



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:28 AM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

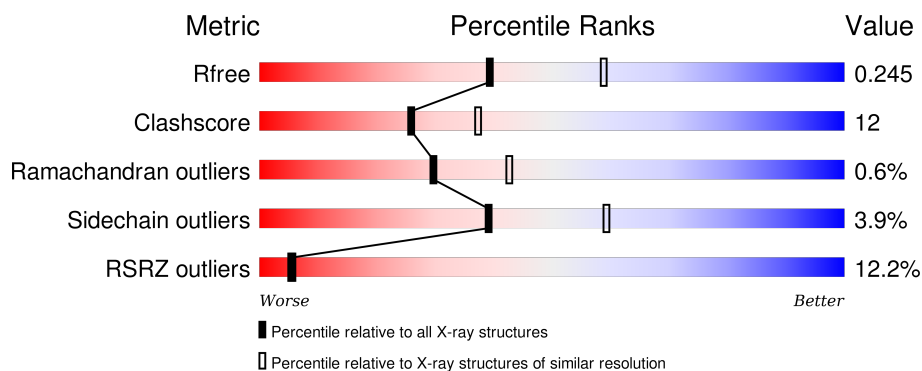
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	445	<div> <div>2%</div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
1	D	445	<div> <div>3%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	G	445	<div> <div>7%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	J	445	<div> <div>8%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	M	445	<div> <div>11%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	445	
2	B	269	
2	E	269	
2	H	269	
2	K	269	
2	N	269	
2	Q	269	
3	C	187	
3	F	187	
3	I	187	
3	L	187	
3	O	187	
3	R	187	

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

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

2 Entry composition

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

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

- Molecule 1 is a protein called Cytochrome b.

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Cytochrome c1.

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

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

There are 36 discrepancies between the modelled and reference sequences:

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

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

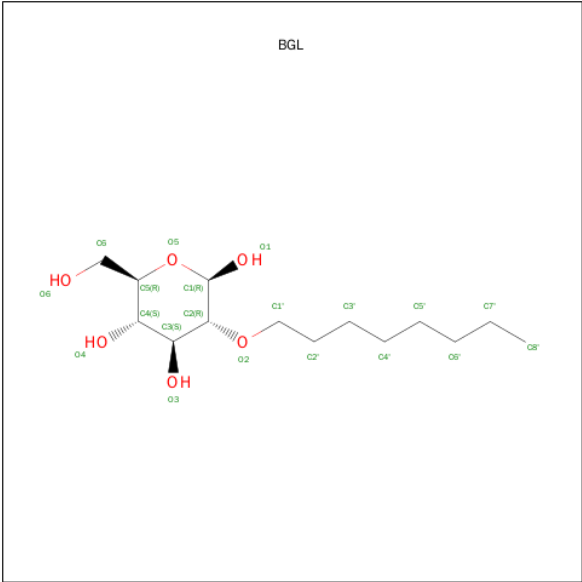
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is beta-octyl glucopyranoside (three-letter code: BGL) (formula: C₁₄H₂₈O₆).



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

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

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

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

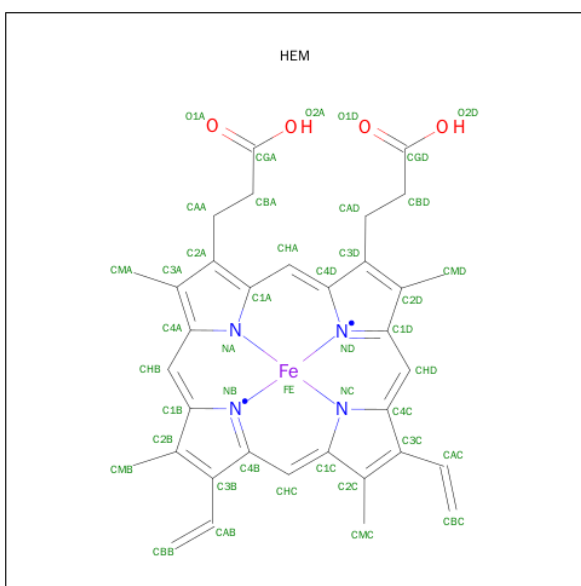
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

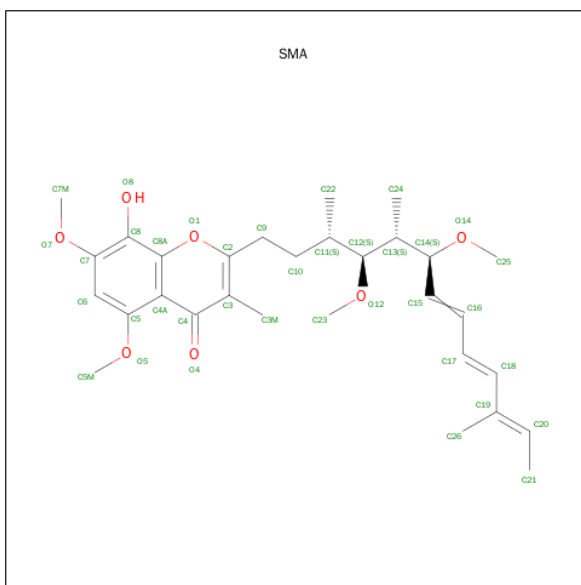
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	R	1	Total	Na	0	0
			1	1		

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



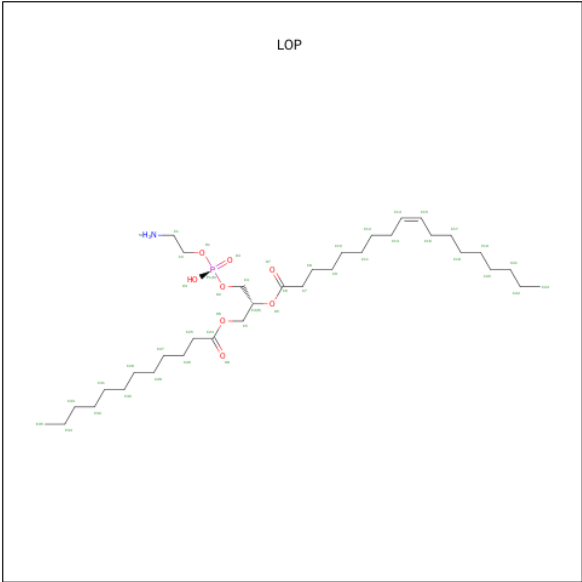
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 9 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



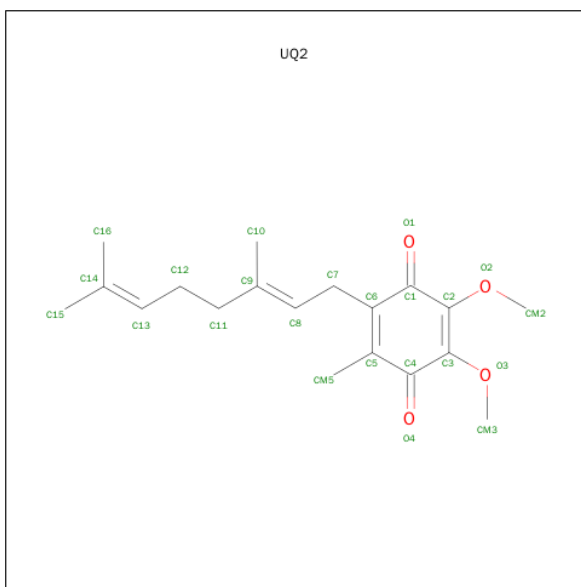
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 37	C 30	O 7	0	0
9	D	1	Total 37	C 30	O 7	0	0
9	G	1	Total 37	C 30	O 7	0	0
9	J	1	Total 37	C 30	O 7	0	0
9	M	1	Total 37	C 30	O 7	0	0
9	P	1	Total 37	C 30	O 7	0	0

- Molecule 10 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C₃₅H₆₈N₁O₈P).



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

- Molecule 11 is UBIQUINONE-2 (three-letter code: UQ2) (formula: C₁₉H₂₆O₄).



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

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 13 is water.

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

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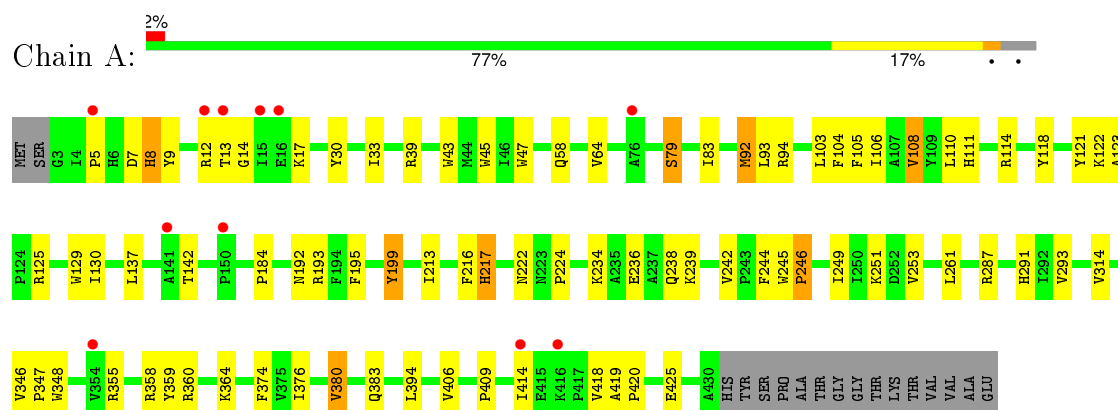
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	G	68	Total 68	O 68	0	0
13	H	35	Total 35	O 35	0	0
13	I	42	Total 42	O 42	0	0
13	J	55	Total 55	O 55	0	0
13	K	17	Total 17	O 17	0	0
13	L	42	Total 42	O 42	0	0
13	M	34	Total 34	O 34	0	0
13	N	11	Total 11	O 11	0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

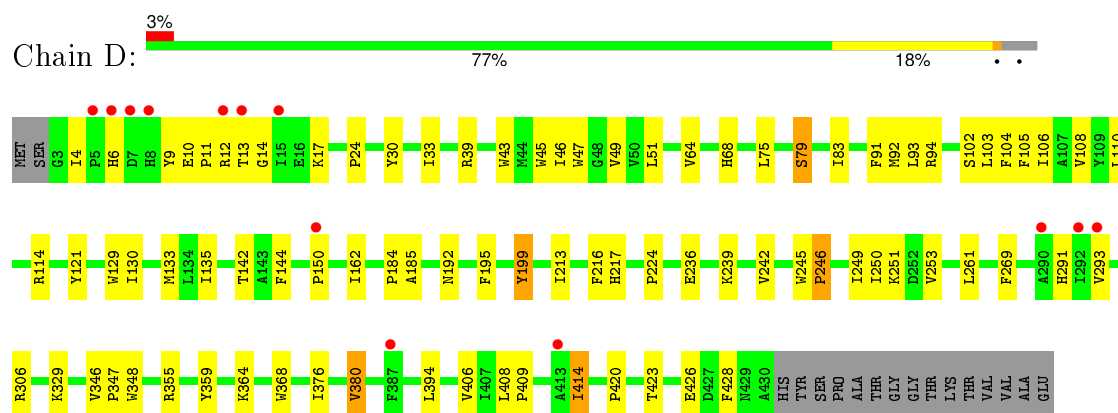
3 Residue-property plots [i](#)

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

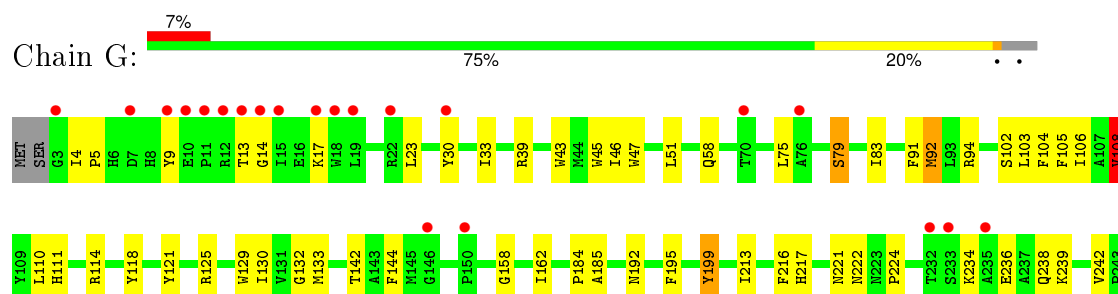
• Molecule 1: Cytochrome b

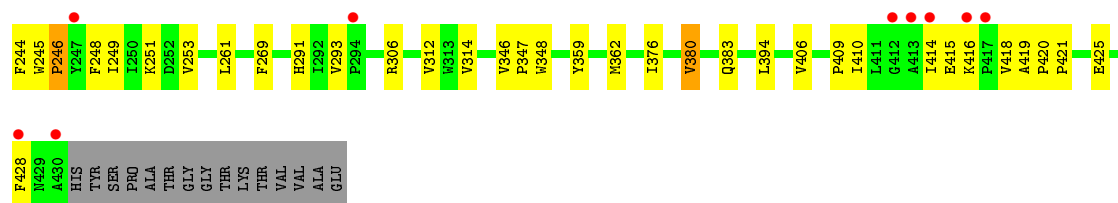


• Molecule 1: Cytochrome b

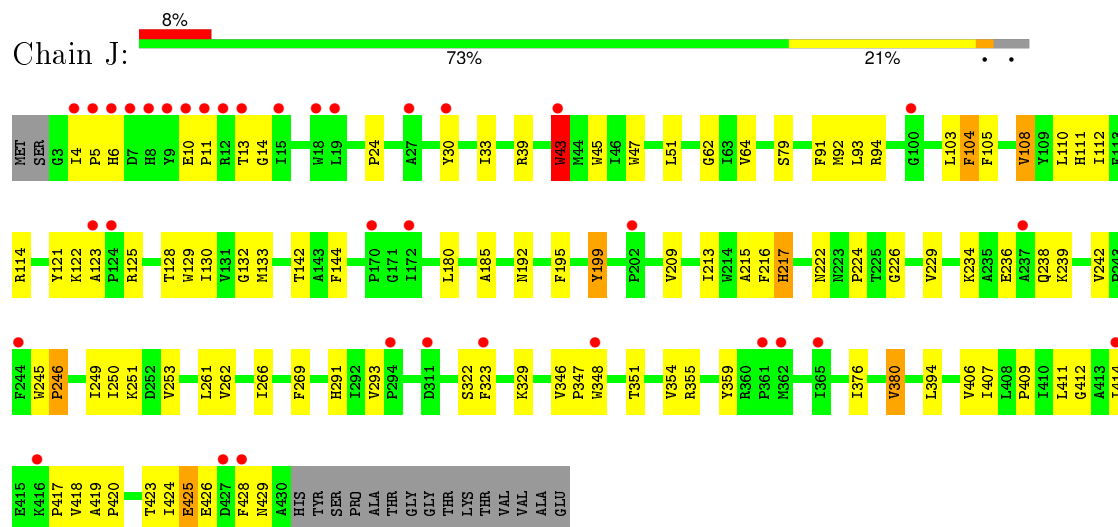


• Molecule 1: Cytochrome b

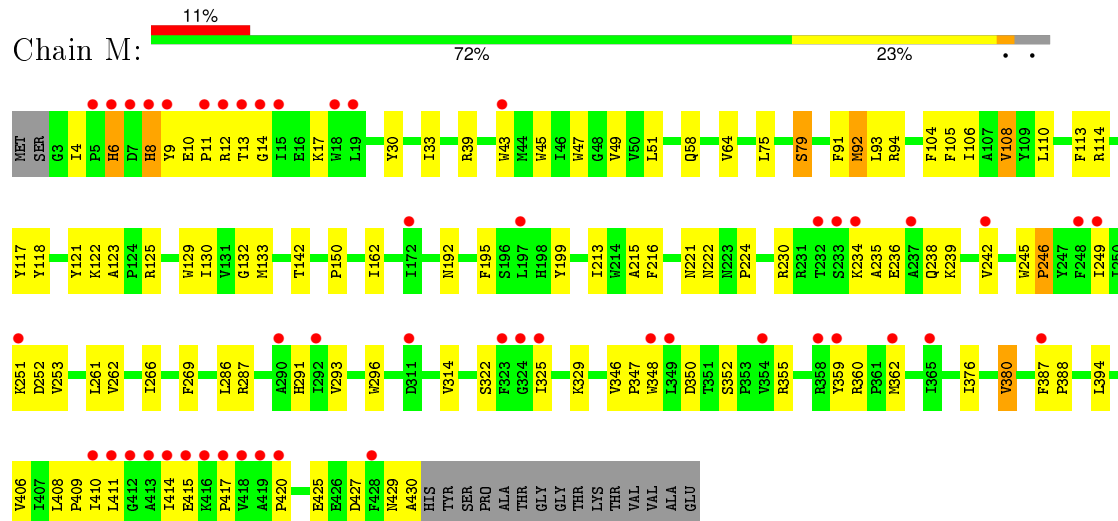




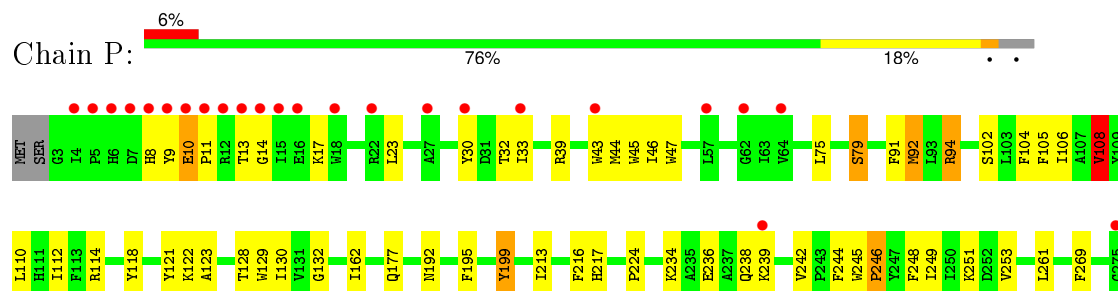
• Molecule 1: Cytochrome b

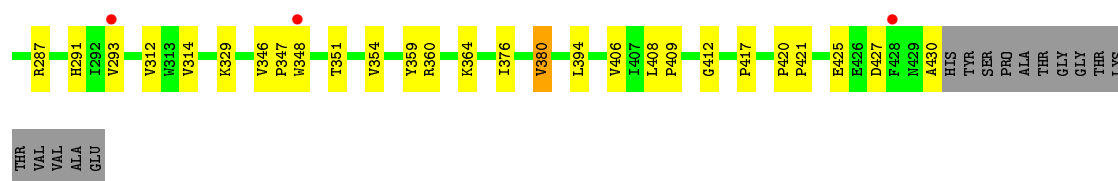


• Molecule 1: Cytochrome b

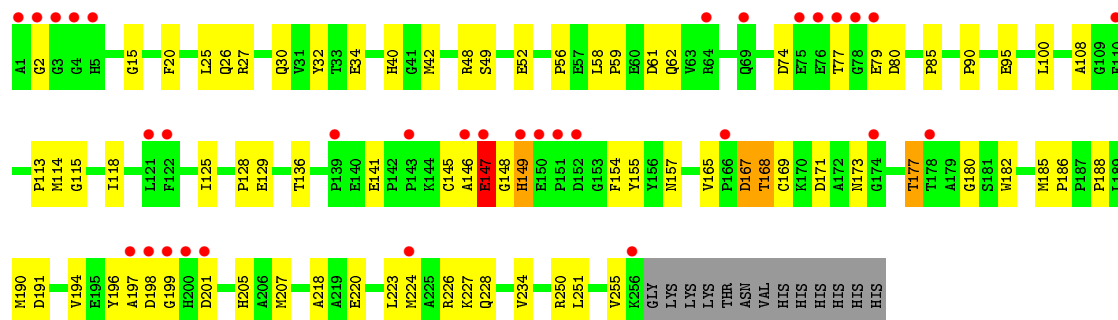


• Molecule 1: Cytochrome b

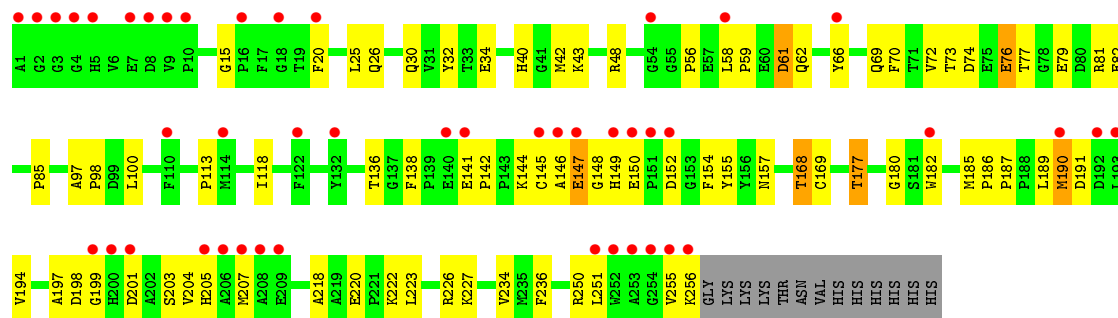




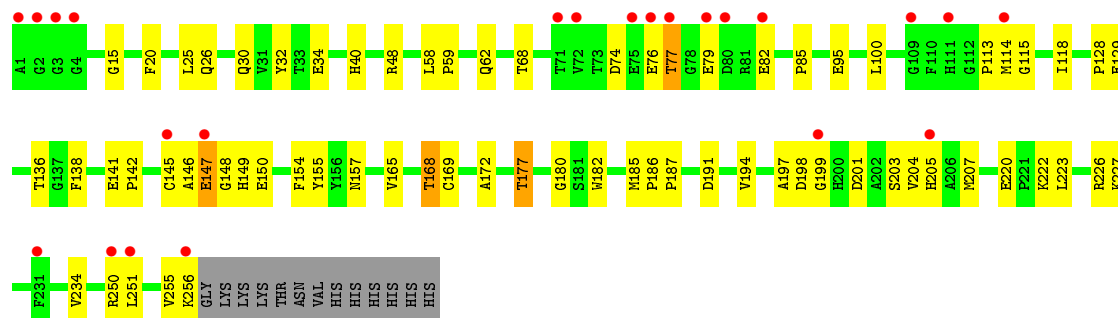
• Molecule 2: Cytochrome c1



• Molecule 2: Cytochrome c1

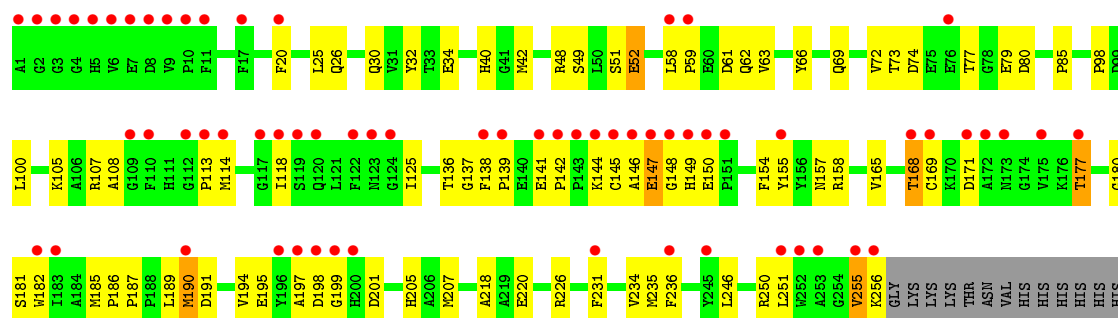


• Molecule 2: Cytochrome c1

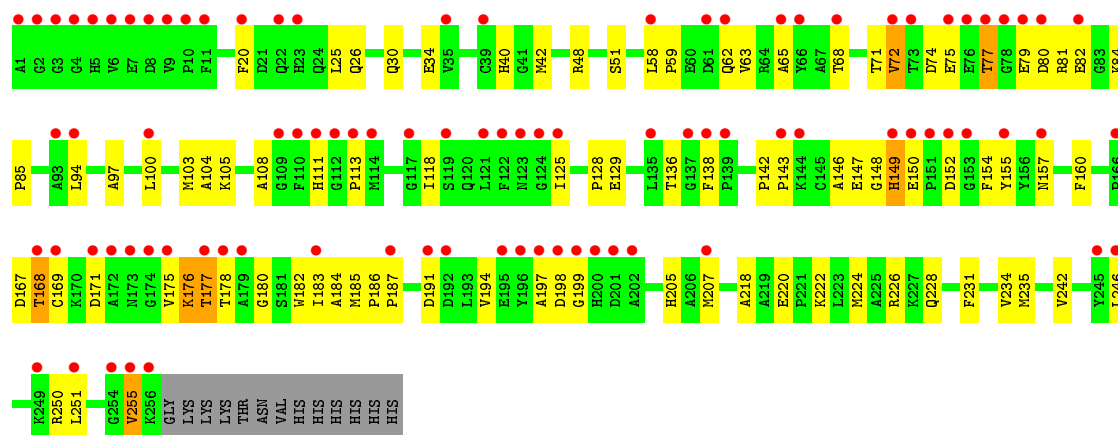


• Molecule 2: Cytochrome c1

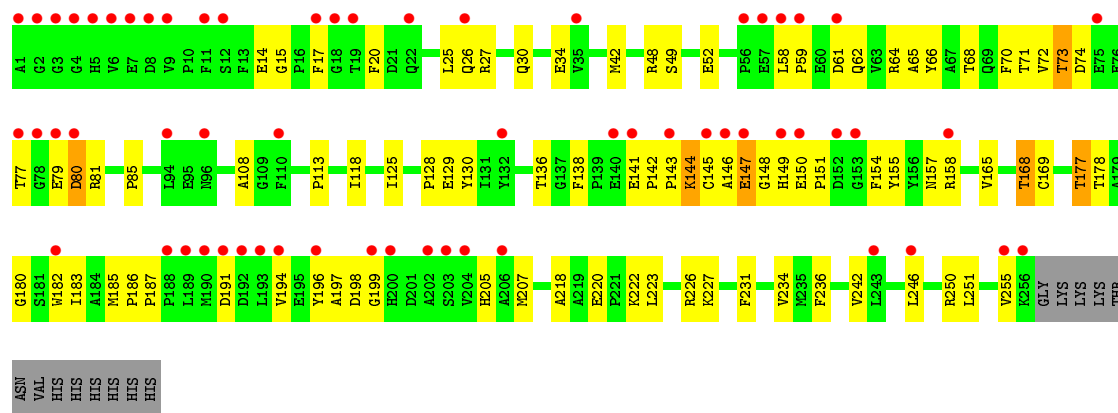




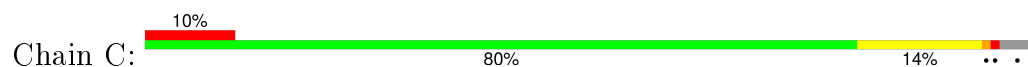
• Molecule 2: Cytochrome c1

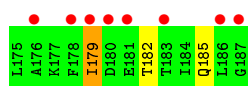


• Molecule 2: Cytochrome c1

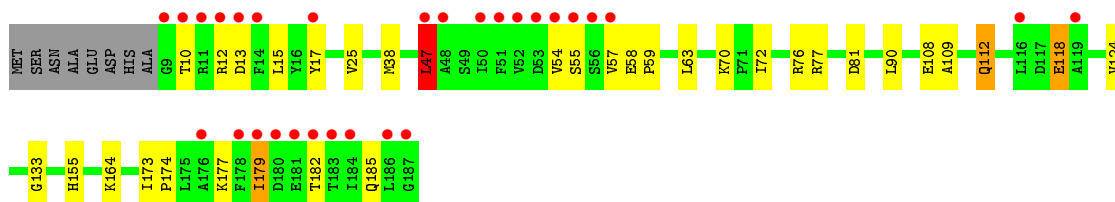
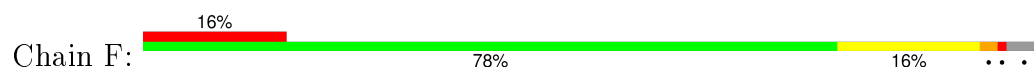


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

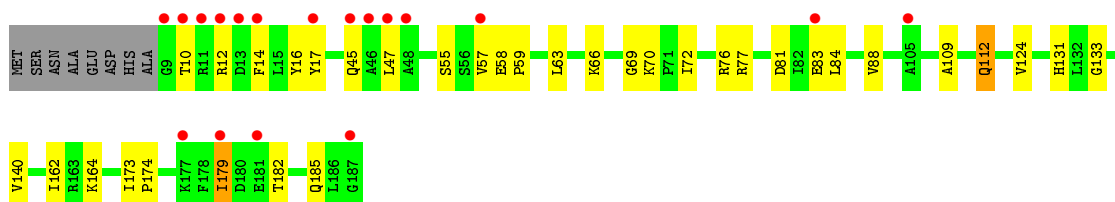
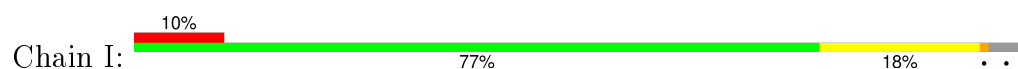




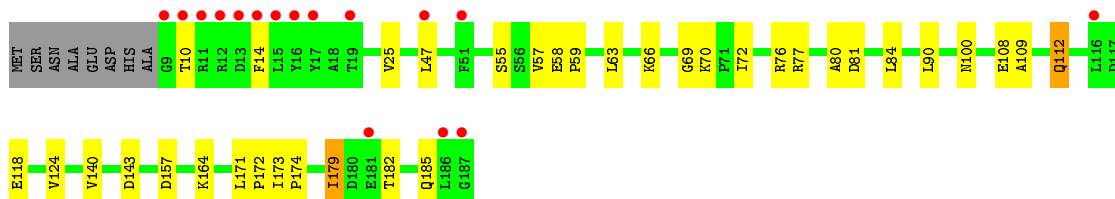
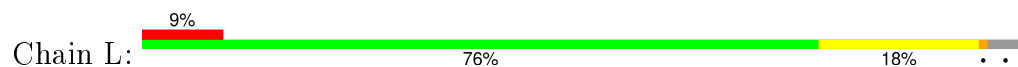
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



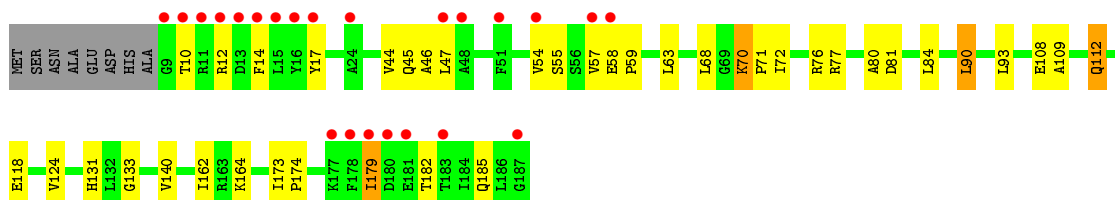
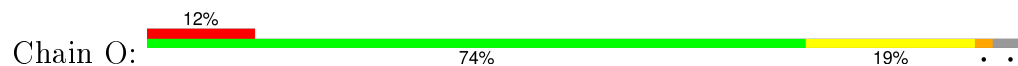
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



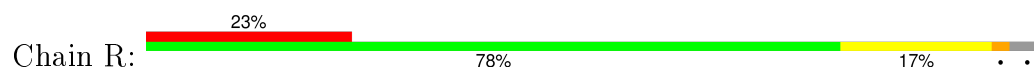
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- 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, α , β , γ	351.89Å 147.04Å 161.31Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	18.00 – 2.40 47.10 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.7 (18.00-2.40) 91.9 (47.10-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.251 0.229 , 0.245	Depositor DCC
R_{free} test set	4928 reflections (1.74%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 574713 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42656	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/3570	0.66	0/4897
1	D	0.39	0/3570	0.66	0/4897
1	G	0.38	0/3570	0.66	1/4897 (0.0%)
1	J	0.40	0/3570	0.66	0/4897
1	M	0.38	0/3570	0.65	0/4897
1	P	0.38	0/3570	0.65	1/4897 (0.0%)
2	B	0.37	0/2010	0.67	0/2733
2	E	0.36	0/2010	0.68	0/2733
2	H	0.37	0/2010	0.68	0/2733
2	K	0.36	0/2010	0.67	0/2733
2	N	0.36	0/2010	0.67	0/2733
2	Q	0.35	0/2010	0.66	0/2733
3	C	0.38	0/1370	0.74	1/1866 (0.1%)
3	F	0.39	0/1370	0.74	2/1866 (0.1%)
3	I	0.39	0/1370	0.76	1/1866 (0.1%)
3	L	0.38	0/1370	0.72	1/1866 (0.1%)
3	O	0.38	0/1370	0.72	1/1866 (0.1%)
3	R	0.38	0/1370	0.73	2/1866 (0.1%)
All	All	0.38	0/41700	0.68	10/56976 (0.0%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

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

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:LYS:HE2	1:J:425:GLU:OE1	1.90	0.70
1:D:92:MET:HE1	2:E:226:ARG:HG3	1.72	0.70
1:G:130:ILE:HD11	1:G:348:TRP:HH2	1.57	0.70
1:G:246:PRO:HG2	2:H:251:LEU:HD21	1.74	0.70
1:D:261:LEU:HD11	2:E:234:VAL:HG13	1.73	0.70
2:Q:194:VAL:HB	2:Q:207:MET:CE	2.22	0.70
1:A:261:LEU:HD11	2:B:234:VAL:HG13	1.71	0.70
1:M:376:ILE:O	1:M:380:VAL:HG22	1.92	0.70
3:C:84:LEU:HD23	3:L:84:LEU:HD23	1.74	0.70
2:N:194:VAL:HB	2:N:207:MET:HE3	1.72	0.69
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.27	0.69
2:H:59:PRO:HD2	2:H:62:GLN:NE2	2.07	0.69
1:P:130:ILE:HD11	1:P:348:TRP:HH2	1.57	0.69
3:F:47:LEU:O	3:F:47:LEU:HD23	1.92	0.69
1:M:269:PHE:HB3	4:N:1045:BGL:H1'2	1.75	0.69
2:K:59:PRO:HD2	2:K:62:GLN:NE2	2.06	0.69
2:H:194:VAL:HB	2:H:207:MET:CE	2.23	0.69
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.56	0.69
2:E:59:PRO:HD2	2:E:62:GLN:NE2	2.07	0.69
2:K:194:VAL:HB	2:K:207:MET:CE	2.23	0.69
1:J:130:ILE:HD11	1:J:348:TRP:HH2	1.57	0.69
3:F:112:GLN:H	3:F:112:GLN:NE2	1.91	0.69
1:M:8:HIS:H	1:M:8:HIS:CD2	2.09	0.69
1:A:287:ARG:HG2	1:A:287:ARG:HH11	1.57	0.69
2:B:59:PRO:HD2	2:B:62:GLN:NE2	2.07	0.69
1:P:91:PHE:CD1	2:Q:222:LYS:HG2	2.28	0.69
2:E:77:THR:HG22	2:E:79:GLU:H	1.58	0.69
8:A:501:HEM:HBC2	8:A:501:HEM:HMC2	1.75	0.68
2:N:40:HIS:CE1	2:N:97:ALA:HB1	2.28	0.68
1:A:374:PHE:HD2	10:A:1021:LOP:H321	1.57	0.68
1:P:376:ILE:O	1:P:380:VAL:HG22	1.92	0.68
1:A:376:ILE:O	1:A:380:VAL:HG22	1.93	0.68
1:P:261:LEU:HD11	2:Q:234:VAL:HG13	1.76	0.68
1:D:130:ILE:HD11	1:D:348:TRP:HH2	1.57	0.68
1:J:376:ILE:O	1:J:380:VAL:HG22	1.92	0.68
1:D:376:ILE:O	1:D:380:VAL:HG22	1.93	0.68
1:G:376:ILE:O	1:G:380:VAL:HG22	1.93	0.68
2:K:49:SER:HA	2:K:52:GLU:HG3	1.76	0.68
1:M:130:ILE:HD11	1:M:348:TRP:HH2	1.57	0.68
1:A:105:PHE:HA	1:A:108:VAL:HG22	1.76	0.67
1:J:104:PHE:O	1:J:108:VAL:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LYS:HE3	1:D:184:PRO:O	1.95	0.67
2:E:194:VAL:HB	2:E:207:MET:CE	2.24	0.67
2:H:250:ARG:CZ	3:I:12:ARG:CB	2.72	0.67
1:G:103:LEU:HD13	10:G:1023:LOP:H211	1.76	0.67
1:P:43:TRP:CZ3	1:P:251:LYS:HE3	2.30	0.67
1:M:230:ARG:HA	13:M:528:HOH:O	1.94	0.67
1:M:118:TYR:OH	10:M:1025:LOP:H31	1.96	0.66
2:B:74:ASP:HB3	2:B:77:THR:HB	1.76	0.66
2:N:138:PHE:HD2	2:N:187:PRO:HG3	1.56	0.66
2:B:194:VAL:HB	2:B:207:MET:CE	2.24	0.66
1:A:246:PRO:HG2	2:B:251:LEU:HD21	1.76	0.66
1:M:261:LEU:HD11	2:N:234:VAL:HG13	1.78	0.66
2:E:77:THR:HG22	2:E:79:GLU:N	2.11	0.65
3:L:112:GLN:NE2	3:L:112:GLN:H	1.93	0.65
1:M:142:THR:HG21	8:M:502:HEM:HBB2	1.76	0.65
2:N:224:MET:O	2:N:228:GLN:HG3	1.95	0.65
1:A:125:ARG:CZ	1:A:222:ASN:HB2	2.25	0.65
2:K:105:LYS:HD3	2:K:220:GLU:HG2	1.78	0.65
1:D:39:ARG:HH12	2:E:255:VAL:CG1	2.09	0.65
2:Q:20:PHE:HB3	2:Q:25:LEU:HD11	1.78	0.65
1:J:199:TYR:HA	8:J:502:HEM:HBC2	1.78	0.65
1:M:39:ARG:HG2	1:M:242:VAL:HG13	1.79	0.65
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.79	0.65
2:B:26:GLN:HG2	2:B:58:LEU:HD21	1.79	0.65
1:D:39:ARG:HG2	1:D:242:VAL:HG13	1.78	0.65
1:P:39:ARG:HG2	1:P:242:VAL:HG13	1.78	0.65
3:R:112:GLN:H	3:R:112:GLN:NE2	1.95	0.65
1:J:24:PRO:HA	13:J:1105:HOH:O	1.96	0.65
2:E:26:GLN:HG2	2:E:58:LEU:HD21	1.79	0.65
2:K:26:GLN:HG2	2:K:58:LEU:HD21	1.79	0.65
1:J:105:PHE:HA	1:J:108:VAL:HG23	1.78	0.64
2:Q:128:PRO:HG2	2:Q:129:GLU:OE1	1.98	0.64
1:G:105:PHE:HA	1:G:108:VAL:HG22	1.78	0.64
3:C:112:GLN:H	3:C:112:GLN:NE2	1.95	0.64
2:H:74:ASP:HB3	2:H:77:THR:HB	1.80	0.64
1:M:105:PHE:HA	1:M:108:VAL:CG2	2.26	0.64
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.80	0.64
1:J:180:LEU:HD22	9:J:1004:SMA:H26	1.78	0.64
2:N:20:PHE:HB3	2:N:25:LEU:HD11	1.78	0.64
2:N:26:GLN:HG2	2:N:58:LEU:HD21	1.80	0.64
1:D:103:LEU:HD13	10:D:1022:LOP:H201	1.79	0.64

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:10:THR:O	3:O:10:THR:HG22	2.04	0.58
1:A:92:MET:CE	2:B:226:ARG:HG3	2.33	0.58
1:D:68:HIS:ND1	13:D:1105:HOH:O	2.32	0.58
1:D:249:ILE:O	1:D:253:VAL:HG23	2.04	0.58
3:I:55:SER:HB3	3:I:182:THR:OG1	2.04	0.58
3:R:10:THR:O	3:R:10:THR:HG22	2.04	0.58
1:A:249:ILE:O	1:A:253:VAL:HG23	2.04	0.57
1:D:43:TRP:CH2	1:D:251:LYS:HG2	2.39	0.57
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.04	0.57
2:E:194:VAL:HB	2:E:207:MET:HE1	1.85	0.57
3:L:55:SER:HB3	3:L:182:THR:OG1	2.04	0.57
3:O:55:SER:HB3	3:O:182:THR:OG1	2.04	0.57
1:M:39:ARG:HH12	2:N:255:VAL:CG1	2.17	0.57
1:A:92:MET:HE1	2:B:226:ARG:HG3	1.86	0.57
3:F:55:SER:HB3	3:F:182:THR:OG1	2.04	0.57
2:B:42:MET:HE2	2:B:218:ALA:HB1	1.86	0.57
3:C:55:SER:HB3	3:C:182:THR:OG1	2.05	0.57
3:F:10:THR:HG22	3:F:10:THR:O	2.04	0.57
1:M:132:GLY:C	8:M:501:HEM:HBC2	2.25	0.57
2:K:51:SER:OG	2:K:63:VAL:HG21	2.05	0.57
1:J:105:PHE:HA	1:J:108:VAL:CG2	2.35	0.57
2:N:71:THR:HG22	2:N:80:ASP:HB3	1.87	0.57
1:D:105:PHE:HA	1:D:108:VAL:HG22	1.86	0.57
1:J:261:LEU:HD11	2:K:234:VAL:HG13	1.87	0.57
1:G:199:TYR:CE2	8:G:502:HEM:HBC1	2.40	0.57
2:E:42:MET:HE2	2:E:218:ALA:HB1	1.86	0.57
2:Q:49:SER:HA	2:Q:52:GLU:HG3	1.87	0.56
3:R:55:SER:HB3	3:R:182:THR:OG1	2.05	0.56
1:M:411:LEU:O	1:M:415:GLU:HG2	2.04	0.56
2:N:138:PHE:CE1	2:N:157:ASN:ND2	2.73	0.56
1:G:248:PHE:HA	1:G:251:LYS:HG2	1.87	0.56
2:B:42:MET:HE1	2:B:218:ALA:CB	2.35	0.56
1:A:5:PRO:HB2	1:A:234:LYS:HA	1.87	0.56
1:G:158:GLY:O	1:G:162:ILE:HD12	2.04	0.56
1:D:406:VAL:O	1:D:409:PRO:HD2	2.05	0.56
3:L:10:THR:O	3:L:10:THR:HG22	2.05	0.56
3:I:10:THR:O	3:I:10:THR:HG22	2.04	0.56
3:C:10:THR:HG22	3:C:10:THR:O	2.05	0.56
2:H:77:THR:CG2	2:H:79:GLU:HB2	2.36	0.56
1:J:5:PRO:HB2	1:J:234:LYS:HA	1.86	0.56
2:Q:72:VAL:HG12	2:Q:73:THR:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:246:PRO:HG2	2:K:251:LEU:HD21	1.86	0.56
1:M:125:ARG:CZ	1:M:222:ASN:HB2	2.35	0.56
1:D:217:HIS:NE2	11:D:1102:UQ2:O4	2.26	0.56
1:P:351:THR:OG1	1:P:412:GLY:HA3	2.05	0.56
2:B:145:CYS:O	2:B:168:THR:OG1	2.21	0.56
2:N:220:GLU:OE2	2:N:226:ARG:NH1	2.39	0.56
1:A:359:TYR:CD2	1:A:420:PRO:HB3	2.41	0.56
1:A:12:ARG:O	1:A:17:LYS:HE2	2.05	0.56
2:N:42:MET:HE2	2:N:218:ALA:HB1	1.88	0.56
1:G:184:PRO:O	3:L:70:LYS:HE3	2.05	0.56
2:Q:81:ARG:HH11	2:Q:81:ARG:HG3	1.70	0.56
1:P:43:TRP:HZ3	1:P:251:LYS:HE3	1.69	0.56
3:C:131:HIS:O	1:D:329:LYS:HE3	2.06	0.56
1:G:383:GLN:HE22	2:H:115:GLY:HA3	1.71	0.56
1:P:236:GLU:HA	1:P:239:LYS:CD	2.36	0.55
1:J:249:ILE:O	1:J:253:VAL:HG23	2.06	0.55
1:J:199:TYR:CD2	8:J:502:HEM:HBC1	2.42	0.55
2:E:194:VAL:HB	2:E:207:MET:HE3	1.88	0.55
2:K:114:MET:HG2	2:K:114:MET:O	2.05	0.55
1:D:144:PHE:CD1	1:D:162:ILE:HD12	2.40	0.55
1:G:4:ILE:N	1:G:4:ILE:HD12	2.19	0.55
2:K:194:VAL:HB	2:K:207:MET:HE3	1.89	0.55
1:A:358:ARG:HH21	10:A:1021:LOP:H21	1.71	0.55
1:P:199:TYR:CD2	8:P:502:HEM:HBC1	2.41	0.55
2:E:56:PRO:HD2	13:E:1045:HOH:O	2.06	0.55
1:A:58:GLN:CB	8:A:502:HEM:HAB	2.37	0.55
2:E:42:MET:HE1	2:E:218:ALA:CB	2.37	0.55
2:B:250:ARG:CD	3:C:12:ARG:HG2	2.28	0.55
1:P:287:ARG:NH1	1:P:287:ARG:HG2	2.21	0.55
1:D:13:THR:HG22	1:D:14:GLY:N	2.22	0.55
1:A:195:PHE:CE2	1:D:195:PHE:HE2	2.10	0.55
2:H:194:VAL:HB	2:H:207:MET:HE3	1.87	0.55
2:B:27:ARG:HD2	2:B:196:TYR:CE2	2.42	0.55
2:Q:246:LEU:O	2:Q:250:ARG:HG2	2.07	0.55
1:D:92:MET:CE	2:E:226:ARG:HG3	2.35	0.55
1:G:92:MET:HE2	1:G:92:MET:HA	1.89	0.55
2:B:194:VAL:HB	2:B:207:MET:HE1	1.88	0.54
1:P:244:PHE:CE1	11:P:1106:UQ2:H2M2	2.42	0.54
1:M:246:PRO:HG2	2:N:251:LEU:HD21	1.88	0.54
3:R:89:GLN:O	3:R:92:GLN:HB2	2.07	0.54
2:Q:66:TYR:CE1	2:Q:70:PHE:HE2	2.24	0.54

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:HIS:NE2	11:G:1103:UQ2:O4	2.36	0.52
1:D:150:PRO:HG3	8:D:502:HEM:O2D	2.10	0.52
1:J:229:VAL:HG22	1:J:424:ILE:HD12	1.92	0.52
2:E:74:ASP:CB	2:E:77:THR:HB	2.35	0.52
3:C:70:LYS:HG3	1:D:185:ALA:HB2	1.92	0.52
1:P:32:THR:HG23	1:P:217:HIS:HE1	1.74	0.52
3:O:80:ALA:O	3:O:84:LEU:HG	2.09	0.52
2:E:250:ARG:CZ	3:F:12:ARG:HG2	2.40	0.52
1:P:13:THR:HG22	1:P:14:GLY:H	1.74	0.52
2:K:185:MET:HB2	8:K:301:HEM:C1D	2.45	0.52
2:B:171:ASP:OD1	2:B:173:ASN:N	2.37	0.52
1:J:269:PHE:HB3	4:K:1044:BGL:H1'2	1.92	0.52
1:A:114:ARG:HD2	1:A:114:ARG:C	2.30	0.52
1:G:346:VAL:HG12	1:G:347:PRO:HD3	1.91	0.52
1:J:132:GLY:C	8:J:501:HEM:HBC2	2.31	0.52
1:J:114:ARG:HD2	1:J:114:ARG:C	2.31	0.52
1:M:236:GLU:HA	1:M:239:LYS:HD3	1.92	0.52
1:M:236:GLU:HA	1:M:239:LYS:CD	2.40	0.52
1:M:58:GLN:CB	8:M:502:HEM:HAB	2.39	0.52
1:P:39:ARG:NH1	2:Q:255:VAL:CG1	2.72	0.52
1:P:114:ARG:C	1:P:114:ARG:HD2	2.31	0.52
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.91	0.51
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.13	0.51
1:J:33:ILE:HG13	1:J:245:TRP:CB	2.39	0.51
2:H:114:MET:O	2:H:114:MET:HG2	2.10	0.51
2:N:160:PHE:CE2	2:N:183:ILE:HG13	2.44	0.51
1:M:114:ARG:C	1:M:114:ARG:HD2	2.31	0.51
2:E:77:THR:HG22	2:E:79:GLU:HB2	1.92	0.51
1:J:142:THR:HG21	8:J:502:HEM:HBB2	1.92	0.51
1:G:114:ARG:C	1:G:114:ARG:HD2	2.30	0.51
2:H:250:ARG:CZ	3:I:12:ARG:HB3	2.40	0.51
2:B:224:MET:O	2:B:228:GLN:HG3	2.11	0.51
1:G:125:ARG:NE	1:G:222:ASN:HB2	2.25	0.51
2:E:42:MET:CE	2:E:218:ALA:CB	2.89	0.51
1:D:114:ARG:HD2	1:D:114:ARG:C	2.31	0.51
8:D:501:HEM:CMB	8:D:501:HEM:HBB2	2.41	0.51
2:H:169:CYS:O	2:H:177:THR:HB	2.11	0.51
2:K:40:HIS:HE1	2:K:98:PRO:HD2	1.76	0.51
2:K:42:MET:HE1	2:K:218:ALA:CB	2.41	0.51
1:M:92:MET:CE	2:N:226:ARG:HG3	2.42	0.50
2:Q:66:TYR:CE1	2:Q:70:PHE:CE2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ARG:HD2	13:G:1118:HOH:O	2.11	0.50
2:H:250:ARG:NH1	3:I:12:ARG:CB	2.73	0.50
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.25	0.50
1:M:133:MET:N	8:M:501:HEM:HBC2	2.27	0.50
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.44	0.50
1:G:5:PRO:HB3	1:G:234:LYS:HG2	1.93	0.50
1:A:383:GLN:HE22	2:B:115:GLY:HA3	1.76	0.50
1:D:91:PHE:CD1	2:E:222:LYS:HG2	2.46	0.50
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.93	0.50
2:N:176:LYS:HD3	2:N:176:LYS:O	2.11	0.50
2:E:66:TYR:CE1	2:E:70:PHE:CE2	2.99	0.50
1:P:312:VAL:HG12	1:P:314:VAL:HG12	1.94	0.50
3:C:57:VAL:HG22	3:C:63:LEU:HD13	1.94	0.50
1:M:125:ARG:NH1	1:M:222:ASN:HB2	2.27	0.50
2:Q:236:PHE:CE1	3:R:25:VAL:HG12	2.46	0.50
2:N:149:HIS:CD2	2:N:168:THR:HG21	2.46	0.50
3:I:70:LYS:HE3	1:J:185:ALA:HB2	1.92	0.50
2:E:42:MET:CE	2:E:218:ALA:HB1	2.42	0.50
2:H:149:HIS:CE1	2:H:168:THR:HG21	2.47	0.50
1:P:11:PRO:HB2	1:P:17:LYS:HG2	1.94	0.50
1:G:236:GLU:HA	1:G:239:LYS:HG3	1.92	0.49
2:H:154:PHE:HB3	2:H:182:TRP:HB3	1.94	0.49
3:L:157:ASP:HB2	13:L:505:HOH:O	2.12	0.49
2:E:40:HIS:CE1	2:E:97:ALA:HB1	2.47	0.49
2:Q:220:GLU:OE2	2:Q:226:ARG:NH1	2.45	0.49
3:R:70:LYS:NZ	3:R:70:LYS:HB2	2.27	0.49
1:P:406:VAL:C	1:P:409:PRO:HD2	2.33	0.49
1:P:128:THR:HG21	8:P:501:HEM:HBD1	1.94	0.49
1:G:5:PRO:CB	1:G:234:LYS:HG2	2.42	0.49
1:J:236:GLU:HA	1:J:239:LYS:CD	2.41	0.49
1:P:248:PHE:CD1	1:P:251:LYS:HD3	2.48	0.49
2:N:143:PRO:HG3	2:N:178:THR:CG2	2.42	0.49
1:P:354:VAL:HG21	1:P:417:PRO:CB	2.42	0.49
2:K:236:PHE:CE1	3:L:25:VAL:HG12	2.47	0.49
2:N:149:HIS:CG	2:N:168:THR:HG21	2.47	0.49
2:Q:151:PRO:HD2	2:Q:182:TRP:CD1	2.47	0.49
2:K:154:PHE:HB3	2:K:182:TRP:HB3	1.94	0.49
3:C:59:PRO:HD3	3:C:76:ARG:NH1	2.28	0.49
2:N:183:ILE:HG23	2:N:185:MET:N	2.24	0.49
1:D:92:MET:HE1	2:E:226:ARG:CG	2.41	0.49
1:D:43:TRP:CE3	1:D:43:TRP:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:ALA:O	1:M:239:LYS:HG3	2.13	0.49
1:M:122:LYS:O	1:M:123:ALA:C	2.51	0.49
3:F:57:VAL:HG22	3:F:63:LEU:HD13	1.95	0.49
3:R:59:PRO:HD3	3:R:76:ARG:NH1	2.28	0.49
2:K:49:SER:HA	2:K:52:GLU:CG	2.43	0.49
1:G:362:MET:N	1:G:415:GLU:OE2	2.45	0.49
2:K:231:PHE:O	2:K:235:MET:HG2	2.13	0.49
1:D:39:ARG:HH12	2:E:255:VAL:HG12	1.76	0.48
1:P:32:THR:HG23	1:P:217:HIS:CE1	2.48	0.48
2:H:250:ARG:NH1	3:I:16:TYR:CZ	2.81	0.48
1:D:102:SER:O	1:D:106:ILE:HG13	2.13	0.48
1:M:406:VAL:O	1:M:409:PRO:HD2	2.12	0.48
11:G:1103:UQ2:C8	11:G:1103:UQ2:H5M1	2.43	0.48
1:D:4:ILE:HD12	1:D:4:ILE:N	2.28	0.48
2:Q:130:TYR:OH	8:Q:301:HEM:O2A	2.17	0.48
3:R:57:VAL:HG22	3:R:63:LEU:HD13	1.94	0.48
3:I:59:PRO:HD3	3:I:76:ARG:NH1	2.28	0.48
4:G:1043:BGL:H5	2:H:15:GLY:H	1.77	0.48
2:N:72:VAL:O	2:N:80:ASP:HA	2.13	0.48
1:G:125:ARG:CZ	1:G:222:ASN:HB2	2.43	0.48
2:N:184:ALA:HB3	8:N:301:HEM:HBD2	1.95	0.48
3:F:47:LEU:O	3:F:47:LEU:CD2	2.61	0.48
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.76	0.48
2:B:149:HIS:NE2	2:B:168:THR:HG21	2.28	0.48
1:G:58:GLN:HB3	8:G:502:HEM:HAB	1.95	0.48
1:G:105:PHE:HA	1:G:108:VAL:CG2	2.44	0.48
1:J:355:ARG:HG3	1:J:355:ARG:HH11	1.79	0.48
1:J:91:PHE:HE2	1:J:92:MET:CE	2.26	0.48
3:L:57:VAL:HG22	3:L:63:LEU:HD13	1.94	0.48
2:N:154:PHE:HB3	2:N:182:TRP:HB3	1.95	0.48
1:M:51:LEU:HB3	8:M:501:HEM:HMB1	1.96	0.48
2:Q:73:THR:HG23	2:Q:80:ASP:OD1	2.13	0.48
2:N:42:MET:CE	2:N:218:ALA:CB	2.91	0.48
3:F:90:LEU:HD11	3:F:108:GLU:HB3	1.95	0.48
1:M:346:VAL:CG1	1:M:347:PRO:HD3	2.44	0.48
1:G:312:VAL:HG12	1:G:314:VAL:HG12	1.96	0.48
2:E:72:VAL:CG1	2:E:73:THR:N	2.76	0.48
2:Q:185:MET:HB2	8:Q:301:HEM:C1D	2.49	0.48
3:I:57:VAL:HG22	3:I:63:LEU:HD13	1.95	0.48
3:L:59:PRO:HD3	3:L:76:ARG:NH1	2.29	0.48
3:L:90:LEU:HD11	3:L:108:GLU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:108:ALA:HA	2:N:125:ILE:O	2.14	0.48
2:B:77:THR:C	2:B:79:GLU:H	2.16	0.47
1:D:43:TRP:O	1:D:46:ILE:HG12	2.14	0.47
2:Q:81:ARG:HG3	2:Q:81:ARG:NH1	2.29	0.47
2:Q:141:GLU:H	2:Q:141:GLU:HG2	1.49	0.47
1:J:51:LEU:HB3	8:J:501:HEM:HMB1	1.96	0.47
1:P:92:MET:HE2	1:P:92:MET:HA	1.96	0.47
3:O:59:PRO:HD3	3:O:76:ARG:NH1	2.29	0.47
1:M:4:ILE:H	1:M:4:ILE:CD1	2.24	0.47
1:P:43:TRP:HA	1:P:43:TRP:CE3	2.49	0.47
1:G:346:VAL:CG1	1:G:347:PRO:HD3	2.44	0.47
1:M:425:GLU:O	1:M:429:ASN:ND2	2.47	0.47
1:A:236:GLU:HA	1:A:239:LYS:HD3	1.97	0.47
1:G:248:PHE:CE1	1:G:251:LYS:HD3	2.48	0.47
1:D:246:PRO:CG	2:E:251:LEU:HD21	2.41	0.47
2:E:142:PRO:CG	2:E:150:GLU:OE2	2.62	0.47
1:J:91:PHE:CE2	1:J:92:MET:CE	2.97	0.47
1:P:346:VAL:CG1	1:P:347:PRO:HD3	2.44	0.47
3:I:66:LYS:HE2	3:I:69:GLY:HA2	1.96	0.47
3:F:59:PRO:HD3	3:F:76:ARG:NH1	2.30	0.47
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.48	0.47
2:E:40:HIS:HE1	2:E:98:PRO:HD2	1.79	0.47
1:A:346:VAL:CG1	1:A:347:PRO:HD3	2.45	0.47
1:M:43:TRP:CZ3	1:M:251:LYS:HE2	2.50	0.47
3:I:84:LEU:O	3:I:88:VAL:HG23	2.14	0.47
3:R:62:GLN:NE2	3:R:73:PHE:CD1	2.83	0.47
3:O:57:VAL:HG22	3:O:63:LEU:HD13	1.95	0.47
1:M:10:GLU:HA	1:M:11:PRO:HD3	1.70	0.47
1:A:360:ARG:O	1:A:364:LYS:HG3	2.14	0.47
1:P:177:GLN:NE2	13:P:611:HOH:O	2.40	0.47
2:B:205:HIS:ND1	2:B:205:HIS:C	2.68	0.47
1:M:113:PHE:HB3	10:M:1025:LOP:H261	1.95	0.47
1:M:92:MET:HE1	2:N:226:ARG:HG3	1.97	0.47
2:Q:236:PHE:CE1	3:R:25:VAL:HG11	2.49	0.47
1:D:346:VAL:CG1	1:D:347:PRO:HD3	2.44	0.47
1:A:43:TRP:CZ3	1:A:251:LYS:HE3	2.50	0.47
1:J:407:ILE:O	1:J:411:LEU:HG	2.14	0.47
1:A:199:TYR:CD2	8:A:502:HEM:HBC1	2.50	0.47
1:G:39:ARG:HD3	1:G:428:PHE:CD2	2.50	0.47
1:J:346:VAL:CG1	1:J:347:PRO:HD3	2.44	0.47
1:J:217:HIS:NE2	11:J:1104:UQ2:O4	2.46	0.47

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:HIS:O	1:D:293:VAL:HG23	2.16	0.44
1:P:102:SER:O	1:P:106:ILE:HG13	2.16	0.44
1:G:47:TRP:CZ2	1:G:110:LEU:HD13	2.53	0.44
1:G:121:TYR:HB3	1:G:129:TRP:CE3	2.53	0.44
1:G:416:LYS:HA	1:G:416:LYS:HD3	1.63	0.44
1:G:106:ILE:HD12	10:G:1023:LOP:H212	1.99	0.44
1:D:47:TRP:CZ2	1:D:110:LEU:HD13	2.53	0.44
1:A:418:VAL:CG1	1:A:419:ALA:N	2.80	0.44
2:B:223:LEU:CD2	2:B:227:LYS:HD2	2.46	0.44
2:H:138:PHE:CD2	2:H:187:PRO:HG3	2.51	0.44
1:J:130:ILE:HD11	1:J:348:TRP:CH2	2.46	0.44
1:J:209:VAL:CG2	8:J:501:HEM:HBB2	2.48	0.44
3:I:14:PHE:O	3:I:17:TYR:HB3	2.17	0.44
3:R:140:VAL:HG12	3:R:140:VAL:O	2.16	0.44
1:M:39:ARG:NH1	2:N:255:VAL:CG1	2.80	0.44
1:G:428:PHE:CZ	2:H:256:LYS:HB3	2.52	0.44
1:J:406:VAL:O	1:J:409:PRO:HD2	2.18	0.44
1:A:47:TRP:CZ2	1:A:110:LEU:HD13	2.53	0.44
2:Q:17:PHE:CE1	2:Q:231:PHE:CZ	3.04	0.44
1:P:427:ASP:O	1:P:430:ALA:HB3	2.18	0.44
1:P:132:GLY:C	8:P:501:HEM:HBC2	2.38	0.44
2:K:236:PHE:HE1	3:L:25:VAL:CG1	2.30	0.44
3:O:47:LEU:CD2	3:O:47:LEU:O	2.64	0.44
1:G:133:MET:SD	8:G:501:HEM:HBC1	2.58	0.44
2:Q:48:ARG:HB3	2:Q:85:PRO:O	2.17	0.44
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.52	0.44
2:K:144:LYS:HA	2:K:147:GLU:HG3	1.99	0.44
2:Q:74:ASP:HB3	2:Q:77:THR:HB	2.00	0.44
1:D:49:VAL:HG23	11:D:1102:UQ2:H2M3	1.99	0.44
3:L:143:ASP:OD2	3:L:164:LYS:NZ	2.51	0.44
1:M:387:PHE:CE1	1:M:388:PRO:HB3	2.53	0.44
2:N:197:ALA:C	2:N:199:GLY:H	2.22	0.44
1:A:8:HIS:CD2	1:A:8:HIS:H	2.36	0.44
2:B:113:PRO:HD2	2:B:118:ILE:HB	1.99	0.44
1:M:425:GLU:HG2	1:M:429:ASN:HD21	1.82	0.43
2:H:222:LYS:HB2	13:H:347:HOH:O	2.18	0.43
1:D:121:TYR:HB3	1:D:129:TRP:CE3	2.53	0.43
3:I:12:ARG:H	3:I:12:ARG:HG2	1.60	0.43
1:A:106:ILE:HD12	10:A:1021:LOP:H212	1.99	0.43
1:P:248:PHE:HD1	1:P:251:LYS:HD3	1.82	0.43
1:J:226:GLY:CA	1:J:355:ARG:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:10:GLU:HA	1:P:11:PRO:HD3	1.69	0.43
2:B:15:GLY:H	4:B:1041:BGL:H1	1.82	0.43
2:E:113:PRO:HD2	2:E:118:ILE:HB	2.00	0.43
2:N:111:HIS:HE1	13:N:552:HOH:O	2.00	0.43
3:R:77:ARG:HB3	3:R:81:ASP:HB2	2.00	0.43
1:G:406:VAL:C	1:G:409:PRO:HD2	2.38	0.43
2:H:223:LEU:HD21	2:H:227:LYS:CE	2.49	0.43
1:J:43:TRP:HA	1:J:43:TRP:HE3	1.83	0.43
1:M:195:PHE:CE2	1:P:195:PHE:HE2	2.12	0.43
2:E:34:GLU:OE1	2:E:194:VAL:HG22	2.19	0.43
1:P:105:PHE:HA	1:P:108:VAL:CG2	2.48	0.43
8:P:502:HEM:HHD	8:P:502:HEM:CBC	2.48	0.43
1:G:92:MET:CE	1:G:92:MET:HA	2.47	0.43
1:J:262:VAL:HG13	4:K:1044:BGL:HB8'1	1.99	0.43
2:K:48:ARG:HB3	2:K:85:PRO:O	2.17	0.43
3:C:84:LEU:HD23	3:C:84:LEU:HA	1.81	0.43
1:P:43:TRP:HA	1:P:43:TRP:HE3	1.84	0.43
2:K:141:GLU:HA	2:K:142:PRO:HD3	1.76	0.43
3:R:10:THR:O	3:R:14:PHE:HB3	2.18	0.43
2:K:40:HIS:HB3	2:K:100:LEU:HG	2.00	0.43
3:R:62:GLN:NE2	3:R:73:PHE:CG	2.87	0.43
1:P:44:MET:CE	10:P:1026:LOP:H92	2.48	0.43
1:D:355:ARG:CD	13:D:1155:HOH:O	2.66	0.43
3:I:179:ILE:HA	3:I:179:ILE:HD13	1.74	0.43
2:H:141:GLU:HG2	13:H:338:HOH:O	2.19	0.43
1:A:92:MET:HE2	1:A:92:MET:HA	2.01	0.43
2:N:149:HIS:CD2	2:N:168:THR:OG1	2.70	0.43
1:P:359:TYR:CD2	1:P:420:PRO:HB3	2.53	0.43
2:Q:144:LYS:NZ	2:Q:147:GLU:OE1	2.51	0.43
2:H:77:THR:HG23	2:H:79:GLU:OE2	2.19	0.43
11:M:1105:UQ2:H3M3	11:M:1105:UQ2:H2M2	2.01	0.43
1:J:43:TRP:HA	1:J:43:TRP:CE3	2.54	0.43
2:Q:197:ALA:C	2:Q:199:GLY:H	2.21	0.43
1:P:47:TRP:CZ2	1:P:110:LEU:HD13	2.53	0.43
2:N:74:ASP:CG	2:N:77:THR:HB	2.39	0.43
1:A:105:PHE:HA	1:A:108:VAL:CG2	2.45	0.43
2:B:34:GLU:OE1	2:B:194:VAL:HG22	2.18	0.43
2:K:42:MET:CE	2:K:218:ALA:CB	2.97	0.43
2:K:165:VAL:CG1	2:K:169:CYS:HB2	2.48	0.43
2:K:155:TYR:CD1	2:K:155:TYR:N	2.87	0.43
2:B:155:TYR:N	2:B:155:TYR:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:427:ASP:O	1:M:430:ALA:HB3	2.18	0.43
1:P:360:ARG:O	1:P:364:LYS:HG3	2.19	0.43
1:J:359:TYR:CD2	1:J:420:PRO:HB3	2.54	0.43
2:E:144:LYS:HD3	2:E:147:GLU:OE2	2.18	0.43
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.52	0.43
1:M:92:MET:HE2	1:M:92:MET:HA	2.00	0.43
2:K:113:PRO:HD2	2:K:118:ILE:HB	2.01	0.43
2:H:155:TYR:CD1	2:H:155:TYR:N	2.87	0.43
1:J:121:TYR:HB3	1:J:129:TRP:CE3	2.53	0.43
1:P:45:TRP:CZ3	1:P:224:PRO:HG3	2.54	0.43
1:G:45:TRP:CZ3	1:G:224:PRO:HG3	2.54	0.43
3:C:14:PHE:O	3:C:17:TYR:HB3	2.18	0.43
3:L:77:ARG:HB3	3:L:81:ASP:HB2	2.01	0.43
1:A:45:TRP:CZ3	1:A:224:PRO:HG3	2.53	0.43
1:J:47:TRP:CZ2	1:J:110:LEU:HD13	2.53	0.43
2:N:34:GLU:OE1	2:N:194:VAL:HG22	2.19	0.43
8:M:502:HEM:CMC	8:M:502:HEM:HBC2	2.49	0.43
1:G:306:ARG:NH2	1:G:383:GLN:O	2.40	0.43
1:J:111:HIS:CD2	8:J:501:HEM:NC	2.87	0.43
3:R:59:PRO:HD3	3:R:76:ARG:HH11	1.83	0.43
1:M:47:TRP:CZ2	1:M:110:LEU:HD13	2.53	0.43
1:M:6:HIS:C	1:M:6:HIS:ND1	2.71	0.43
1:A:406:VAL:O	1:A:409:PRO:HD2	2.19	0.43
1:J:45:TRP:CZ3	1:J:224:PRO:HG3	2.54	0.43
8:D:501:HEM:HBC2	8:D:501:HEM:HMC2	2.01	0.42
2:K:107:ARG:HH21	8:K:301:HEM:CGA	2.32	0.42
3:L:59:PRO:HD3	3:L:76:ARG:HH11	1.84	0.42
1:M:10:GLU:OE2	1:M:11:PRO:HD2	2.19	0.42
2:E:155:TYR:N	2:E:155:TYR:CD1	2.86	0.42
1:D:428:PHE:CZ	2:E:256:LYS:HB2	2.53	0.42
1:M:350:ASP:HB2	1:M:408:LEU:HD13	2.01	0.42
2:N:103:MET:C	2:N:105:LYS:H	2.21	0.42
2:Q:34:GLU:OE1	2:Q:194:VAL:HG22	2.19	0.42
2:H:34:GLU:OE1	2:H:194:VAL:HG22	2.19	0.42
2:Q:42:MET:CE	2:Q:218:ALA:CB	2.97	0.42
3:C:59:PRO:HD3	3:C:76:ARG:HH11	1.84	0.42
2:B:48:ARG:HB3	2:B:85:PRO:O	2.19	0.42
3:C:138:GLY:O	3:C:141:SER:OG	2.32	0.42
1:D:79:SER:O	1:D:83:ILE:HG13	2.20	0.42
1:D:133:MET:SD	8:D:501:HEM:HBC1	2.59	0.42
1:M:123:ALA:O	1:M:355:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:PHE:CD1	2:H:222:LYS:HG2	2.54	0.42
1:A:79:SER:O	1:A:83:ILE:HG13	2.19	0.42
3:R:124:VAL:O	3:R:173:ILE:HG23	2.19	0.42
2:K:34:GLU:OE1	2:K:194:VAL:HG22	2.19	0.42
1:J:112:ILE:HG12	8:J:501:HEM:HAC	2.00	0.42
2:K:197:ALA:C	2:K:199:GLY:H	2.23	0.42
3:R:179:ILE:HD13	3:R:179:ILE:HA	1.74	0.42
2:B:185:MET:HB2	8:B:301:HEM:C1D	2.54	0.42
1:M:394:LEU:HA	1:M:394:LEU:HD23	1.89	0.42
3:O:47:LEU:C	3:O:47:LEU:HD23	2.39	0.42
2:H:113:PRO:HD2	2:H:118:ILE:HB	2.00	0.42
1:D:236:GLU:HA	1:D:239:LYS:HD2	2.02	0.42
3:L:124:VAL:O	3:L:173:ILE:HG23	2.20	0.42
1:M:121:TYR:HB3	1:M:129:TRP:CE3	2.54	0.42
2:E:236:PHE:CE2	3:F:25:VAL:CG1	2.95	0.42
2:Q:183:ILE:HG12	2:Q:185:MET:H	1.85	0.42
1:D:45:TRP:CZ3	1:D:224:PRO:HG3	2.54	0.42
1:J:418:VAL:CG1	1:J:419:ALA:N	2.83	0.42
3:C:179:ILE:CG1	3:C:185:GLN:HE21	2.33	0.42
1:G:394:LEU:HD23	1:G:394:LEU:HA	1.89	0.42
1:J:4:ILE:HA	1:J:5:PRO:HD3	1.88	0.42
1:D:39:ARG:NH1	2:E:255:VAL:HG12	2.34	0.42
2:Q:155:TYR:N	2:Q:155:TYR:CD1	2.87	0.42
3:I:59:PRO:HD3	3:I:76:ARG:HH11	1.84	0.42
2:N:155:TYR:N	2:N:155:TYR:CD1	2.87	0.42
2:N:250:ARG:NH1	3:O:12:ARG:HA	2.33	0.42
3:R:179:ILE:CG1	3:R:185:GLN:HE21	2.33	0.42
2:N:68:THR:HG23	2:N:82:GLU:HB3	2.01	0.42
1:P:121:TYR:HB3	1:P:129:TRP:CE3	2.54	0.42
1:M:105:PHE:O	1:M:108:VAL:HG23	2.20	0.42
1:G:92:MET:CE	2:H:226:ARG:HG3	2.50	0.42
2:Q:165:VAL:CG1	2:Q:169:CYS:HB2	2.50	0.42
1:M:239:LYS:HE2	1:M:425:GLU:OE2	2.20	0.42
2:N:94:LEU:HD22	8:N:301:HEM:HAC	2.01	0.42
1:G:359:TYR:CD2	1:G:420:PRO:HB3	2.55	0.42
1:P:234:LYS:O	1:P:238:GLN:HG3	2.19	0.42
3:L:58:GLU:N	3:L:58:GLU:CD	2.73	0.42
1:M:215:ALA:HA	1:P:23:LEU:HD13	2.01	0.42
2:E:76:GLU:O	2:E:77:THR:C	2.57	0.42
2:E:250:ARG:NH1	2:E:250:ARG:CG	2.82	0.42
2:E:30:GLN:HG2	2:E:34:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:SER:O	1:G:106:ILE:HG13	2.20	0.42
1:M:362:MET:HB3	1:M:411:LEU:HD21	2.02	0.42
1:D:406:VAL:C	1:D:409:PRO:HD2	2.40	0.42
2:N:143:PRO:HG3	2:N:178:THR:HG21	2.02	0.42
2:H:145:CYS:O	2:H:168:THR:OG1	2.28	0.42
1:A:291:HIS:CE1	2:B:2:GLY:HA2	2.54	0.42
3:F:13:ASP:O	3:F:17:TYR:HD2	2.02	0.42
3:I:77:ARG:HB3	3:I:81:ASP:HB2	2.01	0.42
3:L:179:ILE:HA	3:L:179:ILE:HD13	1.74	0.42
1:M:262:VAL:O	1:M:266:ILE:HG12	2.20	0.42
2:K:72:VAL:CG1	2:K:73:THR:N	2.83	0.42
1:M:45:TRP:CZ3	1:M:224:PRO:HG3	2.54	0.42
3:F:77:ARG:HB3	3:F:81:ASP:HB2	2.01	0.42
1:D:364:LYS:O	1:D:368:TRP:HD1	2.02	0.42
2:N:20:PHE:CB	2:N:25:LEU:HD11	2.48	0.41
1:M:239:LYS:HB3	1:M:425:GLU:OE2	2.20	0.41
3:L:179:ILE:CG1	3:L:185:GLN:HE21	2.33	0.41
1:P:122:LYS:O	1:P:123:ALA:C	2.58	0.41
1:M:314:VAL:HG23	1:M:314:VAL:H	1.63	0.41
2:N:160:PHE:CG	2:N:183:ILE:HD12	2.55	0.41
1:G:39:ARG:HH12	2:H:255:VAL:HG12	1.82	0.41
2:H:141:GLU:HA	2:H:142:PRO:HD3	1.87	0.41
1:A:355:ARG:HD3	13:A:1122:HOH:O	2.19	0.41
2:E:154:PHE:HB3	2:E:182:TRP:HB3	2.01	0.41
3:O:44:VAL:O	3:O:46:ALA:N	2.53	0.41
3:F:124:VAL:O	3:F:173:ILE:HG23	2.20	0.41
3:C:77:ARG:HB3	3:C:81:ASP:HB2	2.02	0.41
2:E:48:ARG:HB3	2:E:85:PRO:O	2.19	0.41
2:B:40:HIS:HB3	2:B:100:LEU:HG	2.02	0.41
3:I:58:GLU:N	3:I:58:GLU:CD	2.73	0.41
1:P:394:LEU:HA	1:P:394:LEU:HD23	1.89	0.41
1:D:135:ILE:CG2	8:D:501:HEM:HAB	2.42	0.41
1:D:261:LEU:CD1	2:E:234:VAL:HG13	2.46	0.41
2:N:94:LEU:CD2	8:N:301:HEM:HAC	2.49	0.41
2:K:48:ARG:HG3	2:K:48:ARG:HH11	1.86	0.41
3:I:124:VAL:O	3:I:173:ILE:HG23	2.19	0.41
3:O:58:GLU:N	3:O:58:GLU:CD	2.74	0.41
1:A:111:HIS:CD2	8:A:501:HEM:NC	2.89	0.41
2:Q:20:PHE:CB	2:Q:25:LEU:HD11	2.48	0.41
1:A:122:LYS:O	1:A:123:ALA:C	2.59	0.41
3:O:124:VAL:O	3:O:173:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:162:ILE:HD11	3:I:164:LYS:O	2.21	0.41
2:N:113:PRO:HD2	2:N:118:ILE:HB	2.02	0.41
1:D:394:LEU:HD23	1:D:394:LEU:HA	1.90	0.41
1:P:408:LEU:HA	1:P:408:LEU:HD23	1.91	0.41
1:D:408:LEU:HD23	1:D:408:LEU:HA	1.89	0.41
1:M:322:SER:O	1:M:325:ILE:HD12	2.21	0.41
2:Q:149:HIS:CG	2:Q:168:THR:HG21	2.53	0.41
3:C:47:LEU:CD2	3:C:47:LEU:O	2.63	0.41
2:H:30:GLN:HG2	2:H:34:GLU:OE2	2.20	0.41
1:P:132:GLY:HA3	8:P:501:HEM:HBC2	2.02	0.41
2:E:189:LEU:O	2:E:190:MET:CB	2.68	0.41
2:N:176:LYS:HG2	2:N:178:THR:O	2.19	0.41
3:O:77:ARG:HB3	3:O:81:ASP:HB2	2.01	0.41
2:K:30:GLN:HG2	2:K:34:GLU:OE2	2.21	0.41
1:J:262:VAL:O	1:J:266:ILE:HG12	2.21	0.41
2:N:143:PRO:HG3	2:N:178:THR:HG22	2.03	0.41
2:Q:154:PHE:C	2:Q:155:TYR:CD1	2.94	0.41
2:Q:48:ARG:HH11	2:Q:48:ARG:HG3	1.86	0.41
1:D:306:ARG:HG3	13:D:1150:HOH:O	2.19	0.41
1:J:10:GLU:HA	1:J:11:PRO:HD3	1.87	0.41
3:R:58:GLU:N	3:R:58:GLU:CD	2.73	0.41
2:Q:30:GLN:HG2	2:Q:34:GLU:OE2	2.21	0.41
1:J:199:TYR:CG	8:J:502:HEM:HBC1	2.56	0.41
1:J:250:ILE:HD12	2:K:251:LEU:CD2	2.51	0.41
2:N:42:MET:HE2	2:N:218:ALA:CB	2.51	0.41
2:Q:242:VAL:O	2:Q:246:LEU:HG	2.21	0.41
1:P:354:VAL:HG21	1:P:417:PRO:HB2	2.03	0.41
3:O:162:ILE:HD11	3:O:164:LYS:O	2.20	0.41
2:H:197:ALA:C	2:H:199:GLY:H	2.23	0.41
1:J:133:MET:N	8:J:501:HEM:HBC2	2.36	0.41
1:A:239:LYS:HE2	1:A:425:GLU:OE1	2.21	0.41
1:G:51:LEU:HB3	8:G:501:HEM:HMB1	2.03	0.41
2:N:48:ARG:HH11	2:N:48:ARG:HG3	1.86	0.41
1:J:43:TRP:CZ3	1:J:251:LYS:HD3	2.55	0.41
1:J:64:VAL:HG11	1:J:93:LEU:HD13	2.02	0.41
1:J:122:LYS:O	1:J:123:ALA:C	2.59	0.41
3:O:54:VAL:O	3:O:54:VAL:HG13	2.20	0.41
3:F:58:GLU:N	3:F:58:GLU:CD	2.74	0.41
1:D:250:ILE:HD12	2:E:251:LEU:CD2	2.50	0.41
2:Q:77:THR:C	2:Q:79:GLU:N	2.73	0.41
2:N:40:HIS:HB3	2:N:100:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:130:ILE:HD11	1:P:348:TRP:CH2	2.47	0.41
1:A:130:ILE:HD11	1:A:348:TRP:CH2	2.46	0.41
2:B:77:THR:HG22	2:B:79:GLU:HG3	2.02	0.41
2:B:30:GLN:HG2	2:B:34:GLU:OE2	2.20	0.41
2:K:189:LEU:O	2:K:190:MET:CB	2.69	0.41
2:H:129:GLU:OE1	2:H:129:GLU:N	2.42	0.41
1:J:51:LEU:HD13	8:J:501:HEM:C3B	2.55	0.41
2:H:223:LEU:HD21	2:H:227:LYS:HE3	2.03	0.41
3:L:171:LEU:HA	3:L:172:PRO:HD3	1.95	0.41
1:M:64:VAL:HG11	1:M:93:LEU:HD13	2.03	0.41
3:C:124:VAL:O	3:C:173:ILE:HG23	2.21	0.41
1:M:75:LEU:O	1:M:79:SER:HB3	2.21	0.41
3:C:58:GLU:CD	3:C:58:GLU:N	2.73	0.41
2:H:74:ASP:CB	2:H:77:THR:HB	2.51	0.41
1:P:287:ARG:NH1	1:P:287:ARG:CG	2.83	0.41
1:J:425:GLU:HG3	1:J:429:ASN:ND2	2.33	0.41
1:P:43:TRP:O	1:P:46:ILE:HG12	2.20	0.41
2:B:77:THR:HG22	2:B:79:GLU:CB	2.51	0.41
2:N:154:PHE:C	2:N:155:TYR:CD1	2.94	0.41
2:B:154:PHE:C	2:B:155:TYR:CD1	2.94	0.41
3:I:179:ILE:CG1	3:I:185:GLN:HE21	2.33	0.41
2:N:242:VAL:O	2:N:246:LEU:HG	2.21	0.41
1:A:193:ARG:NH1	3:F:38:MET:HG2	2.36	0.41
2:Q:113:PRO:HD2	2:Q:118:ILE:HB	2.03	0.41
2:E:61:ASP:N	2:E:61:ASP:OD1	2.53	0.41
3:F:54:VAL:O	3:F:54:VAL:HG13	2.20	0.41
1:G:75:LEU:O	1:G:79:SER:HB3	2.21	0.41
1:G:43:TRP:O	1:G:46:ILE:HG12	2.22	0.40
2:H:250:ARG:NH2	3:I:12:ARG:HB2	2.35	0.40
1:G:92:MET:HE1	2:H:226:ARG:HG3	2.03	0.40
1:G:125:ARG:HH21	1:G:221:ASN:C	2.23	0.40
3:O:59:PRO:HD3	3:O:76:ARG:HH11	1.85	0.40
1:M:106:ILE:HG13	1:M:296:TRP:CZ2	2.56	0.40
2:B:154:PHE:HB3	2:B:182:TRP:HB3	2.03	0.40
1:D:236:GLU:O	1:D:239:LYS:HB2	2.20	0.40
2:Q:108:ALA:HA	2:Q:125:ILE:O	2.20	0.40
3:O:93:LEU:HB3	13:O:574:HOH:O	2.20	0.40
2:H:40:HIS:HB3	2:H:100:LEU:HG	2.03	0.40
3:O:179:ILE:CG1	3:O:185:GLN:HE21	2.33	0.40
1:A:64:VAL:HG11	1:A:93:LEU:HD13	2.02	0.40
2:N:152:ASP:OD1	2:N:152:ASP:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:156:TYR:HA	3:R:161:ARG:O	2.21	0.40
3:F:59:PRO:HD3	3:F:76:ARG:HH11	1.86	0.40
2:E:154:PHE:C	2:E:155:TYR:CD1	2.94	0.40
1:M:286:LEU:HD21	3:R:66:LYS:HB2	2.04	0.40
1:D:64:VAL:HG11	1:D:93:LEU:HD13	2.02	0.40
2:B:197:ALA:C	2:B:199:GLY:H	2.24	0.40
2:Q:143:PRO:HG3	2:Q:178:THR:CG2	2.52	0.40
2:E:146:ALA:O	2:E:147:GLU:C	2.59	0.40
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.44	0.40
2:N:30:GLN:HG2	2:N:34:GLU:OE2	2.21	0.40
1:G:130:ILE:HD11	1:G:348:TRP:CH2	2.46	0.40
2:K:154:PHE:C	2:K:155:TYR:CD1	2.94	0.40
1:M:122:LYS:HZ1	1:M:360:ARG:NH1	2.19	0.40
1:J:43:TRP:HH2	1:J:251:LYS:HG2	1.86	0.40
1:D:75:LEU:O	1:D:79:SER:HB3	2.21	0.40
1:G:79:SER:O	1:G:83:ILE:HG13	2.21	0.40
3:F:155:HIS:CD2	3:F:164:LYS:HD3	2.56	0.40
3:O:70:LYS:HB3	3:O:71:PRO:HD2	2.02	0.40
3:F:179:ILE:CG1	3:F:185:GLN:HE21	2.33	0.40
2:H:203:SER:O	2:H:204:VAL:C	2.60	0.40
2:B:113:PRO:O	2:B:114:MET:HB2	2.21	0.40
2:Q:65:ALA:O	2:Q:68:THR:HB	2.22	0.40
2:E:203:SER:O	2:E:204:VAL:C	2.60	0.40
1:J:6:HIS:ND1	1:J:6:HIS:C	2.75	0.40
3:L:118:GLU:CD	3:L:118:GLU:N	2.75	0.40
1:A:394:LEU:HA	1:A:394:LEU:HD23	1.90	0.40
2:K:137:GLY:O	2:K:139:PRO:HD3	2.20	0.40
2:E:250:ARG:HD3	3:F:12:ARG:CG	2.51	0.40
2:N:40:HIS:HD1	2:N:97:ALA:HB1	1.83	0.40
2:K:113:PRO:O	2:K:114:MET:HB3	2.21	0.40
2:E:141:GLU:HA	2:E:142:PRO:HD3	1.77	0.40
2:Q:141:GLU:HA	2:Q:142:PRO:HD3	1.88	0.40
2:H:154:PHE:C	2:H:155:TYR:CD1	2.95	0.40
3:L:100:ASN:HA	3:L:173:ILE:HB	2.03	0.40
2:N:65:ALA:O	2:N:68:THR:HB	2.22	0.40
2:E:197:ALA:C	2:E:199:GLY:H	2.23	0.40
1:P:75:LEU:O	1:P:79:SER:HB3	2.21	0.40
1:J:423:THR:OG1	1:J:426:GLU:HB2	2.22	0.40
1:J:394:LEU:HA	1:J:394:LEU:HD23	1.90	0.40
1:D:414:ILE:HG23	1:D:414:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	D	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
1	G	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	J	426/445 (96%)	407 (96%)	18 (4%)	1 (0%)	52	69
1	M	426/445 (96%)	407 (96%)	19 (4%)	0	100	100
1	P	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
2	B	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	16	23
2	E	254/269 (94%)	231 (91%)	20 (8%)	3 (1%)	16	23
2	H	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	16	23
2	K	254/269 (94%)	231 (91%)	18 (7%)	5 (2%)	9	11
2	N	254/269 (94%)	229 (90%)	20 (8%)	5 (2%)	9	11
2	Q	254/269 (94%)	231 (91%)	21 (8%)	2 (1%)	24	35
3	C	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	30	43
3	F	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	30	43
3	I	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	11	14
3	L	177/187 (95%)	161 (91%)	14 (8%)	2 (1%)	17	25
3	O	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	11	14
3	R	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	30	43
All	All	5142/5406 (95%)	4817 (94%)	292 (6%)	33 (1%)	30	43

All (33) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/366 (96%)	338 (96%)	15 (4%)	36	56
1	D	353/366 (96%)	345 (98%)	8 (2%)	58	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	353/366 (96%)	343 (97%)	10 (3%)	51	72
1	J	353/366 (96%)	342 (97%)	11 (3%)	47	69
1	M	353/366 (96%)	340 (96%)	13 (4%)	41	62
1	P	353/366 (96%)	341 (97%)	12 (3%)	44	65
2	B	203/215 (94%)	191 (94%)	12 (6%)	24	38
2	E	203/215 (94%)	193 (95%)	10 (5%)	31	48
2	H	203/215 (94%)	197 (97%)	6 (3%)	48	70
2	K	203/215 (94%)	192 (95%)	11 (5%)	27	43
2	N	203/215 (94%)	194 (96%)	9 (4%)	35	53
2	Q	203/215 (94%)	193 (95%)	10 (5%)	31	48
3	C	138/144 (96%)	133 (96%)	5 (4%)	42	63
3	F	138/144 (96%)	131 (95%)	7 (5%)	29	46
3	I	138/144 (96%)	132 (96%)	6 (4%)	35	55
3	L	138/144 (96%)	133 (96%)	5 (4%)	42	63
3	O	138/144 (96%)	131 (95%)	7 (5%)	29	46
3	R	138/144 (96%)	133 (96%)	5 (4%)	42	63
All	All	4164/4350 (96%)	4002 (96%)	162 (4%)	39	59

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SMA	A	1001	-	35,38,38	1.89	5 (14%)	40,52,52	1.94	7 (17%)
10	LOP	A	1021	-	43,44,44	0.63	0	44,49,49	1.17	6 (13%)
11	UQ2	A	1101	-	23,23,23	1.48	5 (21%)	28,31,31	1.15	2 (7%)
8	HEM	A	501	1	30,50,50	2.80	10 (33%)	24,82,82	3.19	8 (33%)
8	HEM	A	502	1	30,50,50	2.92	9 (30%)	24,82,82	3.27	8 (33%)
4	BGL	B	1041	-	19,20,20	0.70	0	23,25,25	0.88	1 (4%)
8	HEM	B	301	2	30,50,50	3.12	12 (40%)	24,82,82	3.40	8 (33%)
12	FES	C	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	D	1002	-	35,38,38	1.82	6 (17%)	40,52,52	1.92	9 (22%)
10	LOP	D	1022	-	43,44,44	0.72	0	44,49,49	1.18	4 (9%)
11	UQ2	D	1102	-	23,23,23	1.33	6 (26%)	28,31,31	1.18	3 (10%)
8	HEM	D	501	1	30,50,50	2.69	10 (33%)	24,82,82	3.16	8 (33%)
8	HEM	D	502	1	30,50,50	2.78	12 (40%)	24,82,82	3.30	9 (37%)
4	BGL	E	1042	-	19,20,20	0.69	0	23,25,25	0.95	1 (4%)
8	HEM	E	301	2	30,50,50	2.96	12 (40%)	24,82,82	3.34	8 (33%)
12	FES	F	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	G	1003	-	35,38,38	1.87	5 (14%)	40,52,52	1.82	9 (22%)
10	LOP	G	1023	-	43,44,44	0.72	0	44,49,49	1.17	4 (9%)
4	BGL	G	1043	-	19,20,20	0.88	1 (5%)	23,25,25	0.79	0
11	UQ2	G	1103	-	23,23,23	1.38	5 (21%)	28,31,31	1.07	2 (7%)
8	HEM	G	501	1	30,50,50	2.77	11 (36%)	24,82,82	3.25	8 (33%)
8	HEM	G	502	1	30,50,50	3.11	9 (30%)	24,82,82	3.39	8 (33%)
8	HEM	H	301	2	30,50,50	2.76	10 (33%)	24,82,82	3.40	8 (33%)
12	FES	I	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	J	1004	-	35,38,38	1.80	5 (14%)	40,52,52	1.84	7 (17%)
10	LOP	J	1024	-	43,44,44	0.66	0	44,49,49	1.26	6 (13%)
11	UQ2	J	1104	-	23,23,23	1.23	2 (8%)	28,31,31	1.07	1 (3%)
8	HEM	J	501	1	30,50,50	2.86	11 (36%)	24,82,82	3.32	8 (33%)
8	HEM	J	502	1	30,50,50	3.03	11 (36%)	24,82,82	3.44	8 (33%)
4	BGL	K	1044	-	19,20,20	0.84	1 (5%)	23,25,25	1.07	2 (8%)
8	HEM	K	301	2	30,50,50	2.73	11 (36%)	24,82,82	3.39	8 (33%)
12	FES	L	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	M	1005	-	35,38,38	1.92	5 (14%)	40,52,52	1.88	8 (20%)
10	LOP	M	1025	-	43,44,44	0.69	0	44,49,49	1.15	3 (6%)
11	UQ2	M	1105	-	23,23,23	1.45	5 (21%)	28,31,31	1.15	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	HEM	M	501	1	30,50,50	2.83	12 (40%)	24,82,82	3.25	8 (33%)
8	HEM	M	502	1	30,50,50	2.90	10 (33%)	24,82,82	3.26	8 (33%)
4	BGL	N	1045	-	19,20,20	0.94	1 (5%)	23,25,25	0.78	0
8	HEM	N	301	2	30,50,50	2.98	11 (36%)	24,82,82	3.37	8 (33%)
12	FES	O	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	P	1006	-	35,38,38	1.85	6 (17%)	40,52,52	2.11	11 (27%)
10	LOP	P	1026	-	43,44,44	0.62	0	44,49,49	1.19	5 (11%)
4	BGL	P	1046	-	19,20,20	0.86	0	23,25,25	0.92	1 (4%)
11	UQ2	P	1106	-	23,23,23	1.52	6 (26%)	28,31,31	1.21	4 (14%)
8	HEM	P	501	1	30,50,50	2.74	11 (36%)	24,82,82	3.25	8 (33%)
8	HEM	P	502	1	30,50,50	2.82	11 (36%)	24,82,82	3.19	8 (33%)
8	HEM	Q	301	2	30,50,50	2.93	13 (43%)	24,82,82	3.34	8 (33%)
12	FES	R	200	3	0,4,4	0.00	-	0,4,4	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (260) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	502	HEM	C3B-C4B	-9.05	1.43	1.51
8	J	502	HEM	C3C-CAC	-7.90	1.36	1.51
8	P	502	HEM	C3B-C4B	-7.47	1.45	1.51
8	A	502	HEM	C3B-C4B	-7.29	1.45	1.51
8	B	301	HEM	C3B-C4B	-7.26	1.45	1.51
8	E	301	HEM	C3B-C4B	-7.14	1.45	1.51
8	Q	301	HEM	C3B-C4B	-6.98	1.45	1.51
8	H	301	HEM	C2D-C3D	-6.79	1.34	1.54
8	J	502	HEM	C3B-C4B	-6.76	1.45	1.51
8	B	301	HEM	C2D-C3D	-6.72	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	502	HEM	C3C-CAC	-6.60	1.38	1.51
8	N	301	HEM	C3C-CAC	-6.58	1.39	1.51
8	M	501	HEM	C3B-C4B	-6.53	1.46	1.51
8	D	502	HEM	C2D-C3D	-6.49	1.35	1.54
8	M	502	HEM	C2D-C3D	-6.47	1.35	1.54
8	Q	301	HEM	C2D-C3D	-6.42	1.35	1.54
8	J	502	HEM	C2D-C3D	-6.42	1.35	1.54
8	P	502	HEM	C2D-C3D	-6.40	1.35	1.54
8	A	501	HEM	C2D-C3D	-6.38	1.35	1.54
8	E	301	HEM	C2D-C3D	-6.36	1.35	1.54
8	D	501	HEM	C2D-C3D	-6.34	1.35	1.54
8	M	501	HEM	C2D-C3D	-6.32	1.35	1.54
8	P	501	HEM	C2D-C3D	-6.30	1.35	1.54
8	G	501	HEM	C2D-C3D	-6.30	1.35	1.54
8	M	502	HEM	C3B-C4B	-6.30	1.46	1.51
8	J	501	HEM	C3B-C4B	-6.29	1.46	1.51
8	N	301	HEM	C2D-C3D	-6.28	1.35	1.54
8	J	501	HEM	C2D-C3D	-6.27	1.35	1.54
8	B	301	HEM	C3D-C4D	-6.24	1.43	1.51
8	N	301	HEM	C3B-C4B	-6.22	1.46	1.51
8	A	502	HEM	C2D-C3D	-6.21	1.35	1.54
8	A	501	HEM	C3B-C4B	-6.16	1.46	1.51
8	A	502	HEM	C3B-CAB	-6.13	1.39	1.51
8	G	502	HEM	C2D-C3D	-6.13	1.36	1.54
8	J	501	HEM	C3B-CAB	-6.11	1.39	1.51
8	M	502	HEM	C3B-CAB	-6.08	1.39	1.51
8	B	301	HEM	C3C-CAC	-6.04	1.40	1.51
8	K	301	HEM	C2D-C3D	-6.01	1.36	1.54
8	D	501	HEM	C3B-C4B	-5.96	1.46	1.51
8	A	502	HEM	C3D-C4D	-5.94	1.43	1.51
8	D	502	HEM	C3B-C4B	-5.82	1.46	1.51
8	P	502	HEM	C3C-CAC	-5.74	1.40	1.51
8	H	301	HEM	C3B-C4B	-5.73	1.46	1.51
8	P	501	HEM	C3B-C4B	-5.69	1.46	1.51
8	G	501	HEM	C3B-C4B	-5.69	1.46	1.51
8	A	501	HEM	C3D-C4D	-5.66	1.44	1.51
8	N	301	HEM	C3D-C4D	-5.64	1.44	1.51
8	Q	301	HEM	C3B-CAB	-5.64	1.40	1.51
8	A	501	HEM	C3B-CAB	-5.61	1.40	1.51
8	B	301	HEM	C3B-CAB	-5.56	1.40	1.51
8	D	502	HEM	C3C-CAC	-5.53	1.40	1.51
8	J	502	HEM	C3B-CAB	-5.51	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	301	HEM	C3D-C4D	-5.51	1.44	1.51
8	M	502	HEM	C3D-C4D	-5.51	1.44	1.51
8	M	501	HEM	C3C-CAC	-5.49	1.41	1.51
8	E	301	HEM	C3C-CAC	-5.47	1.41	1.51
8	M	501	HEM	C3B-CAB	-5.45	1.41	1.51
8	Q	301	HEM	C3D-C4D	-5.43	1.44	1.51
8	P	501	HEM	C3C-CAC	-5.31	1.41	1.51
8	M	502	HEM	C3C-CAC	-5.28	1.41	1.51
8	G	501	HEM	C3D-C4D	-5.26	1.44	1.51
8	H	301	HEM	C3C-CAC	-5.25	1.41	1.51
8	G	502	HEM	C3B-CAB	-5.24	1.41	1.51
8	K	301	HEM	C3D-C4D	-5.24	1.44	1.51
8	D	502	HEM	C3B-CAB	-5.23	1.41	1.51
8	D	502	HEM	C3D-C4D	-5.23	1.44	1.51
8	P	501	HEM	C3B-CAB	-5.18	1.41	1.51
8	G	502	HEM	C2C-C1C	-5.16	1.42	1.52
8	J	502	HEM	C3D-C4D	-5.16	1.45	1.51
8	K	301	HEM	C3C-CAC	-5.14	1.41	1.51
8	J	501	HEM	C3C-CAC	-5.08	1.41	1.51
8	K	301	HEM	C3B-C4B	-5.06	1.47	1.51
8	G	501	HEM	C3B-CAB	-5.06	1.41	1.51
8	E	301	HEM	C3B-CAB	-5.05	1.41	1.51
8	G	501	HEM	C3C-CAC	-5.03	1.41	1.51
8	D	501	HEM	C3D-C4D	-4.97	1.45	1.51
8	G	502	HEM	C3D-C4D	-4.96	1.45	1.51
8	H	301	HEM	C3B-CAB	-4.94	1.42	1.51
8	M	501	HEM	C3D-C4D	-4.85	1.45	1.51
8	P	502	HEM	C3B-CAB	-4.82	1.42	1.51
8	D	501	HEM	C3B-CAB	-4.82	1.42	1.51
8	Q	301	HEM	C3C-CAC	-4.79	1.42	1.51
8	J	501	HEM	C3D-C4D	-4.74	1.45	1.51
8	A	502	HEM	C3C-CAC	-4.73	1.42	1.51
8	N	301	HEM	C3B-CAB	-4.68	1.42	1.51
8	N	301	HEM	C2C-C1C	-4.62	1.43	1.52
8	D	501	HEM	C3C-CAC	-4.60	1.42	1.51
8	M	502	HEM	C2C-C1C	-4.49	1.44	1.52
8	K	301	HEM	C3B-CAB	-4.49	1.42	1.51
8	P	501	HEM	C3D-C4D	-4.43	1.45	1.51
8	A	501	HEM	C3C-CAC	-4.33	1.43	1.51
8	J	502	HEM	C2C-C1C	-4.21	1.44	1.52
8	P	502	HEM	C3D-C4D	-4.21	1.46	1.51
8	B	301	HEM	C2C-C1C	-4.12	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	301	HEM	C2C-C1C	-4.01	1.45	1.52
8	H	301	HEM	C3D-C4D	-4.00	1.46	1.51
8	G	501	HEM	C2C-C1C	-3.92	1.45	1.52
8	H	301	HEM	C2C-C1C	-3.91	1.45	1.52
8	A	502	HEM	C2C-C1C	-3.89	1.45	1.52
8	D	501	HEM	C2C-C1C	-3.80	1.45	1.52
8	A	501	HEM	C2C-C1C	-3.77	1.45	1.52
8	P	502	HEM	C2C-C1C	-3.75	1.45	1.52
8	D	502	HEM	C2C-C1C	-3.63	1.45	1.52
8	P	501	HEM	C2C-C1C	-3.55	1.45	1.52
8	Q	301	HEM	C2C-C1C	-3.54	1.45	1.52
8	J	501	HEM	C2C-C1C	-3.53	1.45	1.52
8	M	501	HEM	C2C-C1C	-3.49	1.46	1.52
9	D	1002	SMA	C7-C8	-3.27	1.35	1.40
8	K	301	HEM	C2C-C1C	-3.26	1.46	1.52
9	P	1006	SMA	C7-C8	-2.91	1.36	1.40
8	J	502	HEM	C2D-C1D	-2.76	1.42	1.51
8	D	502	HEM	C2D-C1D	-2.72	1.42	1.51
8	A	501	HEM	C2D-C1D	-2.62	1.43	1.51
8	Q	301	HEM	C2B-C1B	-2.53	1.43	1.51
8	E	301	HEM	C2B-C1B	-2.53	1.43	1.51
8	B	301	HEM	C2B-C1B	-2.51	1.43	1.51
9	J	1004	SMA	C7-C8	-2.50	1.36	1.40
9	G	1003	SMA	C7-C8	-2.47	1.37	1.40
8	D	501	HEM	C2D-C1D	-2.46	1.43	1.51
8	J	501	HEM	C2B-C1B	-2.37	1.44	1.51
8	M	501	HEM	C2B-C1B	-2.33	1.44	1.51
9	M	1005	SMA	C7-C8	-2.30	1.37	1.40
8	Q	301	HEM	C2D-C1D	-2.30	1.44	1.51
8	M	502	HEM	C2D-C1D	-2.28	1.44	1.51
8	B	301	HEM	C2D-C1D	-2.27	1.44	1.51
8	P	502	HEM	C2B-C1B	-2.27	1.44	1.51
8	P	501	HEM	C2B-C1B	-2.26	1.44	1.51
9	A	1001	SMA	C7-C8	-2.26	1.37	1.40
8	K	301	HEM	C2B-C1B	-2.24	1.44	1.51
8	D	501	HEM	C2B-C1B	-2.23	1.44	1.51
8	A	501	HEM	C2B-C1B	-2.23	1.44	1.51
8	M	501	HEM	C2D-C1D	-2.16	1.44	1.51
8	N	301	HEM	C2B-C1B	-2.12	1.44	1.51
8	E	301	HEM	C2D-C1D	-2.10	1.45	1.51
8	Q	301	HEM	CAD-C3D	-2.09	1.49	1.54
8	A	502	HEM	C2D-C1D	-2.09	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	HEM	C2B-C1B	-2.09	1.45	1.51
8	G	501	HEM	C2D-C1D	-2.01	1.45	1.51
4	G	1043	BGL	O5-C1	2.01	1.46	1.43
11	P	1106	UQ2	O2-C2	2.01	1.42	1.37
8	P	502	HEM	C1C-NC	2.04	1.38	1.36
11	D	1102	UQ2	C7-C6	2.05	1.55	1.51
11	M	1105	UQ2	O3-C3	2.05	1.42	1.37
8	E	301	HEM	C4C-NC	2.06	1.38	1.36
11	D	1102	UQ2	O2-C2	2.09	1.42	1.37
11	D	1102	UQ2	C8-C9	2.09	1.37	1.33
8	P	502	HEM	C4C-NC	2.10	1.38	1.36
4	K	1044	BGL	O5-C1	2.11	1.47	1.43
9	P	1006	SMA	O12-C12	2.11	1.48	1.42
9	D	1002	SMA	O12-C12	2.14	1.48	1.42
11	J	1104	UQ2	C6-C5	2.15	1.40	1.35
11	P	1106	UQ2	O3-C3	2.17	1.42	1.37
4	N	1045	BGL	O5-C1	2.20	1.47	1.43
8	B	301	HEM	C4C-NC	2.20	1.38	1.36
8	G	502	HEM	C1C-NC	2.21	1.38	1.36
8	J	502	HEM	C4C-NC	2.22	1.38	1.36
11	P	1106	UQ2	C8-C9	2.22	1.37	1.33
11	G	1103	UQ2	O2-C2	2.25	1.42	1.37
11	A	1101	UQ2	O2-C2	2.25	1.42	1.37
11	G	1103	UQ2	O3-C3	2.27	1.43	1.37
11	D	1102	UQ2	O3-C3	2.31	1.43	1.37
9	D	1002	SMA	O5-C5M	2.32	1.49	1.42
8	D	502	HEM	C4C-NC	2.34	1.38	1.36
8	N	301	HEM	C4C-NC	2.34	1.38	1.36
8	Q	301	HEM	C1C-NC	2.35	1.38	1.36
8	D	502	HEM	C1C-NC	2.36	1.38	1.36
9	A	1001	SMA	O1-C2	2.36	1.38	1.35
9	G	1003	SMA	O8-C8	2.37	1.44	1.35
11	A	1101	UQ2	C7-C6	2.38	1.55	1.51
8	Q	301	HEM	C4C-NC	2.39	1.38	1.36
9	J	1004	SMA	O8-C8	2.39	1.44	1.35
8	G	501	HEM	C4C-NC	2.40	1.39	1.36
9	J	1004	SMA	O1-C2	2.42	1.38	1.35
9	P	1006	SMA	O8-C8	2.43	1.44	1.35
8	J	502	HEM	C1C-NC	2.43	1.39	1.36
11	A	1101	UQ2	C6-C5	2.43	1.41	1.35
8	B	301	HEM	C1C-NC	2.44	1.39	1.36
9	D	1002	SMA	O8-C8	2.44	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	1103	UQ2	C7-C6	2.45	1.55	1.51
8	P	501	HEM	C4C-NC	2.45	1.39	1.36
11	D	1102	UQ2	C6-C5	2.45	1.41	1.35
11	A	1101	UQ2	C8-C9	2.47	1.37	1.33
9	M	1005	SMA	O8-C8	2.48	1.44	1.35
8	K	301	HEM	C4C-NC	2.54	1.39	1.36
11	M	1105	UQ2	C8-C9	2.55	1.38	1.33
11	M	1105	UQ2	C7-C6	2.58	1.56	1.51
8	J	501	HEM	C1C-NC	2.65	1.39	1.36
8	H	301	HEM	C1C-NC	2.65	1.39	1.36
11	M	1105	UQ2	C6-C5	2.66	1.41	1.35
8	M	501	HEM	C1C-NC	2.67	1.39	1.36
8	P	501	HEM	C1C-NC	2.67	1.39	1.36
11	J	1104	UQ2	C7-C8	2.71	1.55	1.50
8	J	501	HEM	C4C-NC	2.71	1.39	1.36
8	M	501	HEM	C4C-NC	2.74	1.39	1.36
8	M	502	HEM	C1C-NC	2.75	1.39	1.36
9	A	1001	SMA	O8-C8	2.77	1.45	1.35
8	H	301	HEM	C4C-NC	2.78	1.39	1.36
11	D	1102	UQ2	C7-C8	2.80	1.55	1.50
8	G	501	HEM	C1C-NC	2.81	1.39	1.36
11	P	1106	UQ2	C6-C5	2.94	1.42	1.35
11	G	1103	UQ2	C6-C5	2.95	1.42	1.35
11	G	1103	UQ2	C7-C8	3.04	1.55	1.50
11	P	1106	UQ2	C7-C8	3.14	1.55	1.50
9	G	1003	SMA	O1-C2	3.19	1.39	1.35
8	E	301	HEM	C1C-NC	3.23	1.40	1.36
9	P	1006	SMA	O1-C2	3.23	1.39	1.35
11	P	1106	UQ2	C7-C6	3.31	1.57	1.51
8	J	502	HEM	CBC-CAC	3.32	1.48	1.29
11	A	1101	UQ2	C7-C8	3.35	1.56	1.50
11	M	1105	UQ2	C7-C8	3.39	1.56	1.50
8	N	301	HEM	C1C-NC	3.62	1.40	1.36
9	M	1005	SMA	O1-C2	3.64	1.39	1.35
8	G	502	HEM	CBC-CAC	3.64	1.50	1.29
8	P	502	HEM	CBC-CAC	3.76	1.51	1.29
8	D	502	HEM	CBC-CAC	3.81	1.51	1.29
8	M	502	HEM	CBB-CAB	3.88	1.51	1.29
8	K	301	HEM	C1C-NC	3.88	1.40	1.36
8	D	502	HEM	CBB-CAB	3.90	1.51	1.29
8	G	502	HEM	CBB-CAB	3.92	1.51	1.29
8	P	501	HEM	CBC-CAC	3.93	1.52	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	501	HEM	CBB-CAB	3.93	1.52	1.29
8	M	501	HEM	CBC-CAC	3.95	1.52	1.29
8	D	501	HEM	CBB-CAB	3.96	1.52	1.29
8	A	502	HEM	CBC-CAC	3.96	1.52	1.29
8	G	501	HEM	CBB-CAB	3.97	1.52	1.29
8	A	502	HEM	CBB-CAB	3.97	1.52	1.29
8	M	502	HEM	CBC-CAC	3.97	1.52	1.29
8	P	501	HEM	CBB-CAB	3.98	1.52	1.29
8	J	501	HEM	CBB-CAB	4.00	1.52	1.29
8	A	501	HEM	CBC-CAC	4.01	1.52	1.29
8	J	501	HEM	CBC-CAC	4.06	1.52	1.29
8	J	502	HEM	CBB-CAB	4.07	1.52	1.29
8	A	501	HEM	CBB-CAB	4.10	1.52	1.29
8	D	501	HEM	CBC-CAC	4.11	1.53	1.29
8	P	502	HEM	CBB-CAB	4.15	1.53	1.29
8	G	501	HEM	CBC-CAC	4.15	1.53	1.29
8	E	301	HEM	CBC-CAC	4.17	1.53	1.29
8	N	301	HEM	CBC-CAC	4.24	1.53	1.29
8	K	301	HEM	CBC-CAC	4.25	1.53	1.29
8	Q	301	HEM	CBC-CAC	4.25	1.53	1.29
8	B	301	HEM	CBB-CAB	4.25	1.53	1.29
8	E	301	HEM	CBB-CAB	4.26	1.53	1.29
8	N	301	HEM	CBB-CAB	4.26	1.53	1.29
8	H	301	HEM	CBC-CAC	4.31	1.54	1.29
8	Q	301	HEM	CBB-CAB	4.31	1.54	1.29
8	B	301	HEM	CBC-CAC	4.34	1.54	1.29
8	H	301	HEM	CBB-CAB	4.36	1.54	1.29
8	K	301	HEM	CBB-CAB	4.47	1.55	1.29
9	D	1002	SMA	O7-C7	5.14	1.45	1.37
9	P	1006	SMA	O7-C7	5.31	1.45	1.37
9	P	1006	SMA	O5-C5	5.38	1.47	1.36
9	M	1005	SMA	O5-C5	5.48	1.47	1.36
9	G	1003	SMA	O7-C7	5.52	1.46	1.37
9	D	1002	SMA	O5-C5	5.80	1.47	1.36
9	J	1004	SMA	O7-C7	5.85	1.46	1.37
9	J	1004	SMA	O5-C5	5.88	1.47	1.36
9	A	1001	SMA	O5-C5	6.14	1.48	1.36
9	G	1003	SMA	O5-C5	6.37	1.48	1.36
9	A	1001	SMA	O7-C7	6.49	1.47	1.37
9	M	1005	SMA	O7-C7	6.63	1.47	1.37

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	502	HEM	C3C-CAC-CBC	-10.52	108.32	124.46
8	G	502	HEM	C3C-CAC-CBC	-9.91	109.25	124.46
8	K	301	HEM	C3B-CAB-CBB	-9.51	109.86	124.46
8	H	301	HEM	C3B-CAB-CBB	-9.51	109.87	124.46
8	E	301	HEM	C3B-CAB-CBB	-9.40	110.04	124.46
8	B	301	HEM	C3B-CAB-CBB	-9.38	110.06	124.46
8	J	501	HEM	C3B-CAB-CBB	-9.32	110.16	124.46
8	D	502	HEM	C3B-CAB-CBB	-9.31	110.17	124.46
8	N	301	HEM	C3C-CAC-CBC	-9.29	110.20	124.46
8	Q	301	HEM	C3B-CAB-CBB	-9.27	110.24	124.46
8	B	301	HEM	C3C-CAC-CBC	-9.22	110.31	124.46
8	A	502	HEM	C3B-CAB-CBB	-9.18	110.38	124.46
8	P	501	HEM	C3C-CAC-CBC	-9.13	110.45	124.46
8	N	301	HEM	C3B-CAB-CBB	-9.12	110.46	124.46
8	K	301	HEM	C3C-CAC-CBC	-9.12	110.47	124.46
8	H	301	HEM	C3C-CAC-CBC	-9.07	110.54	124.46
8	J	501	HEM	C3C-CAC-CBC	-8.99	110.67	124.46
8	E	301	HEM	C3C-CAC-CBC	-8.98	110.68	124.46
8	Q	301	HEM	C3C-CAC-CBC	-8.98	110.68	124.46
8	M	501	HEM	C3B-CAB-CBB	-8.96	110.71	124.46
8	A	502	HEM	C3C-CAC-CBC	-8.95	110.72	124.46
8	M	502	HEM	C3B-CAB-CBB	-8.94	110.74	124.46
8	G	502	HEM	C3B-CAB-CBB	-8.94	110.75	124.46
8	G	501	HEM	C3C-CAC-CBC	-8.89	110.81	124.46
8	M	501	HEM	C3C-CAC-CBC	-8.79	110.98	124.46
8	G	501	HEM	C3B-CAB-CBB	-8.76	111.02	124.46
8	J	502	HEM	C3B-CAB-CBB	-8.69	111.13	124.46
8	P	501	HEM	C3B-CAB-CBB	-8.68	111.14	124.46
8	M	502	HEM	C3C-CAC-CBC	-8.67	111.15	124.46
8	P	502	HEM	C3C-CAC-CBC	-8.67	111.15	124.46
8	A	501	HEM	C3B-CAB-CBB	-8.52	111.39	124.46
8	D	502	HEM	C3C-CAC-CBC	-8.44	111.51	124.46
8	P	502	HEM	C3B-CAB-CBB	-8.42	111.54	124.46
8	D	501	HEM	C3C-CAC-CBC	-8.31	111.70	124.46
8	A	501	HEM	C3C-CAC-CBC	-8.20	111.88	124.46
8	D	501	HEM	C3B-CAB-CBB	-8.17	111.92	124.46
9	J	1004	SMA	C9-C10-C11	-6.36	107.25	114.75
9	D	1002	SMA	C9-C10-C11	-5.33	108.47	114.75
9	A	1001	SMA	C9-C10-C11	-5.21	108.61	114.75
9	M	1005	SMA	C5M-O5-C5	-5.12	110.27	117.77
9	P	1006	SMA	C9-C10-C11	-4.95	108.92	114.75
9	G	1003	SMA	C9-C10-C11	-4.91	108.97	114.75
9	D	1002	SMA	C5M-O5-C5	-4.21	111.61	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	1006	SMA	C5M-O5-C5	-4.09	111.78	117.77
9	J	1004	SMA	C5M-O5-C5	-4.08	111.79	117.77
9	A	1001	SMA	C5M-O5-C5	-3.83	112.16	117.77
9	M	1005	SMA	C9-C10-C11	-3.83	110.24	114.75
9	G	1003	SMA	C5M-O5-C5	-3.73	112.31	117.77
9	A	1001	SMA	O5-C5-C6	-3.72	117.72	123.60
9	D	1002	SMA	C17-C18-C19	-3.11	117.17	126.32
9	D	1002	SMA	O5-C5-C6	-2.95	118.94	123.60
4	K	1044	BGL	C1'-O2-C2	-2.95	106.31	114.40
10	G	1023	LOP	C19-C18-C17	-2.91	99.52	114.53
9	P	1006	SMA	C7M-O7-C7	-2.91	113.14	117.54
9	M	1005	SMA	O5-C5-C6	-2.89	119.02	123.60
10	D	1022	LOP	C27-C26-C25	-2.89	102.69	113.29
10	A	1021	LOP	C19-C18-C17	-2.80	100.09	114.53
9	M	1005	SMA	C7M-O7-C7	-2.78	113.33	117.54
10	P	1026	LOP	C9-C8-C7	-2.74	103.22	113.29
10	P	1026	LOP	C27-C26-C25	-2.70	103.37	113.29
9	M	1005	SMA	C17-C18-C19	-2.69	118.41	126.32
10	G	1023	LOP	C21-C20-C19	-2.65	100.87	114.53
9	D	1002	SMA	C7M-O7-C7	-2.63	113.55	117.54
4	P	1046	BGL	C1'-O2-C2	-2.57	107.34	114.40
9	J	1004	SMA	C7M-O7-C7	-2.57	113.65	117.54
9	G	1003	SMA	C7M-O7-C7	-2.55	113.67	117.54
10	M	1025	LOP	C21-C20-C19	-2.50	101.60	114.53
11	A	1101	UQ2	C7-C8-C9	-2.50	122.46	126.70
9	A	1001	SMA	C7M-O7-C7	-2.50	113.75	117.54
10	M	1025	LOP	C19-C18-C17	-2.49	101.67	114.53
9	P	1006	SMA	O5-C5-C6	-2.47	119.69	123.60
10	D	1022	LOP	C19-C18-C17	-2.46	101.81	114.53
4	E	1042	BGL	C1'-O2-C2	-2.46	107.65	114.40
9	P	1006	SMA	O7-C7-C6	-2.46	120.01	124.21
9	G	1003	SMA	O5-C5-C6	-2.45	119.72	123.60
10	A	1021	LOP	C21-C20-C19	-2.40	102.16	114.53
10	J	1024	LOP	C19-C18-C17	-2.36	102.34	114.53
9	J	1004	SMA	C17-C18-C19	-2.34	119.44	126.32
9	J	1004	SMA	O5-C5-C6	-2.28	119.99	123.60
11	M	1105	UQ2	C7-C8-C9	-2.27	122.84	126.70
11	P	1106	UQ2	C5-C6-C1	-2.25	117.56	120.12
4	K	1044	BGL	C3'-C2'-C1'	-2.25	103.43	113.47
9	A	1001	SMA	C16-C17-C18	-2.22	119.74	124.66
10	A	1021	LOP	C31-C30-C29	-2.21	103.10	114.53
4	B	1041	BGL	C1'-O2-C2	-2.21	108.33	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1021	LOP	C29-C28-C27	-2.19	103.21	114.53
10	J	1024	LOP	C21-C20-C19	-2.18	103.25	114.53
11	D	1102	UQ2	C7-C8-C9	-2.17	123.02	126.70
10	J	1024	LOP	C29-C28-C27	-2.17	103.35	114.53
10	J	1024	LOP	C27-C26-C25	-2.11	105.55	113.29
9	P	1006	SMA	C17-C18-C19	-2.11	120.11	126.32
10	P	1026	LOP	C19-C18-C17	-2.10	103.67	114.53
11	G	1103	UQ2	C7-C8-C9	-2.05	123.22	126.70
11	P	1106	UQ2	C7-C8-C9	-2.03	123.25	126.70
9	G	1003	SMA	C17-C18-C19	-2.03	120.34	126.32
11	D	1102	UQ2	C11-C12-C13	-2.03	106.38	111.69
8	D	502	HEM	CAA-C2A-C1A	-2.01	124.83	127.01
9	D	1002	SMA	C26-C19-C18	2.02	121.46	118.10
10	A	1021	LOP	O6-C24-C25	2.04	118.12	111.90
11	G	1103	UQ2	C10-C9-C11	2.11	118.62	115.41
11	P	1106	UQ2	C8-C7-C6	2.23	118.35	111.64
9	P	1006	SMA	C26-C19-C18	2.26	121.86	118.10
9	G	1003	SMA	C26-C19-C18	2.32	121.96	118.10
10	P	1026	LOP	O6-C24-C25	2.39	119.17	111.90
11	P	1106	UQ2	C10-C9-C11	2.42	119.10	115.41
10	P	1026	LOP	O5-C6-C7	2.43	116.82	111.53
10	D	1022	LOP	O6-C24-C25	2.48	119.46	111.90
9	M	1005	SMA	C14-C15-C16	2.57	131.62	125.66
10	G	1023	LOP	O6-C24-C25	2.59	119.79	111.90
9	D	1002	SMA	C14-C15-C16	2.59	131.68	125.66
11	D	1102	UQ2	C10-C9-C11	2.63	119.43	115.41
9	P	1006	SMA	C13-C14-C15	2.64	118.13	111.79
11	M	1105	UQ2	C10-C9-C11	2.68	119.49	115.41
8	P	501	HEM	CMD-C2D-C3D	2.68	126.20	114.35
8	K	301	HEM	C2D-C3D-C4D	2.69	106.06	101.50
8	G	501	HEM	CMD-C2D-C3D	2.72	126.37	114.35
8	J	501	HEM	CMD-C2D-C3D	2.72	126.38	114.35
8	N	301	HEM	CMD-C2D-C3D	2.73	126.42	114.35
8	D	501	HEM	CMD-C2D-C3D	2.74	126.48	114.35
10	J	1024	LOP	O6-C24-C25	2.75	120.29	111.90
8	G	502	HEM	C2D-C3D-C4D	2.76	106.17	101.50
8	B	301	HEM	CMD-C2D-C3D	2.77	126.59	114.35
11	J	1104	UQ2	C10-C9-C11	2.77	119.64	115.41
8	M	501	HEM	CMD-C2D-C3D	2.78	126.62	114.35
8	M	502	HEM	C2D-C3D-C4D	2.81	106.26	101.50
8	Q	301	HEM	CMD-C2D-C3D	2.81	126.80	114.35
8	J	502	HEM	C2D-C3D-C4D	2.82	106.28	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	501	HEM	CMD-C2D-C3D	2.82	126.83	114.35
8	K	301	HEM	CMD-C2D-C3D	2.83	126.86	114.35
8	E	301	HEM	C2D-C3D-C4D	2.83	106.30	101.50
10	D	1022	LOP	O5-C6-C7	2.84	117.69	111.53
8	P	502	HEM	C2D-C3D-C4D	2.86	106.35	101.50
8	H	301	HEM	CMD-C2D-C3D	2.86	127.02	114.35
8	E	301	HEM	CMD-C2D-C3D	2.87	127.04	114.35
10	M	1025	LOP	O5-C6-C7	2.87	117.77	111.53
8	N	301	HEM	C2D-C3D-C4D	2.88	106.38	101.50
8	H	301	HEM	C2D-C3D-C4D	2.88	106.39	101.50
8	D	502	HEM	CMD-C2D-C3D	2.90	127.16	114.35
8	A	502	HEM	C2D-C3D-C4D	2.90	106.42	101.50
8	M	502	HEM	CMD-C2D-C3D	2.91	127.23	114.35
8	D	502	HEM	C2D-C3D-C4D	2.92	106.46	101.50
8	A	502	HEM	CMD-C2D-C3D	2.94	127.34	114.35
10	G	1023	LOP	O5-C6-C7	2.95	117.93	111.53
8	D	501	HEM	C2D-C3D-C4D	2.96	106.52	101.50
8	P	502	HEM	CMD-C2D-C3D	2.99	127.57	114.35
8	J	502	HEM	CMD-C2D-C3D	2.99	127.58	114.35
10	A	1021	LOP	O5-C6-C7	2.99	118.03	111.53
8	G	502	HEM	CMD-C2D-C3D	2.99	127.59	114.35
8	M	501	HEM	C2D-C3D-C4D	3.06	106.68	101.50
8	G	501	HEM	C2D-C3D-C4D	3.07	106.71	101.50
8	B	301	HEM	C2D-C3D-C4D	3.07	106.71	101.50
11	A	1101	UQ2	C10-C9-C11	3.11	120.15	115.41
8	Q	301	HEM	C2D-C3D-C4D	3.12	106.78	101.50
9	G	1003	SMA	C14-C15-C16	3.19	133.06	125.66
8	A	501	HEM	C2D-C3D-C4D	3.22	106.96	101.50
8	J	501	HEM	C2D-C3D-C4D	3.30	107.09	101.50
8	P	501	HEM	C2D-C3D-C4D	3.38	107.22	101.50
9	P	1006	SMA	O5-C5-C4A	3.51	121.43	115.89
9	J	1004	SMA	O5-C5-C4A	3.57	121.53	115.89
10	J	1024	LOP	O5-C6-C7	3.66	119.49	111.53
8	G	502	HEM	CAD-C3D-C4D	3.77	125.75	112.47
9	G	1003	SMA	O5-C5-C4A	3.77	121.85	115.89
8	P	502	HEM	CMC-C2C-C3C	3.80	126.01	116.53
8	A	502	HEM	CMC-C2C-C3C	3.80	126.01	116.53
8	B	301	HEM	CAD-C3D-C4D	3.86	126.08	112.47
8	A	502	HEM	CMB-C2B-C3B	3.86	126.18	116.53
9	M	1005	SMA	O5-C5-C4A	3.88	122.01	115.89
8	N	301	HEM	CAD-C3D-C4D	3.89	126.19	112.47
8	G	501	HEM	CAD-C3D-C4D	3.90	126.22	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	501	HEM	CAD-C3D-C4D	3.92	126.31	112.47
8	A	502	HEM	CAD-C3D-C4D	3.93	126.33	112.47
8	G	502	HEM	CMC-C2C-C3C	3.93	126.35	116.53
9	D	1002	SMA	O7-C7-C8	3.94	118.43	114.47
9	D	1002	SMA	O5-C5-C4A	3.95	122.12	115.89
8	J	502	HEM	CMC-C2C-C3C	3.96	126.42	116.53
8	A	501	HEM	CAD-C3D-C4D	3.98	126.52	112.47
8	Q	301	HEM	CAD-C3D-C4D	3.99	126.53	112.47
9	G	1003	SMA	O7-C7-C8	4.00	118.49	114.47
8	P	501	HEM	CMC-C2C-C3C	4.01	126.55	116.53
8	G	502	HEM	CMB-C2B-C3B	4.02	126.56	116.53
8	M	502	HEM	CAD-C3D-C4D	4.03	126.67	112.47
8	P	502	HEM	CAD-C3D-C4D	4.06	126.79	112.47
8	P	501	HEM	CAD-C3D-C4D	4.09	126.89	112.47
8	M	501	HEM	CAD-C3D-C4D	4.10	126.94	112.47
9	J	1004	SMA	O7-C7-C8	4.10	118.60	114.47
8	E	301	HEM	CAD-C3D-C4D	4.11	126.98	112.47
8	M	501	HEM	CMC-C2C-C3C	4.12	126.82	116.53
8	J	501	HEM	CMC-C2C-C3C	4.15	126.88	116.53
8	M	501	HEM	CMB-C2B-C3B	4.18	126.97	116.53
8	K	301	HEM	CAD-C3D-C4D	4.18	127.23	112.47
8	J	502	HEM	CAD-C3D-C4D	4.19	127.26	112.47
8	H	301	HEM	CAD-C3D-C4D	4.21	127.31	112.47
8	D	502	HEM	CAD-C3D-C4D	4.21	127.33	112.47
8	D	502	HEM	CMB-C2B-C3B	4.23	127.09	116.53
8	J	501	HEM	CMB-C2B-C3B	4.23	127.09	116.53
8	P	501	HEM	CMB-C2B-C3B	4.25	127.13	116.53
8	Q	301	HEM	CMC-C2C-C3C	4.25	127.15	116.53
9	A	1001	SMA	O5-C5-C4A	4.27	122.63	115.89
8	K	301	HEM	CMC-C2C-C3C	4.27	127.19	116.53
8	M	502	HEM	CMB-C2B-C3B	4.28	127.22	116.53
8	D	501	HEM	CAD-C3D-C2D	4.30	125.59	113.22
8	E	301	HEM	CMB-C2B-C3B	4.31	127.30	116.53
8	E	301	HEM	CMC-C2C-C3C	4.34	127.36	116.53
8	D	502	HEM	CMC-C2C-C3C	4.35	127.40	116.53
9	M	1005	SMA	O7-C7-C8	4.36	118.86	114.47
8	D	501	HEM	CAD-C3D-C4D	4.36	127.86	112.47
8	N	301	HEM	CMB-C2B-C3B	4.37	127.43	116.53
8	J	502	HEM	CMB-C2B-C3B	4.37	127.45	116.53
8	G	501	HEM	CMC-C2C-C3C	4.40	127.50	116.53
8	P	501	HEM	CAD-C3D-C2D	4.40	125.86	113.22
8	H	301	HEM	CMC-C2C-C3C	4.41	127.53	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	501	HEM	CMB-C2B-C3B	4.41	127.53	116.53
8	N	301	HEM	CMC-C2C-C3C	4.44	127.60	116.53
8	B	301	HEM	CMB-C2B-C3B	4.44	127.62	116.53
8	K	301	HEM	CMB-C2B-C3B	4.46	127.66	116.53
8	P	502	HEM	CMB-C2B-C3B	4.47	127.69	116.53
8	Q	301	HEM	CMB-C2B-C3B	4.48	127.71	116.53
8	D	502	HEM	CAD-C3D-C2D	4.52	126.21	113.22
8	B	301	HEM	CMC-C2C-C3C	4.52	127.82	116.53
8	D	501	HEM	CMC-C2C-C3C	4.53	127.83	116.53
8	H	301	HEM	CMB-C2B-C3B	4.54	127.85	116.53
8	M	502	HEM	CMC-C2C-C3C	4.54	127.87	116.53
8	H	301	HEM	CAD-C3D-C2D	4.55	126.29	113.22
8	M	501	HEM	CAD-C3D-C2D	4.56	126.31	113.22
8	J	502	HEM	CAD-C3D-C2D	4.59	126.40	113.22
8	A	501	HEM	CAD-C3D-C2D	4.60	126.44	113.22
8	Q	301	HEM	CAD-C3D-C2D	4.61	126.48	113.22
8	A	501	HEM	CMC-C2C-C3C	4.63	128.10	116.53
8	J	501	HEM	CAD-C3D-C2D	4.66	126.61	113.22
8	E	301	HEM	CAD-C3D-C2D	4.68	126.67	113.22
8	K	301	HEM	CAD-C3D-C2D	4.68	126.67	113.22
8	P	502	HEM	CAD-C3D-C2D	4.71	126.77	113.22
8	A	501	HEM	CMB-C2B-C3B	4.75	128.39	116.53
9	A	1001	SMA	O7-C7-C8	4.79	119.29	114.47
8	G	501	HEM	CAD-C3D-C2D	4.81	127.05	113.22
8	M	502	HEM	CAD-C3D-C2D	4.81	127.06	113.22
8	A	502	HEM	CAD-C3D-C2D	4.84	127.13	113.22
8	B	301	HEM	CAD-C3D-C2D	4.86	127.18	113.22
8	D	501	HEM	CMB-C2B-C3B	4.88	128.71	116.53
8	N	301	HEM	CAD-C3D-C2D	4.89	127.27	113.22
8	G	502	HEM	CAD-C3D-C2D	5.17	128.07	113.22
9	P	1006	SMA	O7-C7-C8	5.21	119.71	114.47
9	P	1006	SMA	C14-C15-C16	5.42	138.23	125.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1021	LOP	6	0
11	A	1101	UQ2	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	501	HEM	3	0
8	A	502	HEM	4	0
4	B	1041	BGL	1	0
8	B	301	HEM	1	0
10	D	1022	LOP	1	0
11	D	1102	UQ2	2	0
8	D	501	HEM	5	0
8	D	502	HEM	3	0
4	E	1042	BGL	3	0
8	E	301	HEM	1	0
10	G	1023	LOP	3	0
4	G	1043	BGL	2	0
11	G	1103	UQ2	3	0
8	G	501	HEM	4	0
8	G	502	HEM	5	0
8	H	301	HEM	1	0
9	J	1004	SMA	1	0
10	J	1024	LOP	1	0
11	J	1104	UQ2	1	0
8	J	501	HEM	9	0
8	J	502	HEM	6	0
4	K	1044	BGL	2	0
8	K	301	HEM	2	0
10	M	1025	LOP	3	0
11	M	1105	UQ2	2	0
8	M	501	HEM	3	0
8	M	502	HEM	5	0
4	N	1045	BGL	1	0
8	N	301	HEM	3	0
9	P	1006	SMA	1	0
10	P	1026	LOP	2	0
4	P	1046	BGL	2	0
11	P	1106	UQ2	4	0
8	P	501	HEM	4	0
8	P	502	HEM	3	0
8	Q	301	HEM	2	0

5.7 Other polymers

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, 95th 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 ²)	Q<0.9
1	A	428/445 (96%)	0.48	11 (2%) 59 58	35, 53, 90, 117	0
1	D	428/445 (96%)	0.40	13 (3%) 54 53	35, 53, 93, 124	0
1	G	428/445 (96%)	0.65	30 (7%) 19 19	35, 56, 100, 124	0
1	J	428/445 (96%)	0.71	35 (8%) 14 14	36, 62, 101, 125	0
1	M	428/445 (96%)	0.77	49 (11%) 7 7	38, 67, 107, 130	0
1	P	428/445 (96%)	0.56	27 (6%) 23 24	35, 56, 100, 127	0
2	B	256/269 (95%)	0.85	33 (12%) 5 5	47, 78, 112, 134	0
2	E	256/269 (95%)	0.99	46 (17%) 2 2	50, 80, 117, 133	0
2	H	256/269 (95%)	0.64	23 (8%) 12 11	40, 72, 113, 135	0
2	K	256/269 (95%)	1.39	65 (25%) 1 1	49, 87, 120, 136	0
2	N	256/269 (95%)	1.81	91 (35%) 0 0	59, 95, 121, 135	0
2	Q	256/269 (95%)	1.23	61 (23%) 1 1	51, 87, 119, 134	0
3	C	179/187 (95%)	0.75	19 (10%) 8 8	37, 59, 101, 139	0
3	F	179/187 (95%)	0.77	29 (16%) 3 2	38, 63, 102, 140	0
3	I	179/187 (95%)	0.61	18 (10%) 9 8	41, 58, 105, 139	0
3	L	179/187 (95%)	0.61	16 (8%) 12 12	37, 59, 104, 139	0
3	O	179/187 (95%)	0.82	23 (12%) 5 5	34, 64, 108, 138	0
3	R	179/187 (95%)	1.17	43 (24%) 1 1	46, 70, 108, 138	0
All	All	5178/5406 (95%)	0.80	632 (12%) 5 5	34, 66, 112, 140	0

All (632) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	9	GLY	18.8
2	Q	2	GLY	18.7
2	E	3	GLY	18.1

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Mol	Chain	Res	Type	RSRZ
3	I	9	GLY	18.1
2	K	3	GLY	16.2
2	E	2	GLY	14.5
2	N	2	GLY	12.5
2	N	3	GLY	12.4
2	K	2	GLY	11.9
3	I	46	ALA	11.5
3	R	9	GLY	11.3
3	F	12	ARG	11.0
2	K	172	ALA	10.6
2	N	1	ALA	10.5
3	O	10	THR	10.3
3	O	9	GLY	10.1
3	O	12	ARG	10.0
3	R	11	ARG	9.9
3	C	10	THR	9.9
3	C	11	ARG	9.7
3	L	12	ARG	9.7
3	O	11	ARG	9.5
2	N	4	GLY	9.4
3	I	10	THR	9.3
3	O	16	TYR	9.2
2	E	1	ALA	9.0
3	C	12	ARG	8.5
2	N	199	GLY	8.5
2	N	109	GLY	8.2
3	O	179	ILE	8.0
2	K	4	GLY	7.9
2	H	1	ALA	7.7
3	L	10	THR	7.7
2	K	169	CYS	7.5
2	K	114	MET	7.4
3	R	10	THR	7.3
2	H	3	GLY	7.3
3	R	179	ILE	7.2
2	N	174	GLY	7.1
3	L	11	ARG	7.1
3	F	179	ILE	7.0
1	M	354	VAL	7.0
1	D	12	ARG	7.0
2	K	145	CYS	6.9
1	J	8	HIS	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	1	ALA	6.9
2	Q	1	ALA	6.6
3	F	9	GLY	6.5
2	N	122	PHE	6.5
2	E	4	GLY	6.5
2	N	6	VAL	6.4
2	K	256	LYS	6.4
2	B	256	LYS	6.3
1	P	12	ARG	6.3
2	K	138	PHE	6.2
2	K	5	HIS	6.2
1	J	5	PRO	6.2
2	H	2	GLY	6.2
1	M	232	THR	6.1
3	F	187	GLY	6.1
3	I	47	LEU	6.0
3	F	10	THR	6.0
3	R	184	ILE	6.0
3	L	14	PHE	5.9
2	B	199	GLY	5.9
2	B	121	LEU	5.9
2	N	178	THR	5.8
2	K	143	PRO	5.8
1	J	7	ASP	5.8
2	K	173	ASN	5.8
3	R	12	ARG	5.7
2	N	173	ASN	5.7
2	Q	255	VAL	5.7
1	M	5	PRO	5.6
2	K	6	VAL	5.6
2	N	172	ALA	5.5
3	L	19	THR	5.5
2	B	4	GLY	5.5
2	E	199	GLY	5.5
3	C	179	ILE	5.5
2	N	110	PHE	5.4
2	N	200	HIS	5.4
1	M	416	LYS	5.4
1	M	417	PRO	5.4
1	M	359	TYR	5.4
2	Q	58	LEU	5.4
1	J	11	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	2	GLY	5.3
2	N	198	ASP	5.3
3	R	13	ASP	5.3
1	J	12	ARG	5.2
2	N	196	TYR	5.2
1	G	12	ARG	5.2
3	F	47	LEU	5.2
3	I	12	ARG	5.2
3	R	52	VAL	5.2
2	N	175	VAL	5.1
1	J	9	TYR	5.1
1	J	10	GLU	5.1
2	N	121	LEU	5.0
2	K	253	ALA	5.0
1	J	348	TRP	5.0
2	Q	7	GLU	5.0
1	M	418	VAL	4.9
1	M	12	ARG	4.9
2	N	201	ASP	4.9
2	K	144	LYS	4.9
2	N	10	PRO	4.9
2	N	77	THR	4.9
1	M	15	ILE	4.9
3	R	47	LEU	4.9
2	Q	5	HIS	4.8
2	K	122	PHE	4.8
2	N	78	GLY	4.8
3	I	179	ILE	4.8
2	N	169	CYS	4.8
3	L	116	LEU	4.8
3	R	14	PHE	4.8
1	J	362	MET	4.8
2	B	146	ALA	4.7
3	C	48	ALA	4.7
3	L	13	ASP	4.7
2	K	124	GLY	4.7
2	K	150	GLU	4.7
3	R	17	TYR	4.7
2	E	200	HIS	4.7
2	K	9	VAL	4.7
1	P	8	HIS	4.6
3	I	17	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
2	Q	147	GLU	4.6
1	J	6	HIS	4.6
3	O	15	LEU	4.6
2	Q	204	VAL	4.6
3	R	187	GLY	4.6
1	J	416	LYS	4.6
3	O	187	GLY	4.5
2	Q	79	GLU	4.5
1	G	18	TRP	4.5
2	N	256	LYS	4.5
2	Q	193	LEU	4.5
2	Q	190	MET	4.5
1	G	15	ILE	4.5
2	N	152	ASP	4.5
2	N	171	ASP	4.5
3	F	54	VAL	4.5
3	O	47	LEU	4.5
2	K	110	PHE	4.5
1	A	416	LYS	4.5
2	K	11	PHE	4.4
3	O	13	ASP	4.4
3	C	47	LEU	4.4
2	Q	152	ASP	4.4
2	Q	9	VAL	4.4
2	N	197	ALA	4.4
2	Q	110	PHE	4.4
2	K	171	ASP	4.4
2	N	149	HIS	4.4
2	Q	194	VAL	4.3
3	F	48	ALA	4.3
2	H	109	GLY	4.3
1	P	6	HIS	4.3
3	I	11	ARG	4.3
3	L	9	GLY	4.3
2	B	200	HIS	4.3
2	Q	196	TYR	4.3
3	F	53	ASP	4.3
2	Q	3	GLY	4.3
2	N	7	GLU	4.3
2	N	123	ASN	4.2
2	K	118	ILE	4.2
2	B	5	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
2	N	202	ALA	4.2
1	P	5	PRO	4.1
3	F	11	ARG	4.1
1	P	4	ILE	4.1
2	K	149	HIS	4.1
3	F	17	TYR	4.1
1	G	416	LYS	4.1
2	E	251	LEU	4.1
2	Q	35	VAL	4.1
2	N	192	ASP	4.1
2	E	7	GLU	4.0
2	N	111	HIS	4.0
1	G	414	ILE	4.0
2	B	151	PRO	4.0
1	M	323	PHE	4.0
2	Q	80	ASP	4.0
3	F	186	LEU	4.0
2	E	140	GLU	4.0
2	N	153	GLY	4.0
2	B	143	PRO	4.0
2	Q	59	PRO	4.0
3	L	181	GLU	3.9
1	P	11	PRO	3.9
3	R	186	LEU	3.9
1	J	311	ASP	3.9
3	R	50	ILE	3.9
3	R	181	GLU	3.9
1	A	12	ARG	3.9
2	N	138	PHE	3.9
1	D	13	THR	3.9
1	G	17	LYS	3.9
3	R	183	THR	3.8
3	L	17	TYR	3.8
2	E	58	LEU	3.8
3	R	51	PHE	3.8
2	B	149	HIS	3.8
2	K	139	PRO	3.8
3	L	15	LEU	3.8
3	O	17	TYR	3.8
3	O	51	PHE	3.8
1	M	8	HIS	3.8
1	G	19	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	P	13	THR	3.7
2	K	10	PRO	3.7
2	B	197	ALA	3.7
2	E	149	HIS	3.7
1	M	365	ILE	3.7
2	E	114	MET	3.7
2	E	5	HIS	3.7
2	K	17	PHE	3.7
3	R	116	LEU	3.7
1	D	5	PRO	3.7
2	K	113	PRO	3.7
1	M	11	PRO	3.7
2	N	255	VAL	3.6
2	K	112	GLY	3.6
3	F	183	THR	3.6
3	O	14	PHE	3.6
2	N	82	GLU	3.6
1	P	7	ASP	3.6
3	I	48	ALA	3.6
3	R	18	ALA	3.6
2	K	141	GLU	3.6
2	B	75	GLU	3.6
2	N	179	ALA	3.6
2	K	59	PRO	3.6
3	R	178	PHE	3.5
3	C	180	ASP	3.5
3	I	45	GLN	3.5
1	M	428	PHE	3.5
2	Q	192	ASP	3.5
3	I	14	PHE	3.5
2	Q	78	GLY	3.5
2	H	79	GLU	3.5
2	Q	191	ASP	3.5
2	Q	145	CYS	3.5
1	D	8	HIS	3.5
1	J	4	ILE	3.5
1	M	234	LYS	3.5
2	B	79	GLU	3.5
2	B	150	GLU	3.5
2	N	125	ILE	3.5
1	G	13	THR	3.4
2	Q	146	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	114	MET	3.4
2	N	151	PRO	3.4
2	E	201	ASP	3.4
1	G	14	GLY	3.4
2	N	58	LEU	3.4
2	B	122	PHE	3.4
2	Q	57	GLU	3.4
1	M	233	SER	3.4
1	M	414	ILE	3.4
2	N	177	THR	3.4
1	P	30	TYR	3.4
2	B	198	ASP	3.4
1	M	362	MET	3.4
2	N	68	THR	3.4
2	Q	256	LYS	3.4
2	K	197	ALA	3.4
1	J	365	ILE	3.4
2	N	66	TYR	3.4
2	N	39	CYS	3.4
2	E	205	HIS	3.3
2	Q	149	HIS	3.3
2	E	10	PRO	3.3
3	O	24	ALA	3.3
2	Q	182	TRP	3.3
1	M	248	PHE	3.3
1	A	414	ILE	3.3
3	R	61	VAL	3.3
3	C	181	GLU	3.3
2	E	190	MET	3.3
2	E	182	TRP	3.3
2	E	256	LYS	3.3
2	H	199	GLY	3.3
3	F	52	VAL	3.3
2	K	7	GLU	3.3
3	C	187	GLY	3.3
2	Q	8	ASP	3.3
1	M	13	THR	3.3
3	O	183	THR	3.3
2	K	175	VAL	3.2
2	N	79	GLU	3.2
2	K	146	ALA	3.2
2	Q	11	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	256	LYS	3.2
3	F	181	GLU	3.2
1	D	292	ILE	3.2
2	N	139	PRO	3.2
1	M	249	ILE	3.2
2	E	141	GLU	3.2
1	G	9	TYR	3.2
2	B	3	GLY	3.2
2	K	199	GLY	3.2
3	F	51	PHE	3.2
1	M	358	ARG	3.2
2	K	148	GLY	3.2
2	N	72	VAL	3.2
3	I	187	GLY	3.2
2	K	190	MET	3.2
2	E	193	LEU	3.1
2	K	142	PRO	3.1
2	Q	4	GLY	3.1
2	K	120	GLN	3.1
2	N	246	LEU	3.1
1	J	414	ILE	3.1
3	R	19	THR	3.1
1	J	428	PHE	3.1
2	K	147	GLU	3.1
2	Q	200	HIS	3.1
1	D	7	ASP	3.1
2	E	8	ASP	3.1
1	M	242	VAL	3.1
2	N	155	TYR	3.1
2	Q	189	LEU	3.1
3	C	183	THR	3.1
2	H	251	LEU	3.0
1	G	10	GLU	3.0
2	H	75	GLU	3.0
2	Q	6	VAL	3.0
1	G	417	PRO	3.0
3	R	15	LEU	3.0
2	E	206	ALA	3.0
2	Q	143	PRO	3.0
3	C	13	ASP	3.0
2	N	9	VAL	3.0
3	I	13	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	N	245	TYR	3.0
2	N	195	GLU	3.0
2	N	166	PRO	3.0
1	M	411	LEU	3.0
2	Q	94	LEU	3.0
1	M	415	GLU	3.0
1	G	30	TYR	3.0
1	G	247	TYR	3.0
1	D	290	ALA	3.0
2	E	255	VAL	3.0
2	Q	56	PRO	3.0
1	G	413	ALA	3.0
2	N	80	ASP	3.0
2	N	150	GLU	3.0
2	N	249	LYS	2.9
2	Q	153	GLY	2.9
1	M	419	ALA	2.9
1	P	239	LYS	2.9
2	H	72	VAL	2.9
2	N	75	GLU	2.9
1	G	11	PRO	2.9
3	C	104	ASP	2.9
1	P	14	GLY	2.9
2	E	151	PRO	2.8
2	E	110	PHE	2.8
1	D	413	ALA	2.8
2	Q	188	PRO	2.8
2	K	231	PHE	2.8
2	E	252	TRP	2.8
1	M	6	HIS	2.8
2	N	100	LEU	2.8
2	E	122	PHE	2.8
3	L	187	GLY	2.8
1	M	348	TRP	2.8
2	Q	96	ASN	2.8
3	R	58	GLU	2.8
1	J	30	TYR	2.8
3	C	16	TYR	2.8
1	M	14	GLY	2.8
1	M	412	GLY	2.8
2	K	119	SER	2.8
2	K	182	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
2	Q	199	GLY	2.7
3	F	182	THR	2.7
1	G	7	ASP	2.7
3	O	180	ASP	2.7
2	N	124	GLY	2.7
1	A	13	THR	2.7
2	H	82	GLU	2.7
2	N	119	SER	2.7
3	F	184	ILE	2.7
3	L	47	LEU	2.7
2	E	18	GLY	2.7
2	N	114	MET	2.7
1	A	76	ALA	2.7
1	J	123	ALA	2.7
3	C	103	ILE	2.7
2	B	76	GLU	2.7
2	B	110	PHE	2.7
2	N	11	PHE	2.7
3	F	14	PHE	2.7
1	J	27	ALA	2.7
1	M	413	ALA	2.7
1	P	10	GLU	2.7
2	Q	202	ALA	2.7
3	R	180	ASP	2.6
3	O	181	GLU	2.6
1	G	412	GLY	2.6
2	K	1	ALA	2.6
3	O	48	ALA	2.6
3	F	13	ASP	2.6
3	R	82	ILE	2.6
1	J	361	PRO	2.6
2	E	16	PRO	2.6
2	Q	12	SER	2.6
1	J	237	ALA	2.6
2	Q	140	GLU	2.6
3	I	57	VAL	2.6
3	R	65	VAL	2.6
3	F	55	SER	2.6
3	R	57	VAL	2.6
1	P	9	TYR	2.6
2	N	5	HIS	2.6
1	J	124	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	19	LEU	2.6
2	N	61	ASP	2.6
3	R	103	ILE	2.6
2	E	147	GLU	2.6
2	Q	18	GLY	2.6
2	K	58	LEU	2.6
2	K	255	VAL	2.5
3	R	56	SER	2.5
2	N	251	LEU	2.5
1	J	323	PHE	2.5
1	M	387	PHE	2.5
2	K	20	PHE	2.5
2	E	9	VAL	2.5
2	Q	61	ASP	2.5
3	F	57	VAL	2.5
2	N	113	PRO	2.5
3	C	178	PHE	2.5
2	H	250	ARG	2.5
2	K	251	LEU	2.5
2	N	94	LEU	2.5
2	Q	158	ARG	2.5
1	J	172	ILE	2.5
1	J	244	PHE	2.5
1	P	428	PHE	2.5
3	R	177	LYS	2.5
2	N	35	VAL	2.5
1	P	22	ARG	2.5
2	Q	141	GLU	2.5
2	Q	243	LEU	2.5
1	G	232	THR	2.5
1	M	18	TRP	2.5
2	B	139	PRO	2.5
2	K	183	ILE	2.5
3	F	50	ILE	2.5
1	M	9	TYR	2.5
2	K	117	GLY	2.5
2	Q	75	GLU	2.5
3	R	79	GLU	2.5
1	P	293	VAL	2.5
2	N	207	MET	2.5
2	K	252	TRP	2.4
2	E	253	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	236	PHE	2.4
2	N	20	PHE	2.4
2	E	145	CYS	2.4
2	H	145	CYS	2.4
2	B	64	ARG	2.4
3	O	57	VAL	2.4
1	P	348	TRP	2.4
3	L	186	LEU	2.4
2	K	168	THR	2.4
3	F	180	ASP	2.4
3	O	54	VAL	2.4
1	M	237	ALA	2.4
2	K	8	ASP	2.4
2	Q	150	GLU	2.4
1	G	294	PRO	2.4
2	K	177	THR	2.4
2	N	62	GLN	2.4
2	N	65	ALA	2.4
3	F	176	ALA	2.4
2	K	245	TYR	2.4
1	M	197	LEU	2.4
3	C	14	PHE	2.4
2	N	168	THR	2.4
1	M	325	ILE	2.4
1	P	15	ILE	2.4
2	E	146	ALA	2.4
2	K	123	ASN	2.3
2	N	143	PRO	2.3
1	G	22	ARG	2.3
2	H	231	PHE	2.3
2	B	178	THR	2.3
2	N	73	THR	2.3
2	E	208	ALA	2.3
2	B	174	GLY	2.3
2	N	112	GLY	2.3
3	R	120	GLY	2.3
2	Q	132	TYR	2.3
2	N	135	LEU	2.3
2	H	205	HIS	2.3
1	A	15	ILE	2.3
1	A	5	PRO	2.3
1	G	3	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	R	105	ALA	2.3
2	N	76	GLU	2.3
3	L	51	PHE	2.3
3	R	122	TRP	2.3
2	H	71	THR	2.3
1	A	150	PRO	2.3
1	M	7	ASP	2.3
1	P	16	GLU	2.3
2	N	183	ILE	2.3
2	Q	206	ALA	2.3
3	F	116	LEU	2.3
2	Q	77	THR	2.3
3	I	181	GLU	2.3
2	B	78	GLY	2.3
2	B	69	GLN	2.3
2	K	155	TYR	2.3
2	K	200	HIS	2.3
2	E	254	GLY	2.3
2	H	80	ASP	2.3
1	J	170	PRO	2.3
1	G	428	PHE	2.3
2	Q	22	GLN	2.3
2	N	191	ASP	2.3
3	L	16	TYR	2.3
3	R	139	GLY	2.3
1	D	293	VAL	2.3
2	N	187	PRO	2.3
1	A	141	ALA	2.2
1	M	292	ILE	2.2
2	N	93	ALA	2.2
2	K	109	GLY	2.2
2	N	137	GLY	2.2
1	M	251	LYS	2.2
3	F	56	SER	2.2
2	B	201	ASP	2.2
1	G	146	GLY	2.2
2	N	117	GLY	2.2
2	E	150	GLU	2.2
3	C	176	ALA	2.2
3	F	119	ALA	2.2
1	P	18	TRP	2.2
3	R	137	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	427	ASP	2.2
2	H	111	HIS	2.2
1	J	100	GLY	2.2
3	C	186	LEU	2.2
2	Q	19	THR	2.2
2	K	196	TYR	2.2
1	M	43	TRP	2.2
1	P	43	TRP	2.2
2	Q	203	SER	2.2
1	D	150	PRO	2.2
2	E	192	ASP	2.2
2	K	198	ASP	2.2
3	R	16	TYR	2.2
3	O	177	LYS	2.2
2	B	166	PRO	2.2
2	N	8	ASP	2.2
1	G	233	SER	2.2
2	N	254	GLY	2.2
2	Q	26	GLN	2.2
1	J	18	TRP	2.2
2	H	77	THR	2.2
1	G	235	ALA	2.1
2	H	4	GLY	2.1
2	B	224	MET	2.1
1	G	70	THR	2.1
1	D	6	HIS	2.1
3	R	185	GLN	2.1
1	P	27	ALA	2.1
3	I	105	ALA	2.1
2	E	207	MET	2.1
1	J	15	ILE	2.1
2	E	152	ASP	2.1
2	E	209	GLU	2.1
2	N	157	ASN	2.1
2	K	151	PRO	2.1
1	A	354	VAL	2.1
1	M	311	ASP	2.1
3	R	53	ASP	2.1
1	J	19	LEU	2.1
1	P	57	LEU	2.1
3	F	178	PHE	2.1
1	P	62	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	290	ALA	2.1
3	R	54	VAL	2.1
1	J	13	THR	2.1
2	E	54	GLY	2.1
2	H	147	GLU	2.1
2	K	76	GLU	2.1
1	M	172	ILE	2.1
2	E	132	TYR	2.1
1	D	387	PHE	2.1
1	M	324	GLY	2.1
1	P	275	GLY	2.1
2	B	147	GLU	2.1
3	O	58	GLU	2.1
2	B	152	ASP	2.1
1	M	410	ILE	2.1
1	A	16	GLU	2.1
1	J	202	PRO	2.1
1	J	43	TRP	2.0
1	G	150	PRO	2.0
2	E	66	TYR	2.0
2	Q	17	PHE	2.0
2	Q	246	LEU	2.0
2	N	22	GLN	2.0
3	I	83	GLU	2.0
2	N	144	LYS	2.0
3	I	177	LYS	2.0
2	N	23	HIS	2.0
1	D	15	ILE	2.0
1	J	294	PRO	2.0
2	B	77	THR	2.0
3	O	178	PHE	2.0
3	R	148	PHE	2.0
2	H	76	GLU	2.0
3	R	100	ASN	2.0
1	G	76	ALA	2.0
1	G	430	ALA	2.0
1	P	64	VAL	2.0
1	M	420	PRO	2.0
1	P	33	ILE	2.0
1	M	349	LEU	2.0
2	E	20	PHE	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, 95th 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(\AA^2)	Q<0.9
11	UQ2	A	1101	23/23	0.66	0.42	11.67	102,105,108,109	0
11	UQ2	D	1102	23/23	0.64	0.37	7.62	92,98,107,107	0
11	UQ2	G	1103	23/23	0.69	0.38	6.84	109,116,117,118	0
11	UQ2	M	1105	23/23	0.64	0.44	6.23	112,123,125,125	0
11	UQ2	J	1104	23/23	0.53	0.49	5.86	107,115,116,117	0
10	LOP	J	1024	45/45	0.82	0.36	5.73	93,113,125,126	0
11	UQ2	P	1106	23/23	0.70	0.32	3.73	101,104,107,108	0
10	LOP	P	1026	45/45	0.83	0.28	2.87	69,95,99,100	0
10	LOP	G	1023	45/45	0.77	0.27	2.84	88,102,112,113	0
10	LOP	D	1022	45/45	0.87	0.25	2.34	63,88,98,102	0
4	BGL	G	1043	20/20	0.78	0.27	1.75	89,91,101,101	0
10	LOP	M	1025	45/45	0.80	0.28	1.55	89,114,123,123	0
10	LOP	A	1021	45/45	0.89	0.22	1.50	72,86,94,99	0
12	FES	L	200	4/4	0.99	0.20	1.32	40,41,41,42	0
4	BGL	P	1046	20/20	0.88	0.26	1.29	87,93,95,95	0
9	SMA	J	1004	37/37	0.95	0.24	1.12	40,49,79,85	0
8	HEM	A	502	43/43	0.98	0.25	1.11	32,37,49,49	0
8	HEM	B	301	43/43	0.95	0.20	0.79	51,56,70,73	0
9	SMA	P	1006	37/37	0.95	0.21	0.76	34,45,76,77	0
9	SMA	D	1002	37/37	0.94	0.22	0.73	39,44,76,78	0
8	HEM	P	502	43/43	0.98	0.24	0.73	35,40,49,53	0
8	HEM	G	502	43/43	0.98	0.23	0.68	32,36,45,49	0
4	BGL	B	1041	20/20	0.80	0.23	0.50	87,97,101,102	0
9	SMA	G	1003	37/37	0.96	0.22	0.48	35,43,60,65	0
8	HEM	J	502	43/43	0.98	0.22	0.48	37,41,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	HEM	H	301	43/43	0.96	0.17	0.41	33,42,47,50	0
4	BGL	N	1045	20/20	0.71	0.31	0.40	107,111,113,114	0
8	HEM	D	502	43/43	0.97	0.22	0.38	32,37,49,58	0
4	BGL	E	1042	20/20	0.90	0.20	0.37	80,85,102,102	0
12	FES	F	200	4/4	0.99	0.18	0.36	43,43,44,45	0
9	SMA	M	1005	37/37	0.96	0.20	0.36	56,66,73,73	0
8	HEM	M	502	43/43	0.98	0.21	0.29	47,49,59,63	0
8	HEM	J	501	43/43	0.95	0.18	0.26	67,75,79,81	0
8	HEM	M	501	43/43	0.97	0.17	0.23	63,69,75,78	0
12	FES	O	200	4/4	0.98	0.18	0.17	42,43,43,43	0
12	FES	C	200	4/4	0.99	0.18	0.12	41,42,42,43	0
9	SMA	A	1001	37/37	0.95	0.21	0.11	38,47,54,56	0
6	CL	I	2004	1/1	0.93	0.16	0.10	67,67,67,67	0
8	HEM	A	501	43/43	0.98	0.18	0.01	43,47,51,53	0
8	HEM	G	501	43/43	0.97	0.17	-0.03	50,59,62,62	0
8	HEM	E	301	43/43	0.96	0.17	-0.07	53,62,73,76	0
8	HEM	D	501	43/43	0.97	0.15	-0.09	40,48,53,55	0
8	HEM	K	301	43/43	0.96	0.17	-0.20	49,55,67,69	0
4	BGL	K	1044	20/20	0.86	0.20	-0.25	95,99,101,101	0
8	HEM	N	301	43/43	0.94	0.20	-0.26	65,72,79,84	0
8	HEM	P	501	43/43	0.98	0.16	-0.42	48,54,57,57	0
12	FES	I	200	4/4	0.97	0.17	-0.49	47,48,48,48	0
12	FES	R	200	4/4	0.98	0.15	-0.60	55,57,58,58	0
8	HEM	Q	301	43/43	0.96	0.15	-0.83	56,65,73,78	0
6	CL	R	2005	1/1	0.94	0.09	-1.46	67,67,67,67	0
7	NA	R	2001	1/1	0.95	0.10	-1.46	62,62,62,62	0
5	SR	H	1013	1/1	0.89	0.08	-2.18	113,113,113,113	0
5	SR	Q	1016	1/1	0.70	0.08	-2.60	137,137,137,137	0
5	SR	E	1012	1/1	0.79	0.04	-2.65	138,138,138,138	0
5	SR	B	1011	1/1	0.79	0.04	-2.66	132,132,132,132	0
5	SR	K	1014	1/1	0.77	0.11	-2.92	145,145,145,145	0
5	SR	N	1015	1/1	0.94	0.06	-4.08	153,153,153,153	0
5	SR	G	1018	1/1	0.80	0.19	-	98,98,98,98	0
5	SR	M	1019	1/1	0.85	0.08	-	154,154,154,154	0
5	SR	A	1017	1/1	0.94	0.17	-	114,114,114,114	0

6.5 Other polymers

There are no such residues in this entry.