:O	2.18	0.43
3:L:179:ILE:HA	3:L:179:ILE:HD13	1.86	0.43
1:M:43:TRP:CZ3	1:M:251:LYS:HE3	2.53	0.43
1:M:365:ILE:HA	1:M:365:ILE:HD13	1.78	0.43
1:M:39:ARG:HB3	1:M:428:PHE:CE1	2.54	0.43
2:N:235:MET:HE2	2:N:235:MET:HA	2.00	0.43
3:O:112:GLN:H	3:O:112:GLN:NE2	2.17	0.43
3:O:30:ALA:O	3:O:33:PRO:HD2	2.18	0.43
1:P:248:PHE:O	1:P:249:ILE:C	2.56	0.43
1:P:408:LEU:HB2	1:P:409:PRO:HD3	1.99	0.43
1:A:276:HIS:ND1	1:A:278:ASP:HB2	2.33	0.43
1:A:394:LEU:HA	1:A:394:LEU:HD23	1.75	0.43
2:B:127:GLY:O	2:B:131:ILE:HG13	2.18	0.43
3:C:90:LEU:CD1	3:C:108:GLU:HB3	2.49	0.43
2:E:205:HIS:C	2:E:205:HIS:ND1	2.72	0.43
3:F:82:ILE:O	3:F:86:ARG:HG3	2.19	0.43
1:J:79:SER:O	1:J:82:HIS:HB3	2.17	0.43
2:K:127:GLY:O	2:K:131:ILE:HG13	2.19	0.43
6:K:301:HEM:CBB	6:K:301:HEM:HMB1	2.48	0.43
1:M:83:ILE:O	1:M:90:GLY:HA3	2.19	0.43
1:P:135:ILE:HG21	6:P:501:HEM:CBB	2.48	0.43
1:P:278:ASP:OD2	1:P:289:PRO:HB3	2.19	0.43
1:P:379:TRP:CE3	1:P:380:VAL:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:TRP:O	1:A:395:ILE:HG13	2.18	0.43
1:A:72:HIS:C	1:A:72:HIS:ND1	2.72	0.43
3:C:41:SER:HB2	3:C:43:ASP:OD1	2.19	0.43
3:F:58:GLU:HB3	3:F:59:PRO:HD2	1.99	0.43
1:G:58:GLN:OE1	1:G:100:GLY:HA3	2.18	0.43
1:G:214:TRP:HH2	1:J:25:ILE:HA	1.84	0.43
3:I:137:ILE:HD11	1:J:290:ALA:HA	1.99	0.43
2:K:240:LEU:HG	2:K:244:LEU:HD12	2.01	0.43
3:R:162:ILE:HD12	3:R:163:ARG:N	2.33	0.43
1:A:22:ARG:HG3	1:A:22:ARG:HH11	1.83	0.43
1:A:9:TYR:CD2	1:A:27:ALA:HA	2.54	0.43
3:C:32:TRP:HB3	3:C:33:PRO:CD	2.49	0.43
3:C:30:ALA:O	3:C:33:PRO:HG2	2.18	0.43
1:D:379:TRP:CE3	1:D:380:VAL:HG13	2.54	0.43
1:G:137:LEU:HA	1:G:137:LEU:HD23	1.70	0.43
1:J:255:ALA:O	1:J:259:VAL:HG23	2.18	0.43
3:L:76:ARG:HG2	3:L:121:GLU:HG2	2.00	0.43
3:L:30:ALA:O	3:L:33:PRO:HG2	2.19	0.43
1:M:188:ASN:O	1:M:189:ALA:C	2.56	0.43
2:N:69:GLN:HG3	2:N:70:PHE:N	2.33	0.43
1:P:202:PRO:O	1:P:205:ILE:HB	2.18	0.43
1:P:362:MET:HB2	1:P:415:GLU:OE2	2.18	0.43
2:Q:144:LYS:O	2:Q:147:GLU:HB2	2.19	0.43
1:A:139:MET:O	1:A:142:THR:HB	2.19	0.43
1:D:135:ILE:O	1:D:139:MET:HG3	2.18	0.43
1:D:22:ARG:HH11	1:D:22:ARG:HG3	1.84	0.43
1:D:39:ARG:NH1	2:E:255:VAL:CG1	2.79	0.43
3:F:41:SER:HB2	3:F:43:ASP:OD1	2.19	0.43
3:F:66:LYS:HG2	3:F:67:PHE:N	2.33	0.43
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.49	0.43
1:J:135:ILE:HG21	6:J:501:HEM:CBB	2.48	0.43
1:J:51:LEU:HD13	6:J:501:HEM:C4B	2.53	0.43
1:M:207:ALA:O	1:M:210:ALA:HB3	2.19	0.43
1:M:299:LEU:O	1:M:302:TYR:HB3	2.18	0.43
2:N:81:ARG:NH1	2:N:84:LYS:HG3	2.34	0.43
3:R:174:PRO:O	3:R:175:LEU:C	2.57	0.43
1:D:248:PHE:O	1:D:249:ILE:C	2.57	0.43
1:D:276:HIS:ND1	1:D:278:ASP:HB2	2.34	0.43
1:D:150:PRO:HG2	6:D:502:HEM:O1A	2.19	0.43
1:G:135:ILE:HG21	6:G:501:HEM:CBB	2.48	0.43
1:G:63:ILE:N	6:G:502:HEM:HAC	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:PHE:HA	1:J:169:ILE:HD12	2.00	0.43
1:J:425:GLU:O	1:J:429:ASN:ND2	2.52	0.43
8:M:503:SMA:H11	8:M:503:SMA:H30	1.76	0.43
2:Q:108:ALA:HA	2:Q:125:ILE:HG22	2.01	0.43
2:Q:186:PRO:O	2:Q:187:PRO:C	2.57	0.43
3:R:148:PHE:HE1	3:R:153:GLY:HA2	1.81	0.43
2:B:154:PHE:HB3	2:B:182:TRP:HB3	2.01	0.43
2:B:230:GLY:O	2:B:231:PHE:C	2.57	0.43
1:D:72:HIS:HE1	1:D:74:ASP:OD2	2.01	0.43
1:D:91:PHE:CG	1:D:92:MET:N	2.87	0.43
1:G:262:VAL:O	1:G:266:ILE:HG12	2.18	0.43
3:I:135:SER:HA	3:I:136:PRO:HD3	1.76	0.43
1:J:83:ILE:O	1:J:90:GLY:HA3	2.19	0.43
1:M:425:GLU:CG	1:M:429:ASN:HD21	2.29	0.43
1:P:428:PHE:CZ	2:Q:256:LYS:HB2	2.54	0.43
2:B:30:GLN:NE2	2:B:194:VAL:HG13	2.34	0.42
2:B:243:LEU:HB3	3:C:19:THR:OG1	2.19	0.42
2:E:42:MET:HE1	2:E:214:PHE:CZ	2.54	0.42
3:F:152:HIS:HB2	7:F:200:FES:S1	2.59	0.42
1:G:139:MET:O	1:G:142:THR:HB	2.18	0.42
1:J:370:LEU:HD22	1:J:403:TYR:CD2	2.54	0.42
1:M:164:GLY:O	1:M:165:LEU:C	2.58	0.42
2:N:43:LYS:HE3	2:N:44:PHE:CZ	2.54	0.42
3:O:59:PRO:HD3	3:O:76:ARG:NH1	2.34	0.42
1:P:207:ALA:O	1:P:210:ALA:HB3	2.19	0.42
3:R:154:SER:OG	3:R:166:PRO:HD2	2.18	0.42
1:G:51:LEU:HD13	6:G:501:HEM:C3B	2.54	0.42
1:J:55:LEU:HA	1:J:55:LEU:HD12	1.84	0.42
2:K:185:MET:HB2	6:K:301:HEM:C1D	2.53	0.42
1:M:312:VAL:O	1:M:315:VAL:HB	2.19	0.42
2:N:61:ASP:HA	2:N:64:ARG:CZ	2.50	0.42
3:O:38:MET:HG2	1:P:193:ARG:NH1	2.34	0.42
1:P:46:ILE:HG13	1:P:47:TRP:N	2.33	0.42
3:C:132:LEU:HA	3:C:132:LEU:HD23	1.81	0.42
1:D:213:ILE:HG22	1:D:217:HIS:HD2	1.84	0.42
1:D:71:PRO:O	1:D:72:HIS:HB2	2.19	0.42
3:L:95:ASP:HB3	3:L:170:ASN:ND2	2.35	0.42
1:M:315:VAL:O	1:M:318:ALA:HB3	2.19	0.42
2:N:23:HIS:O	2:N:26:GLN:HB2	2.19	0.42
3:R:85:GLY:HA3	3:R:111:ASP:OD2	2.19	0.42
1:A:166:PHE:HA	1:A:169:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:O	1:A:302:TYR:HB3	2.20	0.42
1:A:69:TYR:HA	1:A:79:SER:OG	2.19	0.42
2:B:223:LEU:CD2	2:B:227:LYS:HE3	2.39	0.42
2:B:235:MET:O	2:B:236:PHE:C	2.57	0.42
1:D:278:ASP:OD2	1:D:289:PRO:HB3	2.19	0.42
1:D:312:VAL:O	1:D:315:VAL:HB	2.19	0.42
1:D:299:LEU:HB2	1:D:378:THR:HG23	2.02	0.42
3:F:26:ALA:O	3:F:27:THR:C	2.58	0.42
3:I:41:SER:HB2	3:I:43:ASP:OD1	2.18	0.42
3:L:135:SER:HA	3:L:136:PRO:HD3	1.84	0.42
1:M:105:PHE:O	1:M:106:ILE:C	2.57	0.42
1:M:131:VAL:HA	1:M:134:LEU:HD12	2.02	0.42
1:M:394:LEU:HA	1:M:394:LEU:HD23	1.73	0.42
1:P:18:TRP:NE1	1:P:22:ARG:CZ	2.82	0.42
1:P:410:ILE:O	1:P:412:GLY:N	2.52	0.42
1:D:213:ILE:CG2	1:D:217:HIS:CD2	3.02	0.42
1:D:367:PHE:O	1:D:370:LEU:HB3	2.20	0.42
3:F:137:ILE:N	3:F:137:ILE:HD12	2.35	0.42
3:F:32:TRP:CZ2	3:F:36:ASN:HB2	2.54	0.42
1:G:125:ARG:NH2	1:G:221:ASN:C	2.73	0.42
1:G:223:ASN:N	1:G:223:ASN:HD22	2.17	0.42
1:G:317:ILE:HG22	1:G:321:ILE:CD1	2.50	0.42
2:H:102:LEU:O	2:H:103:MET:C	2.57	0.42
1:J:187:ASP:CG	1:J:188:ASN:H	2.23	0.42
2:K:51:SER:OG	2:K:63:VAL:HG21	2.20	0.42
1:M:410:ILE:O	1:M:412:GLY:N	2.53	0.42
2:N:24:GLN:HG3	2:N:210:ASP:OD1	2.19	0.42
1:P:312:VAL:HB	1:P:315:VAL:CG2	2.49	0.42
2:Q:27:ARG:HD2	2:Q:196:TYR:CE2	2.55	0.42
1:A:367:PHE:O	1:A:370:LEU:HB3	2.19	0.42
2:B:114:MET:HG2	2:B:114:MET:O	2.20	0.42
1:A:39:ARG:NH1	2:B:255:VAL:HG12	2.31	0.42
1:D:60:VAL:HG23	1:D:61:THR:N	2.33	0.42
1:D:73:VAL:HG23	1:D:74:ASP:H	1.83	0.42
1:D:92:MET:HB2	1:D:92:MET:HE3	1.98	0.42
2:E:66:TYR:HE1	2:E:70:PHE:HE2	1.67	0.42
3:F:94:VAL:HG23	3:F:162:ILE:O	2.19	0.42
1:G:156:PHE:HE2	1:G:285:PRO:HA	1.82	0.42
1:G:428:PHE:CZ	2:H:256:LYS:HB2	2.55	0.42
1:J:379:TRP:CE3	1:J:380:VAL:HG13	2.55	0.42
1:J:250:ILE:HD12	2:K:251:LEU:CD2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:26:ALA:O	3:L:27:THR:C	2.57	0.42
2:N:105:LYS:HE2	2:N:220:GLU:HG2	2.02	0.42
3:O:126:TRP:NE1	3:O:174:PRO:HB3	2.34	0.42
1:P:164:GLY:O	1:P:165:LEU:C	2.56	0.42
3:R:59:PRO:HD3	3:R:76:ARG:NH1	2.34	0.42
1:A:156:PHE:O	1:A:159:ALA:HB3	2.20	0.42
2:B:49:SER:HA	2:B:52:GLU:CD	2.40	0.42
1:D:39:ARG:HG2	1:D:242:VAL:CG1	2.46	0.42
1:D:53:PHE:CE2	1:D:260:LEU:HD21	2.55	0.42
1:D:69:TYR:HA	1:D:79:SER:OG	2.19	0.42
1:D:91:PHE:CE1	1:D:92:MET:HB2	2.55	0.42
2:E:137:GLY:O	2:E:139:PRO:HD3	2.20	0.42
1:G:22:ARG:HG3	1:G:22:ARG:HH11	1.84	0.42
2:H:187:PRO:HA	2:H:188:PRO:HD2	1.85	0.42
1:J:388:PRO:O	1:J:392:ILE:HG13	2.20	0.42
2:K:32:TYR:CD1	2:K:36:CYS:HB2	2.54	0.42
1:M:114:ARG:HD2	1:M:114:ARG:O	2.20	0.42
1:M:258:VAL:O	1:M:261:LEU:HB3	2.20	0.42
1:M:269:PHE:CB	4:M:431:BGL:H1'2	2.49	0.42
1:M:278:ASP:OD2	1:M:289:PRO:HB3	2.20	0.42
2:N:6:VAL:O	2:N:6:VAL:HG23	2.20	0.42
3:O:32:TRP:CE2	3:O:36:ASN:HB2	2.55	0.42
1:P:51:LEU:HB3	6:P:501:HEM:HMB1	2.02	0.42
1:A:299:LEU:HB2	1:A:378:THR:HG23	2.00	0.42
1:A:269:PHE:HB3	4:A:431:BGL:H1'2	2.02	0.42
3:C:30:ALA:O	3:C:33:PRO:HD2	2.20	0.42
1:D:390:ASP:OD1	1:D:390:ASP:N	2.53	0.42
1:D:394:LEU:HA	1:D:394:LEU:HD23	1.73	0.42
2:E:190:MET:O	2:E:191:ASP:C	2.58	0.42
3:F:93:LEU:CD1	3:F:161:ARG:HD2	2.45	0.42
1:G:295:GLU:O	1:G:298:PHE:N	2.37	0.42
1:G:60:VAL:O	1:G:64:VAL:HG23	2.20	0.42
2:H:48:ARG:CG	2:H:48:ARG:NH1	2.83	0.42
3:I:151:CYS:SG	1:J:292:ILE:HD13	2.60	0.42
1:J:321:ILE:O	1:J:321:ILE:HG22	2.19	0.42
1:J:199:TYR:CZ	6:J:502:HEM:HBC1	2.55	0.42
2:K:146:ALA:HB2	2:K:169:CYS:SG	2.60	0.42
3:L:174:PRO:O	3:L:175:LEU:C	2.58	0.42
1:M:152:GLY:H	1:M:155:SER:HB2	1.85	0.42
1:M:22:ARG:HG3	1:M:22:ARG:HH11	1.85	0.42
1:M:296:TRP:CD2	1:M:297:TYR:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:250:ARG:CZ	3:O:12:ARG:HB3	2.50	0.42
3:O:152:HIS:HB2	7:O:200:FES:S1	2.60	0.42
1:P:132:GLY:CA	6:P:501:HEM:HBC2	2.49	0.42
2:Q:20:PHE:CZ	2:Q:217:TRP:HA	2.55	0.42
2:Q:48:ARG:NH1	2:Q:48:ARG:CG	2.81	0.42
1:A:18:TRP:CD1	1:A:22:ARG:NH1	2.88	0.42
1:A:346:VAL:N	1:A:347:PRO:CD	2.83	0.42
2:B:185:MET:HA	2:B:186:PRO:HD2	1.97	0.42
3:C:63:LEU:HB3	3:C:74:ILE:HB	2.01	0.42
1:D:410:ILE:O	1:D:412:GLY:N	2.53	0.42
2:E:151:PRO:HD2	2:E:182:TRP:CD1	2.55	0.42
1:G:391:TRP:O	1:G:395:ILE:HG13	2.20	0.42
2:H:110:PHE:HE2	2:H:129:GLU:OE2	2.02	0.42
2:H:197:ALA:C	2:H:199:GLY:H	2.24	0.42
2:H:72:VAL:O	2:H:80:ASP:HA	2.20	0.42
1:J:391:TRP:O	1:J:395:ILE:HG13	2.20	0.42
2:K:47:ILE:O	2:K:49:SER:N	2.53	0.42
3:L:152:HIS:HB2	7:L:200:FES:S1	2.59	0.42
3:L:26:ALA:O	3:L:29:ALA:N	2.53	0.42
1:M:366:TYR:CD2	1:M:411:LEU:HD11	2.55	0.42
1:M:52:ALA:HB2	10:M:505:ANJ:C16	2.50	0.42
1:P:118:TYR:CD1	1:P:224:PRO:HA	2.55	0.42
1:P:387:PHE:HA	1:P:390:ASP:OD1	2.20	0.42
1:P:111:HIS:CE1	6:P:501:HEM:C1A	3.07	0.42
3:C:87:SER:HB2	3:L:84:LEU:HD21	2.02	0.42
3:C:89:GLN:HG3	3:C:92:GLN:OE1	2.20	0.42
1:D:102:SER:O	1:D:103:LEU:C	2.58	0.42
1:D:427:ASP:O	1:D:430:ALA:HB3	2.19	0.42
1:D:56:VAL:O	1:D:57:LEU:C	2.58	0.42
3:F:32:TRP:HB3	3:F:33:PRO:CD	2.50	0.42
1:G:105:PHE:O	1:G:106:ILE:C	2.57	0.42
1:G:111:HIS:HE1	6:G:501:HEM:C1A	2.38	0.42
1:G:284:ASN:HA	1:G:285:PRO:HD3	1.88	0.42
2:H:235:MET:O	2:H:236:PHE:C	2.57	0.42
2:H:240:LEU:HG	2:H:244:LEU:HD12	2.02	0.42
1:J:360:ARG:HB2	1:J:363:PHE:HB3	2.02	0.42
2:K:186:PRO:O	2:K:187:PRO:C	2.56	0.42
1:M:105:PHE:HA	1:M:108:VAL:HG23	1.97	0.42
1:M:166:PHE:HA	1:M:169:ILE:HD12	2.01	0.42
1:M:287:ARG:HH11	1:M:287:ARG:HG2	1.84	0.42
6:M:502:HEM:CMB	6:M:502:HEM:CBB	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:141:GLU:HA	2:N:142:PRO:HD3	1.95	0.42
3:O:32:TRP:CZ2	3:O:36:ASN:HB2	2.55	0.42
1:P:114:ARG:O	1:P:114:ARG:HD2	2.19	0.42
1:P:157:TRP:O	1:P:158:GLY:C	2.58	0.42
1:P:296:TRP:CD2	1:P:297:TYR:N	2.88	0.42
1:P:425:GLU:HG2	1:P:429:ASN:ND2	2.35	0.42
1:A:125:ARG:NE	1:A:222:ASN:HB2	2.35	0.41
2:B:197:ALA:C	2:B:199:GLY:H	2.23	0.41
3:C:126:TRP:NE1	3:C:174:PRO:HB3	2.35	0.41
1:D:341:LEU:HD11	1:D:345:LEU:HD11	2.01	0.41
3:F:110:THR:O	3:F:111:ASP:C	2.57	0.41
2:H:51:SER:OG	2:H:63:VAL:HG21	2.20	0.41
3:I:179:ILE:HA	3:I:179:ILE:HD13	1.90	0.41
2:K:66:TYR:HE1	2:K:70:PHE:HE2	1.67	0.41
3:L:155:HIS:CD2	3:L:164:LYS:HD3	2.56	0.41
1:M:43:TRP:HA	1:M:43:TRP:HE3	1.86	0.41
1:P:258:VAL:O	1:P:261:LEU:HB3	2.20	0.41
2:Q:137:GLY:O	2:Q:139:PRO:HD3	2.20	0.41
3:R:131:HIS:CD2	3:R:132:LEU:HG	2.55	0.41
3:R:31:VAL:O	3:R:32:TRP:C	2.58	0.41
1:A:183:GLY:HA2	3:F:40:PRO:HG3	2.01	0.41
1:A:214:TRP:CH2	1:D:25:ILE:HA	2.55	0.41
1:A:60:VAL:O	1:A:64:VAL:HG23	2.20	0.41
2:B:217:TRP:O	2:B:218:ALA:C	2.59	0.41
2:E:77:THR:CG2	2:E:79:GLU:HB2	2.50	0.41
3:F:54:VAL:CG2	3:F:54:VAL:O	2.68	0.41
3:F:76:ARG:HG3	3:F:122:TRP:CH2	2.55	0.41
1:G:172:ILE:HG13	1:G:173:GLY:N	2.35	0.41
1:G:207:ALA:O	1:G:210:ALA:HB3	2.20	0.41
1:G:327:ASP:C	1:G:327:ASP:OD1	2.59	0.41
1:G:379:TRP:CE3	1:G:380:VAL:HG13	2.54	0.41
1:G:213:ILE:HD13	10:G:505:ANJ:H14	2.01	0.41
3:I:138:GLY:O	3:I:141:SER:OG	2.35	0.41
3:I:95:ASP:OD2	3:I:169:GLU:HA	2.21	0.41
1:J:374:PHE:HD2	9:J:504:LOP:H322	1.85	0.41
1:J:407:ILE:O	1:J:411:LEU:HG	2.20	0.41
3:L:180:ASP:OD1	3:L:181:GLU:N	2.53	0.41
1:M:248:PHE:O	1:M:249:ILE:C	2.58	0.41
3:O:77:ARG:NH2	3:O:115:THR:HG21	2.35	0.41
1:P:153:GLN:HB3	1:P:289:PRO:HG2	2.02	0.41
1:P:223:ASN:HD22	1:P:223:ASN:N	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:187:PRO:HA	2:Q:188:PRO:HD3	1.91	0.41
3:R:58:GLU:HB3	3:R:59:PRO:HD2	2.01	0.41
3:R:83:GLU:O	3:R:84:LEU:C	2.58	0.41
1:D:140:MET:O	1:D:141:ALA:C	2.58	0.41
1:D:360:ARG:HB2	1:D:363:PHE:HB3	2.02	0.41
1:G:223:ASN:N	1:G:223:ASN:ND2	2.67	0.41
2:H:165:VAL:HA	2:H:166:PRO:HD3	1.96	0.41
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.78	0.41
3:I:26:ALA:O	3:I:27:THR:C	2.58	0.41
1:J:114:ARG:HD2	1:J:114:ARG:O	2.20	0.41
3:L:41:SER:HB2	3:L:43:ASP:OD1	2.20	0.41
1:M:360:ARG:HB2	1:M:363:PHE:HB3	2.03	0.41
1:M:8:HIS:CD2	1:M:8:HIS:N	2.88	0.41
2:N:13:PHE:O	2:N:227:LYS:NZ	2.53	0.41
2:N:22:GLN:HB2	2:N:22:GLN:HE21	1.68	0.41
3:O:84:LEU:N	3:O:84:LEU:HD12	2.34	0.41
2:Q:146:ALA:HB2	2:Q:169:CYS:SG	2.60	0.41
1:A:248:PHE:O	1:A:249:ILE:C	2.59	0.41
3:C:93:LEU:HD23	3:C:163:ARG:HD3	2.01	0.41
1:D:153:GLN:HB3	1:D:289:PRO:HG2	2.02	0.41
2:E:143:PRO:HD3	2:E:156:TYR:CD2	2.56	0.41
3:F:137:ILE:CD1	3:F:150:PRO:HD3	2.47	0.41
1:G:18:TRP:NE1	1:G:22:ARG:CZ	2.83	0.41
1:G:56:VAL:O	1:G:57:LEU:C	2.58	0.41
2:H:145:CYS:SG	2:H:168:THR:O	2.78	0.41
2:K:144:LYS:O	2:K:147:GLU:HB2	2.20	0.41
3:L:177:LYS:HG2	3:L:177:LYS:O	2.20	0.41
1:M:55:LEU:HD12	1:M:55:LEU:HA	1.81	0.41
1:P:201:LEU:HA	1:P:201:LEU:HD23	1.83	0.41
2:Q:251:LEU:O	2:Q:251:LEU:HD12	2.21	0.41
2:B:22:GLN:HE21	2:B:22:GLN:HB2	1.72	0.41
1:D:4:ILE:CD1	1:D:4:ILE:N	2.82	0.41
2:E:110:PHE:O	2:E:120:GLN:HG2	2.20	0.41
2:E:197:ALA:C	2:E:199:GLY:H	2.24	0.41
2:E:203:SER:O	2:E:204:VAL:C	2.58	0.41
2:E:24:GLN:HG3	2:E:210:ASP:OD1	2.20	0.41
1:G:114:ARG:HD2	1:G:114:ARG:O	2.21	0.41
1:G:111:HIS:CE1	6:G:501:HEM:C1A	3.08	0.41
2:H:127:GLY:O	2:H:131:ILE:HG13	2.21	0.41
2:H:251:LEU:O	2:H:251:LEU:HD12	2.21	0.41
1:J:40:ASN:HD21	1:J:223:ASN:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:358:ARG:HA	1:J:364:LYS:HE2	2.03	0.41
1:P:139:MET:O	1:P:142:THR:HB	2.21	0.41
1:P:322:SER:O	1:P:323:PHE:HB2	2.20	0.41
1:P:39:ARG:HG2	1:P:242:VAL:CG1	2.48	0.41
1:P:91:PHE:CE1	1:P:92:MET:HB2	2.54	0.41
1:A:172:ILE:HG13	1:A:173:GLY:N	2.35	0.41
2:B:149:HIS:NE2	2:B:168:THR:HG21	2.36	0.41
2:B:77:THR:HG22	2:B:79:GLU:H	1.85	0.41
1:D:157:TRP:O	1:D:158:GLY:C	2.57	0.41
1:D:18:TRP:CD1	1:D:22:ARG:NH1	2.88	0.41
1:D:209:VAL:HG22	6:D:501:HEM:HBB2	2.03	0.41
2:E:135:LEU:HD21	6:E:301:HEM:C2B	2.56	0.41
1:G:125:ARG:NH2	1:G:222:ASN:CA	2.83	0.41
1:G:39:ARG:HD3	1:G:428:PHE:CE2	2.55	0.41
1:G:72:HIS:C	1:G:72:HIS:ND1	2.74	0.41
1:J:153:GLN:HB3	1:J:289:PRO:HG2	2.02	0.41
3:L:72:ILE:HG13	3:L:126:TRP:CE3	2.56	0.41
1:M:40:ASN:HD21	1:M:223:ASN:HB2	1.86	0.41
1:M:91:PHE:CG	1:M:92:MET:N	2.88	0.41
1:M:91:PHE:HD2	2:N:222:LYS:HG2	1.84	0.41
3:R:12:ARG:CG	3:R:13:ASP:N	2.83	0.41
1:A:410:ILE:O	1:A:412:GLY:N	2.54	0.41
1:A:91:PHE:CG	1:A:92:MET:N	2.89	0.41
1:A:261:LEU:HD11	2:B:234:VAL:HG13	2.01	0.41
1:D:299:LEU:O	1:D:302:TYR:HB3	2.21	0.41
2:E:189:LEU:O	2:E:190:MET:HB2	2.21	0.41
1:G:157:TRP:O	1:G:158:GLY:C	2.59	0.41
1:G:153:GLN:HB3	1:G:289:PRO:HG2	2.02	0.41
2:H:66:TYR:CE1	2:H:70:PHE:CE2	3.07	0.41
3:I:131:HIS:CD2	3:I:132:LEU:HG	2.56	0.41
1:J:18:TRP:NE1	1:J:22:ARG:CZ	2.83	0.41
1:J:72:HIS:HE1	1:J:74:ASP:OD2	2.03	0.41
1:M:118:TYR:CD1	1:M:224:PRO:HA	2.56	0.41
1:M:322:SER:O	1:M:323:PHE:HB2	2.20	0.41
1:M:395:ILE:O	1:M:398:ALA:HB3	2.20	0.41
1:M:43:TRP:HA	1:M:43:TRP:CE3	2.55	0.41
1:P:299:LEU:HB2	1:P:378:THR:HG23	2.02	0.41
2:Q:234:VAL:HG12	2:Q:235:MET:HE1	2.03	0.41
2:Q:40:HIS:CE1	2:Q:97:ALA:HB1	2.55	0.41
3:R:164:LYS:HG2	3:R:165:GLY:N	2.35	0.41
1:A:77:PHE:CD2	1:A:282:GLU:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:GLN:HG3	2:B:210:ASP:OD1	2.21	0.41
2:B:251:LEU:HD12	2:B:251:LEU:O	2.20	0.41
1:G:317:ILE:CG2	1:G:321:ILE:HD11	2.51	0.41
1:J:37:THR:HA	1:J:38:PRO:HD2	1.93	0.41
3:L:59:PRO:HD3	3:L:76:ARG:NH1	2.36	0.41
2:N:116:THR:HG22	2:N:116:THR:O	2.20	0.41
1:P:29:ALA:CB	10:P:505:ANJ:H233	2.51	0.41
2:Q:76:GLU:CD	2:Q:76:GLU:N	2.74	0.41
2:Q:250:ARG:NE	3:R:12:ARG:HB3	2.35	0.41
1:A:114:ARG:HD2	1:A:114:ARG:O	2.20	0.41
1:A:410:ILE:HG22	1:A:411:LEU:N	2.35	0.41
2:B:185:MET:HB2	6:B:301:HEM:C4D	2.56	0.41
1:D:403:TYR:CE2	1:D:408:LEU:HD11	2.56	0.41
1:D:362:MET:N	1:D:415:GLU:OE2	2.52	0.41
1:D:199:TYR:CZ	6:D:502:HEM:HBC1	2.55	0.41
1:D:55:LEU:O	1:D:59:ILE:HG13	2.21	0.41
2:E:104:ALA:CB	2:E:216:MET:HA	2.51	0.41
2:E:251:LEU:O	2:E:251:LEU:HD12	2.20	0.41
1:G:112:ILE:HG12	6:G:501:HEM:HAC	2.02	0.41
1:G:69:TYR:HA	1:G:79:SER:OG	2.20	0.41
2:H:142:PRO:CG	2:H:150:GLU:OE2	2.69	0.41
1:J:201:LEU:HA	1:J:201:LEU:HD23	1.80	0.41
1:J:207:ALA:O	1:J:210:ALA:HB3	2.21	0.41
2:N:186:PRO:O	2:N:187:PRO:C	2.59	0.41
1:A:252:ASP:O	1:A:256:LEU:HB2	2.21	0.41
2:B:240:LEU:HG	2:B:244:LEU:HD12	2.02	0.41
2:B:32:TYR:CD1	2:B:36:CYS:HB2	2.56	0.41
1:D:207:ALA:O	1:D:210:ALA:HB3	2.20	0.41
2:E:186:PRO:O	2:E:187:PRO:C	2.58	0.41
3:F:179:ILE:HD13	3:F:179:ILE:HA	1.87	0.41
1:G:367:PHE:O	1:G:370:LEU:HB3	2.21	0.41
1:J:188:ASN:O	1:J:189:ALA:C	2.58	0.41
1:J:262:VAL:O	1:J:265:ALA:HB3	2.20	0.41
1:J:72:HIS:ND1	1:J:72:HIS:C	2.74	0.41
3:L:185:GLN:HG2	3:L:185:GLN:O	2.20	0.41
1:M:408:LEU:N	1:M:409:PRO:CD	2.84	0.41
2:N:147:GLU:HG3	2:N:147:GLU:O	2.21	0.41
2:N:197:ALA:C	2:N:199:GLY:H	2.24	0.41
3:O:12:ARG:CG	3:O:13:ASP:N	2.83	0.41
1:P:122:LYS:NZ	1:P:360:ARG:HH11	2.19	0.41
2:Q:150:GLU:HA	2:Q:151:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:203:SER:O	2:Q:204:VAL:C	2.60	0.41
2:Q:235:MET:O	2:Q:236:PHE:C	2.57	0.41
3:R:12:ARG:HG3	3:R:13:ASP:N	2.36	0.41
3:R:26:ALA:O	3:R:27:THR:C	2.59	0.41
1:A:209:VAL:O	1:A:213:ILE:HG13	2.21	0.41
1:A:360:ARG:HB2	1:A:363:PHE:HB3	2.03	0.41
2:B:246:LEU:HB2	3:C:15:LEU:HD21	2.03	0.41
1:D:141:ALA:O	1:D:145:MET:HE2	2.21	0.41
3:F:180:ASP:OD1	3:F:181:GLU:N	2.54	0.41
3:F:32:TRP:N	3:F:33:PRO:HD2	2.36	0.41
1:G:365:ILE:HA	1:G:365:ILE:HD13	1.79	0.41
2:H:76:GLU:O	2:H:78:GLY:N	2.54	0.41
1:J:223:ASN:H	1:J:223:ASN:ND2	2.18	0.41
1:J:118:TYR:CD1	1:J:224:PRO:HA	2.56	0.41
1:J:46:ILE:HG13	1:J:47:TRP:N	2.36	0.41
1:M:91:PHE:C	1:M:91:PHE:CD1	2.93	0.41
1:M:91:PHE:CE1	1:M:92:MET:CE	3.04	0.41
2:N:103:MET:C	2:N:105:LYS:N	2.74	0.41
3:O:26:ALA:O	3:O:27:THR:C	2.58	0.41
1:P:180:LEU:HD23	1:P:180:LEU:HA	1.85	0.41
1:P:262:VAL:O	1:P:266:ILE:HG12	2.21	0.41
2:Q:86:THR:CG2	3:R:46:ALA:HB1	2.51	0.41
1:A:134:LEU:HA	1:A:134:LEU:HD23	1.92	0.40
2:B:206:ALA:O	2:B:207:MET:C	2.59	0.40
3:C:84:LEU:CD1	3:C:84:LEU:H	2.34	0.40
1:D:30:TYR:CZ	1:D:34:MET:HG3	2.55	0.40
2:E:165:VAL:HA	2:E:166:PRO:HD3	1.98	0.40
3:F:132:LEU:HB2	7:F:200:FES:S2	2.61	0.40
1:G:40:ASN:HD21	1:G:223:ASN:HB2	1.86	0.40
1:G:213:ILE:HD11	10:G:505:ANJ:H14	2.00	0.40
1:J:276:HIS:HA	1:J:277:PRO:HD3	1.90	0.40
2:K:205:HIS:ND1	2:K:205:HIS:C	2.73	0.40
2:K:235:MET:O	2:K:236:PHE:C	2.59	0.40
3:L:131:HIS:HB3	7:L:200:FES:S2	2.61	0.40
3:L:84:LEU:N	3:L:84:LEU:HD12	2.34	0.40
1:M:18:TRP:NE1	1:M:22:ARG:CZ	2.84	0.40
1:M:264:PHE:O	1:M:268:GLY:N	2.51	0.40
2:N:143:PRO:HD3	2:N:156:TYR:CD2	2.56	0.40
2:N:64:ARG:HA	2:N:85:PRO:HG3	2.03	0.40
1:P:131:VAL:HA	1:P:134:LEU:HD12	2.02	0.40
2:Q:64:ARG:HA	2:Q:85:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:39:ASN:HD22	3:R:39:ASN:HA	1.72	0.40
2:B:27:ARG:HB3	2:B:196:TYR:CE1	2.56	0.40
3:F:26:ALA:O	3:F:29:ALA:N	2.54	0.40
1:G:164:GLY:O	1:G:167:GLY:N	2.54	0.40
1:G:363:PHE:O	1:G:364:LYS:C	2.58	0.40
1:J:248:PHE:O	1:J:249:ILE:C	2.58	0.40
1:J:278:ASP:OD2	1:J:289:PRO:HB3	2.21	0.40
1:J:56:VAL:O	1:J:57:LEU:C	2.59	0.40
1:J:69:TYR:HA	1:J:79:SER:OG	2.21	0.40
2:K:226:ARG:O	2:K:229:ALA:HB3	2.21	0.40
3:L:31:VAL:O	3:L:32:TRP:C	2.60	0.40
1:M:157:TRP:O	1:M:158:GLY:C	2.59	0.40
1:M:213:ILE:HD13	10:M:505:ANJ:H14	2.01	0.40
1:P:114:ARG:C	1:P:114:ARG:CD	2.89	0.40
3:O:38:MET:CE	1:P:193:ARG:HH11	2.34	0.40
1:P:91:PHE:CE1	1:P:92:MET:HE3	2.52	0.40
2:Q:197:ALA:C	2:Q:199:GLY:H	2.24	0.40
2:Q:205:HIS:ND1	2:Q:205:HIS:C	2.73	0.40
3:R:152:HIS:HB2	7:R:200:FES:S1	2.61	0.40
1:A:284:ASN:HA	1:A:285:PRO:HD3	1.85	0.40
1:A:51:LEU:HD13	6:A:501:HEM:C4B	2.56	0.40
3:C:26:ALA:O	3:C:29:ALA:N	2.54	0.40
1:D:416:LYS:HA	1:D:417:PRO:HD2	1.93	0.40
2:E:226:ARG:O	2:E:229:ALA:HB3	2.21	0.40
2:E:240:LEU:HG	2:E:244:LEU:HD12	2.02	0.40
3:F:14:PHE:CD2	3:F:15:LEU:N	2.89	0.40
1:G:140:MET:O	1:G:141:ALA:C	2.59	0.40
2:H:137:GLY:O	2:H:139:PRO:HD3	2.22	0.40
2:H:189:LEU:HD23	2:H:189:LEU:HA	1.88	0.40
3:I:132:LEU:HA	3:I:132:LEU:HD23	1.89	0.40
3:I:59:PRO:HD3	3:I:76:ARG:HH11	1.86	0.40
1:J:262:VAL:O	1:J:266:ILE:HG12	2.21	0.40
1:J:327:ASP:OD1	1:J:327:ASP:C	2.59	0.40
1:J:410:ILE:O	1:J:412:GLY:N	2.54	0.40
3:L:90:LEU:O	3:L:90:LEU:HG	2.22	0.40
1:P:299:LEU:O	1:P:302:TYR:HB3	2.21	0.40
3:R:137:ILE:O	3:R:147:TRP:HA	2.21	0.40
1:A:72:HIS:HE1	1:A:74:ASP:OD2	2.03	0.40
1:A:8:HIS:N	1:A:8:HIS:CD2	2.86	0.40
3:C:73:PHE:CZ	3:C:127:GLY:HA3	2.56	0.40
1:D:114:ARG:O	1:D:114:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:185:MET:HA	2:E:186:PRO:HD2	1.99	0.40
1:G:248:PHE:HD1	1:G:251:LYS:CD	2.20	0.40
1:J:425:GLU:HG2	1:J:429:ASN:HD21	1.85	0.40
2:K:197:ALA:C	2:K:199:GLY:H	2.25	0.40
2:K:32:TYR:CD2	2:K:42:MET:HE2	2.56	0.40
1:M:110:LEU:HD23	1:M:110:LEU:HA	1.92	0.40
8:P:503:SMA:H11	8:P:503:SMA:H30	1.82	0.40
2:Q:160:PHE:CD2	2:Q:183:ILE:HB	2.56	0.40
2:Q:192:ASP:HA	2:Q:202:ALA:HB3	2.03	0.40
1:A:56:VAL:O	1:A:57:LEU:C	2.58	0.40
3:C:135:SER:HA	3:C:136:PRO:HD3	1.79	0.40
3:C:32:TRP:HB3	3:C:33:PRO:HD3	2.04	0.40
1:D:188:ASN:O	1:D:189:ALA:C	2.60	0.40
1:D:46:ILE:O	1:D:50:VAL:HG23	2.22	0.40
2:E:150:GLU:HA	2:E:151:PRO:HD3	1.96	0.40
1:G:187:ASP:CG	1:G:188:ASN:H	2.24	0.40
1:J:223:ASN:N	1:J:223:ASN:ND2	2.69	0.40
2:K:203:SER:O	2:K:204:VAL:C	2.60	0.40
2:K:223:LEU:HD21	2:K:227:LYS:HE3	2.04	0.40
1:M:163:THR:O	1:M:177:GLN:HG3	2.22	0.40
1:M:327:ASP:C	1:M:327:ASP:OD1	2.60	0.40
2:Q:17:PHE:CE1	2:Q:231:PHE:CE1	3.09	0.40
2:Q:236:PHE:CZ	3:R:25:VAL:HG12	2.56	0.40
2:Q:32:TYR:CD1	2:Q:36:CYS:HB2	2.56	0.40
3:R:26:ALA:O	3:R:29:ALA:N	2.54	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	426/428 (100%)	366 (86%)	54 (13%)	6 (1%)	13 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	426/428 (100%)	365 (86%)	57 (13%)	4 (1%)	20	60
1	G	426/428 (100%)	368 (86%)	53 (12%)	5 (1%)	15	51
1	J	426/428 (100%)	361 (85%)	58 (14%)	7 (2%)	11	43
1	M	426/428 (100%)	364 (85%)	54 (13%)	8 (2%)	9	39
1	P	426/428 (100%)	364 (85%)	54 (13%)	8 (2%)	9	39
2	B	254/256 (99%)	210 (83%)	38 (15%)	6 (2%)	7	32
2	E	254/256 (99%)	210 (83%)	37 (15%)	7 (3%)	6	29
2	H	254/256 (99%)	205 (81%)	42 (16%)	7 (3%)	6	29
2	K	254/256 (99%)	205 (81%)	41 (16%)	8 (3%)	5	26
2	N	254/256 (99%)	210 (83%)	36 (14%)	8 (3%)	5	26
2	Q	254/256 (99%)	212 (84%)	34 (13%)	8 (3%)	5	26
3	C	177/179 (99%)	143 (81%)	28 (16%)	6 (3%)	4	24
3	F	177/179 (99%)	148 (84%)	23 (13%)	6 (3%)	4	24
3	I	177/179 (99%)	145 (82%)	24 (14%)	8 (4%)	3	17
3	L	177/179 (99%)	144 (81%)	29 (16%)	4 (2%)	7	33
3	O	177/179 (99%)	148 (84%)	22 (12%)	7 (4%)	3	20
3	R	177/179 (99%)	143 (81%)	28 (16%)	6 (3%)	4	24
All	All	5142/5178 (99%)	4311 (84%)	712 (14%)	119 (2%)	7	33

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
3	C	109	ALA
1	D	73	VAL
1	D	76	ALA
3	F	45	GLN
3	F	107	ALA
3	F	109	ALA
1	G	73	VAL
1	G	76	ALA
3	I	45	GLN
3	I	109	ALA
1	J	73	VAL
1	J	76	ALA
3	L	107	ALA

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Mol	Chain	Res	Type
3	L	109	ALA
1	M	73	VAL
1	M	76	ALA
3	O	107	ALA
3	O	109	ALA
1	P	73	VAL
1	P	76	ALA
3	R	45	GLN
3	R	107	ALA
3	R	109	ALA
1	A	76	ALA
1	A	173	GLY
2	B	43	LYS
3	C	107	ALA
1	D	173	GLY
2	E	43	LYS
2	E	190	MET
1	G	173	GLY
1	G	411	LEU
3	I	107	ALA
3	I	143	ASP
1	J	173	GLY
2	K	104	ALA
2	K	145	CYS
2	K	190	MET
3	L	45	GLN
1	M	173	GLY
1	M	411	LEU
2	N	43	LYS
2	N	104	ALA
3	O	90	LEU
1	P	173	GLY
2	Q	43	LYS
2	Q	137	GLY
3	R	83	GLU
3	R	90	LEU
3	R	140	VAL
1	A	411	LEU
2	B	198	ASP
2	E	137	GLY
2	E	198	ASP
2	H	43	LYS

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Mol	Chain	Res	Type
2	H	77	THR
2	H	188	PRO
2	H	198	ASP
2	K	77	THR
2	K	137	GLY
2	K	198	ASP
2	N	198	ASP
3	O	45	GLN
3	O	134	CYS
1	P	143	ALA
1	P	411	LEU
2	Q	77	THR
2	Q	188	PRO
2	Q	198	ASP
2	B	137	GLY
3	C	90	LEU
1	D	411	LEU
2	E	95	GLU
3	F	140	VAL
2	H	137	GLY
1	J	143	ALA
1	J	411	LEU
2	K	48	ARG
1	M	143	ALA
1	M	355	ARG
2	N	48	ARG
2	N	137	GLY
2	N	188	PRO
2	Q	48	ARG
2	Q	75	GLU
1	A	6	HIS
1	A	143	ALA
2	B	95	GLU
2	B	188	PRO
2	B	190	MET
2	E	48	ARG
2	H	48	ARG
2	H	78	GLY
3	I	83	GLU
3	I	134	CYS
3	I	140	VAL
2	K	81	ARG

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Mol	Chain	Res	Type
2	Q	95	GLU
3	C	83	GLU
3	F	134	CYS
1	G	143	ALA
2	N	95	GLU
2	N	190	MET
3	C	168	PRO
2	E	188	PRO
3	L	140	VAL
3	O	140	VAL
3	C	140	VAL
1	J	123	ALA
1	M	421	PRO
3	O	168	PRO
1	P	421	PRO
3	F	168	PRO
3	I	168	PRO
1	M	325	ILE
1	J	421	PRO
1	P	123	ALA
1	P	249	ILE

### 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	353/353 (100%)	333 (94%)	20 (6%)	24	60
1	D	353/353 (100%)	340 (96%)	13 (4%)	39	75
1	G	353/353 (100%)	332 (94%)	21 (6%)	23	58
1	J	353/353 (100%)	338 (96%)	15 (4%)	34	71
1	M	353/353 (100%)	338 (96%)	15 (4%)	34	71
1	P	353/353 (100%)	337 (96%)	16 (4%)	32	68
2	B	203/203 (100%)	195 (96%)	8 (4%)	37	73
2	E	203/203 (100%)	197 (97%)	6 (3%)	46	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	203/203 (100%)	192 (95%)	11 (5%)	26	62
2	K	203/203 (100%)	197 (97%)	6 (3%)	46	79
2	N	203/203 (100%)	197 (97%)	6 (3%)	46	79
2	Q	203/203 (100%)	198 (98%)	5 (2%)	53	83
3	C	138/138 (100%)	129 (94%)	9 (6%)	20	55
3	F	138/138 (100%)	127 (92%)	11 (8%)	14	47
3	I	138/138 (100%)	125 (91%)	13 (9%)	10	38
3	L	138/138 (100%)	128 (93%)	10 (7%)	17	51
3	O	138/138 (100%)	127 (92%)	11 (8%)	14	47
3	R	138/138 (100%)	126 (91%)	12 (9%)	12	43
All	All	4164/4164 (100%)	3956 (95%)	208 (5%)	28	65

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	7	ASP
1	A	8	HIS
1	A	49	VAL
1	A	60	VAL
1	A	92	MET
1	A	94	ARG
1	A	104	PHE
1	A	190	THR
1	A	192	ASN
1	A	199	TYR
1	A	217	HIS
1	A	223	ASN
1	A	246	PRO
1	A	295	GLU
1	A	311	ASP
1	A	314	VAL
1	A	316	GLN
1	A	319	ASN
1	A	385	THR
2	B	61	ASP
2	B	80	ASP
2	B	147	GLU

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Mol	Chain	Res	Type
2	B	154	PHE
2	B	155	TYR
2	B	158	ARG
2	B	168	THR
2	B	220	GLU
3	C	12	ARG
3	C	19	THR
3	C	41	SER
3	C	72	ILE
3	C	112	GLN
3	C	135	SER
3	C	168	PRO
3	C	174	PRO
3	C	179	ILE
1	D	7	ASP
1	D	8	HIS
1	D	60	VAL
1	D	92	MET
1	D	94	ARG
1	D	104	PHE
1	D	190	THR
1	D	192	ASN
1	D	223	ASN
1	D	246	PRO
1	D	252	ASP
1	D	385	THR
1	D	421	PRO
2	E	61	ASP
2	E	155	TYR
2	E	168	THR
2	E	176	LYS
2	E	188	PRO
2	E	220	GLU
3	F	19	THR
3	F	41	SER
3	F	72	ILE
3	F	90	LEU
3	F	111	ASP
3	F	112	GLN
3	F	118	GLU
3	F	125	MET
3	F	168	PRO

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Mol	Chain	Res	Type
3	F	177	LYS
3	F	179	ILE
1	G	4	ILE
1	G	7	ASP
1	G	8	HIS
1	G	49	VAL
1	G	60	VAL
1	G	92	MET
1	G	94	ARG
1	G	104	PHE
1	G	108	VAL
1	G	125	ARG
1	G	190	THR
1	G	192	ASN
1	G	199	TYR
1	G	217	HIS
1	G	223	ASN
1	G	246	PRO
1	G	287	ARG
1	G	311	ASP
1	G	315	VAL
1	G	385	THR
1	G	421	PRO
2	H	60	GLU
2	H	73	THR
2	H	75	GLU
2	H	80	ASP
2	H	95	GLU
2	H	141	GLU
2	H	145	CYS
2	H	167	ASP
2	H	168	THR
2	H	220	GLU
2	H	236	PHE
3	I	12	ARG
3	I	14	PHE
3	I	19	THR
3	I	41	SER
3	I	44	VAL
3	I	72	ILE
3	I	92	GLN
3	I	112	GLN

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Mol	Chain	Res	Type
3	I	118	GLU
3	I	168	PRO
3	I	174	PRO
3	I	177	LYS
3	I	179	ILE
1	J	7	ASP
1	J	8	HIS
1	J	43	TRP
1	J	49	VAL
1	J	60	VAL
1	J	94	ARG
1	J	104	PHE
1	J	108	VAL
1	J	190	THR
1	J	192	ASN
1	J	217	HIS
1	J	223	ASN
1	J	246	PRO
1	J	385	THR
1	J	421	PRO
2	K	80	ASP
2	K	154	PHE
2	K	168	THR
2	K	171	ASP
2	K	188	PRO
2	K	220	GLU
3	L	19	THR
3	L	41	SER
3	L	72	ILE
3	L	90	LEU
3	L	112	GLN
3	L	118	GLU
3	L	168	PRO
3	L	174	PRO
3	L	177	LYS
3	L	179	ILE
1	M	7	ASP
1	M	8	HIS
1	M	43	TRP
1	M	49	VAL
1	M	60	VAL
1	M	94	ARG

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Mol	Chain	Res	Type
1	M	104	PHE
1	M	108	VAL
1	M	190	THR
1	M	192	ASN
1	M	199	TYR
1	M	223	ASN
1	M	246	PRO
1	M	252	ASP
1	M	385	THR
2	N	80	ASP
2	N	154	PHE
2	N	158	ARG
2	N	168	THR
2	N	188	PRO
2	N	220	GLU
3	O	19	THR
3	O	41	SER
3	O	44	VAL
3	O	72	ILE
3	O	94	VAL
3	O	112	GLN
3	O	125	MET
3	O	168	PRO
3	O	174	PRO
3	O	177	LYS
3	O	179	ILE
1	P	7	ASP
1	P	8	HIS
1	P	49	VAL
1	P	60	VAL
1	P	94	ARG
1	P	104	PHE
1	P	108	VAL
1	P	190	THR
1	P	192	ASN
1	P	217	HIS
1	P	223	ASN
1	P	246	PRO
1	P	287	ARG
1	P	309	THR
1	P	385	THR
1	P	421	PRO

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Mol	Chain	Res	Type
2	Q	52	GLU
2	Q	80	ASP
2	Q	90	PRO
2	Q	168	THR
2	Q	220	GLU
3	R	19	THR
3	R	41	SER
3	R	72	ILE
3	R	89	GLN
3	R	92	GLN
3	R	112	GLN
3	R	118	GLU
3	R	121	GLU
3	R	168	PRO
3	R	174	PRO
3	R	177	LYS
3	R	179	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	177	GLN
1	A	192	ASN
1	A	319	ASN
1	A	429	ASN
2	B	22	GLN
2	B	62	GLN
2	B	111	HIS
2	B	228	GLN
3	C	36	ASN
3	C	39	ASN
3	C	112	GLN
3	C	185	GLN
1	D	177	GLN
1	D	192	ASN
1	D	217	HIS
1	D	429	ASN
2	E	22	GLN
2	E	62	GLN
2	E	111	HIS
2	E	228	GLN

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Mol	Chain	Res	Type
3	F	36	ASN
3	F	39	ASN
3	F	112	GLN
3	F	185	GLN
1	G	8	HIS
1	G	192	ASN
1	G	217	HIS
1	G	319	ASN
1	G	383	GLN
1	G	429	ASN
2	H	22	GLN
2	H	62	GLN
2	H	149	HIS
3	I	36	ASN
3	I	39	ASN
3	I	92	GLN
3	I	112	GLN
3	I	185	GLN
1	J	8	HIS
1	J	177	GLN
1	J	192	ASN
1	J	221	ASN
1	J	383	GLN
1	J	429	ASN
2	K	22	GLN
2	K	62	GLN
2	K	111	HIS
2	K	228	GLN
3	L	36	ASN
3	L	39	ASN
3	L	89	GLN
3	L	92	GLN
3	L	112	GLN
3	L	185	GLN
1	M	8	HIS
1	M	177	GLN
1	M	192	ASN
1	M	217	HIS
1	M	429	ASN
2	N	22	GLN
2	N	62	GLN
2	N	96	ASN

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Mol	Chain	Res	Type
3	O	36	ASN
3	O	39	ASN
3	O	112	GLN
3	O	185	GLN
1	P	8	HIS
1	P	177	GLN
1	P	192	ASN
1	P	429	ASN
2	Q	22	GLN
2	Q	62	GLN
2	Q	120	GLN
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 54 ligands modelled in this entry, 6 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
8	SMA	A	1	-	36,38,38	1.75	6 (16%)	44,52,52	2.53	13 (29%)
4	BGL	A	431	-	20,20,20	1.71	2 (10%)	23,25,25	1.06	3 (13%)
6	HEM	A	501	1	28,50,50	1.83	7 (25%)	17,82,82	1.01	1 (5%)
6	HEM	A	502	1	28,50,50	2.08	9 (32%)	17,82,82	1.16	1 (5%)
9	LOP	A	503	-	44,44,44	0.54	0	46,49,49	1.26	5 (10%)
10	ANJ	A	504	-	40,40,40	1.75	12 (30%)	35,54,54	1.73	7 (20%)
6	HEM	B	301	2	28,50,50	1.77	7 (25%)	17,82,82	1.18	1 (5%)
7	FES	C	200	3	0,4,4	0.00	-	0,4,4	0.00	-
8	SMA	D	2	-	36,38,38	2.12	8 (22%)	44,52,52	2.18	12 (27%)
4	BGL	D	431	-	20,20,20	1.47	2 (10%)	23,25,25	1.15	2 (8%)
6	HEM	D	501	1	28,50,50	1.86	7 (25%)	17,82,82	0.99	1 (5%)
6	HEM	D	502	1	28,50,50	1.74	6 (21%)	17,82,82	1.11	1 (5%)
9	LOP	D	503	-	44,44,44	0.55	0	46,49,49	1.32	6 (13%)
10	ANJ	D	504	-	40,40,40	1.80	13 (32%)	35,54,54	1.66	8 (22%)
6	HEM	E	301	2	28,50,50	1.86	7 (25%)	17,82,82	0.98	0
7	FES	F	200	3	0,4,4	0.00	-	0,4,4	0.00	-
4	BGL	G	431	-	20,20,20	1.86	2 (10%)	23,25,25	0.86	0
6	HEM	G	501	1	28,50,50	2.02	6 (21%)	17,82,82	0.85	1 (5%)
6	HEM	G	502	1	28,50,50	2.03	8 (28%)	17,82,82	1.05	1 (5%)
8	SMA	G	503	-	36,38,38	1.80	7 (19%)	44,52,52	2.50	13 (29%)
9	LOP	G	504	-	44,44,44	0.63	0	46,49,49	1.23	4 (8%)
10	ANJ	G	505	-	40,40,40	1.65	9 (22%)	35,54,54	1.82	8 (22%)
6	HEM	H	301	2	28,50,50	2.01	7 (25%)	17,82,82	1.28	2 (11%)
7	FES	I	200	3	0,4,4	0.00	-	0,4,4	0.00	-
4	BGL	J	431	-	20,20,20	1.64	2 (10%)	23,25,25	1.01	3 (13%)
6	HEM	J	501	1	28,50,50	1.98	8 (28%)	17,82,82	0.88	0
6	HEM	J	502	1	28,50,50	2.08	10 (35%)	17,82,82	1.00	1 (5%)
8	SMA	J	503	-	36,38,38	1.75	5 (13%)	44,52,52	2.19	11 (25%)
9	LOP	J	504	-	44,44,44	0.67	1 (2%)	46,49,49	1.17	2 (4%)
10	ANJ	J	505	-	40,40,40	1.89	11 (27%)	35,54,54	1.67	6 (17%)
6	HEM	K	301	2	28,50,50	1.96	6 (21%)	17,82,82	1.24	0
7	FES	L	200	3	0,4,4	0.00	-	0,4,4	0.00	-
4	BGL	M	431	-	20,20,20	1.80	2 (10%)	23,25,25	0.67	0
6	HEM	M	501	1	28,50,50	1.76	6 (21%)	17,82,82	1.05	1 (5%)
6	HEM	M	502	1	28,50,50	1.99	8 (28%)	17,82,82	1.14	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SMA	M	503	-	36,38,38	1.95	5 (13%)	44,52,52	2.21	10 (22%)
9	LOP	M	504	-	44,44,44	0.61	0	46,49,49	1.34	6 (13%)
10	ANJ	M	505	-	40,40,40	1.80	11 (27%)	35,54,54	1.80	9 (25%)
6	HEM	N	301	2	28,50,50	1.69	6 (21%)	17,82,82	1.13	1 (5%)
7	FES	O	200	3	0,4,4	0.00	-	0,4,4	0.00	-
6	HEM	P	501	1	28,50,50	2.05	7 (25%)	17,82,82	0.89	1 (5%)
6	HEM	P	502	1	28,50,50	1.99	6 (21%)	17,82,82	1.19	2 (11%)
8	SMA	P	503	-	36,38,38	1.89	8 (22%)	44,52,52	1.86	6 (13%)
9	LOP	P	504	-	44,44,44	0.61	0	46,49,49	1.29	5 (10%)
10	ANJ	P	505	-	40,40,40	1.77	11 (27%)	35,54,54	1.68	7 (20%)
4	BGL	Q	257	-	20,20,20	1.53	2 (10%)	23,25,25	1.01	1 (4%)
6	HEM	Q	301	2	28,50,50	1.79	6 (21%)	17,82,82	1.11	0
7	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
8	SMA	A	1	-	-	0/33/34/34	0/2/2/2
4	BGL	A	431	-	-	0/11/31/31	0/1/1/1
6	HEM	A	501	1	-	0/6/54/54	0/0/8/8
6	HEM	A	502	1	-	0/6/54/54	0/0/8/8
9	LOP	A	503	-	-	0/48/48/48	0/0/0/0
10	ANJ	A	504	-	-	0/39/55/55	0/1/2/2
6	HEM	B	301	2	-	0/6/54/54	0/0/8/8
7	FES	C	200	3	-	0/0/4/4	0/1/1/1
8	SMA	D	2	-	-	0/33/34/34	0/2/2/2
4	BGL	D	431	-	-	0/11/31/31	0/1/1/1
6	HEM	D	501	1	-	0/6/54/54	0/0/8/8
6	HEM	D	502	1	-	0/6/54/54	0/0/8/8
9	LOP	D	503	-	-	0/48/48/48	0/0/0/0
10	ANJ	D	504	-	-	0/39/55/55	0/1/2/2
6	HEM	E	301	2	-	0/6/54/54	0/0/8/8
7	FES	F	200	3	-	0/0/4/4	0/1/1/1
4	BGL	G	431	-	-	0/11/31/31	0/1/1/1
6	HEM	G	501	1	-	0/6/54/54	0/0/8/8
6	HEM	G	502	1	-	0/6/54/54	0/0/8/8
8	SMA	G	503	-	-	0/33/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LOP	G	504	-	-	0/48/48/48	0/0/0/0
10	ANJ	G	505	-	-	0/39/55/55	0/1/2/2
6	HEM	H	301	2	-	0/6/54/54	0/0/8/8
7	FES	I	200	3	-	0/0/4/4	0/1/1/1
4	BGL	J	431	-	-	0/11/31/31	0/1/1/1
6	HEM	J	501	1	-	0/6/54/54	0/0/8/8
6	HEM	J	502	1	-	0/6/54/54	0/0/8/8
8	SMA	J	503	-	-	0/33/34/34	0/2/2/2
9	LOP	J	504	-	-	0/48/48/48	0/0/0/0
10	ANJ	J	505	-	-	0/39/55/55	0/1/2/2
6	HEM	K	301	2	-	0/6/54/54	0/0/8/8
7	FES	L	200	3	-	0/0/4/4	0/1/1/1
4	BGL	M	431	-	-	0/11/31/31	0/1/1/1
6	HEM	M	501	1	-	0/6/54/54	0/0/8/8
6	HEM	M	502	1	-	0/6/54/54	0/0/8/8
8	SMA	M	503	-	-	0/33/34/34	0/2/2/2
9	LOP	M	504	-	-	0/48/48/48	0/0/0/0
10	ANJ	M	505	-	-	0/39/55/55	0/1/2/2
6	HEM	N	301	2	-	0/6/54/54	0/0/8/8
7	FES	O	200	3	-	0/0/4/4	0/1/1/1
6	HEM	P	501	1	-	0/6/54/54	0/0/8/8
6	HEM	P	502	1	-	0/6/54/54	0/0/8/8
8	SMA	P	503	-	-	0/33/34/34	0/2/2/2
9	LOP	P	504	-	-	0/48/48/48	0/0/0/0
10	ANJ	P	505	-	-	0/39/55/55	0/1/2/2
4	BGL	Q	257	-	-	0/11/31/31	0/1/1/1
6	HEM	Q	301	2	-	0/6/54/54	0/0/8/8
7	FES	R	200	3	-	0/0/4/4	0/1/1/1

All (246) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	502	HEM	C3B-CAB	-5.28	1.37	1.47
6	P	501	HEM	C3C-C2C	-5.13	1.33	1.40
6	G	501	HEM	C3C-C2C	-5.09	1.33	1.40
6	K	301	HEM	C3B-C2B	-5.08	1.33	1.40
6	A	502	HEM	C3C-C2C	-4.87	1.33	1.40
6	J	501	HEM	C3B-CAB	-4.82	1.38	1.47
6	M	502	HEM	C3B-C2B	-4.82	1.34	1.40
6	J	502	HEM	C3C-CAC	-4.61	1.38	1.47
6	G	502	HEM	C3C-C2C	-4.52	1.34	1.40
6	A	502	HEM	C3C-CAC	-4.52	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	301	HEM	C3B-C2B	-4.48	1.34	1.40
6	P	502	HEM	C3C-CAC	-4.40	1.39	1.47
6	G	502	HEM	C3B-CAB	-4.34	1.39	1.47
6	H	301	HEM	C3C-CAC	-4.31	1.39	1.47
6	G	501	HEM	C3B-CAB	-4.30	1.39	1.47
6	K	301	HEM	C3B-CAB	-4.28	1.39	1.47
6	P	501	HEM	C3B-CAB	-4.26	1.39	1.47
6	D	501	HEM	C3C-C2C	-4.23	1.34	1.40
6	D	502	HEM	C3C-C2C	-4.22	1.34	1.40
6	M	502	HEM	C3B-CAB	-4.15	1.39	1.47
6	J	501	HEM	C3B-C2B	-4.06	1.35	1.40
6	J	501	HEM	C3C-C2C	-4.03	1.35	1.40
6	P	502	HEM	C3C-C2C	-4.02	1.35	1.40
6	G	502	HEM	C3B-C2B	-4.01	1.35	1.40
6	P	502	HEM	C3B-CAB	-3.99	1.39	1.47
6	A	501	HEM	C3B-CAB	-3.99	1.40	1.47
6	G	501	HEM	C3B-C2B	-3.97	1.35	1.40
6	Q	301	HEM	C3C-CAC	-3.96	1.39	1.47
6	G	501	HEM	C3C-CAC	-3.95	1.39	1.47
6	A	501	HEM	C3B-C2B	-3.94	1.35	1.40
6	E	301	HEM	C3C-CAC	-3.92	1.39	1.47
6	A	502	HEM	C3B-CAB	-3.92	1.40	1.47
6	P	501	HEM	C3C-CAC	-3.90	1.40	1.47
6	D	501	HEM	C3C-CAC	-3.88	1.40	1.47
6	G	502	HEM	C3C-CAC	-3.81	1.40	1.47
6	P	501	HEM	C3B-C2B	-3.78	1.35	1.40
6	H	301	HEM	C3B-CAB	-3.71	1.40	1.47
6	M	501	HEM	C3B-C2B	-3.70	1.35	1.40
6	P	502	HEM	C3B-C2B	-3.68	1.35	1.40
8	P	503	SMA	C7-C8	-3.60	1.35	1.40
6	E	301	HEM	C3B-C2B	-3.58	1.35	1.40
6	Q	301	HEM	C3B-CAB	-3.57	1.40	1.47
6	M	501	HEM	C3C-C2C	-3.53	1.35	1.40
6	E	301	HEM	C3B-CAB	-3.50	1.40	1.47
6	J	501	HEM	C3C-CAC	-3.47	1.40	1.47
6	A	501	HEM	C3C-C2C	-3.44	1.35	1.40
6	M	502	HEM	C3C-CAC	-3.41	1.40	1.47
6	B	301	HEM	C3B-C2B	-3.40	1.35	1.40
6	B	301	HEM	C3C-C2C	-3.39	1.35	1.40
6	K	301	HEM	C3C-CAC	-3.36	1.41	1.47
6	H	301	HEM	C3C-C2C	-3.32	1.36	1.40
6	A	501	HEM	C3C-CAC	-3.32	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	301	HEM	C3C-CAC	-3.30	1.41	1.47
6	D	502	HEM	C3B-CAB	-3.25	1.41	1.47
6	B	301	HEM	C3C-CAC	-3.23	1.41	1.47
6	D	501	HEM	C3B-CAB	-3.18	1.41	1.47
6	B	301	HEM	C3B-CAB	-3.17	1.41	1.47
6	M	501	HEM	C3B-CAB	-3.15	1.41	1.47
6	Q	301	HEM	C3B-C2B	-3.06	1.36	1.40
6	D	502	HEM	C3C-CAC	-3.05	1.41	1.47
6	J	502	HEM	C3B-C2B	-3.02	1.36	1.40
6	Q	301	HEM	C3C-C2C	-2.96	1.36	1.40
6	D	501	HEM	C3B-C2B	-2.95	1.36	1.40
6	N	301	HEM	C3B-CAB	-2.93	1.42	1.47
6	M	502	HEM	C3C-C2C	-2.89	1.36	1.40
6	M	501	HEM	C3C-CAC	-2.87	1.42	1.47
6	N	301	HEM	C3C-C2C	-2.85	1.36	1.40
10	P	505	ANJ	C6-C8	-2.78	1.44	1.50
8	D	2	SMA	C7-C8	-2.74	1.36	1.40
6	J	502	HEM	C3C-C2C	-2.72	1.36	1.40
10	J	505	ANJ	C6-C8	-2.61	1.44	1.50
6	E	301	HEM	C3C-C2C	-2.60	1.36	1.40
6	N	301	HEM	C3B-C2B	-2.59	1.36	1.40
8	P	503	SMA	C3-C2	-2.59	1.36	1.39
6	A	502	HEM	C3B-C2B	-2.58	1.36	1.40
10	D	504	ANJ	O7-C17	-2.48	1.14	1.21
6	B	301	HEM	C1A-CHA	-2.43	1.33	1.40
6	A	502	HEM	C4D-ND	-2.43	1.33	1.36
6	K	301	HEM	C3C-C2C	-2.42	1.37	1.40
8	G	503	SMA	C6-C7	-2.41	1.34	1.38
6	D	502	HEM	C3B-C2B	-2.41	1.37	1.40
10	A	504	ANJ	O7-C17	-2.31	1.15	1.21
6	P	501	HEM	C1A-CHA	-2.29	1.34	1.40
6	G	502	HEM	C4B-CHC	-2.26	1.34	1.40
8	G	503	SMA	C4A-C8A	-2.23	1.38	1.41
6	J	502	HEM	C4B-CHC	-2.22	1.34	1.40
6	G	502	HEM	C1A-CHA	-2.17	1.34	1.40
6	H	301	HEM	C4B-CHC	-2.13	1.34	1.40
6	A	502	HEM	C4B-CHC	-2.06	1.34	1.40
6	E	301	HEM	C1D-CHD	-2.06	1.34	1.40
6	M	502	HEM	C1A-CHA	-2.05	1.34	1.40
8	P	503	SMA	C4A-C8A	-2.03	1.38	1.41
6	D	501	HEM	C4B-CHC	-2.03	1.34	1.40
9	J	504	LOP	O5-C6	2.02	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	505	ANJ	C1-N1	2.02	1.37	1.34
10	M	505	ANJ	O3-C8	2.04	1.27	1.23
6	J	501	HEM	C1B-NB	2.04	1.39	1.36
6	A	502	HEM	C1B-NB	2.05	1.39	1.36
10	D	504	ANJ	O4-C10	2.06	1.49	1.46
4	M	431	BGL	O2-C2	2.06	1.46	1.43
10	D	504	ANJ	C25-C24	2.07	1.57	1.51
10	A	504	ANJ	C1-N1	2.10	1.37	1.34
4	G	431	BGL	O5-C1	2.11	1.47	1.43
10	A	504	ANJ	C2-N1	2.12	1.44	1.41
8	A	1	SMA	C9-C2	2.12	1.53	1.51
10	A	504	ANJ	C18-C13	2.14	1.58	1.54
6	A	501	HEM	C1C-NC	2.14	1.39	1.36
6	J	502	HEM	CMA-C3A	2.15	1.56	1.51
6	J	501	HEM	C1C-NC	2.15	1.39	1.36
10	G	505	ANJ	C2-N1	2.16	1.44	1.41
10	D	504	ANJ	O3-C8	2.18	1.27	1.23
10	P	505	ANJ	O4-C12	2.19	1.39	1.34
6	J	502	HEM	C4C-NC	2.19	1.39	1.36
10	G	505	ANJ	C1-N1	2.22	1.37	1.34
8	G	503	SMA	O1-C8A	2.24	1.40	1.36
8	D	2	SMA	O12-C12	2.25	1.48	1.42
10	D	504	ANJ	C26-C25	2.29	1.60	1.52
6	J	502	HEM	C1C-NC	2.29	1.39	1.36
10	J	505	ANJ	C1-N1	2.30	1.37	1.34
10	G	505	ANJ	C26-C25	2.31	1.60	1.52
8	A	1	SMA	O1-C8A	2.32	1.40	1.36
10	P	505	ANJ	O8-C14	2.33	1.48	1.44
10	J	505	ANJ	O4-C10	2.35	1.50	1.46
10	G	505	ANJ	O8-C14	2.36	1.48	1.44
10	J	505	ANJ	C26-C25	2.42	1.61	1.52
10	P	505	ANJ	O3-C8	2.42	1.28	1.23
8	M	503	SMA	O1-C8A	2.42	1.40	1.36
6	M	502	HEM	C4C-NC	2.43	1.39	1.36
10	A	504	ANJ	C4-C3	2.48	1.43	1.38
8	P	503	SMA	O8-C8	2.52	1.44	1.35
10	A	504	ANJ	C2-C7	2.52	1.44	1.40
4	J	431	BGL	O5-C1	2.53	1.47	1.43
4	D	431	BGL	O5-C1	2.53	1.47	1.43
8	M	503	SMA	O8-C8	2.54	1.44	1.35
10	M	505	ANJ	O4-C10	2.56	1.50	1.46
8	D	2	SMA	O8-C8	2.56	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	504	ANJ	C10-C9	2.58	1.58	1.53
8	D	2	SMA	C9-C2	2.58	1.54	1.51
10	M	505	ANJ	C26-C25	2.60	1.61	1.52
10	D	504	ANJ	C4-C3	2.61	1.43	1.38
8	J	503	SMA	O8-C8	2.63	1.44	1.35
10	P	505	ANJ	C1-N1	2.73	1.38	1.34
10	M	505	ANJ	C4-C3	2.74	1.44	1.38
10	D	504	ANJ	C2-N1	2.75	1.45	1.41
10	A	504	ANJ	C26-C25	2.75	1.62	1.52
10	M	505	ANJ	C2-N1	2.77	1.45	1.41
8	J	503	SMA	O1-C8A	2.81	1.41	1.36
8	G	503	SMA	O8-C8	2.81	1.45	1.35
4	Q	257	BGL	O5-C1	2.82	1.48	1.43
10	J	505	ANJ	O4-C12	2.82	1.40	1.34
10	P	505	ANJ	C2-N1	2.84	1.45	1.41
8	A	1	SMA	O8-C8	2.85	1.45	1.35
10	M	505	ANJ	O8-C14	2.85	1.49	1.44
10	G	505	ANJ	O4-C12	2.85	1.40	1.34
8	P	503	SMA	O1-C8A	2.86	1.41	1.36
10	G	505	ANJ	C4-C3	2.87	1.44	1.38
8	D	2	SMA	O1-C8A	2.96	1.41	1.36
4	A	431	BGL	O5-C1	2.98	1.48	1.43
10	J	505	ANJ	C2-N1	2.98	1.46	1.41
10	D	504	ANJ	O4-C12	2.99	1.41	1.34
10	D	504	ANJ	C1-N1	3.01	1.38	1.34
10	A	504	ANJ	C13-C12	3.03	1.57	1.51
6	P	502	HEM	CBC-CAC	3.04	1.50	1.28
10	D	504	ANJ	O8-C14	3.05	1.49	1.44
10	P	505	ANJ	C4-C3	3.06	1.44	1.38
6	J	502	HEM	CBC-CAC	3.07	1.50	1.28
10	P	505	ANJ	C13-C12	3.09	1.57	1.51
10	P	505	ANJ	C26-C25	3.09	1.63	1.52
6	A	501	HEM	CBB-CAB	3.15	1.51	1.28
10	J	505	ANJ	C4-C3	3.15	1.44	1.38
6	A	502	HEM	CBC-CAC	3.19	1.51	1.28
6	J	501	HEM	CBC-CAC	3.19	1.51	1.28
6	G	502	HEM	CBC-CAC	3.20	1.51	1.28
10	G	505	ANJ	C10-C9	3.22	1.59	1.53
10	D	504	ANJ	C5-C6	3.23	1.45	1.39
6	G	501	HEM	CBC-CAC	3.23	1.51	1.28
8	P	503	SMA	O1-C2	3.26	1.39	1.35
6	P	501	HEM	CBC-CAC	3.27	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	501	HEM	CBB-CAB	3.27	1.51	1.28
6	J	501	HEM	CBB-CAB	3.28	1.51	1.28
6	G	501	HEM	CBB-CAB	3.28	1.52	1.28
6	M	502	HEM	CBC-CAC	3.28	1.52	1.28
6	J	502	HEM	CBB-CAB	3.31	1.52	1.28
6	D	501	HEM	CBC-CAC	3.34	1.52	1.28
10	P	505	ANJ	C5-C6	3.36	1.45	1.39
6	D	501	HEM	CBB-CAB	3.36	1.52	1.28
6	M	501	HEM	CBB-CAB	3.37	1.52	1.28
6	H	301	HEM	CBC-CAC	3.38	1.52	1.28
6	E	301	HEM	CBC-CAC	3.39	1.52	1.28
6	A	501	HEM	CBC-CAC	3.39	1.52	1.28
10	A	504	ANJ	O4-C10	3.40	1.52	1.46
6	A	502	HEM	CBB-CAB	3.41	1.52	1.28
6	Q	301	HEM	CBC-CAC	3.44	1.53	1.28
6	D	502	HEM	CBC-CAC	3.45	1.53	1.28
6	N	301	HEM	CBB-CAB	3.45	1.53	1.28
10	A	504	ANJ	O4-C12	3.46	1.42	1.34
6	E	301	HEM	CBB-CAB	3.50	1.53	1.28
6	M	501	HEM	CBC-CAC	3.51	1.53	1.28
10	G	505	ANJ	C5-C6	3.52	1.45	1.39
6	Q	301	HEM	CBB-CAB	3.53	1.53	1.28
10	J	505	ANJ	C10-C9	3.53	1.60	1.53
10	M	505	ANJ	O4-C12	3.53	1.42	1.34
10	D	504	ANJ	C10-C9	3.55	1.60	1.53
10	J	505	ANJ	C13-C12	3.56	1.58	1.51
6	K	301	HEM	CBC-CAC	3.57	1.54	1.28
6	K	301	HEM	CBB-CAB	3.58	1.54	1.28
6	B	301	HEM	CBB-CAB	3.59	1.54	1.28
6	P	502	HEM	CBB-CAB	3.61	1.54	1.28
6	N	301	HEM	CBC-CAC	3.61	1.54	1.28
6	B	301	HEM	CBC-CAC	3.62	1.54	1.28
6	H	301	HEM	CBB-CAB	3.62	1.54	1.28
6	M	502	HEM	CBB-CAB	3.63	1.54	1.28
6	D	502	HEM	CBB-CAB	3.65	1.54	1.28
10	M	505	ANJ	C13-C12	3.68	1.58	1.51
6	G	502	HEM	CBB-CAB	3.70	1.54	1.28
10	M	505	ANJ	C10-C9	3.78	1.60	1.53
10	D	504	ANJ	C13-C12	3.82	1.58	1.51
10	J	505	ANJ	O8-C14	3.83	1.50	1.44
10	M	505	ANJ	C5-C6	3.90	1.46	1.39
8	A	1	SMA	O1-C2	4.10	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	505	ANJ	C13-C12	4.12	1.59	1.51
8	J	503	SMA	O1-C2	4.13	1.40	1.35
10	A	504	ANJ	C5-C6	4.38	1.46	1.39
10	J	505	ANJ	C5-C6	4.43	1.46	1.39
8	M	503	SMA	O1-C2	4.52	1.41	1.35
8	A	1	SMA	O5-C5	4.55	1.45	1.36
8	G	503	SMA	O5-C5	4.68	1.45	1.36
10	P	505	ANJ	C10-C9	4.75	1.62	1.53
8	G	503	SMA	O1-C2	4.79	1.41	1.35
8	G	503	SMA	O7-C7	4.92	1.44	1.37
8	D	2	SMA	O1-C2	4.94	1.41	1.35
4	D	431	BGL	C1-C2	4.99	1.56	1.52
8	P	503	SMA	O7-C7	5.00	1.45	1.37
8	J	503	SMA	O5-C5	5.16	1.46	1.36
4	Q	257	BGL	C1-C2	5.21	1.57	1.52
8	M	503	SMA	O5-C5	5.30	1.46	1.36
8	J	503	SMA	O7-C7	5.56	1.45	1.37
4	J	431	BGL	C1-C2	5.64	1.57	1.52
8	P	503	SMA	O5-C5	5.85	1.47	1.36
8	A	1	SMA	O7-C7	5.92	1.46	1.37
4	A	431	BGL	C1-C2	6.05	1.57	1.52
8	D	2	SMA	O5-C5	6.10	1.47	1.36
8	D	2	SMA	O7-C7	6.18	1.46	1.37
4	M	431	BGL	C1-C2	6.40	1.57	1.52
8	M	503	SMA	O7-C7	7.07	1.48	1.37
4	G	431	BGL	C1-C2	7.15	1.58	1.52

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1	SMA	C5M-O5-C5	-6.84	108.04	117.77
8	G	503	SMA	C5M-O5-C5	-5.80	109.51	117.77
8	M	503	SMA	C5M-O5-C5	-5.66	109.72	117.77
10	G	505	ANJ	O6-C17-C9	-5.47	101.68	110.28
8	J	503	SMA	C5M-O5-C5	-5.44	110.02	117.77
10	J	505	ANJ	O6-C17-C9	-5.23	102.05	110.28
10	P	505	ANJ	O6-C17-C9	-5.10	102.26	110.28
10	M	505	ANJ	O6-C17-C9	-4.98	102.44	110.28
10	D	504	ANJ	O6-C17-C9	-4.69	102.90	110.28
10	A	504	ANJ	O6-C17-C9	-4.61	103.02	110.28
8	J	503	SMA	C7M-O7-C7	-4.49	111.08	117.54
8	G	503	SMA	C7M-O7-C7	-4.27	111.40	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1	SMA	C9-C10-C11	-4.16	109.11	114.72
8	G	503	SMA	O7-C7-C6	-4.14	117.19	124.17
8	A	1	SMA	C7M-O7-C7	-4.13	111.60	117.54
8	D	2	SMA	C7M-O7-C7	-3.92	111.89	117.54
8	D	2	SMA	C9-C10-C11	-3.83	109.56	114.72
9	D	503	LOP	C19-C18-C17	-3.61	95.87	114.45
8	P	503	SMA	C7M-O7-C7	-3.58	112.38	117.54
8	A	1	SMA	O7-C7-C6	-3.58	118.14	124.17
9	M	504	LOP	C12-C11-C10	-3.54	96.22	114.45
10	A	504	ANJ	C5-C6-C7	-3.52	115.18	118.70
8	A	1	SMA	C16-C17-C18	-3.35	115.99	124.65
10	M	505	ANJ	C5-C6-C7	-3.31	115.39	118.70
9	A	503	LOP	C19-C18-C17	-3.28	97.53	114.45
8	M	503	SMA	C7M-O7-C7	-3.25	112.86	117.54
10	D	504	ANJ	C5-C6-C7	-3.22	115.48	118.70
10	M	505	ANJ	C19-C18-C13	-3.21	108.37	114.34
9	P	504	LOP	C19-C18-C17	-3.14	98.27	114.45
10	G	505	ANJ	C5-C6-C7	-3.10	115.59	118.70
8	D	2	SMA	C5M-O5-C5	-3.07	113.40	117.77
4	D	431	BGL	C1'-O2-C2	-2.96	106.91	114.32
8	M	503	SMA	O7-C7-C6	-2.95	119.19	124.17
8	D	2	SMA	C17-C18-C19	-2.91	118.25	126.42
9	P	504	LOP	C9-C8-C7	-2.89	102.66	113.24
8	J	503	SMA	O7-C7-C6	-2.88	119.32	124.17
10	A	504	ANJ	O3-C8-N2	-2.86	117.24	122.46
8	M	503	SMA	O5-C5-C6	-2.85	118.78	123.49
4	D	431	BGL	C3'-C2'-C1'	-2.81	100.84	113.48
8	D	2	SMA	O7-C7-C6	-2.79	119.47	124.17
10	G	505	ANJ	O3-C8-N2	-2.77	117.40	122.46
8	G	503	SMA	O5-C5-C6	-2.77	118.91	123.49
10	P	505	ANJ	C5-C6-C7	-2.72	115.98	118.70
9	M	504	LOP	C10-C9-C8	-2.71	100.49	114.45
4	Q	257	BGL	C1'-O2-C2	-2.68	107.60	114.32
10	J	505	ANJ	C5-C6-C7	-2.66	116.04	118.70
8	A	1	SMA	O1-C8A-C4A	-2.65	118.72	121.11
4	A	431	BGL	C1'-O2-C2	-2.64	107.70	114.32
8	A	1	SMA	O5-C5-C6	-2.59	119.21	123.49
8	J	503	SMA	O5-C5-C6	-2.58	119.22	123.49
8	P	503	SMA	C5M-O5-C5	-2.58	114.10	117.77
9	A	503	LOP	C31-C30-C29	-2.57	101.22	114.45
9	A	503	LOP	C21-C20-C19	-2.54	101.39	114.45
10	G	505	ANJ	C19-C18-C13	-2.49	109.72	114.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	503	SMA	C4-C4A-C5	-2.46	121.09	124.94
9	D	503	LOP	C21-C20-C19	-2.45	101.84	114.45
9	G	504	LOP	C31-C30-C29	-2.43	101.95	114.45
8	M	503	SMA	C16-C17-C18	-2.42	118.38	124.65
10	D	504	ANJ	O3-C8-N2	-2.41	118.05	122.46
10	M	505	ANJ	O3-C8-N2	-2.38	118.11	122.46
10	J	505	ANJ	O3-C8-N2	-2.37	118.14	122.46
8	G	503	SMA	O1-C8A-C4A	-2.36	118.98	121.11
4	A	431	BGL	C3'-C2'-C1'	-2.36	102.89	113.48
4	J	431	BGL	C3'-C2'-C1'	-2.31	103.08	113.48
8	J	503	SMA	C9-C10-C11	-2.25	111.69	114.72
8	A	1	SMA	C4-C4A-C5	-2.25	121.42	124.94
8	G	503	SMA	C11-C12-C13	-2.22	108.37	114.29
9	A	503	LOP	C29-C28-C27	-2.18	103.21	114.45
9	J	504	LOP	C19-C18-C17	-2.13	103.50	114.45
8	D	2	SMA	C4-C4A-C5	-2.12	121.63	124.94
10	P	505	ANJ	O3-C8-N2	-2.12	118.59	122.46
9	M	504	LOP	C29-C28-C27	-2.11	103.56	114.45
8	G	503	SMA	C17-C18-C19	-2.10	120.51	126.42
8	G	503	SMA	C9-C10-C11	-2.10	111.89	114.72
9	G	504	LOP	C12-C13-C14	-2.09	101.12	112.50
6	H	301	HEM	CAA-CBA-CGA	-2.07	109.12	112.66
4	J	431	BGL	C1'-O2-C2	-2.06	109.15	114.32
9	D	503	LOP	P1-O1-C2	-2.06	110.83	121.60
8	J	503	SMA	C17-C18-C19	-2.05	120.64	126.42
8	J	503	SMA	C17-C16-C15	-2.05	110.12	125.26
8	D	2	SMA	C22-C11-C12	-2.04	107.85	111.24
9	D	503	LOP	C9-C8-C7	-2.04	105.78	113.24
4	A	431	BGL	C5'-C4'-C3'	-2.03	103.98	114.45
4	J	431	BGL	C5'-C4'-C3'	-2.02	104.06	114.45
9	P	504	LOP	C21-C20-C19	-2.00	104.13	114.45
8	M	503	SMA	C26-C19-C18	2.00	121.29	118.10
6	A	501	HEM	C3B-C4B-NB	2.01	111.81	109.21
10	M	505	ANJ	O6-C15-C16	2.03	110.43	106.83
6	G	501	HEM	C3B-C4B-NB	2.03	111.84	109.21
10	P	505	ANJ	C14-O8-C24	2.03	121.26	117.85
10	D	504	ANJ	O1-C1-N1	2.04	128.47	125.80
9	M	504	LOP	C11-C12-C13	2.04	121.59	113.74
10	D	504	ANJ	C14-O8-C24	2.06	121.30	117.85
10	P	505	ANJ	O1-C1-N1	2.07	128.51	125.80
6	P	502	HEM	CBD-CAD-C3D	2.10	116.48	112.47
6	B	301	HEM	C3B-C4B-NB	2.11	111.93	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	504	ANJ	O1-C1-N1	2.12	128.57	125.80
10	P	505	ANJ	O6-C15-C16	2.13	110.61	106.83
10	M	505	ANJ	O1-C1-N1	2.15	128.61	125.80
6	M	501	HEM	C3B-C4B-NB	2.15	111.99	109.21
10	J	505	ANJ	O6-C15-C16	2.15	110.65	106.83
6	P	501	HEM	C3B-C4B-NB	2.15	112.00	109.21
8	D	2	SMA	C13-C14-C15	2.17	117.42	112.10
6	D	502	HEM	C3B-C4B-NB	2.18	112.03	109.21
6	N	301	HEM	C3B-C4B-NB	2.20	112.06	109.21
10	G	505	ANJ	O1-C1-N1	2.22	128.71	125.80
6	J	502	HEM	C3B-C4B-NB	2.27	112.14	109.21
10	M	505	ANJ	C6-C8-N2	2.27	121.20	116.88
8	A	1	SMA	C26-C19-C18	2.27	121.72	118.10
10	M	505	ANJ	C3-C2-C7	2.28	121.40	119.86
10	D	504	ANJ	C3-C2-C7	2.29	121.41	119.86
6	P	502	HEM	C3B-C4B-NB	2.31	112.19	109.21
6	H	301	HEM	C3B-C4B-NB	2.32	112.21	109.21
10	D	504	ANJ	C6-C8-N2	2.35	121.35	116.88
9	G	504	LOP	O6-C24-C25	2.41	118.90	111.90
6	G	502	HEM	C3B-C4B-NB	2.45	112.37	109.21
10	G	505	ANJ	C3-C2-C7	2.48	121.53	119.86
6	D	501	HEM	C3B-C4B-NB	2.48	112.42	109.21
6	A	502	HEM	C3B-C4B-NB	2.52	112.46	109.21
10	A	504	ANJ	C3-C2-C7	2.52	121.56	119.86
9	M	504	LOP	O6-C24-C25	2.54	119.29	111.90
9	P	504	LOP	O6-C24-C25	2.68	119.69	111.90
10	G	505	ANJ	C6-C8-N2	2.72	122.05	116.88
10	J	505	ANJ	C6-C8-N2	2.74	122.10	116.88
9	P	504	LOP	O5-C6-C7	2.79	117.34	111.55
8	P	503	SMA	O5-C5-C4A	2.84	120.20	115.91
9	D	503	LOP	O5-C6-C7	2.92	117.61	111.55
10	A	504	ANJ	C6-C8-N2	2.93	122.45	116.88
8	D	2	SMA	O5-C5-C4A	3.02	120.47	115.91
8	M	503	SMA	O1-C8A-C8	3.05	119.64	116.03
9	D	503	LOP	O6-C24-C25	3.05	120.77	111.90
9	M	504	LOP	O5-C6-C7	3.06	117.91	111.55
9	A	503	LOP	O5-C6-C7	3.09	117.96	111.55
8	P	503	SMA	O1-C8A-C8	3.35	120.00	116.03
8	G	503	SMA	O5-C5-C4A	3.41	121.05	115.91
8	J	503	SMA	O1-C8A-C8	3.55	120.24	116.03
8	A	1	SMA	O5-C5-C4A	3.55	121.28	115.91
8	J	503	SMA	O5-C5-C4A	3.68	121.47	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2	SMA	O1-C8A-C8	3.74	120.47	116.03
8	M	503	SMA	O5-C5-C4A	3.96	121.88	115.91
8	P	503	SMA	O7-C7-C8	3.96	118.42	114.49
10	D	504	ANJ	O6-C17-O7	4.16	129.33	124.08
8	A	1	SMA	O1-C8A-C8	4.24	121.06	116.03
9	J	504	LOP	O5-C6-C7	4.26	120.40	111.55
10	A	504	ANJ	O6-C17-O7	4.29	129.48	124.08
10	P	505	ANJ	O6-C17-O7	4.31	129.51	124.08
8	G	503	SMA	O1-C8A-C8	4.36	121.20	116.03
10	M	505	ANJ	O6-C17-O7	4.36	129.58	124.08
9	G	504	LOP	O5-C6-C7	4.47	120.83	111.55
10	J	505	ANJ	O6-C17-O7	4.50	129.75	124.08
10	G	505	ANJ	O6-C17-O7	4.54	129.80	124.08
8	M	503	SMA	O1-C2-C9	5.62	118.86	111.94
8	J	503	SMA	O7-C7-C8	6.05	120.48	114.49
8	D	2	SMA	O7-C7-C8	6.16	120.59	114.49
8	J	503	SMA	O1-C2-C9	6.18	119.55	111.94
8	D	2	SMA	O1-C2-C9	6.50	119.95	111.94
8	A	1	SMA	O1-C2-C9	6.83	120.35	111.94
8	M	503	SMA	O7-C7-C8	6.92	121.34	114.49
8	P	503	SMA	O1-C2-C9	6.92	120.46	111.94
8	A	1	SMA	O7-C7-C8	7.07	121.49	114.49
8	G	503	SMA	O1-C2-C9	7.23	120.85	111.94
8	G	503	SMA	O7-C7-C8	7.95	122.36	114.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

45 monomers are involved in 193 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1	SMA	6	0
4	A	431	BGL	1	0
6	A	501	HEM	6	0
6	A	502	HEM	1	0
9	A	503	LOP	5	0
10	A	504	ANJ	7	0
6	B	301	HEM	6	0
7	C	200	FES	2	0
8	D	2	SMA	3	0
4	D	431	BGL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	501	HEM	6	0
6	D	502	HEM	8	0
9	D	503	LOP	3	0
10	D	504	ANJ	7	0
6	E	301	HEM	2	0
7	F	200	FES	2	0
4	G	431	BGL	2	0
6	G	501	HEM	8	0
6	G	502	HEM	4	0
8	G	503	SMA	6	0
9	G	504	LOP	4	0
10	G	505	ANJ	7	0
6	H	301	HEM	1	0
7	I	200	FES	2	0
6	J	501	HEM	7	0
6	J	502	HEM	5	0
8	J	503	SMA	4	0
9	J	504	LOP	3	0
10	J	505	ANJ	7	0
6	K	301	HEM	2	0
7	L	200	FES	2	0
4	M	431	BGL	2	0
6	M	501	HEM	5	0
6	M	502	HEM	1	0
8	M	503	SMA	3	0
9	M	504	LOP	7	0
10	M	505	ANJ	6	0
7	O	200	FES	2	0
6	P	501	HEM	11	0
6	P	502	HEM	6	0
8	P	503	SMA	4	0
9	P	504	LOP	4	0
10	P	505	ANJ	7	0
6	Q	301	HEM	1	0
7	R	200	FES	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	428/428 (100%)	-0.33	5 (1%) 79 61	31, 60, 105, 139	0
1	D	428/428 (100%)	-0.34	5 (1%) 79 61	33, 59, 109, 147	0
1	G	428/428 (100%)	-0.20	14 (3%) 47 24	34, 63, 113, 153	0
1	J	428/428 (100%)	-0.18	18 (4%) 37 18	36, 65, 113, 164	0
1	M	428/428 (100%)	-0.18	16 (3%) 42 21	41, 71, 117, 157	0
1	P	428/428 (100%)	-0.29	7 (1%) 72 51	40, 64, 116, 162	0
2	B	256/256 (100%)	0.33	28 (10%) 6 2	54, 90, 138, 176	0
2	E	256/256 (100%)	0.06	11 (4%) 36 17	47, 89, 141, 172	0
2	H	256/256 (100%)	0.15	17 (6%) 19 7	41, 88, 139, 179	0
2	K	256/256 (100%)	0.12	23 (8%) 10 4	49, 95, 141, 173	0
2	N	256/256 (100%)	0.66	42 (16%) 2 1	64, 104, 148, 177	0
2	Q	256/256 (100%)	0.21	23 (8%) 10 4	59, 99, 148, 174	0
3	C	179/179 (100%)	-0.23	9 (5%) 30 13	38, 67, 125, 186	0
3	F	179/179 (100%)	-0.20	4 (2%) 62 41	42, 70, 127, 184	0
3	I	179/179 (100%)	-0.07	12 (6%) 19 7	44, 70, 124, 183	0
3	L	179/179 (100%)	-0.25	4 (2%) 62 41	39, 68, 129, 183	0
3	O	179/179 (100%)	-0.06	10 (5%) 25 11	44, 75, 131, 184	0
3	R	179/179 (100%)	0.36	16 (8%) 10 4	49, 86, 130, 181	0
All	All	5178/5178 (100%)	-0.07	264 (5%) 29 13	31, 75, 132, 186	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	GLY	12.7
2	B	4	GLY	11.5
2	E	3	GLY	10.4

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Mol	Chain	Res	Type	RSRZ
2	Q	4	GLY	10.4
3	R	9	GLY	10.2
2	B	3	GLY	9.8
3	R	10	THR	8.7
1	M	232	THR	8.6
2	Q	5	HIS	8.0
2	Q	2	GLY	7.6
2	H	3	GLY	7.3
3	R	13	ASP	6.9
1	J	11	PRO	6.8
3	I	10	THR	6.8
2	N	2	GLY	6.3
2	E	2	GLY	6.3
2	B	2	GLY	6.3
3	R	11	ARG	6.1
2	K	143	PRO	6.0
2	Q	3	GLY	6.0
3	O	16	TYR	5.8
1	J	8	HIS	5.7
3	I	9	GLY	5.6
3	I	181	GLU	5.5
2	N	150	GLU	5.4
2	K	145	CYS	5.4
1	G	10	GLU	5.3
3	R	17	TYR	5.3
2	N	123	ASN	5.2
1	J	10	GLU	5.1
3	F	17	TYR	5.1
2	E	4	GLY	5.1
2	K	147	GLU	5.0
2	N	7	GLU	4.9
1	M	233	SER	4.9
2	B	5	HIS	4.9
2	B	122	PHE	4.9
1	D	8	HIS	4.9
2	H	1	ALA	4.9
2	N	178	THR	4.7
1	M	5	PRO	4.7
2	N	143	PRO	4.7
2	N	149	HIS	4.6
1	G	12	ARG	4.6
1	J	9	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	124	GLY	4.4
3	I	17	TYR	4.4
1	A	11	PRO	4.4
2	N	146	ALA	4.4
2	K	142	PRO	4.4
2	K	5	HIS	4.4
2	K	150	GLU	4.3
2	N	4	GLY	4.3
2	N	256	LYS	4.2
2	E	1	ALA	4.2
1	P	12	ARG	4.2
2	K	256	LYS	4.1
1	M	12	ARG	4.0
2	B	111	HIS	4.0
2	B	256	LYS	4.0
2	K	141	GLU	4.0
3	R	181	GLU	3.9
3	O	17	TYR	3.9
2	N	3	GLY	3.8
1	G	417	PRO	3.8
2	B	147	GLU	3.7
1	D	10	GLU	3.7
3	L	10	THR	3.7
2	Q	6	VAL	3.7
2	Q	147	GLU	3.7
2	E	76	GLU	3.6
2	Q	95	GLU	3.6
2	N	122	PHE	3.6
2	H	114	MET	3.6
2	H	95	GLU	3.6
2	Q	1	ALA	3.6
3	I	14	PHE	3.6
3	C	10	THR	3.5
2	K	2	GLY	3.5
2	K	144	LYS	3.5
2	B	123	ASN	3.5
3	L	17	TYR	3.5
1	A	10	GLU	3.5
3	I	13	ASP	3.5
2	K	3	GLY	3.5
1	G	11	PRO	3.5
1	A	12	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
3	O	179	ILE	3.4
1	J	12	ARG	3.4
2	N	147	GLU	3.3
2	B	121	LEU	3.3
1	M	385	THR	3.3
2	B	1	ALA	3.3
2	Q	94	LEU	3.3
1	D	12	ARG	3.3
1	G	418	VAL	3.3
3	C	104	ASP	3.3
2	E	118	ILE	3.3
2	H	4	GLY	3.3
2	N	198	ASP	3.3
2	N	151	PRO	3.3
1	J	362	MET	3.2
2	N	121	LEU	3.2
1	J	7	ASP	3.2
1	D	13	THR	3.2
1	M	387	PHE	3.1
2	H	71	THR	3.1
3	R	14	PHE	3.1
1	G	9	TYR	3.1
1	G	416	LYS	3.1
2	B	7	GLU	3.1
1	M	384	GLN	3.1
1	J	428	PHE	3.1
2	B	140	GLU	3.1
2	H	72	VAL	3.1
3	R	12	ARG	3.1
2	N	200	HIS	3.1
3	O	22	ALA	3.0
3	C	105	ALA	3.0
1	M	236	GLU	3.0
2	Q	96	ASN	3.0
2	N	168	THR	3.0
2	N	16	PRO	3.0
3	I	46	ALA	3.0
3	R	114	ARG	3.0
1	J	361	PRO	2.9
1	J	414	ILE	2.9
2	B	149	HIS	2.9
3	I	12	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
3	F	9	GLY	2.9
2	B	110	PHE	2.9
3	F	47	LEU	2.9
2	K	146	ALA	2.9
2	N	114	MET	2.9
1	J	5	PRO	2.9
3	C	9	GLY	2.8
2	B	71	THR	2.8
2	H	147	GLU	2.8
2	N	8	ASP	2.8
2	N	142	PRO	2.8
2	Q	91	HIS	2.8
3	O	105	ALA	2.8
2	Q	150	GLU	2.8
3	I	180	ASP	2.8
1	J	6	HIS	2.8
3	O	181	GLU	2.7
2	E	122	PHE	2.7
2	N	110	PHE	2.7
2	H	123	ASN	2.7
1	M	419	ALA	2.7
2	N	93	ALA	2.7
1	G	17	LYS	2.7
2	N	169	CYS	2.7
2	N	6	VAL	2.7
2	Q	7	GLU	2.7
3	C	90	LEU	2.7
2	K	4	GLY	2.7
3	O	9	GLY	2.6
2	N	82	GLU	2.6
1	G	30	TYR	2.6
3	R	65	VAL	2.6
2	B	6	VAL	2.6
2	N	111	HIS	2.6
1	D	11	PRO	2.6
2	B	148	GLY	2.5
2	N	158	ARG	2.5
3	C	11	ARG	2.5
2	B	114	MET	2.5
1	J	311	ASP	2.5
2	B	119	SER	2.5
1	P	6	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	245	TYR	2.5
1	J	419	ALA	2.5
2	H	109	GLY	2.5
1	P	239	LYS	2.5
3	F	10	THR	2.5
2	Q	98	PRO	2.5
3	O	103	ILE	2.5
2	B	150	GLU	2.5
1	M	386	THR	2.5
2	Q	141	GLU	2.5
2	N	174	GLY	2.4
1	J	427	ASP	2.4
1	G	13	THR	2.4
1	G	172	ILE	2.4
1	P	428	PHE	2.4
1	P	11	PRO	2.4
2	H	93	ALA	2.4
1	J	384	GLN	2.4
2	N	199	GLY	2.4
2	Q	190	MET	2.4
1	M	428	PHE	2.4
2	N	197	ALA	2.4
1	P	9	TYR	2.4
2	Q	80	ASP	2.4
3	R	112	GLN	2.4
3	R	145	GLY	2.4
2	K	140	GLU	2.4
2	H	80	ASP	2.4
1	G	247	TYR	2.3
2	K	148	GLY	2.3
2	K	114	MET	2.3
3	I	179	ILE	2.3
3	L	13	ASP	2.3
2	Q	149	HIS	2.3
1	J	418	VAL	2.3
1	M	234	LYS	2.3
2	K	187	PRO	2.3
2	N	172	ALA	2.3
1	G	171	GLY	2.3
2	K	139	PRO	2.3
3	C	103	ILE	2.2
2	N	242	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	414	ILE	2.2
3	C	22	ALA	2.2
2	N	20	PHE	2.2
2	B	178	THR	2.2
1	M	13	THR	2.2
3	C	18	ALA	2.2
3	I	11	ARG	2.2
2	K	8	ASP	2.2
3	R	18	ALA	2.2
2	N	109	GLY	2.2
2	H	96	ASN	2.2
2	E	71	THR	2.2
1	P	13	THR	2.2
2	N	139	PRO	2.2
2	Q	184	ALA	2.1
2	E	123	ASN	2.1
2	B	141	GLU	2.1
2	N	166	PRO	2.1
2	K	59	PRO	2.1
2	Q	193	LEU	2.1
2	K	1	ALA	2.1
3	L	14	PHE	2.1
3	R	52	VAL	2.1
2	B	143	PRO	2.1
2	H	79	GLU	2.1
2	N	145	CYS	2.1
2	E	94	LEU	2.1
3	O	108	GLU	2.1
1	G	429	ASN	2.1
2	B	8	ASP	2.1
3	R	180	ASP	2.1
1	A	359	TYR	2.1
2	N	144	LYS	2.1
2	B	182	TRP	2.1
2	Q	8	ASP	2.1
3	R	83	GLU	2.1
1	A	17	LYS	2.0
1	M	366	TYR	2.0
2	B	146	ALA	2.0
1	M	349	LEU	2.0
1	J	358	ARG	2.0
2	N	138	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	82	GLU	2.0
2	Q	92	SER	2.0
3	I	16	TYR	2.0
2	E	117	GLY	2.0
2	H	83	GLY	2.0
2	Q	110	PHE	2.0
2	K	149	HIS	2.0
2	K	155	TYR	2.0
3	O	12	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	LOP	P	504	45/45	0.84	0.38	4.29	63,98,114,118	0
9	LOP	J	504	45/45	0.79	0.60	4.20	105,143,157,158	0
9	LOP	M	504	45/45	0.83	0.36	3.06	91,121,132,133	0
9	LOP	G	504	45/45	0.78	0.35	2.85	91,111,130,131	0
10	ANJ	M	505	39/39	0.93	0.24	2.49	82,96,101,103	0
4	BGL	G	431	20/20	0.80	0.48	2.31	93,98,109,109	0
9	LOP	D	503	45/45	0.89	0.28	1.92	49,102,111,113	0
4	BGL	M	431	20/20	0.67	0.66	1.60	120,124,128,129	0
10	ANJ	G	505	39/39	0.94	0.26	1.52	52,75,95,98	0
8	SMA	J	503	37/37	0.94	0.22	1.40	42,60,69,72	0
10	ANJ	P	505	39/39	0.93	0.24	1.29	63,74,89,96	0
6	HEM	J	501	43/43	0.96	0.22	0.88	74,84,95,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SMA	P	503	37/37	0.96	0.22	0.82	33,47,68,70	0
10	ANJ	A	504	39/39	0.93	0.21	0.79	57,73,93,96	0
6	HEM	G	501	43/43	0.97	0.24	0.72	58,71,84,91	0
6	HEM	M	501	43/43	0.96	0.23	0.71	73,78,88,91	0
10	ANJ	J	505	39/39	0.92	0.23	0.68	88,96,102,104	0
10	ANJ	D	504	39/39	0.94	0.21	0.58	57,69,84,85	0
8	SMA	M	503	37/37	0.93	0.20	0.50	50,68,78,80	0
6	HEM	P	501	43/43	0.98	0.22	0.47	58,67,79,85	0
9	LOP	A	503	45/45	0.90	0.25	0.36	62,89,101,105	0
6	HEM	J	502	43/43	0.98	0.18	0.20	27,37,52,60	0
6	HEM	M	502	43/43	0.98	0.19	0.15	49,54,64,66	0
8	SMA	G	503	37/37	0.95	0.22	0.13	37,47,64,67	0
6	HEM	B	301	43/43	0.96	0.21	0.12	54,59,74,78	0
7	FES	L	200	4/4	0.99	0.17	0.11	32,34,36,39	0
6	HEM	N	301	43/43	0.91	0.24	0.10	71,81,87,89	0
6	HEM	A	501	43/43	0.97	0.21	0.06	39,56,61,62	0
4	BGL	Q	257	20/20	0.85	0.21	0.06	94,99,103,103	0
4	BGL	A	431	20/20	0.86	0.32	0.04	90,98,102,104	0
7	FES	F	200	4/4	0.99	0.18	0.02	42,42,42,45	0
6	HEM	E	301	43/43	0.97	0.23	-0.03	55,63,79,80	0
6	HEM	D	501	43/43	0.97	0.20	-0.04	50,56,68,73	0
8	SMA	D	2	37/37	0.96	0.19	-0.14	32,44,52,54	0
4	BGL	D	431	20/20	0.89	0.21	-0.20	79,86,88,89	0
6	HEM	P	502	43/43	0.98	0.18	-0.29	25,36,48,59	0
7	FES	O	200	4/4	0.99	0.15	-0.33	40,43,43,50	0
8	SMA	A	1	37/37	0.94	0.20	-0.40	34,49,61,66	0
6	HEM	H	301	43/43	0.97	0.20	-0.47	39,50,58,60	0
6	HEM	G	502	43/43	0.98	0.17	-0.47	22,34,45,51	0
7	FES	R	200	4/4	0.99	0.17	-0.48	56,57,58,59	0
6	HEM	D	502	43/43	0.98	0.17	-0.49	16,29,46,53	0
7	FES	I	200	4/4	0.99	0.14	-0.52	45,47,48,50	0
6	HEM	K	301	43/43	0.97	0.17	-0.55	49,60,74,75	0
7	FES	C	200	4/4	0.99	0.15	-0.57	33,36,40,42	0
4	BGL	J	431	20/20	0.86	0.17	-0.59	94,99,103,104	0
6	HEM	Q	301	43/43	0.96	0.23	-0.61	64,75,81,82	0
6	HEM	A	502	43/43	0.98	0.16	-0.75	14,29,45,49	0
5	SR	Q	258	1/1	0.87	0.07	-1.52	139,139,139,139	0
5	SR	B	257	1/1	0.92	0.04	-1.75	136,136,136,136	0
5	SR	K	257	1/1	0.88	0.07	-1.86	134,134,134,134	0
5	SR	H	257	1/1	0.95	0.06	-1.96	106,106,106,106	0
5	SR	E	257	1/1	0.92	0.05	-2.30	111,111,111,111	0
5	SR	N	257	1/1	0.75	0.07	-2.32	153,153,153,153	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.