



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 07:52 PM EDT

PDB ID : 3Q08  
Title : Crystal Structure of Chlorite Dismutase from *D. Aromatica* at pH 6.5  
Authors : Goblirsch, B.R.; Wilmot, C.M.  
Deposited on : unknown  
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

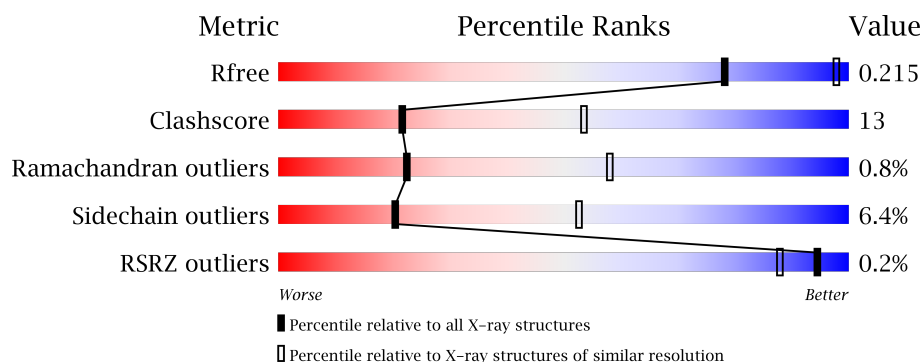
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	248	
1	B	248	
1	C	248	
1	D	248	
1	E	248	

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Mol	Chain	Length	Quality of chain
1	F	248	 71%24% . .
1	G	248	 71%24% . .
1	H	248	 74%20% . .
1	I	248	 71%25% . .
1	J	248	 70%23% . .
1	K	248	 75%20% . .
1	L	248	 72%21% . .
1	M	248	 72%23% . .
1	N	248	 69%25% . .
1	O	248	 76%20% . .
1	P	248	 72%24% . .
1	Q	248	 69%25% . .
1	R	248	 75%20% . .
1	S	248	 70%25% . .
1	T	248	 66%29% . .

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
2	HEM	G	1000	-	-	-	X
3	NO2	A	2000	-	-	-	X
3	NO2	B	2000	-	-	-	X
3	NO2	K	2000	-	-	-	X
3	NO2	M	2000	-	-	-	X
3	NO2	R	2000	-	-	-	X
4	MES	A	2001	-	-	-	X
4	MES	B	2001	-	-	-	X
4	MES	F	2001	-	-	-	X
4	MES	G	2001	-	-	-	X
4	MES	H	2001	-	-	-	X
4	MES	M	2001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MES	N	2001	-	-	-	X
4	MES	O	2001	-	-	-	X
4	MES	P	2001	-	-	-	X
4	MES	Q	2001	-	-	-	X
4	MES	S	2001	-	-	-	X
4	MES	T	2001	-	-	-	X
5	CA	M	1001	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39760 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 Chlorite dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	B	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	C	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	D	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	E	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	F	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	G	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	H	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	I	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	J	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	K	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	L	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	M	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	N	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	O	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			
1	P	241	Total	C	N	O	S	0	0	0
			1928	1239	325	359	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	241	Total 1928	C 1239	N 325	O 359	S 5	0	0	0
1	R	241	Total 1928	C 1239	N 325	O 359	S 5	0	0	0
1	S	241	Total 1928	C 1239	N 325	O 359	S 5	0	0	0
1	T	241	Total 1928	C 1239	N 325	O 359	S 5	0	0	0

- # HEM

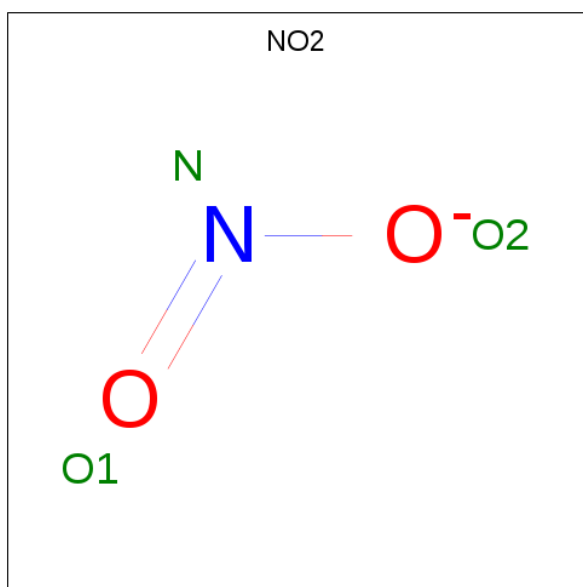
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			3	1	2		
3	B	1	Total	N	O	0	0
			3	1	2		
3	C	1	Total	N	O	0	0
			3	1	2		
3	D	1	Total	N	O	0	0
			3	1	2		
3	E	1	Total	N	O	0	0
			3	1	2		
3	F	1	Total	N	O	0	0
			3	1	2		
3	G	1	Total	N	O	0	0
			3	1	2		
3	H	1	Total	N	O	0	0
			3	1	2		
3	I	1	Total	N	O	0	0
			3	1	2		
3	J	1	Total	N	O	0	0
			3	1	2		
3	K	1	Total	N	O	0	0
			3	1	2		
3	L	1	Total	N	O	0	0
			3	1	2		
3	M	1	Total	N	O	0	0
			3	1	2		
3	N	1	Total	N	O	0	0
			3	1	2		

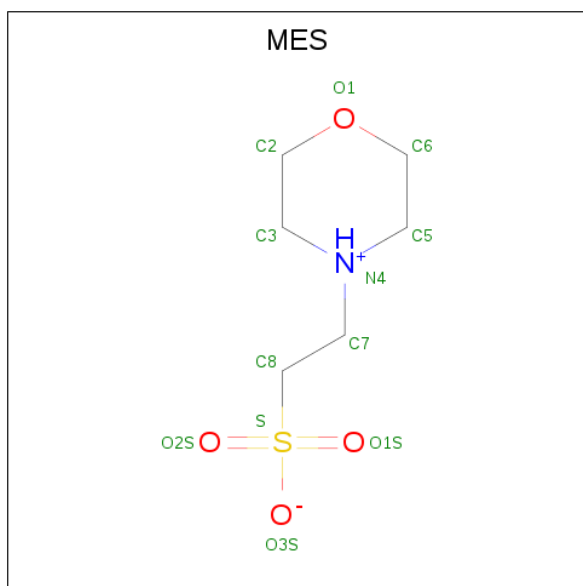
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	N	O	0	0
			3	1	2		
3	P	1	Total	N	O	0	0
			3	1	2		
3	Q	1	Total	N	O	0	0
			3	1	2		
3	R	1	Total	N	O	0	0
			3	1	2		
3	S	1	Total	N	O	0	0
			3	1	2		
3	T	1	Total	N	O	0	0
			3	1	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	L	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	N	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	O	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	P	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	Q	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	R	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	S	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	T	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Ca	0	0
			1	1		
5	G	1	Total	Ca	0	0
			1	1		
5	J	1	Total	Ca	0	0
			1	1		
5	Q	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Ca 1 1	0	0
5	K	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0
5	H	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	I	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0
5	T	1	Total Ca 1 1	0	0
5	N	1	Total Ca 1 1	0	0
5	O	1	Total Ca 1 1	0	0
5	R	1	Total Ca 1 1	0	0
5	L	1	Total Ca 1 1	0	0
5	S	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0
5	M	1	Total Ca 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0

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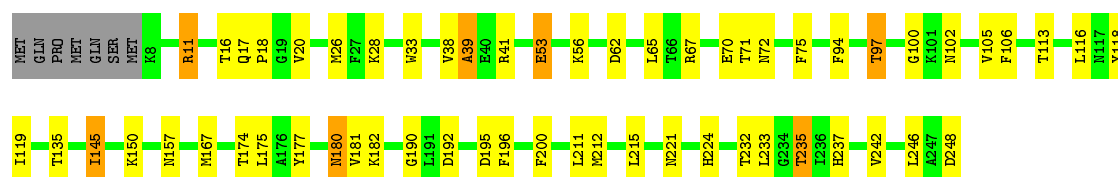
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0
6	F	1	Total O 1 1	0	0
6	G	1	Total O 1 1	0	0
6	H	1	Total O 1 1	0	0
6	I	1	Total O 1 1	0	0
6	J	1	Total O 1 1	0	0
6	K	1	Total O 1 1	0	0
6	L	1	Total O 1 1	0	0
6	M	1	Total O 1 1	0	0
6	N	1	Total O 1 1	0	0
6	O	1	Total O 1 1	0	0
6	P	1	Total O 1 1	0	0
6	Q	1	Total O 1 1	0	0
6	R	1	Total O 1 1	0	0
6	S	1	Total O 1 1	0	0
6	T	1	Total O 1 1	0	0



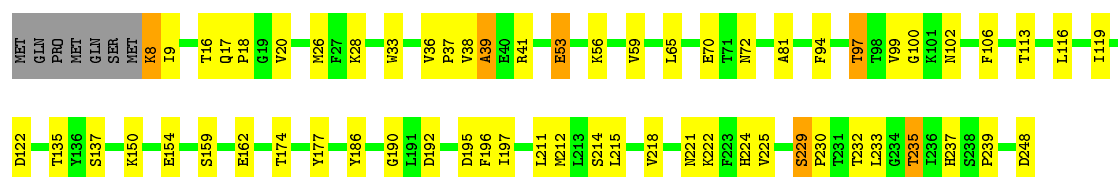
- Molecule 1: Chlorite dismutase





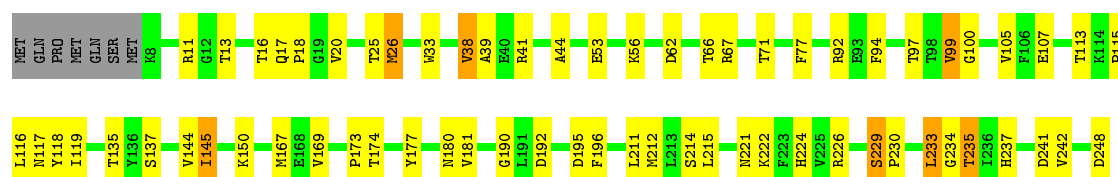
- Molecule 1: Chlorite dismutase

Chain E: 72% 23%



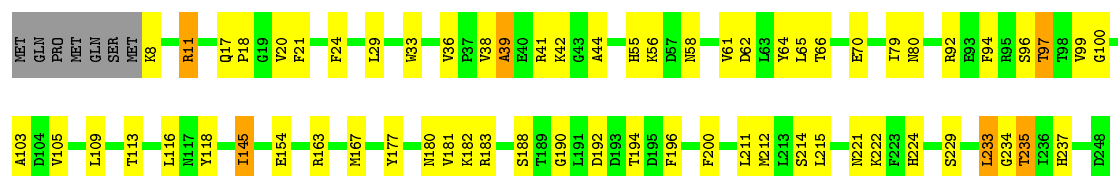
- Molecule 1: Chlorite dismutase

Chain F: 71% 24%



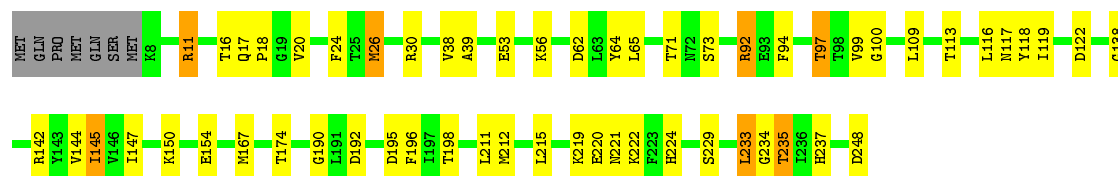
- Molecule 1: Chlorite dismutase

Chain G: 71% 24%



- Molecule 1: Chlorite dismutase

Chain H: 74% 20%



- Molecule 1: Chlorite dismutase

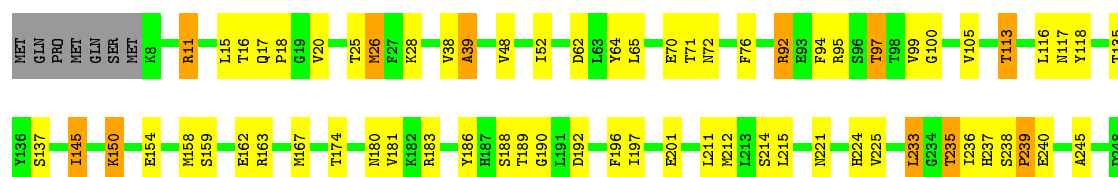
Chain I: 71% 25%





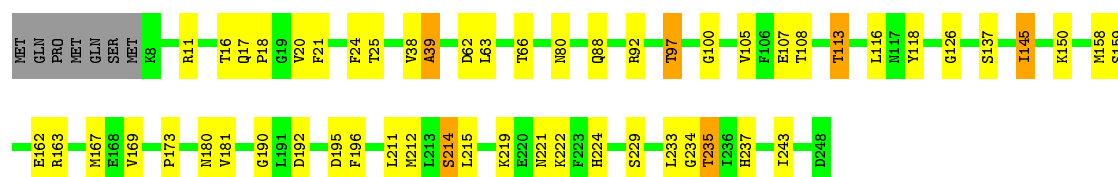
- Molecule 1: Chlorite dismutase

Chain J: 70% 23%



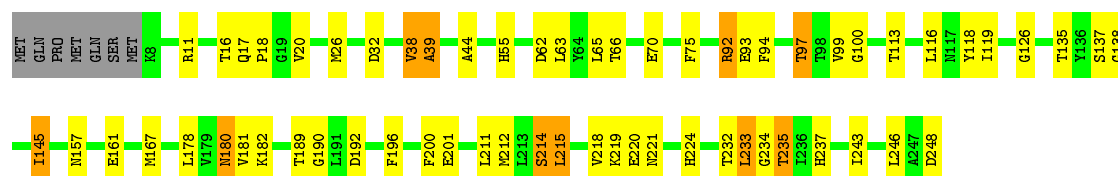
- Molecule 1: Chlorite dismutase

Chain K: 75% 20%



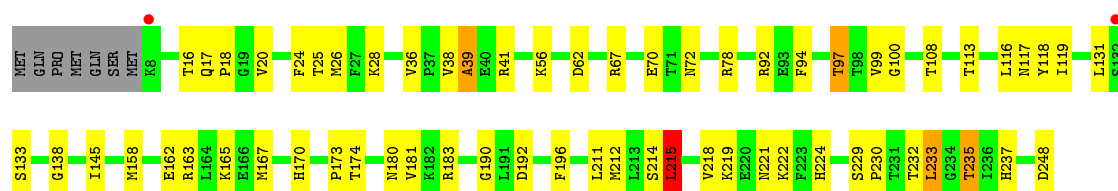
- Molecule 1: Chlorite dismutase

Chain L: 72% 21%



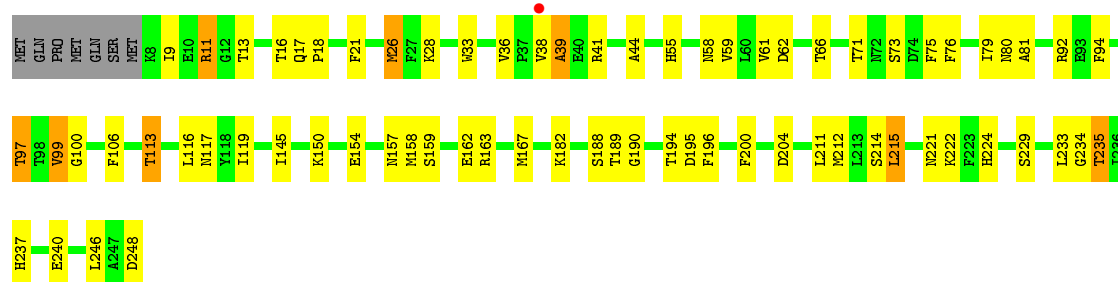
- Molecule 1: Chlorite dismutase

Chain M: 72% 23%



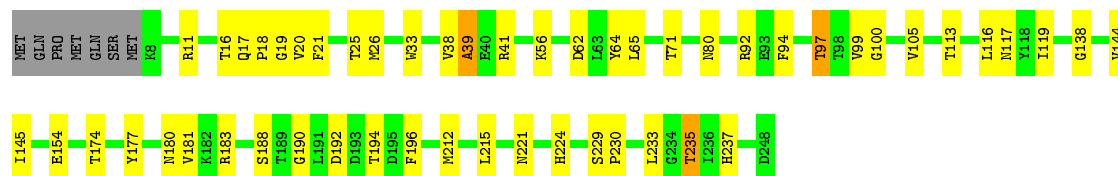
- Molecule 1: Chlorite dismutase

Chain N: 69% 25%



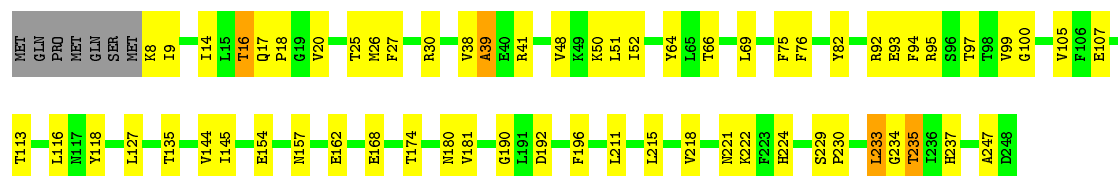
- Molecule 1: Chlorite dismutase

Chain O: 76% 20% 2%



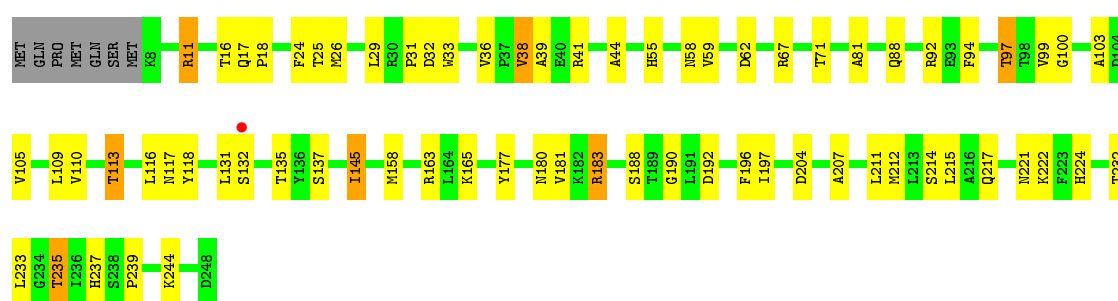
- Molecule 1: Chlorite dismutase

Chain P: 72% 24% 2%



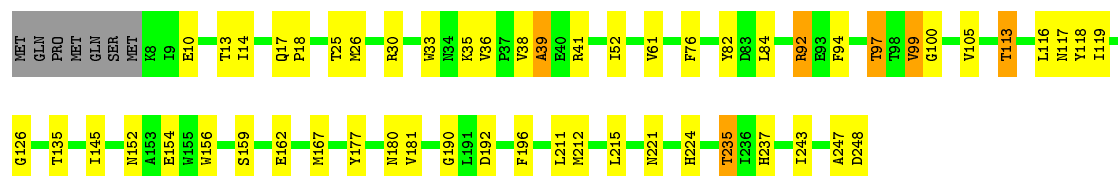
- Molecule 1: Chlorite dismutase

Chain Q: 69% 25% 6%



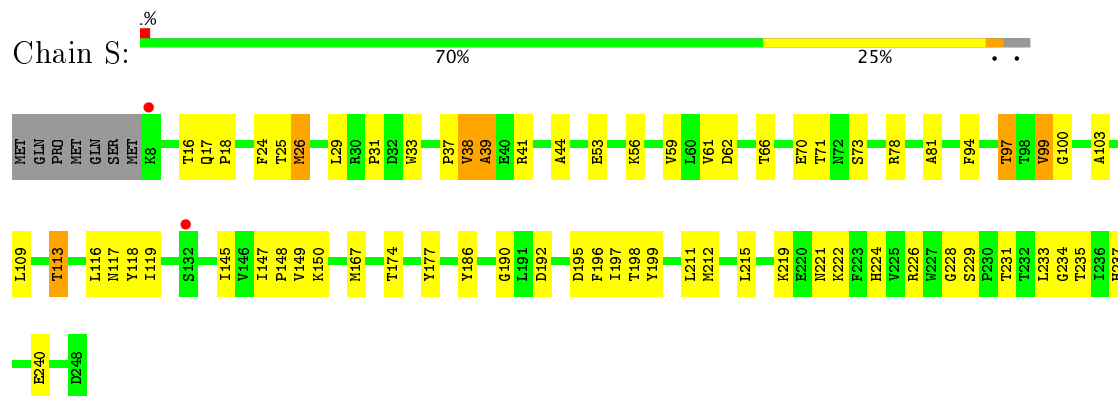
- Molecule 1: Chlorite dismutase

Chain R: 75% 20% 5%

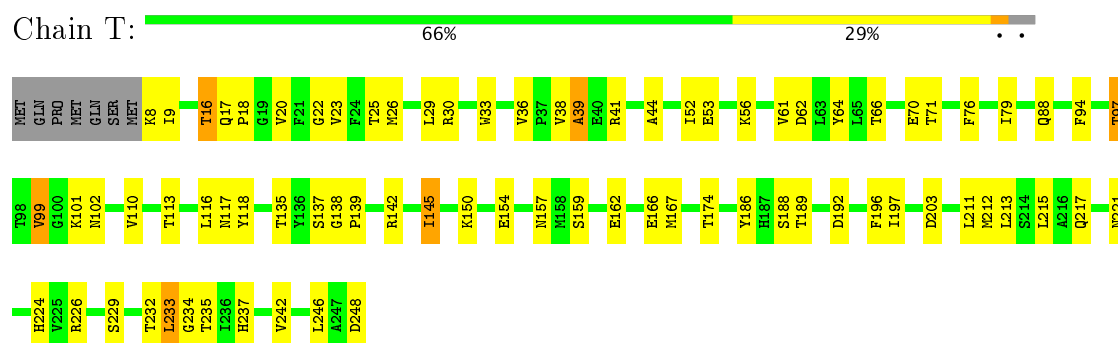




- Molecule 1: Chlorite dismutase



- Molecule 1: Chlorite dismutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.70 Å   202.85 Å   247.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	46.91 – 3.05 46.91 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.91-3.05) 98.0 (46.91-3.04)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.65 (at 3.06 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.178   ,   0.221 0.175   ,   0.215	Depositor DCC
$R_{free}$ test set	5827 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 15.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	39760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CA, MES, NO2

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	0.90	3/1973 (0.2%)	0.91	3/2676 (0.1%)
1	B	0.91	2/1973 (0.1%)	0.89	2/2676 (0.1%)
1	C	0.88	0/1973	0.87	2/2676 (0.1%)
1	D	0.86	1/1973 (0.1%)	0.87	0/2676
1	E	0.90	0/1973	0.90	1/2676 (0.0%)
1	F	0.75	0/1973	0.82	1/2676 (0.0%)
1	G	0.81	0/1973	0.83	2/2676 (0.1%)
1	H	0.83	0/1973	0.87	3/2676 (0.1%)
1	I	0.85	1/1973 (0.1%)	0.88	0/2676
1	J	0.77	0/1973	0.84	0/2676
1	K	0.81	0/1973	0.83	0/2676
1	L	0.80	1/1973 (0.1%)	0.84	0/2676
1	M	0.83	1/1973 (0.1%)	0.88	1/2676 (0.0%)
1	N	0.79	0/1973	0.84	1/2676 (0.0%)
1	O	0.76	0/1973	0.80	2/2676 (0.1%)
1	P	0.68	1/1973 (0.1%)	0.74	0/2676
1	Q	0.75	0/1973	0.78	2/2676 (0.1%)
1	R	0.68	0/1973	0.76	0/2676
1	S	0.66	0/1973	0.71	0/2676
1	T	0.65	0/1973	0.75	0/2676
All	All	0.80	10/39460 (0.0%)	0.83	20/53520 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	H	0	1
1	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	2
1	O	0	1
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	GLU	CG-CD	5.94	1.60	1.51
1	I	162	GLU	CG-CD	5.87	1.60	1.51
1	M	162	GLU	CG-CD	5.81	1.60	1.51
1	L	161	GLU	CG-CD	5.74	1.60	1.51
1	A	53	GLU	CG-CD	5.39	1.60	1.51
1	P	162	GLU	CG-CD	5.30	1.59	1.51
1	A	56	LYS	CD-CE	5.17	1.64	1.51
1	D	53	GLU	CG-CD	5.12	1.59	1.51
1	B	133	SER	CA-CB	5.09	1.60	1.52
1	A	161	GLU	CG-CD	5.02	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	131	LEU	CA-CB-CG	6.75	130.81	115.30
1	E	122	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	30	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	N	204	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	H	142	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	56	LYS	CD-CE-NZ	5.59	124.57	111.70
1	Q	183	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	C	215	LEU	CB-CG-CD1	5.51	120.36	111.00
1	H	122	ASP	CB-CG-OD1	5.47	123.23	118.30
1	C	92	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	M	215	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	142	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	O	92	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	F	241	ASP	CB-CG-OD1	5.13	122.92	118.30
1	G	183	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	G	163	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	122	ASP	CB-CG-OD1	5.08	122.87	118.30
1	H	30	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	O	92	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	137	SER	C-N-CA	-5.00	111.79	122.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	SER	Peptide
1	H	138	GLY	Peptide
1	L	138	GLY	Peptide
1	M	133	SER	Peptide
1	M	138	GLY	Peptide
1	O	138	GLY	Peptide

## 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	1928	0	1938	68	0
1	B	1928	0	1938	62	0
1	C	1928	0	1938	61	0
1	D	1928	0	1938	52	0
1	E	1928	0	1938	57	0
1	F	1928	0	1938	58	0
1	G	1928	0	1938	60	0
1	H	1928	0	1938	49	0
1	I	1928	0	1938	59	0
1	J	1928	0	1938	70	0
1	K	1928	0	1938	48	0
1	L	1928	0	1938	55	0
1	M	1928	0	1938	49	0
1	N	1928	0	1938	60	0
1	O	1928	0	1938	47	0
1	P	1928	0	1938	55	0
1	Q	1928	0	1938	53	0
1	R	1928	0	1938	56	0
1	S	1928	0	1938	58	0
1	T	1928	0	1938	60	0
2	A	43	0	30	13	0
2	B	43	0	30	8	0
2	C	43	0	30	14	0
2	D	43	0	30	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	43	0	30	10	0
2	F	43	0	30	13	0
2	G	43	0	30	10	0
2	H	43	0	30	14	0
2	I	43	0	30	8	0
2	J	43	0	30	14	0
2	K	43	0	30	11	0
2	L	43	0	30	12	0
2	M	43	0	30	13	0
2	N	43	0	30	11	0
2	O	43	0	30	10	0
2	P	43	0	30	10	0
2	Q	43	0	30	10	0
2	R	43	0	30	9	0
2	S	43	0	30	15	0
2	T	43	0	30	10	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	1	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0
3	N	3	0	0	0	0
3	O	3	0	0	0	0
3	P	3	0	0	0	0
3	Q	3	0	0	0	0
3	R	3	0	0	0	0
3	S	3	0	0	0	0
3	T	3	0	0	0	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0
4	C	12	0	12	1	0
4	D	12	0	12	0	0
4	E	12	0	12	1	0
4	F	12	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	12	0	12	0	0
4	H	12	0	12	1	0
4	I	12	0	12	0	0
4	J	12	0	12	0	0
4	K	12	0	12	0	0
4	L	12	0	12	0	0
4	M	12	0	12	0	0
4	N	12	0	12	1	0
4	O	12	0	12	1	0
4	P	12	0	12	1	0
4	Q	12	0	12	0	0
4	R	12	0	12	0	0
4	S	12	0	12	1	0
4	T	12	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	2	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	1	0	0	1	0
6	J	1	0	0	1	0
6	K	1	0	0	0	0
6	L	1	0	0	2	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
All	All	39760	0	39600	1064	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 13.

All (1064) 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)
1:D:196:PHE:CZ	2:D:1000:HEM:O2D	1.77	1.37
1:K:196:PHE:CZ	2:K:1000:HEM:O2D	1.80	1.35
1:C:196:PHE:CZ	2:C:1000:HEM:O2D	1.89	1.25
1:H:196:PHE:CZ	2:H:1000:HEM:O2D	1.90	1.25
1:F:196:PHE:CZ	2:F:1000:HEM:O2D	1.94	1.21
1:A:196:PHE:CZ	2:A:1000:HEM:O2D	1.96	1.17
1:E:18:PRO:HA	1:E:113:THR:HG22	1.29	1.15
1:H:97:THR:HG22	1:H:100:GLY:H	1.11	1.15
1:T:196:PHE:CZ	2:T:1000:HEM:O2D	2.00	1.15
1:E:196:PHE:CZ	2:E:1000:HEM:O2D	2.00	1.14
1:R:196:PHE:CZ	2:R:1000:HEM:O2D	2.02	1.13
1:G:18:PRO:HA	1:G:113:THR:HG22	1.32	1.11
1:C:18:PRO:HA	1:C:113:THR:HG22	1.30	1.10
1:L:196:PHE:CZ	2:L:1000:HEM:O2D	2.03	1.09
1:C:18:PRO:HA	1:C:113:THR:CG2	1.82	1.09
1:N:18:PRO:HA	1:N:113:THR:HG22	1.31	1.07
1:L:18:PRO:HA	1:L:113:THR:HG22	1.33	1.07
1:M:18:PRO:HA	1:M:113:THR:HG22	1.36	1.07
1:H:18:PRO:HA	1:H:113:THR:HG22	1.35	1.06
1:D:97:THR:HG22	1:D:100:GLY:H	1.17	1.06
1:J:18:PRO:HA	1:J:113:THR:HG22	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:HA	1:A:113:THR:CG2	1.87	1.04
1:M:97:THR:HG22	1:M:100:GLY:H	1.22	1.04
1:B:138:GLY:HA2	1:F:115:PRO:HG2	1.04	1.04
1:G:196:PHE:CZ	2:G:1000:HEM:O2D	2.11	1.04
1:G:18:PRO:HA	1:G:113:THR:CG2	1.86	1.04
1:A:97:THR:HG22	1:A:100:GLY:H	1.20	1.04
1:L:17:GLN:O	1:L:113:THR:HG21	1.57	1.03
1:O:196:PHE:CZ	2:O:1000:HEM:O2D	2.11	1.03
1:D:18:PRO:HA	1:D:113:THR:HG22	1.39	1.02
1:E:221:ASN:HD22	1:E:224:HIS:CD2	1.78	1.02
1:C:221:ASN:HD22	1:C:224:HIS:HD2	1.04	1.01
1:H:221:ASN:HD22	1:H:224:HIS:HD2	1.07	1.01
1:S:221:ASN:HD22	1:S:224:HIS:HD2	1.08	1.01
1:B:53:GLU:OE2	1:B:56:LYS:NZ	1.94	1.00
1:C:97:THR:HG22	1:C:100:GLY:H	1.26	1.00
1:B:196:PHE:CZ	2:B:1000:HEM:O2D	2.15	1.00
1:B:18:PRO:HA	1:B:113:THR:HG22	1.41	0.99
1:G:221:ASN:HD22	1:G:224:HIS:CD2	1.81	0.99
1:R:18:PRO:HA	1:R:113:THR:HG22	1.44	0.99
1:I:196:PHE:CZ	2:I:1000:HEM:O2D	2.16	0.99
1:T:221:ASN:HD22	1:T:224:HIS:HD2	1.11	0.99
1:K:17:GLN:O	1:K:113:THR:HG21	1.63	0.98
1:O:97:THR:HG22	1:O:100:GLY:H	1.27	0.98
1:K:221:ASN:HD22	1:K:224:HIS:HD2	1.07	0.98
1:N:18:PRO:HA	1:N:113:THR:CG2	1.94	0.97
1:I:18:PRO:HA	1:I:113:THR:HG22	1.43	0.97
1:J:221:ASN:HD22	1:J:224:HIS:CD2	1.82	0.97
1:J:221:ASN:HD22	1:J:224:HIS:HD2	1.01	0.97
1:B:221:ASN:HD22	1:B:224:HIS:HD2	1.02	0.96
1:L:221:ASN:HD22	1:L:224:HIS:HD2	1.11	0.96
1:T:18:PRO:HA	1:T:113:THR:HG22	1.42	0.96
1:A:18:PRO:HA	1:A:113:THR:HG22	1.43	0.96
1:D:18:PRO:HA	1:D:113:THR:CG2	1.94	0.96
1:N:221:ASN:HD22	1:N:224:HIS:HD2	0.99	0.96
1:K:196:PHE:HZ	2:K:1000:HEM:O2D	1.45	0.96
1:M:17:GLN:O	1:M:113:THR:HG21	1.65	0.96
1:N:221:ASN:HD22	1:N:224:HIS:CD2	1.83	0.96
1:J:196:PHE:CZ	2:J:1000:HEM:O2D	2.19	0.95
1:G:17:GLN:O	1:G:113:THR:HG21	1.64	0.95
1:O:17:GLN:O	1:O:113:THR:HG21	1.65	0.95
1:T:17:GLN:O	1:T:113:THR:HG21	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:LEU:HD11	2:K:1000:HEM:HBB2	1.49	0.94
1:L:18:PRO:HA	1:L:113:THR:CG2	1.98	0.94
1:C:221:ASN:HD22	1:C:224:HIS:CD2	1.83	0.94
1:D:221:ASN:HD22	1:D:224:HIS:HD2	0.97	0.94
1:I:221:ASN:HD22	1:I:224:HIS:HD2	0.95	0.94
1:E:221:ASN:ND2	1:E:224:HIS:HD2	1.66	0.94
1:J:18:PRO:HA	1:J:113:THR:CG2	1.96	0.94
1:B:97:THR:HG22	1:B:100:GLY:H	1.30	0.94
1:F:221:ASN:HD22	1:F:224:HIS:HD2	0.97	0.93
1:E:18:PRO:HA	1:E:113:THR:CG2	1.99	0.93
1:M:196:PHE:CZ	2:M:1000:HEM:O2D	2.21	0.92
1:B:17:GLN:O	1:B:113:THR:HG21	1.70	0.92
1:R:235:THR:HG23	1:R:237:HIS:NE2	1.84	0.92
1:A:221:ASN:HD22	1:A:224:HIS:HD2	1.07	0.92
1:D:221:ASN:HD22	1:D:224:HIS:CD2	1.87	0.92
1:H:221:ASN:HD22	1:H:224:HIS:CD2	1.87	0.92
1:I:221:ASN:HD22	1:I:224:HIS:CD2	1.87	0.92
1:P:18:PRO:HA	1:P:113:THR:HG22	1.51	0.92
1:B:138:GLY:CA	1:F:115:PRO:HG2	1.98	0.91
1:J:97:THR:HG22	1:J:100:GLY:H	1.34	0.91
1:K:18:PRO:HA	1:K:113:THR:HG22	1.48	0.91
1:O:221:ASN:HD22	1:O:224:HIS:HD2	0.98	0.91
1:G:221:ASN:HD22	1:G:224:HIS:HD2	0.98	0.91
1:G:221:ASN:ND2	1:G:224:HIS:HD2	1.68	0.90
1:O:18:PRO:HA	1:O:113:THR:HG22	1.54	0.90
1:E:17:GLN:O	1:E:113:THR:HG21	1.71	0.90
1:E:235:THR:HG23	1:E:237:HIS:NE2	1.86	0.90
1:G:97:THR:HG22	1:G:100:GLY:H	1.37	0.90
1:K:221:ASN:HD22	1:K:224:HIS:CD2	1.90	0.89
1:Q:97:THR:HG22	1:Q:100:GLY:H	1.38	0.89
1:Q:18:PRO:HA	1:Q:113:THR:HG22	1.53	0.89
1:M:221:ASN:HD22	1:M:224:HIS:HD2	1.16	0.89
1:I:97:THR:HG22	1:I:100:GLY:H	1.37	0.89
1:N:17:GLN:O	1:N:113:THR:HG21	1.71	0.89
1:R:221:ASN:HD22	1:R:224:HIS:HD2	1.19	0.89
1:N:97:THR:HG22	1:N:100:GLY:H	1.36	0.88
1:A:221:ASN:HD22	1:A:224:HIS:CD2	1.91	0.88
1:N:221:ASN:ND2	1:N:224:HIS:HD2	1.71	0.88
1:E:221:ASN:HD22	1:E:224:HIS:HD2	0.91	0.87
1:B:221:ASN:HD22	1:B:224:HIS:CD2	1.92	0.87
1:P:196:PHE:CZ	2:P:1000:HEM:O2D	2.27	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:196:PHE:CZ	2:Q:1000:HEM:O2D	2.26	0.87
1:D:94:PHE:O	1:D:97:THR:HB	1.75	0.87
1:I:18:PRO:HA	1:I:113:THR:CG2	2.03	0.87
1:S:221:ASN:HD22	1:S:224:HIS:CD2	1.93	0.86
1:J:221:ASN:ND2	1:J:224:HIS:HD2	1.72	0.86
1:O:221:ASN:HD22	1:O:224:HIS:CD2	1.90	0.86
1:C:221:ASN:ND2	1:C:224:HIS:HD2	1.70	0.86
1:N:196:PHE:CZ	2:N:1000:HEM:O2D	2.28	0.86
1:S:18:PRO:HA	1:S:113:THR:HG22	1.55	0.86
1:B:235:THR:HG23	1:B:237:HIS:NE2	1.90	0.85
1:I:17:GLN:O	1:I:113:THR:HG21	1.77	0.85
1:Q:17:GLN:O	1:Q:113:THR:HG21	1.77	0.85
1:J:235:THR:HG23	1:J:237:HIS:NE2	1.90	0.85
1:R:17:GLN:O	1:R:113:THR:HG21	1.76	0.85
1:M:18:PRO:HA	1:M:113:THR:CG2	2.06	0.85
1:B:18:PRO:HA	1:B:113:THR:CG2	2.06	0.85
1:M:221:ASN:HD22	1:M:224:HIS:CD2	1.94	0.85
1:F:221:ASN:HD22	1:F:224:HIS:CD2	1.90	0.84
1:G:211:LEU:HD11	2:G:1000:HEM:HBB2	1.56	0.84
1:Q:55:HIS:HD2	1:Q:58:ASN:HD22	1.23	0.84
1:P:221:ASN:HD22	1:P:224:HIS:HD2	1.26	0.84
1:J:97:THR:CG2	1:J:100:GLY:H	1.90	0.84
1:D:221:ASN:ND2	1:D:224:HIS:HD2	1.76	0.83
1:P:94:PHE:O	1:P:97:THR:HG22	1.77	0.83
1:Q:221:ASN:HD22	1:Q:224:HIS:HD2	1.22	0.83
1:Q:221:ASN:HD22	1:Q:224:HIS:CD2	1.97	0.83
1:H:221:ASN:ND2	1:H:224:HIS:HD2	1.76	0.83
1:J:17:GLN:O	1:J:113:THR:HG21	1.79	0.83
1:S:196:PHE:CZ	2:S:1000:HEM:O2D	2.30	0.83
1:L:196:PHE:HZ	2:L:1000:HEM:O2D	1.61	0.82
1:O:221:ASN:ND2	1:O:224:HIS:HD2	1.76	0.82
2:L:1000:HEM:HBB2	2:L:1000:HEM:HHC	1.61	0.82
1:I:221:ASN:ND2	1:I:224:HIS:HD2	1.77	0.82
1:H:18:PRO:HA	1:H:113:THR:CG2	2.08	0.82
1:H:196:PHE:HZ	2:H:1000:HEM:O2D	1.61	0.81
1:I:212:MET:HG3	1:J:190:GLY:CA	2.11	0.81
1:I:211:LEU:HD11	2:I:1000:HEM:HBB2	1.61	0.81
1:C:17:GLN:O	1:C:113:THR:HG21	1.79	0.81
1:F:18:PRO:HA	1:F:113:THR:HG22	1.61	0.81
1:A:17:GLN:O	1:A:113:THR:HG21	1.79	0.80
1:K:18:PRO:HA	1:K:113:THR:CG2	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HG22	1:A:100:GLY:N	1.97	0.80
1:A:196:PHE:HZ	2:A:1000:HEM:O2D	1.65	0.80
1:C:196:PHE:HZ	2:C:1000:HEM:O2D	1.61	0.80
1:L:221:ASN:HD22	1:L:224:HIS:CD2	1.99	0.80
1:L:235:THR:HG23	1:L:237:HIS:NE2	1.97	0.79
1:A:97:THR:CG2	1:A:100:GLY:H	1.92	0.79
1:H:97:THR:HG22	1:H:100:GLY:N	1.93	0.79
1:F:212:MET:HG3	1:G:190:GLY:HA3	1.64	0.79
1:R:18:PRO:HA	1:R:113:THR:CG2	2.12	0.79
1:F:190:GLY:HA3	1:J:212:MET:HG3	1.66	0.78
1:O:18:PRO:HA	1:O:113:THR:CG2	2.13	0.78
1:D:196:PHE:CE1	2:D:1000:HEM:O2D	2.36	0.78
1:O:97:THR:CG2	1:O:100:GLY:H	1.96	0.78
1:A:174:THR:HB	2:A:1000:HEM:HBB2	1.63	0.78
1:B:221:ASN:ND2	1:B:224:HIS:HD2	1.80	0.78
1:F:196:PHE:HZ	2:F:1000:HEM:O2D	1.63	0.78
1:T:221:ASN:HD22	1:T:224:HIS:CD2	2.00	0.78
1:N:159:SER:OG	1:N:162:GLU:HG3	1.83	0.77
1:K:235:THR:HG23	1:K:237:HIS:NE2	1.99	0.77
1:A:221:ASN:ND2	1:A:224:HIS:HD2	1.83	0.77
1:T:116:LEU:HA	2:T:1000:HEM:O1A	1.85	0.77
1:E:211:LEU:HD11	2:E:1000:HEM:HBB2	1.67	0.77
1:P:105:VAL:HG12	1:S:71:THR:HG23	1.65	0.77
1:A:174:THR:HG22	1:A:211:LEU:HD11	1.67	0.76
1:M:211:LEU:HD11	2:M:1000:HEM:HBB2	1.66	0.76
1:S:221:ASN:ND2	1:S:224:HIS:HD2	1.83	0.76
1:R:196:PHE:HZ	2:R:1000:HEM:O2D	1.62	0.76
1:H:17:GLN:O	1:H:113:THR:HG21	1.86	0.75
1:H:196:PHE:CE1	2:H:1000:HEM:O2D	2.38	0.75
1:Q:55:HIS:CD2	1:Q:58:ASN:HD22	2.04	0.75
1:S:17:GLN:O	1:S:113:THR:HG21	1.84	0.75
1:R:211:LEU:HD11	2:R:1000:HEM:HBB2	1.69	0.75
1:Q:11:ARG:NH2	1:Q:62:ASP:OD1	2.20	0.75
1:D:177:TYR:HB2	2:D:1000:HEM:HBB1	1.68	0.75
1:M:221:ASN:ND2	1:M:224:HIS:HD2	1.84	0.75
1:D:97:THR:HG22	1:D:100:GLY:N	1.99	0.75
1:A:70:GLU:OE2	1:A:232:THR:HA	1.87	0.74
1:R:212:MET:HG3	1:S:190:GLY:HA3	1.69	0.74
1:K:97:THR:HG22	1:K:100:GLY:H	1.51	0.74
1:M:211:LEU:HD11	2:M:1000:HEM:CBB	2.16	0.74
1:P:190:GLY:HA3	1:S:212:MET:HG3	1.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:97:THR:HG22	1:M:100:GLY:N	2.01	0.74
1:N:11:ARG:NH2	1:N:62:ASP:OD1	2.21	0.74
1:O:116:LEU:HA	2:O:1000:HEM:O1A	1.88	0.74
1:F:235:THR:HG23	1:F:237:HIS:NE2	2.01	0.74
1:F:221:ASN:ND2	1:F:224:HIS:HD2	1.81	0.74
1:M:97:THR:CG2	1:M:100:GLY:H	1.98	0.74
1:E:97:THR:HG22	1:E:100:GLY:H	1.51	0.74
1:G:212:MET:HG3	1:H:190:GLY:HA3	1.68	0.74
1:E:97:THR:CG2	1:E:100:GLY:H	2.00	0.73
1:B:94:PHE:O	1:B:97:THR:HB	1.86	0.73
1:I:119:ILE:HG13	2:I:1000:HEM:HMA3	1.70	0.73
1:H:116:LEU:HA	2:H:1000:HEM:O1A	1.88	0.73
1:A:235:THR:HG23	1:A:237:HIS:NE2	2.04	0.73
1:P:17:GLN:O	1:P:113:THR:HG21	1.89	0.73
1:O:174:THR:HB	2:O:1000:HEM:HBB2	1.71	0.73
1:B:235:THR:CG2	1:B:237:HIS:NE2	2.51	0.72
1:K:221:ASN:ND2	1:K:224:HIS:HD2	1.82	0.72
1:L:221:ASN:ND2	1:L:224:HIS:HD2	1.86	0.72
1:C:212:MET:HG3	1:E:190:GLY:HA3	1.71	0.72
1:A:65:LEU:HB3	1:A:235:THR:HG22	1.71	0.72
1:C:235:THR:HG23	1:C:237:HIS:NE2	2.04	0.72
1:A:174:THR:CB	2:A:1000:HEM:HBB2	2.19	0.72
1:F:17:GLN:O	1:F:113:THR:HG21	1.89	0.72
1:T:174:THR:HG22	1:T:211:LEU:CD1	2.20	0.72
1:I:212:MET:HG3	1:J:190:GLY:HA3	1.72	0.72
1:M:116:LEU:HA	2:M:1000:HEM:O1A	1.90	0.71
1:G:196:PHE:HZ	2:G:1000:HEM:O2D	1.67	0.71
1:B:138:GLY:HA2	1:F:115:PRO:CG	2.01	0.71
1:N:18:PRO:CA	1:N:113:THR:HG22	2.14	0.71
1:T:235:THR:HG23	1:T:237:HIS:NE2	2.06	0.71
1:E:196:PHE:HZ	2:E:1000:HEM:O2D	1.70	0.71
1:D:17:GLN:O	1:D:113:THR:HG21	1.91	0.71
1:R:118:TYR:HE2	2:R:1000:HEM:O1D	1.74	0.71
1:E:174:THR:HB	2:E:1000:HEM:CBB	2.21	0.70
1:F:145:ILE:HD13	1:F:233:LEU:HD13	1.73	0.70
1:F:221:ASN:HA	1:F:224:HIS:CD2	2.26	0.70
1:F:38:VAL:HB	1:F:41:ARG:NH1	2.06	0.70
1:D:235:THR:HG23	1:D:237:HIS:NE2	2.06	0.70
1:J:196:PHE:HZ	2:J:1000:HEM:O2D	1.75	0.70
1:A:71:THR:HG23	1:D:105:VAL:HG12	1.72	0.70
1:D:196:PHE:CE2	2:D:1000:HEM:O2D	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:174:THR:HG22	1:P:211:LEU:HD11	1.74	0.70
1:A:177:TYR:HB2	2:A:1000:HEM:HBB1	1.74	0.70
1:P:221:ASN:HD22	1:P:224:HIS:CD2	2.09	0.70
1:Q:116:LEU:HA	2:Q:1000:HEM:O1A	1.92	0.70
1:H:174:THR:HB	2:H:1000:HEM:CBB	2.22	0.70
1:L:70:GLU:OE2	1:L:232:THR:HA	1.91	0.70
1:N:212:MET:HG3	1:O:190:GLY:HA3	1.74	0.70
1:F:211:LEU:HD11	2:F:1000:HEM:HBB2	1.73	0.69
1:I:11:ARG:NH2	1:I:62:ASP:OD1	2.24	0.69
1:A:190:GLY:CA	1:E:212:MET:HG3	2.23	0.69
1:H:212:MET:HG3	1:I:190:GLY:CA	2.23	0.69
1:B:97:THR:HG22	1:B:100:GLY:N	2.07	0.69
1:Q:211:LEU:HD11	2:Q:1000:HEM:HBB2	1.75	0.69
1:Q:18:PRO:HA	1:Q:113:THR:CG2	2.22	0.69
1:D:174:THR:HG22	1:D:211:LEU:HD11	1.74	0.69
1:K:211:LEU:HD11	2:K:1000:HEM:CBB	2.21	0.69
1:G:212:MET:HG3	1:H:190:GLY:CA	2.23	0.68
1:A:174:THR:HG22	1:A:211:LEU:CD1	2.23	0.68
1:B:97:THR:CG2	1:B:100:GLY:H	2.05	0.68
1:S:97:THR:CG2	1:S:100:GLY:H	2.06	0.68
1:J:65:LEU:HB3	1:J:235:THR:HG22	1.74	0.68
1:A:44:ALA:HB1	1:A:99:VAL:HG22	1.75	0.68
1:G:65:LEU:HB3	1:G:235:THR:HG22	1.76	0.68
1:N:222:LYS:HE2	1:O:154:GLU:OE1	1.94	0.68
1:B:65:LEU:HB3	1:B:235:THR:HG22	1.76	0.68
1:I:235:THR:HG23	1:I:237:HIS:NE2	2.08	0.68
1:P:235:THR:HG23	1:P:237:HIS:NE2	2.08	0.68
1:Q:221:ASN:ND2	1:Q:224:HIS:HD2	1.91	0.68
1:K:196:PHE:CE1	2:K:1000:HEM:O2D	2.45	0.67
1:L:11:ARG:NH2	1:L:62:ASP:OD1	2.27	0.67
1:S:116:LEU:HA	2:S:1000:HEM:O1A	1.94	0.67
1:O:97:THR:HG22	1:O:100:GLY:N	2.05	0.67
1:P:16:THR:O	4:P:2001:MES:H52	1.94	0.67
1:S:18:PRO:HA	1:S:113:THR:CG2	2.24	0.67
1:L:20:VAL:H	1:L:113:THR:HB	1.60	0.67
1:N:94:PHE:O	1:N:97:THR:HB	1.95	0.67
1:A:11:ARG:NH2	1:A:62:ASP:OD1	2.28	0.66
1:N:117:ASN:N	2:N:1000:HEM:O1A	2.26	0.66
1:N:211:LEU:HD11	2:N:1000:HEM:HBB2	1.75	0.66
1:Q:105:VAL:HG12	1:T:71:THR:HG23	1.76	0.66
1:B:190:GLY:CA	1:D:212:MET:HG3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:MET:HG3	1:I:190:GLY:HA2	1.76	0.66
1:P:190:GLY:CA	1:S:212:MET:HG3	2.24	0.66
1:D:174:THR:HG22	1:D:211:LEU:CD1	2.26	0.66
1:R:221:ASN:HD22	1:R:224:HIS:CD2	2.09	0.66
1:T:221:ASN:ND2	1:T:224:HIS:HD2	1.88	0.66
1:C:94:PHE:O	1:C:97:THR:HB	1.94	0.66
1:J:118:TYR:HE2	2:J:1000:HEM:O1D	1.78	0.66
1:K:105:VAL:HG12	1:O:71:THR:HG23	1.77	0.66
1:K:212:MET:HG3	1:L:190:GLY:CA	2.26	0.66
1:R:97:THR:CG2	1:R:100:GLY:H	2.09	0.66
1:F:105:VAL:HG12	1:J:71:THR:HG23	1.76	0.66
1:L:224:HIS:CE1	6:L:3000:HOH:O	2.49	0.66
1:N:97:THR:HG22	1:N:100:GLY:N	2.09	0.65
1:A:190:GLY:HA3	1:E:212:MET:HG3	1.77	0.65
1:D:180:ASN:HB3	1:D:181:VAL:HG23	1.77	0.65
1:F:116:LEU:HA	2:F:1000:HEM:O1A	1.95	0.65
1:K:11:ARG:NH2	1:K:62:ASP:OD1	2.27	0.65
1:N:97:THR:CG2	1:N:100:GLY:H	2.07	0.65
1:G:20:VAL:H	1:G:113:THR:HB	1.61	0.65
1:F:174:THR:HB	2:F:1000:HEM:CBB	2.26	0.65
1:C:97:THR:HG22	1:C:100:GLY:N	2.07	0.65
1:I:65:LEU:HB3	1:I:235:THR:HG22	1.78	0.65
1:O:117:ASN:N	2:O:1000:HEM:O1A	2.30	0.65
1:D:116:LEU:HA	2:D:1000:HEM:O1A	1.96	0.65
1:E:211:LEU:O	1:E:214:SER:HB2	1.95	0.65
1:G:145:ILE:HD13	1:G:233:LEU:HD13	1.79	0.65
1:J:116:LEU:HA	2:J:1000:HEM:O1A	1.95	0.65
1:K:180:ASN:HB3	1:K:181:VAL:HG23	1.78	0.65
1:K:212:MET:HG3	1:L:190:GLY:HA2	1.78	0.65
1:M:235:THR:HG23	1:M:237:HIS:NE2	2.11	0.64
1:C:97:THR:CG2	1:C:100:GLY:H	2.06	0.64
1:O:196:PHE:CE2	2:O:1000:HEM:O2D	2.50	0.64
1:C:174:THR:HB	2:C:1000:HEM:HBB2	1.80	0.64
1:F:174:THR:HB	2:F:1000:HEM:HBB2	1.79	0.64
1:I:196:PHE:CE1	2:I:1000:HEM:O2D	2.50	0.64
1:T:174:THR:HG22	1:T:211:LEU:HD11	1.77	0.64
1:C:212:MET:HG3	1:E:190:GLY:CA	2.28	0.64
1:P:18:PRO:HA	1:P:113:THR:CG2	2.26	0.64
1:F:18:PRO:HD3	4:F:2001:MES:H22	1.79	0.64
1:H:118:TYR:CD2	1:H:167:MET:HG3	2.32	0.64
1:M:212:MET:HG3	1:N:190:GLY:CA	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:66:THR:HG22	1:P:234:GLY:HA3	1.78	0.64
1:S:221:ASN:HA	1:S:224:HIS:CD2	2.32	0.64
1:D:150:LYS:HA	1:D:195:ASP:HB2	1.79	0.64
1:M:212:MET:HG3	1:N:190:GLY:HA3	1.80	0.64
1:Q:212:MET:HG3	1:R:190:GLY:HA3	1.78	0.64
1:T:196:PHE:CE1	2:T:1000:HEM:O2D	2.49	0.64
1:C:18:PRO:HA	1:C:113:THR:HG21	1.74	0.63
1:D:20:VAL:H	1:D:113:THR:HB	1.64	0.63
1:P:116:LEU:HA	2:P:1000:HEM:O1A	1.97	0.63
1:R:211:LEU:HD11	2:R:1000:HEM:CBB	2.27	0.63
1:E:235:THR:CG2	1:E:237:HIS:NE2	2.61	0.63
1:J:174:THR:HB	2:J:1000:HEM:HBB2	1.80	0.63
1:H:71:THR:HG23	1:I:105:VAL:HG12	1.81	0.63
1:A:38:VAL:O	1:A:39:ALA:HB2	1.98	0.63
1:P:180:ASN:HB3	1:P:181:VAL:HG23	1.80	0.63
1:C:196:PHE:CE1	2:C:1000:HEM:O2D	2.49	0.62
1:Q:71:THR:HG23	1:R:105:VAL:HG12	1.80	0.62
1:T:196:PHE:HZ	2:T:1000:HEM:O2D	1.79	0.62
1:J:97:THR:HG22	1:J:100:GLY:N	2.11	0.62
1:D:38:VAL:O	1:D:39:ALA:CB	2.47	0.62
2:L:1000:HEM:CBB	2:L:1000:HEM:HHC	2.29	0.62
1:Q:235:THR:HG23	1:Q:237:HIS:NE2	2.14	0.62
1:A:196:PHE:CE1	2:A:1000:HEM:O2D	2.50	0.62
1:B:11:ARG:NH2	1:B:62:ASP:OD1	2.32	0.62
1:L:212:MET:HG3	1:M:190:GLY:HA3	1.80	0.62
1:P:127:LEU:HD12	1:P:168:GLU:HG2	1.79	0.62
1:B:116:LEU:HA	2:B:1000:HEM:O1A	2.00	0.62
1:I:28:LYS:NZ	1:I:72:ASN:HD22	1.98	0.62
1:I:222:LYS:HE2	1:J:154:GLU:OE1	2.00	0.62
1:I:212:MET:HG3	1:J:190:GLY:HA2	1.80	0.62
1:R:97:THR:HG22	1:R:100:GLY:H	1.65	0.62
1:H:94:PHE:O	1:H:97:THR:HB	2.00	0.61
1:C:116:LEU:HA	2:C:1000:HEM:O1A	2.01	0.61
1:N:59:VAL:HG12	1:N:81:ALA:HB2	1.83	0.61
1:R:117:ASN:N	2:R:1000:HEM:O1A	2.33	0.61
1:S:174:THR:HB	2:S:1000:HEM:CBB	2.29	0.61
1:B:53:GLU:CD	1:B:56:LYS:NZ	2.53	0.61
1:F:119:ILE:HG13	2:F:1000:HEM:HMA3	1.80	0.61
1:D:97:THR:CG2	1:D:100:GLY:H	2.04	0.61
1:G:235:THR:HG23	1:G:237:HIS:NE2	2.16	0.61
1:L:97:THR:CG2	1:L:100:GLY:H	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:LEU:CD1	2:I:1000:HEM:HBB2	2.30	0.61
1:Q:36:VAL:O	1:Q:41:ARG:HD3	2.01	0.61
1:G:94:PHE:O	1:G:97:THR:HB	2.00	0.61
1:L:145:ILE:HD13	1:L:233:LEU:HD13	1.82	0.61
1:N:212:MET:HG3	1:O:190:GLY:CA	2.31	0.61
1:H:11:ARG:NH2	1:H:62:ASP:OD1	2.33	0.61
1:S:186:TYR:HB2	1:S:197:ILE:HB	1.82	0.61
1:Q:117:ASN:N	2:Q:1000:HEM:O1A	2.33	0.60
1:Q:145:ILE:HD13	1:Q:233:LEU:HD13	1.83	0.60
1:A:33:TRP:CZ2	1:A:41:ARG:HG2	2.35	0.60
1:E:9:ILE:O	1:E:9:ILE:HG22	2.01	0.60
1:A:38:VAL:O	1:A:39:ALA:CB	2.48	0.60
1:G:211:LEU:HD11	2:G:1000:HEM:CBB	2.31	0.60
1:P:51:LEU:HD11	1:P:93:GLU:HB3	1.82	0.60
1:A:212:MET:HG3	1:D:190:GLY:HA3	1.83	0.60
1:M:119:ILE:O	1:M:119:ILE:HG22	2.02	0.60
1:E:174:THR:HB	2:E:1000:HEM:HBB2	1.83	0.60
1:J:174:THR:HB	2:J:1000:HEM:CBB	2.31	0.60
1:O:65:LEU:HB3	1:O:235:THR:HG22	1.84	0.60
1:K:116:LEU:HA	2:K:1000:HEM:O1A	2.01	0.60
1:F:212:MET:HG3	1:G:190:GLY:CA	2.30	0.60
1:N:38:VAL:O	1:N:39:ALA:CB	2.50	0.60
1:R:41:ARG:NH2	1:R:247:ALA:O	2.35	0.60
1:M:158:MET:O	1:M:163:ARG:NH1	2.35	0.59
1:K:190:GLY:CA	1:O:212:MET:HG3	2.32	0.59
1:R:94:PHE:O	1:R:97:THR:HG22	2.02	0.59
1:S:66:THR:HG22	1:S:234:GLY:HA3	1.84	0.59
1:E:53:GLU:O	1:E:56:LYS:HB2	2.02	0.59
1:R:18:PRO:CA	1:R:113:THR:HG22	2.27	0.59
1:S:211:LEU:HD11	2:S:1000:HEM:HBB2	1.84	0.59
1:T:26:MET:HG3	1:T:76:PHE:HB3	1.85	0.59
1:O:18:PRO:CA	1:O:113:THR:HG22	2.31	0.59
1:N:167:MET:CE	2:N:1000:HEM:HBD1	2.33	0.59
1:N:75:PHE:CD1	1:N:246:LEU:HD11	2.38	0.59
1:B:190:GLY:HA3	1:D:212:MET:HG3	1.84	0.59
1:E:196:PHE:CE1	2:E:1000:HEM:O2D	2.53	0.59
1:A:116:LEU:HA	2:A:1000:HEM:O1A	2.02	0.58
1:M:196:PHE:HZ	2:M:1000:HEM:O2D	1.85	0.58
1:S:97:THR:HG22	1:S:100:GLY:H	1.66	0.58
1:A:145:ILE:HD13	1:A:233:LEU:HD13	1.84	0.58
1:C:158:MET:O	1:C:163:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1000:HEM:HHC	2:H:1000:HEM:HBB2	1.83	0.58
1:F:150:LYS:HA	1:F:195:ASP:HB2	1.83	0.58
1:J:145:ILE:HD13	1:J:233:LEU:HD13	1.85	0.58
1:L:224:HIS:HE1	6:L:3000:HOH:O	1.83	0.58
1:F:118:TYR:HE2	2:F:1000:HEM:O1D	1.86	0.58
1:T:30:ARG:NH2	1:T:101:LYS:O	2.29	0.58
1:C:145:ILE:HD13	1:C:233:LEU:HD13	1.86	0.58
1:I:116:LEU:HA	2:I:1000:HEM:O1A	2.04	0.58
1:O:221:ASN:HA	1:O:224:HIS:CD2	2.38	0.58
1:E:211:LEU:HD11	2:E:1000:HEM:CBB	2.34	0.58
1:H:145:ILE:HD13	1:H:233:LEU:HD13	1.84	0.58
1:E:59:VAL:HG12	1:E:81:ALA:HB2	1.83	0.58
1:L:97:THR:HG22	1:L:100:GLY:H	1.68	0.58
1:P:211:LEU:HD11	2:P:1000:HEM:HBB2	1.85	0.58
1:Q:118:TYR:HE2	2:Q:1000:HEM:O1D	1.85	0.58
1:S:18:PRO:CA	1:S:113:THR:HG22	2.32	0.58
1:K:235:THR:CG2	1:K:237:HIS:NE2	2.66	0.58
1:L:221:ASN:HA	1:L:224:HIS:CD2	2.38	0.58
1:D:18:PRO:HA	1:D:113:THR:HG21	1.86	0.58
1:G:116:LEU:HA	2:G:1000:HEM:O1A	2.03	0.58
1:K:211:LEU:CD1	2:K:1000:HEM:CBB	2.82	0.58
1:P:196:PHE:HZ	2:P:1000:HEM:O2D	1.84	0.58
1:Q:190:GLY:HA3	1:T:212:MET:HG3	1.86	0.58
2:H:1000:HEM:HHC	2:H:1000:HEM:CBB	2.33	0.57
1:H:97:THR:CG2	1:H:100:GLY:H	1.99	0.57
1:I:235:THR:CG2	1:I:237:HIS:NE2	2.67	0.57
1:D:221:ASN:HA	1:D:224:HIS:CD2	2.39	0.57
1:L:18:PRO:CA	1:L:113:THR:HG22	2.22	0.57
1:S:44:ALA:HB1	1:S:99:VAL:HG22	1.85	0.57
1:G:11:ARG:NH2	1:G:62:ASP:OD1	2.36	0.57
1:T:20:VAL:H	1:T:113:THR:HB	1.69	0.57
1:N:235:THR:HG23	1:N:237:HIS:NE2	2.20	0.57
1:R:92:ARG:HH11	1:R:92:ARG:HG2	1.69	0.57
1:E:186:TYR:HB2	1:E:197:ILE:HB	1.85	0.57
1:J:18:PRO:CA	1:J:113:THR:HG22	2.25	0.57
1:Q:97:THR:CG2	1:Q:100:GLY:H	2.15	0.57
1:H:211:LEU:HD11	2:H:1000:HEM:HBB2	1.87	0.57
2:K:1000:HEM:HHC	2:K:1000:HEM:HBB2	1.84	0.57
1:Q:44:ALA:HB1	1:Q:99:VAL:HG22	1.87	0.57
1:D:116:LEU:HD13	1:D:119:ILE:O	2.05	0.57
1:F:180:ASN:HB3	1:F:181:VAL:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:LEU:HB3	1:H:235:THR:HG22	1.87	0.57
1:L:182:LYS:O	1:L:200:PHE:HA	2.05	0.57
1:S:196:PHE:CE1	2:S:1000:HEM:O2D	2.57	0.57
1:T:29:LEU:HD13	1:T:33:TRP:CD1	2.40	0.57
1:B:211:LEU:HD11	2:B:1000:HEM:HBB2	1.86	0.56
1:D:174:THR:HB	2:D:1000:HEM:HBB2	1.87	0.56
1:F:118:TYR:CD2	1:F:167:MET:HG3	2.39	0.56
1:P:41:ARG:NH2	1:P:247:ALA:O	2.35	0.56
1:C:20:VAL:H	1:C:113:THR:HB	1.70	0.56
1:A:18:PRO:CA	1:A:113:THR:HG22	2.27	0.56
1:B:174:THR:HG22	1:B:211:LEU:HD11	1.86	0.56
1:L:116:LEU:HA	2:L:1000:HEM:O1A	2.05	0.56
1:M:235:THR:CG2	1:M:237:HIS:NE2	2.68	0.56
1:Q:94:PHE:O	1:Q:97:THR:HB	2.05	0.56
1:P:221:ASN:ND2	1:P:224:HIS:HD2	2.02	0.56
1:Q:118:TYR:CE2	2:Q:1000:HEM:O1D	2.59	0.56
1:B:182:LYS:O	1:B:200:PHE:HA	2.06	0.56
1:G:97:THR:CG2	1:G:100:GLY:H	2.15	0.56
1:N:38:VAL:O	1:N:39:ALA:HB2	2.05	0.56
1:R:116:LEU:HA	2:R:1000:HEM:O1A	2.06	0.56
1:C:222:LYS:HE3	1:E:154:GLU:OE1	2.05	0.56
1:P:196:PHE:CE1	2:P:1000:HEM:O2D	2.57	0.56
1:K:97:THR:CG2	1:K:100:GLY:H	2.18	0.56
1:L:196:PHE:CE1	2:L:1000:HEM:O2D	2.57	0.56
1:I:71:THR:HG23	1:J:105:VAL:HG12	1.87	0.56
1:B:212:MET:HG3	1:C:190:GLY:CA	2.36	0.56
1:Q:196:PHE:HZ	2:Q:1000:HEM:O2D	1.81	0.56
1:N:167:MET:HE2	2:N:1000:HEM:HBD1	1.88	0.55
1:R:33:TRP:CZ2	1:R:41:ARG:HG2	2.41	0.55
1:A:219:LYS:O	1:A:222:LYS:HB2	2.05	0.55
1:F:145:ILE:CD1	1:F:233:LEU:HD13	2.36	0.55
1:R:221:ASN:ND2	1:R:224:HIS:HD2	1.98	0.55
1:S:118:TYR:HE2	2:S:1000:HEM:O1D	1.89	0.55
1:A:118:TYR:CD2	1:A:167:MET:HG3	2.40	0.55
1:D:70:GLU:OE2	1:D:232:THR:HA	2.06	0.55
1:E:36:VAL:O	1:E:41:ARG:HD3	2.07	0.55
1:K:221:ASN:HA	1:K:224:HIS:CD2	2.41	0.55
1:S:119:ILE:O	1:S:119:ILE:HG22	2.07	0.55
1:B:190:GLY:HA2	1:D:212:MET:HG3	1.88	0.55
1:E:235:THR:HG23	1:E:237:HIS:CD2	2.42	0.55
1:L:92:ARG:HH11	1:L:92:ARG:HG2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:PHE:CE1	2:B:1000:HEM:O2D	2.59	0.55
1:G:182:LYS:O	1:G:200:PHE:HA	2.07	0.54
1:F:190:GLY:CA	1:J:212:MET:HG3	2.35	0.54
1:L:55:HIS:HE1	1:L:93:GLU:OE1	1.90	0.54
1:A:44:ALA:HB1	1:A:99:VAL:CG2	2.37	0.54
1:G:196:PHE:CE1	2:G:1000:HEM:O2D	2.59	0.54
1:L:211:LEU:O	1:L:214:SER:HB2	2.07	0.54
1:D:11:ARG:NH2	1:D:62:ASP:OD1	2.40	0.54
1:G:66:THR:HG22	1:G:234:GLY:HA3	1.89	0.54
1:R:10:GLU:HB2	1:R:13:THR:HB	1.87	0.54
1:N:150:LYS:HA	1:N:195:ASP:HB2	1.89	0.54
1:L:97:THR:HG22	1:L:100:GLY:N	2.22	0.54
1:F:18:PRO:HA	1:F:113:THR:CG2	2.34	0.54
1:O:64:TYR:CD1	1:O:144:VAL:HG11	2.41	0.54
1:T:9:ILE:O	1:T:9:ILE:HG22	2.07	0.54
1:B:145:ILE:HD13	1:B:233:LEU:HD13	1.89	0.54
1:B:92:ARG:HG3	1:D:67:ARG:HG2	1.89	0.54
1:E:150:LYS:HA	1:E:195:ASP:HB2	1.90	0.54
1:M:174:THR:HG22	1:M:211:LEU:HD11	1.89	0.54
1:R:26:MET:HG3	1:R:76:PHE:HB3	1.89	0.54
1:G:38:VAL:O	1:G:39:ALA:HB2	2.08	0.54
1:H:53:GLU:O	1:H:56:LYS:HG3	2.08	0.54
1:K:190:GLY:HA3	1:O:212:MET:HG3	1.90	0.54
1:F:67:ARG:HG2	1:G:92:ARG:HG3	1.90	0.54
1:K:158:MET:O	1:K:163:ARG:NH1	2.38	0.54
1:S:53:GLU:O	1:S:56:LYS:HG3	2.07	0.54
1:S:24:PHE:HB2	1:S:109:LEU:HB2	1.89	0.53
1:F:20:VAL:H	1:F:113:THR:HB	1.73	0.53
1:J:174:THR:HG22	1:J:211:LEU:CD1	2.38	0.53
1:A:157:ASN:HD21	1:E:218:VAL:C	2.12	0.53
1:L:65:LEU:HB3	1:L:235:THR:HG22	1.90	0.53
1:Q:180:ASN:HB3	1:Q:181:VAL:HG23	1.89	0.53
1:A:18:PRO:HA	1:A:113:THR:HG21	1.87	0.53
1:C:18:PRO:CA	1:C:113:THR:HG22	2.21	0.53
1:H:119:ILE:HG13	2:H:1000:HEM:HMA3	1.90	0.53
1:F:211:LEU:HD11	2:F:1000:HEM:CBB	2.38	0.53
1:M:28:LYS:NZ	1:M:72:ASN:HD22	2.07	0.53
1:O:188:SER:HB2	1:O:194:THR:O	2.08	0.53
1:J:235:THR:CG2	1:J:237:HIS:NE2	2.67	0.53
1:S:118:TYR:CE2	2:S:1000:HEM:O1D	2.62	0.53
1:P:221:ASN:HA	1:P:224:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:118:TYR:CD2	1:T:167:MET:HG3	2.44	0.53
1:A:190:GLY:HA2	1:E:212:MET:HG3	1.90	0.53
1:N:26:MET:HB3	1:N:73:SER:HB3	1.91	0.53
1:O:19:GLY:N	1:O:113:THR:HG22	2.24	0.53
1:F:97:THR:HG22	1:F:100:GLY:H	1.74	0.52
1:N:188:SER:HB2	1:N:194:THR:O	2.10	0.52
1:A:235:THR:CG2	1:A:237:HIS:NE2	2.71	0.52
1:C:174:THR:HB	2:C:1000:HEM:CBB	2.38	0.52
1:E:18:PRO:CA	1:E:113:THR:HG22	2.20	0.52
1:L:211:LEU:HD11	2:L:1000:HEM:HBB2	1.91	0.52
1:B:166:GLU:OE1	1:B:166:GLU:HA	2.10	0.52
1:F:196:PHE:CE1	2:F:1000:HEM:O2D	2.57	0.52
1:G:233:LEU:HD12	1:G:234:GLY:N	2.24	0.52
1:H:212:MET:HG3	1:I:190:GLY:HA3	1.91	0.52
1:R:177:TYR:CD2	1:R:211:LEU:HD13	2.44	0.52
1:E:97:THR:HG22	1:E:100:GLY:N	2.23	0.52
1:K:211:LEU:CD1	2:K:1000:HEM:HBB2	2.32	0.52
1:Q:109:LEU:HB3	1:Q:197:ILE:CD1	2.40	0.52
1:T:52:ILE:HG12	1:T:61:VAL:HG21	1.92	0.52
1:G:211:LEU:CD1	2:G:1000:HEM:HBB2	2.33	0.52
1:P:97:THR:CG2	1:P:100:GLY:H	2.22	0.52
1:B:212:MET:HG3	1:C:190:GLY:HA3	1.90	0.52
1:I:20:VAL:H	1:I:113:THR:HB	1.75	0.52
1:J:196:PHE:CE1	2:J:1000:HEM:O2D	2.61	0.52
1:J:235:THR:HG23	1:J:237:HIS:CD2	2.44	0.52
1:R:33:TRP:CH2	1:R:41:ARG:HG2	2.44	0.52
1:B:219:LYS:O	1:B:222:LYS:HB2	2.08	0.52
1:E:221:ASN:HA	1:E:224:HIS:CD2	2.45	0.52
1:N:195:ASP:HB3	1:N:196:PHE:CE2	2.45	0.52
1:O:38:VAL:O	1:O:39:ALA:CB	2.57	0.52
1:Q:110:VAL:O	1:Q:188:SER:OG	2.22	0.52
1:E:20:VAL:H	1:E:113:THR:HB	1.74	0.52
1:H:92:ARG:HH11	1:H:92:ARG:HG2	1.74	0.52
1:H:211:LEU:HD11	2:H:1000:HEM:CBB	2.40	0.52
1:J:38:VAL:O	1:J:39:ALA:HB2	2.10	0.52
1:T:211:LEU:CD1	2:T:1000:HEM:HBB2	2.40	0.52
1:B:105:VAL:HG12	1:D:71:THR:HG23	1.92	0.52
1:E:116:LEU:HA	2:E:1000:HEM:O1A	2.10	0.52
1:J:174:THR:CG2	2:J:1000:HEM:HBB2	2.40	0.52
1:K:38:VAL:O	1:K:39:ALA:CB	2.58	0.52
1:T:33:TRP:HB2	1:T:102:ASN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:TYR:CD2	1:G:167:MET:HG3	2.45	0.51
1:Q:222:LYS:HE2	1:R:154:GLU:OE1	2.08	0.51
1:T:159:SER:OG	1:T:162:GLU:HG3	2.10	0.51
1:A:174:THR:HB	2:A:1000:HEM:CBB	2.35	0.51
1:J:211:LEU:HD11	2:J:1000:HEM:HBB2	1.90	0.51
1:J:221:ASN:HA	1:J:224:HIS:CD2	2.45	0.51
1:L:215:LEU:O	1:L:218:VAL:HG22	2.10	0.51
1:P:97:THR:HG23	1:P:100:GLY:H	1.76	0.51
1:T:221:ASN:HA	1:T:224:HIS:CD2	2.45	0.51
1:B:18:PRO:CA	1:B:113:THR:HG22	2.28	0.51
1:F:177:TYR:HB2	2:F:1000:HEM:HBB1	1.92	0.51
1:P:30:ARG:NH2	1:S:31:PRO:HB3	2.26	0.51
1:J:174:THR:HG22	1:J:211:LEU:HD11	1.91	0.51
1:L:178:LEU:HD21	2:L:1000:HEM:HMB3	1.92	0.51
1:M:70:GLU:OE2	1:M:232:THR:HA	2.11	0.51
1:P:20:VAL:H	1:P:113:THR:HB	1.74	0.51
1:G:18:PRO:HA	1:G:113:THR:HG21	1.84	0.51
1:M:174:THR:HB	2:M:1000:HEM:CBB	2.39	0.51
1:O:116:LEU:CA	2:O:1000:HEM:O1A	2.58	0.51
1:T:23:VAL:HG22	1:T:110:VAL:HG22	1.93	0.51
1:Q:116:LEU:CA	2:Q:1000:HEM:O1A	2.58	0.51
1:A:36:VAL:O	1:A:41:ARG:HD3	2.10	0.51
1:B:61:VAL:HG22	1:B:79:ILE:CD1	2.41	0.51
1:C:11:ARG:NH2	1:C:62:ASP:OD1	2.44	0.51
1:S:147:ILE:HG12	1:S:231:THR:HG23	1.92	0.51
1:G:180:ASN:HB3	1:G:181:VAL:HG23	1.92	0.51
1:G:38:VAL:O	1:G:38:VAL:HG13	2.11	0.51
1:K:159:SER:OG	1:K:162:GLU:HG3	2.10	0.51
1:L:235:THR:HG23	1:L:237:HIS:CD2	2.46	0.51
1:T:211:LEU:HD11	2:T:1000:HEM:HBB2	1.91	0.51
2:B:1000:HEM:HBB2	2:B:1000:HEM:HHC	1.93	0.51
1:C:211:LEU:HD11	2:C:1000:HEM:HBB2	1.93	0.51
1:O:38:VAL:O	1:O:39:ALA:HB2	2.10	0.51
1:P:9:ILE:HG22	1:P:9:ILE:O	2.11	0.51
1:B:196:PHE:HZ	2:B:1000:HEM:O2D	1.86	0.50
1:B:38:VAL:O	1:B:39:ALA:HB2	2.11	0.50
1:E:119:ILE:HG13	2:E:1000:HEM:HMA3	1.93	0.50
2:K:1000:HEM:CBB	2:K:1000:HEM:HHC	2.41	0.50
1:S:94:PHE:O	1:S:97:THR:HG22	2.11	0.50
1:C:174:THR:HG22	1:C:211:LEU:CD1	2.41	0.50
1:C:75:PHE:CD1	1:C:246:LEU:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:TYR:HE2	2:H:1000:HEM:O1D	1.94	0.50
1:N:158:MET:O	1:N:163:ARG:NH1	2.44	0.50
1:R:180:ASN:HB3	1:R:181:VAL:HG23	1.93	0.50
1:C:177:TYR:HB2	2:C:1000:HEM:HBB1	1.92	0.50
1:J:201:GLU:HG2	1:J:236:ILE:HD11	1.92	0.50
1:L:118:TYR:HE2	2:L:1000:HEM:O1D	1.93	0.50
1:J:94:PHE:O	1:J:97:THR:HB	2.11	0.50
1:O:33:TRP:CH2	1:O:41:ARG:HG2	2.45	0.50
1:A:63:LEU:HG	1:A:242:VAL:HG11	1.93	0.50
1:F:44:ALA:HB1	1:F:99:VAL:HG22	1.92	0.50
1:J:211:LEU:HD11	2:J:1000:HEM:CBB	2.42	0.50
1:Q:235:THR:CG2	1:Q:237:HIS:NE2	2.75	0.50
1:N:66:THR:HG22	1:N:234:GLY:HA3	1.94	0.50
1:A:212:MET:HG3	1:D:190:GLY:CA	2.41	0.50
1:D:182:LYS:O	1:D:200:PHE:HA	2.12	0.50
1:L:180:ASN:HB3	1:L:181:VAL:HG23	1.94	0.50
1:S:174:THR:HB	2:S:1000:HEM:HBB2	1.93	0.50
1:L:211:LEU:HD11	2:L:1000:HEM:CBB	2.42	0.50
2:H:1000:HEM:CHC	2:H:1000:HEM:HBB2	2.41	0.49
1:K:145:ILE:HD13	1:K:233:LEU:HD13	1.94	0.49
1:S:177:TYR:HB2	2:S:1000:HEM:HBB1	1.94	0.49
1:S:38:VAL:O	1:S:39:ALA:HB2	2.12	0.49
1:K:169:VAL:O	1:K:173:PRO:HD3	2.11	0.49
1:A:94:PHE:O	1:A:97:THR:HB	2.11	0.49
1:E:33:TRP:O	1:E:41:ARG:HD2	2.13	0.49
1:O:11:ARG:NH2	1:O:62:ASP:OD1	2.45	0.49
1:G:211:LEU:CD1	2:G:1000:HEM:CBB	2.91	0.49
1:I:221:ASN:HA	1:I:224:HIS:CD2	2.47	0.49
1:N:116:LEU:HA	2:N:1000:HEM:O1A	2.12	0.49
1:Q:29:LEU:HD23	1:Q:103:ALA:HB2	1.94	0.49
1:A:117:ASN:N	2:A:1000:HEM:O1A	2.44	0.49
1:G:221:ASN:HA	1:G:224:HIS:CD2	2.48	0.49
2:L:1000:HEM:HBB2	2:L:1000:HEM:CHC	2.33	0.49
1:M:211:LEU:CD1	2:M:1000:HEM:CBB	2.90	0.49
1:S:59:VAL:HG12	1:S:81:ALA:HB2	1.94	0.49
1:A:136:TYR:C	1:A:136:TYR:CD2	2.86	0.49
1:A:41:ARG:HH21	1:A:248:ASP:HA	1.77	0.49
1:D:237:HIS:HB2	1:D:242:VAL:HG23	1.95	0.49
1:J:28:LYS:NZ	1:J:72:ASN:HD22	2.10	0.49
1:M:38:VAL:O	1:M:39:ALA:HB2	2.12	0.49
1:N:36:VAL:O	1:N:41:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:211:LEU:CD2	2:P:1000:HEM:CBB	2.91	0.49
1:T:174:THR:HB	2:T:1000:HEM:C3B	2.48	0.49
1:E:150:LYS:HG2	1:E:225:VAL:HG23	1.94	0.49
1:H:224:HIS:CE1	6:H:3000:HOH:O	2.65	0.49
1:I:119:ILE:HG13	2:I:1000:HEM:CMA	2.42	0.49
1:R:118:TYR:CD2	1:R:167:MET:HG3	2.48	0.49
1:Q:212:MET:HG3	1:R:190:GLY:CA	2.43	0.49
1:A:64:TYR:CD1	1:A:144:VAL:HG11	2.48	0.49
1:A:237:HIS:HB2	1:A:242:VAL:HG23	1.94	0.49
1:F:97:THR:CG2	1:F:100:GLY:H	2.26	0.49
1:F:71:THR:HG23	1:G:105:VAL:HG12	1.95	0.49
1:I:64:TYR:CD2	1:I:76:PHE:CE2	3.01	0.49
1:M:20:VAL:H	1:M:113:THR:HB	1.77	0.49
1:A:219:LYS:N	1:D:157:ASN:HD21	2.11	0.48
1:T:36:VAL:O	1:T:41:ARG:HD3	2.13	0.48
1:B:53:GLU:CD	1:B:56:LYS:HZ3	2.16	0.48
1:H:64:TYR:CD1	1:H:144:VAL:HG11	2.47	0.48
1:I:180:ASN:HB2	1:I:181:VAL:HG23	1.94	0.48
1:M:94:PHE:O	1:M:97:THR:HB	2.12	0.48
1:S:198:THR:HG21	2:S:1000:HEM:HBC2	1.94	0.48
1:T:142:ARG:NE	1:T:203:ASP:OD1	2.45	0.48
1:Q:18:PRO:CA	1:Q:113:THR:HG22	2.36	0.48
1:F:33:TRP:O	1:F:41:ARG:HD2	2.13	0.48
1:L:44:ALA:HB1	1:L:99:VAL:CG2	2.44	0.48
1:N:44:ALA:HB1	1:N:99:VAL:HG22	1.96	0.48
1:P:69:LEU:HG	1:T:88:GLN:HG3	1.96	0.48
1:C:221:ASN:ND2	1:C:224:HIS:CD2	2.59	0.48
1:E:116:LEU:HD13	1:E:119:ILE:O	2.12	0.48
1:I:38:VAL:O	1:I:39:ALA:CB	2.61	0.48
1:C:38:VAL:HB	1:C:41:ARG:HH12	1.79	0.48
4:T:2001:MES:H81	4:T:2001:MES:H51	1.56	0.48
1:O:19:GLY:H	1:O:113:THR:HG22	1.78	0.48
1:Q:158:MET:O	1:Q:163:ARG:NH1	2.47	0.48
1:C:28:LYS:CE	1:C:72:ASN:HA	2.44	0.48
1:Q:211:LEU:HD21	2:Q:1000:HEM:CBB	2.44	0.48
1:S:174:THR:HG22	1:S:211:LEU:CD1	2.44	0.48
1:T:186:TYR:HB2	1:T:197:ILE:HB	1.95	0.48
1:C:118:TYR:CD2	1:C:167:MET:HG3	2.49	0.48
1:D:53:GLU:HG2	1:D:56:LYS:NZ	2.29	0.48
1:J:70:GLU:HA	1:J:70:GLU:OE1	2.13	0.48
1:L:94:PHE:O	1:L:97:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:38:VAL:HB	1:R:41:ARG:NH1	2.28	0.48
1:B:63:LEU:HD23	1:B:239:PRO:HA	1.95	0.47
1:F:117:ASN:N	2:F:1000:HEM:O1A	2.46	0.47
1:I:94:PHE:O	1:I:97:THR:HB	2.14	0.47
1:K:66:THR:HG22	1:K:234:GLY:HA3	1.96	0.47
1:O:94:PHE:O	1:O:97:THR:HB	2.14	0.47
1:N:182:LYS:O	1:N:200:PHE:HA	2.14	0.47
1:P:118:TYR:HE2	2:P:1000:HEM:O1D	1.98	0.47
1:P:145:ILE:CD1	1:P:233:LEU:HD13	2.44	0.47
1:G:70:GLU:HA	1:G:70:GLU:OE1	2.14	0.47
1:J:26:MET:N	1:J:26:MET:SD	2.88	0.47
1:M:18:PRO:CA	1:M:113:THR:HG22	2.25	0.47
1:R:235:THR:CG2	1:R:237:HIS:NE2	2.66	0.47
1:T:44:ALA:HB1	1:T:99:VAL:HG22	1.97	0.47
1:A:145:ILE:CD1	1:A:233:LEU:HD13	2.44	0.47
1:F:26:MET:HB2	1:F:107:GLU:HB2	1.96	0.47
1:H:198:THR:HG21	2:H:1000:HEM:HBC2	1.96	0.47
1:I:70:GLU:OE2	1:I:232:THR:HA	2.14	0.47
1:J:11:ARG:NH2	1:J:62:ASP:OD1	2.47	0.47
1:K:118:TYR:CD2	1:K:167:MET:HG3	2.49	0.47
1:K:190:GLY:HA2	1:O:212:MET:HG3	1.95	0.47
1:M:180:ASN:HB3	1:M:181:VAL:HG23	1.96	0.47
1:P:218:VAL:C	1:T:157:ASN:HD21	2.18	0.47
1:B:235:THR:HG23	1:B:237:HIS:CD2	2.49	0.47
1:E:177:TYR:HB2	2:E:1000:HEM:HBB1	1.97	0.47
1:E:28:LYS:HD2	1:E:106:PHE:CE1	2.50	0.47
1:B:28:LYS:NZ	1:B:72:ASN:HD22	2.12	0.47
1:G:222:LYS:HE3	1:H:154:GLU:OE1	2.15	0.47
1:K:24:PHE:O	1:K:108:THR:HA	2.15	0.47
1:M:211:LEU:O	1:M:214:SER:HB2	2.13	0.47
1:P:38:VAL:O	1:P:39:ALA:CB	2.63	0.47
1:Q:145:ILE:HA	1:Q:232:THR:O	2.15	0.47
1:B:233:LEU:HD12	1:B:234:GLY:N	2.30	0.47
1:Q:211:LEU:HD11	2:Q:1000:HEM:CBB	2.44	0.47
1:R:33:TRP:O	1:R:41:ARG:HD2	2.14	0.47
1:N:9:ILE:O	1:N:9:ILE:HG22	2.15	0.47
1:R:14:ILE:HD12	1:R:82:TYR:CE2	2.48	0.47
1:A:211:LEU:HD11	2:A:1000:HEM:CBB	2.45	0.47
1:A:174:THR:O	2:A:1000:HEM:CBB	2.63	0.47
2:B:1000:HEM:CBB	2:B:1000:HEM:HHC	2.45	0.47
1:B:55:HIS:CD2	1:B:58:ASN:HD22	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:116:LEU:CD2	2:N:1000:HEM:HBA2	2.45	0.47
1:Q:67:ARG:HG2	1:R:92:ARG:HG3	1.96	0.47
1:B:53:GLU:CD	1:B:56:LYS:HZ1	2.14	0.46
1:E:159:SER:OG	1:E:162:GLU:HG3	2.15	0.46
1:K:219:LYS:N	1:L:157:ASN:HD21	2.14	0.46
1:E:70:GLU:OE2	1:E:232:THR:HA	2.14	0.46
1:J:180:ASN:HB3	1:J:181:VAL:HG23	1.97	0.46
1:S:167:MET:CE	2:S:1000:HEM:HBD1	2.46	0.46
1:T:17:GLN:O	1:T:113:THR:CG2	2.51	0.46
1:C:211:LEU:CD1	2:C:1000:HEM:CBB	2.93	0.46
1:D:38:VAL:O	1:D:39:ALA:HB3	2.15	0.46
1:M:212:MET:HG3	1:N:190:GLY:HA2	1.97	0.46
1:M:36:VAL:O	1:M:41:ARG:HD3	2.15	0.46
1:C:59:VAL:HG12	1:C:81:ALA:HB2	1.98	0.46
1:C:66:THR:HG22	1:C:234:GLY:HA3	1.96	0.46
1:E:65:LEU:HB3	1:E:235:THR:HG22	1.96	0.46
1:H:222:LYS:HE2	1:I:154:GLU:OE1	2.15	0.46
1:O:21:PHE:O	1:O:80:ASN:HA	2.16	0.46
1:B:44:ALA:HB1	1:B:99:VAL:HG22	1.98	0.46
4:E:2001:MES:H82	4:E:2001:MES:H51	1.68	0.46
1:J:95:ARG:HA	1:J:100:GLY:HA3	1.96	0.46
1:P:157:ASN:HD21	1:S:219:LYS:N	2.13	0.46
1:R:118:TYR:CE2	2:R:1000:HEM:O1D	2.62	0.46
1:R:235:THR:HG23	1:R:237:HIS:CD2	2.50	0.46
1:M:118:TYR:CD2	1:M:167:MET:HG3	2.50	0.46
1:P:211:LEU:HD21	2:P:1000:HEM:HBB2	1.98	0.46
1:B:55:HIS:HD2	1:B:58:ASN:HD22	1.62	0.46
1:B:61:VAL:HG22	1:B:79:ILE:HD12	1.98	0.46
1:L:118:TYR:CD2	1:L:167:MET:HG3	2.50	0.46
1:M:170:HIS:O	1:M:173:PRO:HD2	2.15	0.46
1:N:28:LYS:HD2	1:N:106:PHE:CE1	2.51	0.46
1:P:14:ILE:HG13	1:P:82:TYR:CZ	2.51	0.46
1:P:211:LEU:CD1	2:P:1000:HEM:HBB2	2.45	0.46
1:A:92:ARG:HG2	1:A:92:ARG:HH11	1.81	0.46
1:E:150:LYS:HG2	1:E:225:VAL:CG2	2.45	0.46
1:G:33:TRP:HA	1:G:36:VAL:HG23	1.97	0.46
1:J:118:TYR:CE2	2:J:1000:HEM:O1D	2.63	0.46
2:M:1000:HEM:HHC	2:M:1000:HEM:CBB	2.45	0.46
1:O:174:THR:HB	2:O:1000:HEM:CBB	2.44	0.46
1:P:66:THR:HG22	1:P:234:GLY:CA	2.45	0.46
1:S:97:THR:HG23	1:S:100:GLY:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:LYS:HB2	1:I:201:GLU:HB2	1.97	0.46
1:A:174:THR:CG2	2:A:1000:HEM:HBB2	2.45	0.45
1:L:119:ILE:HG13	2:L:1000:HEM:HMA3	1.98	0.45
1:C:159:SER:OG	1:C:162:GLU:HG3	2.15	0.45
1:C:224:HIS:HE1	6:C:3000:HOH:O	1.99	0.45
1:F:180:ASN:CB	1:F:181:VAL:HG23	2.45	0.45
1:G:211:LEU:O	1:G:214:SER:HB2	2.15	0.45
1:J:158:MET:O	1:J:163:ARG:NH1	2.48	0.45
1:N:21:PHE:O	1:N:80:ASN:HA	2.16	0.45
1:D:65:LEU:HB3	1:D:235:THR:HG22	1.97	0.45
1:G:233:LEU:HD12	1:G:233:LEU:C	2.37	0.45
1:T:188:SER:O	1:T:189:THR:C	2.53	0.45
1:T:150:LYS:HB3	1:T:226:ARG:HB3	1.97	0.45
1:C:222:LYS:CE	1:E:154:GLU:OE1	2.64	0.45
1:F:222:LYS:HE2	1:G:154:GLU:OE1	2.16	0.45
1:G:118:TYR:HE2	2:G:1000:HEM:O1D	1.98	0.45
1:H:26:MET:HB3	1:H:73:SER:HB3	1.99	0.45
1:L:182:LYS:HB2	1:L:201:GLU:HB2	1.97	0.45
1:L:126:GLY:HA3	1:R:126:GLY:O	2.16	0.45
1:Q:31:PRO:HB3	1:R:30:ARG:NH2	2.31	0.45
1:T:117:ASN:N	2:T:1000:HEM:O1A	2.45	0.45
1:B:221:ASN:HA	1:B:224:HIS:CD2	2.51	0.45
1:B:41:ARG:NH2	1:B:247:ALA:O	2.41	0.45
1:G:44:ALA:HB1	1:G:99:VAL:CG2	2.46	0.45
1:I:91:MET:O	1:I:95:ARG:HG3	2.16	0.45
1:J:174:THR:CB	2:J:1000:HEM:HBB2	2.45	0.45
1:J:48:VAL:O	1:J:52:ILE:HG13	2.17	0.45
1:A:188:SER:HB2	1:A:194:THR:O	2.16	0.45
1:G:188:SER:HB2	1:G:194:THR:HG23	1.98	0.45
1:G:33:TRP:CZ2	1:G:41:ARG:HG2	2.51	0.45
1:L:219:LYS:O	1:L:220:GLU:C	2.55	0.45
1:G:235:THR:CG2	1:G:237:HIS:NE2	2.79	0.45
1:C:75:PHE:CD1	1:C:246:LEU:CD1	2.99	0.45
1:F:229:SER:N	1:F:230:PRO:HA	2.32	0.45
1:H:235:THR:HG23	1:H:237:HIS:CD2	2.52	0.45
1:J:97:THR:HG23	1:J:99:VAL:N	2.32	0.45
1:P:174:THR:HG22	1:P:211:LEU:CD1	2.44	0.45
1:P:211:LEU:HD21	2:P:1000:HEM:CBB	2.46	0.45
1:S:33:TRP:CZ2	1:S:41:ARG:HG2	2.51	0.45
1:L:212:MET:HG3	1:M:190:GLY:CA	2.45	0.45
1:T:145:ILE:CD1	1:T:233:LEU:HD13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:180:ASN:CB	1:I:181:VAL:HG23	2.47	0.45
1:L:38:VAL:O	1:L:39:ALA:CB	2.65	0.45
1:T:62:ASP:HB3	1:T:64:TYR:CZ	2.52	0.45
1:T:22:GLY:HA2	1:T:79:ILE:O	2.16	0.45
1:F:92:ARG:NH1	1:J:245:ALA:HB1	2.31	0.44
1:K:167:MET:CE	2:K:1000:HEM:HBD1	2.47	0.44
1:R:33:TRP:C	1:R:35:LYS:H	2.19	0.44
1:S:150:LYS:HA	1:S:195:ASP:HB2	1.99	0.44
1:T:166:GLU:OE1	1:T:166:GLU:HA	2.16	0.44
1:T:18:PRO:HA	1:T:113:THR:CG2	2.31	0.44
1:H:224:HIS:HE1	6:H:3000:HOH:O	2.00	0.44
1:I:222:LYS:CE	1:J:154:GLU:OE1	2.65	0.44
1:J:159:SER:OG	1:J:162:GLU:HG3	2.17	0.44
1:T:94:PHE:O	1:T:97:THR:HG22	2.18	0.44
1:B:59:VAL:HB	1:B:79:ILE:HG23	1.98	0.44
1:H:117:ASN:H	2:H:1000:HEM:CGA	2.29	0.44
1:H:24:PHE:HB2	1:H:109:LEU:HB2	1.98	0.44
1:I:28:LYS:HZ2	1:I:72:ASN:HD22	1.63	0.44
1:K:211:LEU:O	1:K:214:SER:HB2	2.17	0.44
1:N:119:ILE:N	1:N:119:ILE:HD13	2.31	0.44
1:R:221:ASN:HA	1:R:224:HIS:CD2	2.52	0.44
1:S:29:LEU:HD23	1:S:103:ALA:HB2	2.00	0.44
1:I:212:MET:CG	1:J:190:GLY:HA3	2.43	0.44
1:J:64:TYR:HB2	1:J:76:PHE:CE1	2.53	0.44
1:L:75:PHE:CD1	1:L:246:LEU:HD11	2.53	0.44
1:A:19:GLY:N	1:A:113:THR:HG22	2.32	0.44
1:K:88:GLN:O	1:K:92:ARG:HB2	2.17	0.44
1:N:196:PHE:HZ	2:N:1000:HEM:O2D	1.92	0.44
4:N:2001:MES:H51	4:N:2001:MES:H82	1.61	0.44
1:B:217:GLN:HG2	1:C:156:TRP:O	2.17	0.44
4:F:2001:MES:H51	4:F:2001:MES:H82	1.29	0.44
1:L:66:THR:HG22	1:L:234:GLY:HA3	1.98	0.44
1:M:117:ASN:N	2:M:1000:HEM:O1A	2.48	0.44
1:P:222:LYS:HE2	1:T:154:GLU:OE1	2.18	0.44
1:C:211:LEU:HD11	2:C:1000:HEM:CBB	2.48	0.44
1:D:145:ILE:HA	1:D:232:THR:O	2.18	0.44
1:J:188:SER:O	1:J:189:THR:C	2.55	0.44
1:J:92:ARG:HG2	1:J:92:ARG:HH11	1.82	0.44
1:L:44:ALA:HB1	1:L:99:VAL:HG22	2.00	0.44
1:M:116:LEU:CA	2:M:1000:HEM:O1A	2.64	0.44
1:M:218:VAL:C	1:N:157:ASN:HD21	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:97:THR:HG22	1:Q:100:GLY:N	2.19	0.44
1:E:195:ASP:HB3	1:E:196:PHE:CE2	2.53	0.44
1:F:38:VAL:HB	1:F:41:ARG:HH12	1.83	0.44
1:G:29:LEU:HD23	1:G:103:ALA:HB2	2.00	0.44
1:G:55:HIS:CD2	1:G:58:ASN:HD22	2.36	0.44
1:J:238:SER:O	1:J:239:PRO:C	2.56	0.44
1:K:21:PHE:O	1:K:80:ASN:HA	2.18	0.44
1:O:117:ASN:H	2:O:1000:HEM:CGA	2.30	0.44
1:S:38:VAL:O	1:S:39:ALA:CB	2.65	0.44
1:A:41:ARG:NE	1:A:247:ALA:O	2.46	0.44
1:B:159:SER:OG	1:B:162:GLU:HG3	2.18	0.44
1:G:18:PRO:CA	1:G:113:THR:CG2	2.77	0.44
1:G:21:PHE:O	1:G:80:ASN:HA	2.18	0.44
1:N:211:LEU:HD11	2:N:1000:HEM:CBB	2.47	0.44
1:N:215:LEU:HD12	1:N:215:LEU:HA	1.79	0.44
4:O:2001:MES:H82	4:O:2001:MES:H51	1.61	0.44
4:S:2001:MES:H51	4:S:2001:MES:H82	1.72	0.44
1:S:33:TRP:CH2	1:S:41:ARG:HG2	2.52	0.44
1:T:167:MET:CE	2:T:1000:HEM:HBD1	2.47	0.44
1:C:224:HIS:CE1	6:C:3000:HOH:O	2.71	0.43
1:H:235:THR:HG23	1:H:237:HIS:NE2	2.33	0.43
1:I:118:TYR:CD2	1:I:167:MET:HG3	2.53	0.43
1:K:20:VAL:H	1:K:113:THR:HB	1.82	0.43
1:N:116:LEU:HD22	2:N:1000:HEM:HBA2	1.99	0.43
1:Q:235:THR:HG23	1:Q:237:HIS:CD2	2.53	0.43
1:B:149:VAL:HA	1:B:226:ARG:O	2.18	0.43
1:C:229:SER:HA	1:C:230:PRO:HA	1.76	0.43
1:F:62:ASP:O	1:F:77:PHE:HA	2.18	0.43
1:I:169:VAL:O	1:I:173:PRO:HD2	2.18	0.43
1:M:222:LYS:HE2	1:N:154:GLU:OE1	2.18	0.43
1:P:145:ILE:HD13	1:P:233:LEU:HD13	1.99	0.43
1:B:212:MET:HG3	1:C:190:GLY:HA2	1.99	0.43
4:C:2001:MES:H51	4:C:2001:MES:H82	1.75	0.43
1:G:18:PRO:CA	1:G:113:THR:HG22	2.22	0.43
1:G:61:VAL:HG22	1:G:79:ILE:HD12	2.00	0.43
1:I:38:VAL:O	1:I:39:ALA:HB2	2.18	0.43
1:M:229:SER:HA	1:M:230:PRO:HA	1.84	0.43
1:S:116:LEU:CA	2:S:1000:HEM:O1A	2.64	0.43
1:A:27:PHE:CE1	1:A:95:ARG:HD2	2.53	0.43
1:C:63:LEU:HD23	1:C:239:PRO:HA	2.01	0.43
1:B:67:ARG:HG2	1:C:92:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:180:ASN:CB	1:P:181:VAL:HG23	2.47	0.43
1:S:148:PRO:HD2	1:S:228:GLY:HA2	1.99	0.43
1:S:26:MET:HB3	1:S:73:SER:HB3	2.01	0.43
1:E:8:LYS:HE2	1:E:8:LYS:HB2	1.58	0.43
1:Q:38:VAL:O	1:Q:38:VAL:HG13	2.18	0.43
1:B:20:VAL:H	1:B:113:THR:HB	1.83	0.43
1:G:97:THR:HG22	1:G:100:GLY:N	2.19	0.43
1:H:147:ILE:HD13	1:H:212:MET:HE2	2.01	0.43
1:J:167:MET:CE	2:J:1000:HEM:HBD1	2.48	0.43
1:N:221:ASN:HA	1:N:224:HIS:CD2	2.54	0.43
1:P:235:THR:HG21	1:T:88:GLN:OE1	2.19	0.43
1:R:36:VAL:O	1:R:41:ARG:HD3	2.17	0.43
1:S:78:ARG:NH1	1:S:199:TYR:CE2	2.87	0.43
1:C:118:TYR:HE2	2:C:1000:HEM:O1D	2.01	0.43
1:E:28:LYS:NZ	1:E:72:ASN:HD22	2.16	0.43
1:I:188:SER:HB2	1:I:194:THR:O	2.19	0.43
1:M:219:LYS:N	1:N:157:ASN:HD21	2.16	0.43
1:R:84:LEU:HD12	1:R:84:LEU:HA	1.84	0.43
1:S:61:VAL:HG12	1:S:62:ASP:N	2.33	0.43
1:B:174:THR:HG22	1:B:211:LEU:CD1	2.49	0.43
1:E:37:PRO:O	1:E:39:ALA:N	2.52	0.43
1:C:174:THR:CB	2:C:1000:HEM:HBB2	2.47	0.43
1:C:67:ARG:HD2	1:C:74:ASP:OD1	2.19	0.43
1:F:116:LEU:CA	2:F:1000:HEM:O1A	2.66	0.43
1:M:145:ILE:HD13	1:M:233:LEU:HD13	2.01	0.43
1:O:235:THR:HG23	1:O:237:HIS:NE2	2.34	0.43
1:T:235:THR:HG23	1:T:237:HIS:CD2	2.53	0.43
1:E:229:SER:HA	1:E:230:PRO:HA	1.89	0.43
1:F:169:VAL:O	1:F:173:PRO:HD3	2.19	0.43
1:I:174:THR:HG22	1:I:211:LEU:CD1	2.49	0.43
1:I:24:PHE:O	1:I:108:THR:HA	2.19	0.43
1:N:55:HIS:CD2	1:N:58:ASN:HD22	2.37	0.43
1:O:17:GLN:O	1:O:113:THR:CG2	2.51	0.43
1:Q:204:ASP:O	1:Q:207:ALA:HB3	2.18	0.43
1:S:149:VAL:HA	1:S:226:ARG:O	2.19	0.43
1:A:221:ASN:HA	1:A:224:HIS:CD2	2.54	0.42
1:F:144:VAL:O	1:F:233:LEU:HA	2.18	0.42
1:H:235:THR:HG21	1:I:88:GLN:OE1	2.19	0.42
1:T:66:THR:HG22	1:T:234:GLY:HA3	1.99	0.42
1:C:211:LEU:CD1	2:C:1000:HEM:HBB2	2.49	0.42
1:D:196:PHE:HZ	2:D:1000:HEM:O2D	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:VAL:O	1:G:39:ALA:CB	2.67	0.42
1:I:97:THR:HG23	1:I:98:THR:N	2.34	0.42
1:O:177:TYR:HB2	2:O:1000:HEM:HBB1	2.00	0.42
1:O:180:ASN:HB3	1:O:181:VAL:HG23	2.01	0.42
1:P:27:PHE:HB2	1:P:75:PHE:CZ	2.55	0.42
1:R:38:VAL:HB	1:R:41:ARG:HH12	1.84	0.42
1:R:38:VAL:O	1:R:39:ALA:HB2	2.18	0.42
1:B:130:GLY:O	1:B:131:LEU:C	2.57	0.42
1:D:28:LYS:HD2	1:D:106:PHE:CE1	2.54	0.42
1:H:150:LYS:HA	1:H:195:ASP:HB2	2.02	0.42
1:O:119:ILE:HG13	2:O:1000:HEM:HMA3	2.01	0.42
1:Q:24:PHE:HB2	1:Q:109:LEU:HB2	2.01	0.42
1:R:26:MET:HG3	1:R:76:PHE:CB	2.49	0.42
1:A:182:LYS:O	1:A:200:PHE:HA	2.19	0.42
1:G:235:THR:HG23	1:G:237:HIS:CD2	2.54	0.42
1:H:20:VAL:H	1:H:113:THR:HB	1.85	0.42
1:I:235:THR:HG23	1:I:237:HIS:CD2	2.54	0.42
1:P:235:THR:HG23	1:P:237:HIS:CD2	2.54	0.42
1:T:53:GLU:O	1:T:56:LYS:HG3	2.19	0.42
1:E:70:GLU:HA	1:E:70:GLU:OE1	2.19	0.42
1:F:94:PHE:O	1:F:97:THR:HG22	2.19	0.42
1:J:38:VAL:O	1:J:39:ALA:CB	2.67	0.42
1:K:92:ARG:HG2	1:K:92:ARG:HH11	1.84	0.42
1:P:229:SER:HA	1:P:230:PRO:HA	1.88	0.42
1:R:159:SER:OG	1:R:162:GLU:HG3	2.18	0.42
1:R:177:TYR:CG	1:R:211:LEU:HD13	2.54	0.42
1:P:154:GLU:OE1	1:S:222:LYS:HE2	2.20	0.42
1:C:150:LYS:HA	1:C:195:ASP:HB2	2.02	0.42
1:R:119:ILE:HG13	2:R:1000:HEM:HMA2	2.00	0.42
1:T:242:VAL:O	1:T:246:LEU:HG	2.20	0.42
1:T:70:GLU:OE2	1:T:232:THR:HA	2.20	0.42
1:A:116:LEU:HD13	1:A:119:ILE:O	2.20	0.42
1:J:117:ASN:N	2:J:1000:HEM:O1A	2.48	0.42
1:N:13:THR:O	1:N:16:THR:HB	2.19	0.42
1:O:20:VAL:H	1:O:113:THR:HB	1.85	0.42
1:O:235:THR:HG23	1:O:237:HIS:CD2	2.54	0.42
1:P:144:VAL:O	1:P:233:LEU:HA	2.19	0.42
1:T:38:VAL:O	1:T:39:ALA:HB2	2.20	0.42
1:D:75:PHE:CD1	1:D:246:LEU:HD11	2.55	0.42
1:H:233:LEU:HD12	1:H:234:GLY:N	2.35	0.42
1:Q:59:VAL:HG12	1:Q:81:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:118:TYR:CD2	1:J:167:MET:HG3	2.55	0.42
1:J:183:ARG:NE	3:J:2000:NO2:N	2.55	0.42
1:K:18:PRO:CA	1:K:113:THR:HG22	2.34	0.42
1:K:212:MET:HG3	1:L:190:GLY:HA3	2.01	0.42
1:R:99:VAL:HG21	1:R:243:ILE:HD12	2.02	0.42
1:R:33:TRP:C	1:R:35:LYS:N	2.73	0.42
1:F:66:THR:HG22	1:F:234:GLY:HA3	2.01	0.42
1:I:174:THR:HG22	1:I:211:LEU:HD12	2.01	0.42
1:S:211:LEU:CD1	2:S:1000:HEM:HBB2	2.50	0.42
1:C:166:GLU:HA	1:C:166:GLU:OE1	2.20	0.41
1:I:29:LEU:HD11	1:I:246:LEU:HD22	2.01	0.41
1:K:63:LEU:HD21	1:K:243:ILE:HD11	2.02	0.41
1:Q:88:GLN:OE1	1:T:235:THR:HG21	2.19	0.41
1:S:117:ASN:N	2:S:1000:HEM:O1A	2.48	0.41
1:S:24:PHE:CE2	1:S:197:ILE:HG21	2.55	0.41
1:T:26:MET:HG3	1:T:76:PHE:CB	2.50	0.41
1:D:235:THR:CG2	1:D:237:HIS:NE2	2.78	0.41
1:L:63:LEU:HD21	1:L:243:ILE:HD11	2.03	0.41
1:S:117:ASN:H	2:S:1000:HEM:CGA	2.32	0.41
1:S:70:GLU:OE1	1:S:70:GLU:HA	2.19	0.41
1:A:119:ILE:HG13	2:A:1000:HEM:HMA2	2.01	0.41
1:B:38:VAL:O	1:B:39:ALA:CB	2.68	0.41
1:I:224:HIS:HE1	6:I:3000:HOH:O	2.02	0.41
1:K:150:LYS:HA	1:K:195:ASP:HB2	2.02	0.41
1:T:138:GLY:HA3	1:T:139:PRO:HD3	1.93	0.41
1:A:33:TRP:CH2	1:A:41:ARG:HG2	2.56	0.41
1:F:237:HIS:HB2	1:F:242:VAL:HG23	2.01	0.41
1:G:177:TYR:HB2	2:G:1000:HEM:HBB1	2.02	0.41
1:L:145:ILE:CD1	1:L:233:LEU:HD13	2.50	0.41
1:N:196:PHE:CE1	2:N:1000:HEM:O2D	2.73	0.41
1:Q:217:GLN:HA	1:R:156:TRP:O	2.21	0.41
1:T:116:LEU:CA	2:T:1000:HEM:O1A	2.63	0.41
1:T:213:LEU:O	1:T:217:GLN:HG3	2.20	0.41
1:K:219:LYS:O	1:K:222:LYS:HB2	2.20	0.41
2:M:1000:HEM:HHC	2:M:1000:HEM:HBB2	2.02	0.41
1:N:71:THR:HG23	1:O:105:VAL:HG12	2.02	0.41
1:N:61:VAL:HG22	1:N:79:ILE:HD12	2.03	0.41
1:P:95:ARG:HA	1:P:100:GLY:HA3	2.03	0.41
1:O:229:SER:HA	1:O:230:PRO:HA	1.90	0.41
1:Q:97:THR:HG23	1:Q:99:VAL:H	1.85	0.41
1:A:127:LEU:HD23	1:A:175:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HA	1:A:199:TYR:O	2.20	0.41
1:B:150:LYS:HB3	1:B:226:ARG:HB3	2.03	0.41
1:E:94:PHE:O	1:E:97:THR:HG22	2.20	0.41
1:I:75:PHE:CD1	1:I:246:LEU:HD11	2.56	0.41
1:J:224:HIS:HE1	6:J:3000:HOH:O	2.04	0.41
2:M:1000:HEM:CHC	2:M:1000:HEM:HBB2	2.51	0.41
1:N:33:TRP:CZ2	1:N:41:ARG:HG2	2.56	0.41
1:A:154:GLU:OE1	1:E:222:LYS:HE2	2.21	0.41
2:B:1000:HEM:HBB2	2:B:1000:HEM:CHC	2.51	0.41
1:J:186:TYR:HB2	1:J:197:ILE:HB	2.03	0.41
1:S:235:THR:HG23	1:S:237:HIS:NE2	2.36	0.41
1:C:28:LYS:NZ	1:C:72:ASN:HD22	2.19	0.41
1:E:33:TRP:HB2	1:E:102:ASN:HB3	2.02	0.41
1:G:62:ASP:HB3	1:G:64:TYR:CZ	2.54	0.41
1:J:150:LYS:HG2	1:J:225:VAL:CG2	2.51	0.41
1:P:64:TYR:CD2	1:P:76:PHE:CE2	3.09	0.41
1:C:65:LEU:HB3	1:C:235:THR:HG22	2.02	0.41
1:D:33:TRP:CZ2	1:D:41:ARG:HG2	2.55	0.41
1:F:229:SER:N	1:F:230:PRO:CA	2.84	0.41
1:G:24:PHE:HB2	1:G:109:LEU:HB2	2.03	0.41
1:J:15:LEU:HD23	1:J:15:LEU:HA	1.86	0.41
1:J:221:ASN:ND2	1:J:224:HIS:CD2	2.61	0.41
1:M:215:LEU:HD23	2:M:1000:HEM:HMC3	2.03	0.41
1:M:38:VAL:O	1:M:39:ALA:CB	2.68	0.41
1:M:62:ASP:HB2	1:M:78:ARG:HB3	2.02	0.41
1:Q:177:TYR:CD2	1:Q:211:LEU:HD13	2.56	0.41
1:S:235:THR:HG23	1:S:237:HIS:CD2	2.56	0.41
1:D:118:TYR:CD2	1:D:167:MET:HG3	2.55	0.41
1:I:171:THR:OG1	2:I:1000:HEM:HMA3	2.21	0.41
1:J:20:VAL:H	1:J:113:THR:HB	1.84	0.41
1:D:175:LEU:HD12	1:K:126:GLY:HA2	2.03	0.41
1:O:183:ARG:O	1:O:183:ARG:HG3	2.21	0.41
1:A:169:VAL:O	1:A:173:PRO:HD2	2.22	0.40
1:C:188:SER:O	1:C:189:THR:C	2.59	0.40
1:D:33:TRP:HB2	1:D:102:ASN:HB3	2.03	0.40
1:I:92:ARG:HG2	1:I:92:ARG:HH11	1.87	0.40
1:L:97:THR:CG2	1:L:100:GLY:N	2.82	0.40
1:Q:92:ARG:HH11	1:Q:92:ARG:HG2	1.86	0.40
1:L:235:THR:CG2	1:L:237:HIS:NE2	2.75	0.40
1:P:48:VAL:O	1:P:52:ILE:HG13	2.20	0.40
1:R:52:ILE:HG12	1:R:61:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:16:THR:O	4:T:2001:MES:H52	2.22	0.40
1:C:167:MET:CE	2:C:1000:HEM:HBD1	2.51	0.40
1:D:28:LYS:NZ	1:D:72:ASN:HD22	2.19	0.40
1:F:53:GLU:O	1:F:56:LYS:HG3	2.22	0.40
1:H:195:ASP:HB3	1:H:196:PHE:CE2	2.56	0.40
4:H:2001:MES:H82	4:H:2001:MES:H51	1.71	0.40
1:I:237:HIS:HB2	1:I:242:VAL:HG23	2.03	0.40
1:I:62:ASP:HB2	1:I:78:ARG:HB3	2.04	0.40
1:M:24:PHE:O	1:M:108:THR:HA	2.22	0.40
1:M:67:ARG:HG2	1:N:92:ARG:HG3	2.02	0.40
1:T:145:ILE:HD13	1:T:233:LEU:HD13	2.04	0.40
1:C:69:LEU:HA	1:C:69:LEU:HD23	1.85	0.40
1:J:64:TYR:CD2	1:J:64:TYR:N	2.89	0.40
1:N:26:MET:HG3	1:N:76:PHE:HB3	2.02	0.40
1:P:94:PHE:O	1:P:97:THR:CG2	2.59	0.40
1:F:150:LYS:HB3	1:F:226:ARG:HB3	2.04	0.40
1:H:219:LYS:O	1:H:220:GLU:C	2.58	0.40
1:R:152:ASN:OD1	1:R:154:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/248 (96%)	230 (96%)	7 (3%)	2 (1%)	22	58
1	B	239/248 (96%)	229 (96%)	7 (3%)	3 (1%)	14	45
1	C	239/248 (96%)	228 (95%)	8 (3%)	3 (1%)	14	45
1	D	239/248 (96%)	233 (98%)	5 (2%)	1 (0%)	38	72
1	E	239/248 (96%)	229 (96%)	8 (3%)	2 (1%)	22	58
1	F	239/248 (96%)	227 (95%)	10 (4%)	2 (1%)	22	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	239/248 (96%)	232 (97%)	6 (2%)	1 (0%)	38	72
1	H	239/248 (96%)	226 (95%)	11 (5%)	2 (1%)	22	58
1	I	239/248 (96%)	225 (94%)	12 (5%)	2 (1%)	22	58
1	J	239/248 (96%)	226 (95%)	11 (5%)	2 (1%)	22	58
1	K	239/248 (96%)	230 (96%)	8 (3%)	1 (0%)	38	72
1	L	239/248 (96%)	231 (97%)	6 (2%)	2 (1%)	22	58
1	M	239/248 (96%)	228 (95%)	8 (3%)	3 (1%)	14	45
1	N	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	38	72
1	O	239/248 (96%)	227 (95%)	11 (5%)	1 (0%)	38	72
1	P	239/248 (96%)	225 (94%)	13 (5%)	1 (0%)	38	72
1	Q	239/248 (96%)	223 (93%)	11 (5%)	5 (2%)	8	32
1	R	239/248 (96%)	226 (95%)	12 (5%)	1 (0%)	38	72
1	S	239/248 (96%)	225 (94%)	11 (5%)	3 (1%)	14	45
1	T	239/248 (96%)	228 (95%)	10 (4%)	1 (0%)	38	72
All	All	4780/4960 (96%)	4555 (95%)	186 (4%)	39 (1%)	22	58

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ALA
1	C	39	ALA
1	E	38	VAL
1	E	39	ALA
1	F	38	VAL
1	F	39	ALA
1	G	39	ALA
1	H	39	ALA
1	I	39	ALA
1	J	39	ALA
1	K	39	ALA
1	M	39	ALA
1	O	39	ALA
1	P	39	ALA
1	R	39	ALA
1	A	39	ALA
1	B	56	LYS
1	C	56	LYS

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Mol	Chain	Res	Type
1	D	39	ALA
1	L	39	ALA
1	M	56	LYS
1	N	39	ALA
1	Q	38	VAL
1	Q	39	ALA
1	S	38	VAL
1	S	39	ALA
1	T	39	ALA
1	B	131	LEU
1	Q	32	ASP
1	M	131	LEU
1	Q	132	SER
1	C	38	VAL
1	I	38	VAL
1	A	38	VAL
1	Q	239	PRO
1	S	37	PRO
1	J	239	PRO
1	L	38	VAL
1	H	38	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	212/219 (97%)	198 (93%)	14 (7%)	19	51
1	B	212/219 (97%)	198 (93%)	14 (7%)	19	51
1	C	212/219 (97%)	198 (93%)	14 (7%)	19	51
1	D	212/219 (97%)	200 (94%)	12 (6%)	24	57
1	E	212/219 (97%)	197 (93%)	15 (7%)	17	49
1	F	212/219 (97%)	196 (92%)	16 (8%)	16	46
1	G	212/219 (97%)	200 (94%)	12 (6%)	24	57
1	H	212/219 (97%)	199 (94%)	13 (6%)	22	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	212/219 (97%)	200 (94%)	12 (6%)	24	57
1	J	212/219 (97%)	195 (92%)	17 (8%)	14	44
1	K	212/219 (97%)	200 (94%)	12 (6%)	24	57
1	L	212/219 (97%)	196 (92%)	16 (8%)	16	46
1	M	212/219 (97%)	199 (94%)	13 (6%)	22	55
1	N	212/219 (97%)	198 (93%)	14 (7%)	19	51
1	O	212/219 (97%)	201 (95%)	11 (5%)	27	61
1	P	212/219 (97%)	199 (94%)	13 (6%)	22	55
1	Q	212/219 (97%)	195 (92%)	17 (8%)	14	44
1	R	212/219 (97%)	201 (95%)	11 (5%)	27	61
1	S	212/219 (97%)	200 (94%)	12 (6%)	24	57
1	T	212/219 (97%)	199 (94%)	13 (6%)	22	55
All	All	4240/4380 (97%)	3969 (94%)	271 (6%)	20	53

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	16	THR
1	A	25	THR
1	A	97	THR
1	A	107	GLU
1	A	113	THR
1	A	135	THR
1	A	145	ILE
1	A	174	THR
1	A	192	ASP
1	A	215	LEU
1	A	229	SER
1	A	235	THR
1	A	240	GLU
1	B	11	ARG
1	B	16	THR
1	B	26	MET
1	B	53	GLU
1	B	97	THR
1	B	99	VAL
1	B	107	GLU

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Mol	Chain	Res	Type
1	B	135	THR
1	B	192	ASP
1	B	215	LEU
1	B	229	SER
1	B	235	THR
1	B	240	GLU
1	B	248	ASP
1	C	11	ARG
1	C	16	THR
1	C	25	THR
1	C	26	MET
1	C	38	VAL
1	C	56	LYS
1	C	92	ARG
1	C	97	THR
1	C	145	ILE
1	C	192	ASP
1	C	214	SER
1	C	215	LEU
1	C	229	SER
1	C	235	THR
1	D	11	ARG
1	D	16	THR
1	D	26	MET
1	D	97	THR
1	D	135	THR
1	D	145	ILE
1	D	180	ASN
1	D	192	ASP
1	D	215	LEU
1	D	233	LEU
1	D	235	THR
1	D	248	ASP
1	E	8	LYS
1	E	16	THR
1	E	26	MET
1	E	53	GLU
1	E	97	THR
1	E	99	VAL
1	E	135	THR
1	E	137	SER
1	E	192	ASP

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Mol	Chain	Res	Type
1	E	215	LEU
1	E	229	SER
1	E	233	LEU
1	E	235	THR
1	E	239	PRO
1	E	248	ASP
1	F	11	ARG
1	F	13	THR
1	F	16	THR
1	F	25	THR
1	F	26	MET
1	F	99	VAL
1	F	135	THR
1	F	137	SER
1	F	145	ILE
1	F	192	ASP
1	F	214	SER
1	F	215	LEU
1	F	229	SER
1	F	233	LEU
1	F	235	THR
1	F	248	ASP
1	G	8	LYS
1	G	11	ARG
1	G	42	LYS
1	G	56	LYS
1	G	96	SER
1	G	97	THR
1	G	145	ILE
1	G	192	ASP
1	G	215	LEU
1	G	229	SER
1	G	233	LEU
1	G	235	THR
1	H	11	ARG
1	H	16	THR
1	H	26	MET
1	H	92	ARG
1	H	97	THR
1	H	99	VAL
1	H	145	ILE
1	H	192	ASP

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Mol	Chain	Res	Type
1	H	215	LEU
1	H	229	SER
1	H	233	LEU
1	H	235	THR
1	H	248	ASP
1	I	11	ARG
1	I	26	MET
1	I	41	ARG
1	I	96	SER
1	I	97	THR
1	I	135	THR
1	I	145	ILE
1	I	192	ASP
1	I	215	LEU
1	I	229	SER
1	I	233	LEU
1	I	235	THR
1	J	11	ARG
1	J	16	THR
1	J	25	THR
1	J	26	MET
1	J	92	ARG
1	J	97	THR
1	J	113	THR
1	J	135	THR
1	J	137	SER
1	J	145	ILE
1	J	150	LYS
1	J	192	ASP
1	J	214	SER
1	J	215	LEU
1	J	233	LEU
1	J	235	THR
1	J	240	GLU
1	K	16	THR
1	K	25	THR
1	K	97	THR
1	K	107	GLU
1	K	113	THR
1	K	137	SER
1	K	145	ILE
1	K	192	ASP

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Mol	Chain	Res	Type
1	K	214	SER
1	K	215	LEU
1	K	229	SER
1	K	235	THR
1	L	16	THR
1	L	26	MET
1	L	32	ASP
1	L	92	ARG
1	L	97	THR
1	L	135	THR
1	L	137	SER
1	L	145	ILE
1	L	180	ASN
1	L	189	THR
1	L	192	ASP
1	L	214	SER
1	L	215	LEU
1	L	233	LEU
1	L	235	THR
1	L	248	ASP
1	M	16	THR
1	M	25	THR
1	M	26	MET
1	M	92	ARG
1	M	97	THR
1	M	99	VAL
1	M	165	LYS
1	M	183	ARG
1	M	192	ASP
1	M	215	LEU
1	M	233	LEU
1	M	235	THR
1	M	248	ASP
1	N	11	ARG
1	N	26	MET
1	N	97	THR
1	N	99	VAL
1	N	113	THR
1	N	145	ILE
1	N	189	THR
1	N	214	SER
1	N	215	LEU

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Mol	Chain	Res	Type
1	N	229	SER
1	N	233	LEU
1	N	235	THR
1	N	240	GLU
1	N	248	ASP
1	O	16	THR
1	O	25	THR
1	O	26	MET
1	O	56	LYS
1	O	97	THR
1	O	99	VAL
1	O	145	ILE
1	O	192	ASP
1	O	215	LEU
1	O	233	LEU
1	O	235	THR
1	P	8	LYS
1	P	16	THR
1	P	25	THR
1	P	26	MET
1	P	50	LYS
1	P	92	ARG
1	P	99	VAL
1	P	107	GLU
1	P	135	THR
1	P	192	ASP
1	P	215	LEU
1	P	233	LEU
1	P	235	THR
1	Q	11	ARG
1	Q	16	THR
1	Q	25	THR
1	Q	26	MET
1	Q	33	TRP
1	Q	97	THR
1	Q	113	THR
1	Q	135	THR
1	Q	137	SER
1	Q	145	ILE
1	Q	165	LYS
1	Q	183	ARG
1	Q	192	ASP

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Mol	Chain	Res	Type
1	Q	214	SER
1	Q	215	LEU
1	Q	235	THR
1	Q	244	LYS
1	R	25	THR
1	R	92	ARG
1	R	97	THR
1	R	99	VAL
1	R	113	THR
1	R	135	THR
1	R	145	ILE
1	R	192	ASP
1	R	215	LEU
1	R	235	THR
1	R	248	ASP
1	S	16	THR
1	S	25	THR
1	S	26	MET
1	S	97	THR
1	S	99	VAL
1	S	113	THR
1	S	145	ILE
1	S	192	ASP
1	S	215	LEU
1	S	229	SER
1	S	233	LEU
1	S	240	GLU
1	T	8	LYS
1	T	16	THR
1	T	25	THR
1	T	97	THR
1	T	99	VAL
1	T	135	THR
1	T	137	SER
1	T	145	ILE
1	T	192	ASP
1	T	215	LEU
1	T	229	SER
1	T	233	LEU
1	T	248	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	157	ASN
1	A	221	ASN
1	A	224	HIS
1	B	55	HIS
1	B	72	ASN
1	B	157	ASN
1	B	221	ASN
1	B	224	HIS
1	C	58	ASN
1	C	72	ASN
1	C	157	ASN
1	C	221	ASN
1	C	224	HIS
1	D	55	HIS
1	D	72	ASN
1	D	157	ASN
1	D	217	GLN
1	D	221	ASN
1	D	224	HIS
1	E	55	HIS
1	E	58	ASN
1	E	72	ASN
1	E	80	ASN
1	E	157	ASN
1	E	217	GLN
1	E	221	ASN
1	E	224	HIS
1	F	72	ASN
1	F	157	ASN
1	F	217	GLN
1	F	224	HIS
1	G	55	HIS
1	G	72	ASN
1	G	157	ASN
1	G	217	GLN
1	G	221	ASN
1	G	224	HIS
1	H	72	ASN
1	H	102	ASN
1	H	157	ASN
1	H	221	ASN
1	H	224	HIS

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Mol	Chain	Res	Type
1	I	55	HIS
1	I	72	ASN
1	I	157	ASN
1	I	221	ASN
1	I	224	HIS
1	J	72	ASN
1	J	157	ASN
1	J	217	GLN
1	J	221	ASN
1	J	224	HIS
1	K	58	ASN
1	K	72	ASN
1	K	157	ASN
1	K	221	ASN
1	K	224	HIS
1	L	55	HIS
1	L	72	ASN
1	L	157	ASN
1	L	224	HIS
1	M	55	HIS
1	M	72	ASN
1	M	157	ASN
1	M	217	GLN
1	M	221	ASN
1	M	224	HIS
1	N	55	HIS
1	N	72	ASN
1	N	157	ASN
1	N	217	GLN
1	N	221	ASN
1	N	224	HIS
1	O	157	ASN
1	O	221	ASN
1	O	224	HIS
1	P	157	ASN
1	P	224	HIS
1	Q	55	HIS
1	Q	157	ASN
1	Q	217	GLN
1	Q	221	ASN
1	Q	224	HIS
1	R	157	ASN

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Mol	Chain	Res	Type
1	R	224	HIS
1	S	157	ASN
1	S	217	GLN
1	S	221	ASN
1	S	224	HIS
1	T	58	ASN
1	T	72	ASN
1	T	157	ASN
1	T	221	ASN
1	T	224	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 20 are monoatomic - leaving 60 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
2	HEM	A	1000	1,3	28,50,50	2.28	8 (28%)	17,82,82	1.73	5 (29%)
3	NO2	A	2000	2	1,2,2	4.50	1 (100%)	0,1,1	0.00	-
4	MES	A	2001	-	12,12,12	2.18	1 (8%)	14,16,16	2.56	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	1000	1,3	28,50,50	2.32	7 (25%)	17,82,82	2.03	5 (29%)
3	NO2	B	2000	2	1,2,2	4.81	1 (100%)	0,1,1	0.00	-
4	MES	B	2001	-	12,12,12	1.87	2 (16%)	14,16,16	3.33	9 (64%)
2	HEM	C	1000	1,3	28,50,50	2.48	7 (25%)	17,82,82	2.21	5 (29%)
3	NO2	C	2000	2	1,2,2	4.72	1 (100%)	0,1,1	0.00	-
4	MES	C	2001	-	12,12,12	2.02	1 (8%)	14,16,16	2.56	5 (35%)
2	HEM	D	1000	1,3	28,50,50	2.47	10 (35%)	17,82,82	2.34	5 (29%)
3	NO2	D	2000	2	1,2,2	4.85	1 (100%)	0,1,1	0.00	-
4	MES	D	2001	-	12,12,12	2.03	1 (8%)	14,16,16	3.13	6 (42%)
2	HEM	E	1000	1,3	28,50,50	2.18	7 (25%)	17,82,82	1.94	5 (29%)
3	NO2	E	2000	2	1,2,2	4.50	1 (100%)	0,1,1	0.00	-
4	MES	E	2001	-	12,12,12	2.05	1 (8%)	14,16,16	2.91	9 (64%)
2	HEM	F	1000	1,3	28,50,50	2.28	8 (28%)	17,82,82	1.71	4 (23%)
3	NO2	F	2000	2	1,2,2	4.95	1 (100%)	0,1,1	0.00	-
4	MES	F	2001	-	12,12,12	2.18	1 (8%)	14,16,16	3.06	9 (64%)
2	HEM	G	1000	1,3	28,50,50	2.17	8 (28%)	17,82,82	1.90	4 (23%)
3	NO2	G	2000	2	1,2,2	4.62	1 (100%)	0,1,1	0.00	-
4	MES	G	2001	-	12,12,12	2.08	1 (8%)	14,16,16	2.77	9 (64%)
2	HEM	H	1000	1,3	28,50,50	2.31	10 (35%)	17,82,82	1.66	5 (29%)
3	NO2	H	2000	2	1,2,2	5.05	1 (100%)	0,1,1	0.00	-
4	MES	H	2001	-	12,12,12	2.30	1 (8%)	14,16,16	2.92	7 (50%)
2	HEM	I	1000	1,3	28,50,50	2.38	10 (35%)	17,82,82	2.17	6 (35%)
3	NO2	I	2000	2	1,2,2	4.54	1 (100%)	0,1,1	0.00	-
4	MES	I	2001	-	12,12,12	2.16	1 (8%)	14,16,16	2.96	7 (50%)
2	HEM	J	1000	1,3	28,50,50	2.11	7 (25%)	17,82,82	2.18	6 (35%)
3	NO2	J	2000	2	1,2,2	4.91	1 (100%)	0,1,1	0.00	-
4	MES	J	2001	-	12,12,12	2.19	1 (8%)	14,16,16	2.83	8 (57%)
2	HEM	K	1000	1,3	28,50,50	2.31	7 (25%)	17,82,82	1.78	3 (17%)
3	NO2	K	2000	2	1,2,2	4.77	1 (100%)	0,1,1	0.00	-
4	MES	K	2001	-	12,12,12	2.19	1 (8%)	14,16,16	3.28	9 (64%)
2	HEM	L	1000	1,3	28,50,50	2.23	9 (32%)	17,82,82	1.82	3 (17%)
3	NO2	L	2000	2	1,2,2	5.09	1 (100%)	0,1,1	0.00	-
4	MES	L	2001	-	12,12,12	2.12	1 (8%)	14,16,16	2.87	6 (42%)
2	HEM	M	1000	1,3	28,50,50	2.26	7 (25%)	17,82,82	1.92	4 (23%)
3	NO2	M	2000	2	1,2,2	5.14	1 (100%)	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MES	M	2001	-	12,12,12	2.10	3 (25%)	14,16,16	3.31	9 (64%)
2	HEM	N	1000	1,3	28,50,50	2.24	8 (28%)	17,82,82	1.70	5 (29%)
3	NO2	N	2000	2	1,2,2	4.95	1 (100%)	0,1,1	0.00	-
4	MES	N	2001	-	12,12,12	1.74	1 (8%)	14,16,16	3.15	8 (57%)
2	HEM	O	1000	1,3	28,50,50	2.23	10 (35%)	17,82,82	1.75	3 (17%)
3	NO2	O	2000	2	1,2,2	4.76	1 (100%)	0,1,1	0.00	-
4	MES	O	2001	-	12,12,12	2.03	1 (8%)	14,16,16	2.66	7 (50%)
2	HEM	P	1000	1,3	28,50,50	2.35	6 (21%)	17,82,82	1.58	3 (17%)
3	NO2	P	2000	2	1,2,2	5.15	1 (100%)	0,1,1	0.00	-
4	MES	P	2001	-	12,12,12	2.14	1 (8%)	14,16,16	2.71	6 (42%)
2	HEM	Q	1000	1,3	28,50,50	2.41	9 (32%)	17,82,82	2.16	4 (23%)
3	NO2	Q	2000	2	1,2,2	5.25	1 (100%)	0,1,1	0.00	-
4	MES	Q	2001	-	12,12,12	1.93	2 (16%)	14,16,16	2.78	6 (42%)
2	HEM	R	1000	1,3	28,50,50	2.08	7 (25%)	17,82,82	2.12	4 (23%)
3	NO2	R	2000	2	1,2,2	5.08	1 (100%)	0,1,1	0.00	-
4	MES	R	2001	-	12,12,12	2.03	1 (8%)	14,16,16	2.90	8 (57%)
2	HEM	S	1000	1,3	28,50,50	2.37	10 (35%)	17,82,82	1.93	5 (29%)
3	NO2	S	2000	2	1,2,2	4.95	1 (100%)	0,1,1	0.00	-
4	MES	S	2001	-	12,12,12	2.09	1 (8%)	14,16,16	2.60	7 (50%)
2	HEM	T	1000	1,3	28,50,50	2.32	7 (25%)	17,82,82	1.83	5 (29%)
3	NO2	T	2000	2	1,2,2	4.97	1 (100%)	0,1,1	0.00	-
4	MES	T	2001	-	12,12,12	2.13	1 (8%)	14,16,16	2.70	6 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	A	2000	2	-	0/0/0/0	0/0/0/0
4	MES	A	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	B	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	B	2000	2	-	0/0/0/0	0/0/0/0
4	MES	B	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	C	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	C	2000	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	C	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	D	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	D	2000	2	-	0/0/0/0	0/0/0/0
4	MES	D	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	E	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	E	2000	2	-	0/0/0/0	0/0/0/0
4	MES	E	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	F	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	F	2000	2	-	0/0/0/0	0/0/0/0
4	MES	F	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	G	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	G	2000	2	-	0/0/0/0	0/0/0/0
4	MES	G	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	H	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	H	2000	2	-	0/0/0/0	0/0/0/0
4	MES	H	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	I	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	I	2000	2	-	0/0/0/0	0/0/0/0
4	MES	I	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	J	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	J	2000	2	-	0/0/0/0	0/0/0/0
4	MES	J	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	K	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	K	2000	2	-	0/0/0/0	0/0/0/0
4	MES	K	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	L	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	L	2000	2	-	0/0/0/0	0/0/0/0
4	MES	L	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	M	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	M	2000	2	-	0/0/0/0	0/0/0/0
4	MES	M	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	N	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	N	2000	2	-	0/0/0/0	0/0/0/0
4	MES	N	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	O	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	O	2000	2	-	0/0/0/0	0/0/0/0
4	MES	O	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	P	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	P	2000	2	-	0/0/0/0	0/0/0/0
4	MES	P	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	Q	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	Q	2000	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	Q	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	R	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	R	2000	2	-	0/0/0/0	0/0/0/0
4	MES	R	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	S	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	S	2000	2	-	0/0/0/0	0/0/0/0
4	MES	S	2001	-	-	0/6/14/14	0/1/1/1
2	HEM	T	1000	1,3	-	0/6/54/54	0/0/8/8
3	NO2	T	2000	2	-	0/0/0/0	0/0/0/0
4	MES	T	2001	-	-	0/6/14/14	0/1/1/1

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2001	MES	C8-S	-7.56	1.66	1.77
4	K	2001	MES	C8-S	-7.44	1.66	1.77
4	J	2001	MES	C8-S	-7.21	1.66	1.77
4	A	2001	MES	C8-S	-7.12	1.66	1.77
4	I	2001	MES	C8-S	-7.06	1.66	1.77
2	C	1000	HEM	C3B-C2B	-7.05	1.31	1.40
4	P	2001	MES	C8-S	-7.03	1.67	1.77
4	L	2001	MES	C8-S	-7.00	1.67	1.77
4	T	2001	MES	C8-S	-6.93	1.67	1.77
4	S	2001	MES	C8-S	-6.90	1.67	1.77
4	F	2001	MES	C8-S	-6.86	1.67	1.77
4	D	2001	MES	C8-S	-6.72	1.67	1.77
4	E	2001	MES	C8-S	-6.69	1.67	1.77
4	C	2001	MES	C8-S	-6.67	1.67	1.77
4	O	2001	MES	C8-S	-6.65	1.67	1.77
4	G	2001	MES	C8-S	-6.57	1.67	1.77
2	D	1000	HEM	C3C-C2C	-6.49	1.31	1.40
2	C	1000	HEM	C3C-C2C	-6.45	1.31	1.40
4	R	2001	MES	C8-S	-6.40	1.67	1.77
2	B	1000	HEM	C3B-C2B	-6.30	1.32	1.40
4	M	2001	MES	C8-S	-6.15	1.68	1.77
2	B	1000	HEM	C3C-C2C	-5.97	1.32	1.40
2	T	1000	HEM	C3B-C2B	-5.91	1.32	1.40
2	K	1000	HEM	C3B-C2B	-5.82	1.32	1.40
2	I	1000	HEM	C3B-C2B	-5.81	1.32	1.40
2	D	1000	HEM	C3B-C2B	-5.78	1.32	1.40
2	A	1000	HEM	C3C-C2C	-5.71	1.32	1.40
2	N	1000	HEM	C3C-C2C	-5.67	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1000	HEM	C3B-C2B	-5.65	1.32	1.40
2	Q	1000	HEM	C3B-C2B	-5.64	1.32	1.40
2	A	1000	HEM	C3B-C2B	-5.62	1.32	1.40
4	Q	2001	MES	C8-S	-5.61	1.69	1.77
2	H	1000	HEM	C3C-C2C	-5.58	1.33	1.40
2	P	1000	HEM	C3B-C2B	-5.56	1.33	1.40
2	L	1000	HEM	C3B-C2B	-5.55	1.33	1.40
2	N	1000	HEM	C3B-C2B	-5.55	1.33	1.40
2	M	1000	HEM	C3B-C2B	-5.55	1.33	1.40
2	Q	1000	HEM	C3C-C2C	-5.45	1.33	1.40
4	N	2001	MES	C8-S	-5.41	1.69	1.77
2	F	1000	HEM	C3B-C2B	-5.37	1.33	1.40
2	T	1000	HEM	C3C-C2C	-5.36	1.33	1.40
2	P	1000	HEM	C3C-C2C	-5.26	1.33	1.40
2	G	1000	HEM	C3B-C2B	-5.23	1.33	1.40
2	I	1000	HEM	C3C-C2C	-5.18	1.33	1.40
2	K	1000	HEM	C3C-C2C	-5.16	1.33	1.40
2	R	1000	HEM	C3B-C2B	-5.14	1.33	1.40
2	F	1000	HEM	C3C-C2C	-5.10	1.33	1.40
2	E	1000	HEM	C3C-C2C	-5.08	1.33	1.40
2	M	1000	HEM	C3C-C2C	-5.03	1.33	1.40
2	E	1000	HEM	C3B-C2B	-4.79	1.34	1.40
2	O	1000	HEM	C3B-C2B	-4.72	1.34	1.40
4	B	2001	MES	C8-S	-4.68	1.70	1.77
2	S	1000	HEM	C3B-C2B	-4.66	1.34	1.40
2	G	1000	HEM	C3C-C2C	-4.65	1.34	1.40
2	J	1000	HEM	C3B-C2B	-4.51	1.34	1.40
2	O	1000	HEM	C3C-C2C	-4.50	1.34	1.40
2	L	1000	HEM	C3C-C2C	-4.45	1.34	1.40
2	R	1000	HEM	C3C-C2C	-4.44	1.34	1.40
2	S	1000	HEM	C3C-C2C	-4.27	1.34	1.40
2	J	1000	HEM	C3C-C2C	-4.10	1.34	1.40
2	H	1000	HEM	C4A-CHB	-2.15	1.34	1.40
2	D	1000	HEM	C4B-CHC	-2.03	1.34	1.40
4	M	2001	MES	O2S-S	2.00	1.51	1.45
2	H	1000	HEM	CMA-C3A	2.01	1.55	1.51
2	B	1000	HEM	CMC-C2C	2.02	1.55	1.51
2	A	1000	HEM	CAA-C2A	2.03	1.55	1.52
4	Q	2001	MES	O1S-S	2.04	1.51	1.45
2	L	1000	HEM	C1B-NB	2.04	1.39	1.36
2	G	1000	HEM	CMB-C2B	2.04	1.55	1.51
2	K	1000	HEM	C1A-NA	2.05	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1000	HEM	C3B-CAB	2.05	1.51	1.47
2	A	1000	HEM	CAD-C3D	2.07	1.56	1.52
2	D	1000	HEM	CAA-C2A	2.08	1.55	1.52
2	R	1000	HEM	C1B-NB	2.11	1.39	1.36
2	D	1000	HEM	CMB-C2B	2.12	1.56	1.51
2	I	1000	HEM	C1C-NC	2.12	1.39	1.36
2	S	1000	HEM	C1B-NB	2.12	1.39	1.36
2	O	1000	HEM	CMC-C2C	2.13	1.56	1.51
2	S	1000	HEM	CMB-C2B	2.13	1.56	1.51
2	H	1000	HEM	CMB-C2B	2.14	1.56	1.51
2	N	1000	HEM	CMB-C2B	2.14	1.56	1.51
2	G	1000	HEM	C1B-NB	2.16	1.39	1.36
2	N	1000	HEM	CMA-C3A	2.16	1.56	1.51
4	M	2001	MES	O1S-S	2.17	1.51	1.45
2	N	1000	HEM	CAA-C2A	2.19	1.55	1.52
2	A	1000	HEM	CMB-C2B	2.19	1.56	1.51
2	O	1000	HEM	C1B-NB	2.21	1.39	1.36
2	L	1000	HEM	CMC-C2C	2.22	1.56	1.51
2	Q	1000	HEM	C1C-NC	2.22	1.39	1.36
2	O	1000	HEM	C4D-ND	2.24	1.39	1.36
2	F	1000	HEM	CMB-C2B	2.24	1.56	1.51
2	T	1000	HEM	C4D-ND	2.24	1.39	1.36
2	S	1000	HEM	CMC-C2C	2.25	1.56	1.51
2	M	1000	HEM	C1B-NB	2.26	1.39	1.36
2	O	1000	HEM	C1C-NC	2.26	1.39	1.36
2	B	1000	HEM	C4D-ND	2.27	1.39	1.36
2	L	1000	HEM	C4D-ND	2.28	1.39	1.36
2	C	1000	HEM	CMA-C3A	2.28	1.56	1.51
2	I	1000	HEM	C1B-NB	2.29	1.39	1.36
2	Q	1000	HEM	CAD-C3D	2.29	1.56	1.52
2	C	1000	HEM	C4D-ND	2.29	1.39	1.36
2	C	1000	HEM	C3B-CAB	2.35	1.52	1.47
4	B	2001	MES	O1S-S	2.35	1.52	1.45
2	J	1000	HEM	CMB-C2B	2.36	1.56	1.51
2	Q	1000	HEM	C3C-CAC	2.37	1.52	1.47
2	O	1000	HEM	CAA-C2A	2.44	1.56	1.52
2	J	1000	HEM	C1B-NB	2.44	1.39	1.36
2	F	1000	HEM	C1C-NC	2.45	1.39	1.36
2	I	1000	HEM	CMC-C2C	2.45	1.56	1.51
2	E	1000	HEM	C1C-NC	2.45	1.39	1.36
2	D	1000	HEM	CMA-C3A	2.46	1.56	1.51
2	I	1000	HEM	C3C-CAC	2.46	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1000	HEM	C3C-CAC	2.47	1.52	1.47
2	H	1000	HEM	C1B-NB	2.47	1.39	1.36
2	P	1000	HEM	C4D-ND	2.47	1.39	1.36
2	R	1000	HEM	C1C-NC	2.52	1.39	1.36
2	H	1000	HEM	C4D-ND	2.55	1.39	1.36
2	N	1000	HEM	C3B-CAB	2.57	1.53	1.47
2	S	1000	HEM	C1C-NC	2.58	1.39	1.36
2	T	1000	HEM	C1C-NC	2.59	1.39	1.36
2	M	1000	HEM	C3B-CAB	2.59	1.53	1.47
2	I	1000	HEM	CMA-C3A	2.60	1.56	1.51
2	K	1000	HEM	C3C-CAC	2.60	1.52	1.47
2	E	1000	HEM	C3C-CAC	2.68	1.53	1.47
2	L	1000	HEM	C1C-NC	2.70	1.40	1.36
2	D	1000	HEM	C4D-ND	2.70	1.40	1.36
2	R	1000	HEM	C3C-CAC	2.71	1.53	1.47
2	A	1000	HEM	C3B-CAB	2.72	1.53	1.47
2	D	1000	HEM	C3C-CAC	2.72	1.53	1.47
2	J	1000	HEM	C3B-CAB	2.73	1.53	1.47
2	G	1000	HEM	C3B-CAB	2.73	1.53	1.47
2	E	1000	HEM	C3B-CAB	2.74	1.53	1.47
2	D	1000	HEM	C3B-CAB	2.76	1.53	1.47
2	G	1000	HEM	C3C-CAC	2.76	1.53	1.47
2	H	1000	HEM	C3C-CAC	2.79	1.53	1.47
2	T	1000	HEM	C3B-CAB	2.80	1.53	1.47
2	O	1000	HEM	C3C-CAC	2.81	1.53	1.47
2	F	1000	HEM	C3B-CAB	2.84	1.53	1.47
2	P	1000	HEM	C3C-CAC	2.85	1.53	1.47
2	C	1000	HEM	C3C-CAC	2.86	1.53	1.47
2	Q	1000	HEM	CAA-C2A	2.90	1.56	1.52
2	T	1000	HEM	C3C-CAC	2.91	1.53	1.47
2	M	1000	HEM	C4D-ND	2.91	1.40	1.36
2	N	1000	HEM	C3C-CAC	2.92	1.53	1.47
2	Q	1000	HEM	C4D-ND	2.93	1.40	1.36
2	F	1000	HEM	C4D-ND	2.95	1.40	1.36
2	B	1000	HEM	C3B-CAB	2.96	1.53	1.47
2	K	1000	HEM	C3B-CAB	3.01	1.53	1.47
2	A	1000	HEM	C3C-CAC	3.01	1.53	1.47
2	B	1000	HEM	C3C-CAC	3.01	1.53	1.47
2	E	1000	HEM	C4D-ND	3.04	1.40	1.36
2	G	1000	HEM	C1C-NC	3.09	1.40	1.36
2	F	1000	HEM	C3C-CAC	3.10	1.53	1.47
2	R	1000	HEM	C3B-CAB	3.12	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1000	HEM	C3C-CAC	3.16	1.54	1.47
2	M	1000	HEM	C3C-CAC	3.25	1.54	1.47
2	Q	1000	HEM	C3B-CAB	3.27	1.54	1.47
2	S	1000	HEM	C3B-CAB	3.30	1.54	1.47
2	I	1000	HEM	C3B-CAB	3.31	1.54	1.47
2	O	1000	HEM	C3B-CAB	3.36	1.54	1.47
2	L	1000	HEM	C3B-CAB	3.37	1.54	1.47
2	I	1000	HEM	C4D-ND	3.38	1.40	1.36
2	K	1000	HEM	C4D-ND	3.53	1.40	1.36
2	S	1000	HEM	C3C-CAC	3.85	1.55	1.47
2	P	1000	HEM	C3B-CAB	3.89	1.55	1.47
2	S	1000	HEM	C4D-ND	3.89	1.41	1.36
3	E	2000	NO2	O1-N	4.50	1.43	1.21
3	A	2000	NO2	O1-N	4.50	1.43	1.21
3	I	2000	NO2	O1-N	4.54	1.43	1.21
3	G	2000	NO2	O1-N	4.62	1.43	1.21
3	C	2000	NO2	O1-N	4.72	1.44	1.21
2	R	1000	HEM	C3D-C2D	4.76	1.51	1.37
3	O	2000	NO2	O1-N	4.76	1.44	1.21
3	K	2000	NO2	O1-N	4.77	1.44	1.21
2	G	1000	HEM	C3D-C2D	4.78	1.51	1.37
3	B	2000	NO2	O1-N	4.81	1.44	1.21
3	D	2000	NO2	O1-N	4.85	1.44	1.21
3	J	2000	NO2	O1-N	4.91	1.45	1.21
2	A	1000	HEM	C3D-C2D	4.92	1.52	1.37
3	S	2000	NO2	O1-N	4.95	1.45	1.21
3	N	2000	NO2	O1-N	4.95	1.45	1.21
3	F	2000	NO2	O1-N	4.95	1.45	1.21
2	M	1000	HEM	C3D-C2D	4.96	1.52	1.37
3	T	2000	NO2	O1-N	4.97	1.45	1.21
2	I	1000	HEM	C3D-C2D	4.99	1.52	1.37
2	B	1000	HEM	C3D-C2D	4.99	1.52	1.37
2	F	1000	HEM	C3D-C2D	5.01	1.52	1.37
2	E	1000	HEM	C3D-C2D	5.02	1.52	1.37
3	H	2000	NO2	O1-N	5.05	1.45	1.21
2	H	1000	HEM	C3D-C2D	5.05	1.52	1.37
3	R	2000	NO2	O1-N	5.08	1.45	1.21
3	L	2000	NO2	O1-N	5.09	1.45	1.21
2	C	1000	HEM	C3D-C2D	5.10	1.52	1.37
2	L	1000	HEM	C3D-C2D	5.12	1.52	1.37
3	M	2000	NO2	O1-N	5.14	1.46	1.21
3	P	2000	NO2	O1-N	5.15	1.46	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1000	HEM	C3D-C2D	5.20	1.53	1.37
2	O	1000	HEM	C3D-C2D	5.23	1.53	1.37
3	Q	2000	NO2	O1-N	5.25	1.46	1.21
2	T	1000	HEM	C3D-C2D	5.27	1.53	1.37
2	J	1000	HEM	C3D-C2D	5.30	1.53	1.37
2	K	1000	HEM	C3D-C2D	5.39	1.53	1.37
2	D	1000	HEM	C3D-C2D	5.50	1.54	1.37
2	S	1000	HEM	C3D-C2D	5.51	1.54	1.37
2	P	1000	HEM	C3D-C2D	5.52	1.54	1.37
2	Q	1000	HEM	C3D-C2D	5.62	1.54	1.37

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2001	MES	C6-C5-N4	-6.67	100.75	110.11
4	H	2001	MES	C6-C5-N4	-6.41	101.13	110.11
4	K	2001	MES	C6-C5-N4	-5.71	102.10	110.11
4	R	2001	MES	C6-C5-N4	-5.11	102.94	110.11
4	M	2001	MES	O2S-S-C8	-4.93	102.56	106.79
4	B	2001	MES	O1S-S-C8	-4.66	102.79	106.79
2	D	1000	HEM	CAD-CBD-CGD	-4.49	104.98	112.66
4	L	2001	MES	C6-C5-N4	-4.41	103.92	110.11
4	L	2001	MES	C2-C3-N4	-4.38	103.97	110.11
4	D	2001	MES	C6-C5-N4	-4.24	104.16	110.11
2	D	1000	HEM	C1D-C2D-C3D	-4.11	104.14	107.00
4	J	2001	MES	C2-C3-N4	-3.96	104.55	110.11
2	M	1000	HEM	CBA-CAA-C2A	-3.90	105.03	112.48
4	T	2001	MES	C2-C3-N4	-3.86	104.70	110.11
2	K	1000	HEM	CMA-C3A-C4A	-3.75	122.69	128.46
2	J	1000	HEM	CMA-C3A-C4A	-3.75	122.70	128.46
2	E	1000	HEM	CMA-C3A-C4A	-3.74	122.72	128.46
4	O	2001	MES	C2-C3-N4	-3.68	104.95	110.11
2	S	1000	HEM	CMA-C3A-C4A	-3.68	122.81	128.46
2	C	1000	HEM	CBA-CAA-C2A	-3.63	105.55	112.48
4	P	2001	MES	C2-C3-N4	-3.58	105.09	110.11
2	C	1000	HEM	C1D-C2D-C3D	-3.53	104.54	107.00
2	D	1000	HEM	CBA-CAA-C2A	-3.52	105.75	112.48
4	Q	2001	MES	C6-C5-N4	-3.51	105.18	110.11
2	Q	1000	HEM	CMA-C3A-C4A	-3.51	123.07	128.46
2	B	1000	HEM	CMA-C3A-C4A	-3.44	123.18	128.46
4	J	2001	MES	C6-C5-N4	-3.40	105.34	110.11
4	M	2001	MES	C6-C5-N4	-3.36	105.41	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1000	HEM	CMA-C3A-C4A	-3.33	123.35	128.46
2	R	1000	HEM	CAA-CBA-CGA	-3.32	106.98	112.66
2	F	1000	HEM	CMA-C3A-C4A	-3.30	123.40	128.46
4	E	2001	MES	C6-C5-N4	-3.27	105.53	110.11
2	T	1000	HEM	CMA-C3A-C4A	-3.20	123.55	128.46
4	Q	2001	MES	C2-C3-N4	-3.16	105.67	110.11
4	G	2001	MES	C6-C5-N4	-3.11	105.75	110.11
2	S	1000	HEM	CBA-CAA-C2A	-3.10	106.55	112.48
4	F	2001	MES	C6-C5-N4	-3.09	105.78	110.11
2	J	1000	HEM	C3C-C4C-NC	-3.08	105.12	110.94
4	K	2001	MES	C2-C3-N4	-3.08	105.80	110.11
2	O	1000	HEM	CMA-C3A-C4A	-3.08	123.74	128.46
4	E	2001	MES	C2-C3-N4	-3.06	105.81	110.11
2	L	1000	HEM	CMA-C3A-C4A	-3.00	123.86	128.46
2	H	1000	HEM	CMA-C3A-C4A	-2.99	123.86	128.46
2	C	1000	HEM	CAD-CBD-CGD	-2.94	107.64	112.66
2	A	1000	HEM	CMA-C3A-C4A	-2.93	123.95	128.46
2	I	1000	HEM	CBA-CAA-C2A	-2.93	106.89	112.48
4	S	2001	MES	C6-C5-N4	-2.92	106.01	110.11
2	B	1000	HEM	CBA-CAA-C2A	-2.89	106.96	112.48
2	E	1000	HEM	CBA-CAA-C2A	-2.87	107.00	112.48
4	G	2001	MES	C2-C3-N4	-2.86	106.10	110.11
4	O	2001	MES	C6-C5-N4	-2.79	106.20	110.11
2	R	1000	HEM	CMA-C3A-C4A	-2.78	124.19	128.46
4	R	2001	MES	C2-C3-N4	-2.74	106.28	110.11
4	S	2001	MES	C2-C3-N4	-2.71	106.31	110.11
4	N	2001	MES	C6-C5-N4	-2.70	106.33	110.11
4	N	2001	MES	O2S-S-O1S	-2.70	104.51	113.86
2	N	1000	HEM	CMA-C3A-C4A	-2.69	124.33	128.46
2	I	1000	HEM	CAD-CBD-CGD	-2.66	108.12	112.66
2	I	1000	HEM	CAA-CBA-CGA	-2.65	108.13	112.66
2	Q	1000	HEM	C3C-C4C-NC	-2.65	105.94	110.94
2	S	1000	HEM	CAA-CBA-CGA	-2.62	108.19	112.66
2	R	1000	HEM	C3C-C4C-NC	-2.57	106.10	110.94
4	E	2001	MES	O2S-S-O1S	-2.56	105.00	113.86
2	P	1000	HEM	CMA-C3A-C4A	-2.53	124.57	128.46
2	L	1000	HEM	C3C-C4C-NC	-2.50	106.22	110.94
4	K	2001	MES	O2S-S-O1S	-2.45	105.35	113.86
2	M	1000	HEM	CMA-C3A-C4A	-2.45	124.69	128.46
2	H	1000	HEM	C1D-C2D-C3D	-2.45	105.29	107.00
2	A	1000	HEM	CBA-CAA-C2A	-2.44	107.83	112.48
2	M	1000	HEM	C3C-C4C-NC	-2.43	106.36	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1000	HEM	CBA-CAA-C2A	-2.42	107.86	112.48
2	B	1000	HEM	C1D-C2D-C3D	-2.41	105.32	107.00
4	F	2001	MES	O2S-S-C8	-2.40	104.73	106.79
2	C	1000	HEM	CBD-CAD-C3D	-2.40	107.90	112.47
2	I	1000	HEM	CMA-C3A-C4A	-2.39	124.79	128.46
4	I	2001	MES	C2-C3-N4	-2.35	106.82	110.11
4	H	2001	MES	C2-C3-N4	-2.34	106.83	110.11
2	A	1000	HEM	CAD-CBD-CGD	-2.32	108.69	112.66
4	M	2001	MES	O2S-S-O1S	-2.31	105.86	113.86
2	Q	1000	HEM	CBD-CAD-C3D	-2.29	108.11	112.47
2	H	1000	HEM	CBA-CAA-C2A	-2.26	108.16	112.48
4	G	2001	MES	O2S-S-C8	-2.24	104.87	106.79
2	E	1000	HEM	CBD-CAD-C3D	-2.18	108.31	112.47
2	G	1000	HEM	CAD-CBD-CGD	-2.16	108.97	112.66
2	F	1000	HEM	CBA-CAA-C2A	-2.14	108.40	112.48
2	A	1000	HEM	C3C-C4C-NC	-2.14	106.91	110.94
2	D	1000	HEM	CBD-CAD-C3D	-2.13	108.40	112.47
4	C	2001	MES	C6-C5-N4	-2.13	107.12	110.11
2	J	1000	HEM	CAD-CBD-CGD	-2.13	109.02	112.66
2	P	1000	HEM	CAA-CBA-CGA	-2.13	109.02	112.66
2	N	1000	HEM	C1D-C2D-C3D	-2.08	105.55	107.00
2	T	1000	HEM	CAD-CBD-CGD	-2.08	109.10	112.66
2	T	1000	HEM	CAA-CBA-CGA	-2.08	109.10	112.66
2	O	1000	HEM	CAD-CBD-CGD	-2.07	109.13	112.66
2	N	1000	HEM	C3C-C4C-NC	-2.06	107.05	110.94
4	N	2001	MES	C6-O1-C2	2.02	116.71	109.89
4	G	2001	MES	C6-O1-C2	2.02	116.74	109.89
2	N	1000	HEM	CMA-C3A-C2A	2.03	128.78	124.94
4	B	2001	MES	O1-C2-C3	2.04	116.39	111.83
4	S	2001	MES	C6-O1-C2	2.05	116.83	109.89
4	I	2001	MES	O3S-S-C8	2.05	108.58	106.06
4	B	2001	MES	C6-O1-C2	2.05	116.84	109.89
4	J	2001	MES	C6-O1-C2	2.07	116.90	109.89
2	B	1000	HEM	CMA-C3A-C2A	2.07	128.85	124.94
4	B	2001	MES	O1-C6-C5	2.08	116.48	111.83
4	H	2001	MES	C6-O1-C2	2.09	116.96	109.89
4	R	2001	MES	O3S-S-C8	2.11	108.65	106.06
2	H	1000	HEM	CMA-C3A-C2A	2.13	128.97	124.94
4	F	2001	MES	O1-C2-C3	2.14	116.61	111.83
2	T	1000	HEM	C4A-C3A-C2A	2.14	108.49	107.00
4	A	2001	MES	C6-O1-C2	2.15	117.15	109.89
2	K	1000	HEM	CMA-C3A-C2A	2.21	129.10	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2001	MES	C6-O1-C2	2.23	117.42	109.89
2	I	1000	HEM	CMA-C3A-C2A	2.23	129.14	124.94
4	P	2001	MES	O2S-S-C8	2.32	108.79	106.79
2	E	1000	HEM	CMA-C3A-C2A	2.34	129.36	124.94
2	G	1000	HEM	CMA-C3A-C2A	2.35	129.37	124.94
2	F	1000	HEM	CMA-C3A-C2A	2.39	129.46	124.94
2	J	1000	HEM	CMA-C3A-C2A	2.40	129.47	124.94
2	S	1000	HEM	CMA-C3A-C2A	2.42	129.50	124.94
4	F	2001	MES	C7-N4-C3	2.46	117.56	111.26
4	J	2001	MES	O1S-S-C8	2.46	108.91	106.79
2	S	1000	HEM	C4C-C3C-C2C	2.48	108.63	106.90
4	M	2001	MES	O3S-S-C8	2.50	109.13	106.06
4	O	2001	MES	O1S-S-C8	2.50	108.94	106.79
4	T	2001	MES	C7-N4-C3	2.56	117.83	111.26
4	B	2001	MES	C7-N4-C3	2.60	117.91	111.26
4	G	2001	MES	C7-N4-C3	2.62	117.98	111.26
4	G	2001	MES	O1S-S-C8	2.63	109.05	106.79
4	R	2001	MES	C6-O1-C2	2.64	118.82	109.89
4	F	2001	MES	O1S-S-C8	2.67	109.09	106.79
4	F	2001	MES	C7-N4-C5	2.67	118.11	111.26
4	Q	2001	MES	C7-N4-C3	2.68	118.14	111.26
4	K	2001	MES	O2S-S-C8	2.77	109.17	106.79
4	P	2001	MES	C7-N4-C3	2.77	118.35	111.26
4	E	2001	MES	C7-N4-C3	2.77	118.36	111.26
4	R	2001	MES	C7-N4-C5	2.80	118.44	111.26
4	I	2001	MES	O1S-S-C8	2.88	109.26	106.79
4	H	2001	MES	C7-N4-C3	2.91	118.71	111.26
4	O	2001	MES	C7-N4-C3	2.92	118.75	111.26
4	S	2001	MES	C7-N4-C3	2.95	118.82	111.26
4	J	2001	MES	C7-N4-C3	2.95	118.83	111.26
4	C	2001	MES	C7-N4-C3	2.98	118.89	111.26
4	I	2001	MES	C7-N4-C3	3.03	119.01	111.26
4	M	2001	MES	C7-N4-C3	3.07	119.11	111.26
4	B	2001	MES	O2S-S-C8	3.08	109.44	106.79
4	A	2001	MES	C7-N4-C3	3.09	119.17	111.26
4	T	2001	MES	O2S-S-C8	3.11	109.46	106.79
4	F	2001	MES	C6-O1-C2	3.14	120.50	109.89
4	E	2001	MES	C7-N4-C5	3.14	119.31	111.26
4	D	2001	MES	C7-N4-C3	3.16	119.36	111.26
4	M	2001	MES	C7-N4-C5	3.16	119.36	111.26
4	M	2001	MES	C6-O1-C2	3.18	120.64	109.89
4	E	2001	MES	O1S-S-C8	3.20	109.54	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2001	MES	C7-N4-C5	3.20	119.46	111.26
4	J	2001	MES	C7-N4-C5	3.22	119.52	111.26
4	D	2001	MES	O1S-S-C8	3.28	109.61	106.79
4	L	2001	MES	C7-N4-C3	3.28	119.67	111.26
4	N	2001	MES	C7-N4-C5	3.29	119.69	111.26
4	N	2001	MES	O3S-S-C8	3.31	110.13	106.06
4	A	2001	MES	C7-N4-C5	3.39	119.95	111.26
4	L	2001	MES	C7-N4-C5	3.39	119.95	111.26
4	K	2001	MES	O1S-S-C8	3.41	109.72	106.79
4	P	2001	MES	C7-N4-C5	3.43	120.04	111.26
4	C	2001	MES	C7-N4-C5	3.43	120.05	111.26
4	I	2001	MES	C7-N4-C5	3.46	120.14	111.26
4	O	2001	MES	O3S-S-C8	3.49	110.35	106.06
4	R	2001	MES	C7-N4-C3	3.52	120.29	111.26
4	T	2001	MES	C7-N4-C5	3.53	120.29	111.26
4	K	2001	MES	C7-N4-C5	3.57	120.40	111.26
2	H	1000	HEM	C4C-C3C-C2C	3.65	109.44	106.90
4	S	2001	MES	C7-N4-C5	3.65	120.60	111.26
4	O	2001	MES	C7-N4-C5	3.68	120.68	111.26
2	K	1000	HEM	C4C-C3C-C2C	3.72	109.49	106.90
4	H	2001	MES	C7-N4-C5	3.75	120.86	111.26
4	N	2001	MES	C7-N4-C3	3.80	121.00	111.26
4	H	2001	MES	O3S-S-C8	3.87	110.81	106.06
4	Q	2001	MES	C7-N4-C5	3.91	121.28	111.26
4	T	2001	MES	O3S-S-C8	3.98	110.95	106.06
4	K	2001	MES	C7-N4-C3	4.01	121.53	111.26
2	P	1000	HEM	C4C-C3C-C2C	4.03	109.71	106.90
4	K	2001	MES	C5-N4-C3	4.06	118.06	108.87
4	B	2001	MES	C7-N4-C5	4.11	121.80	111.26
4	R	2001	MES	O1S-S-C8	4.14	110.35	106.79
2	F	1000	HEM	C4C-C3C-C2C	4.21	109.84	106.90
4	G	2001	MES	C7-N4-C5	4.23	122.10	111.26
4	S	2001	MES	O3S-S-C8	4.26	111.29	106.06
4	J	2001	MES	O3S-S-C8	4.26	111.30	106.06
4	L	2001	MES	O3S-S-C8	4.28	111.32	106.06
2	N	1000	HEM	C4C-C3C-C2C	4.29	109.89	106.90
2	A	1000	HEM	C4C-C3C-C2C	4.29	109.89	106.90
2	T	1000	HEM	C4C-C3C-C2C	4.41	109.98	106.90
2	E	1000	HEM	C4C-C3C-C2C	4.43	109.99	106.90
2	D	1000	HEM	C4C-C3C-C2C	4.44	110.00	106.90
2	M	1000	HEM	C4C-C3C-C2C	4.53	110.06	106.90
4	N	2001	MES	C5-N4-C3	4.60	119.30	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1000	HEM	C4C-C3C-C2C	4.64	110.14	106.90
4	E	2001	MES	O3S-S-C8	4.72	111.86	106.06
4	G	2001	MES	O3S-S-C8	4.77	111.93	106.06
2	G	1000	HEM	C4C-C3C-C2C	4.79	110.25	106.90
4	P	2001	MES	O3S-S-C8	4.85	112.03	106.06
4	G	2001	MES	C5-N4-C3	4.88	119.92	108.87
4	A	2001	MES	O3S-S-C8	4.94	112.13	106.06
4	C	2001	MES	O3S-S-C8	4.96	112.15	106.06
4	B	2001	MES	C5-N4-C3	5.04	120.29	108.87
2	C	1000	HEM	C4C-C3C-C2C	5.06	110.43	106.90
4	L	2001	MES	C5-N4-C3	5.08	120.37	108.87
4	H	2001	MES	C5-N4-C3	5.10	120.43	108.87
2	B	1000	HEM	C4C-C3C-C2C	5.13	110.48	106.90
4	O	2001	MES	C5-N4-C3	5.16	120.56	108.87
4	Q	2001	MES	C5-N4-C3	5.17	120.58	108.87
4	S	2001	MES	C5-N4-C3	5.17	120.58	108.87
4	F	2001	MES	O3S-S-C8	5.24	112.50	106.06
4	I	2001	MES	C5-N4-C3	5.29	120.85	108.87
4	A	2001	MES	C5-N4-C3	5.30	120.87	108.87
4	C	2001	MES	C5-N4-C3	5.38	121.06	108.87
4	D	2001	MES	C5-N4-C3	5.44	121.19	108.87
2	J	1000	HEM	C4C-C3C-C2C	5.44	110.70	106.90
4	R	2001	MES	C5-N4-C3	5.47	121.27	108.87
2	L	1000	HEM	C4C-C3C-C2C	5.48	110.73	106.90
4	Q	2001	MES	O3S-S-C8	5.50	112.82	106.06
4	M	2001	MES	C5-N4-C3	5.58	121.52	108.87
4	P	2001	MES	C5-N4-C3	5.62	121.61	108.87
4	J	2001	MES	C5-N4-C3	5.64	121.64	108.87
4	T	2001	MES	C5-N4-C3	5.74	121.88	108.87
2	R	1000	HEM	C4C-C3C-C2C	5.77	110.93	106.90
4	K	2001	MES	O3S-S-C8	5.87	113.28	106.06
4	E	2001	MES	C5-N4-C3	5.94	122.33	108.87
2	I	1000	HEM	C4C-C3C-C2C	5.94	111.05	106.90
4	M	2001	MES	O1S-S-C8	6.08	112.02	106.79
2	Q	1000	HEM	C4C-C3C-C2C	6.27	111.28	106.90
4	D	2001	MES	O3S-S-C8	6.74	114.34	106.06
4	F	2001	MES	C5-N4-C3	6.83	124.33	108.87
4	B	2001	MES	O3S-S-C8	7.42	115.18	106.06
4	N	2001	MES	O1S-S-C8	7.55	113.28	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 234 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	HEM	13	0
2	B	1000	HEM	8	0
2	C	1000	HEM	14	0
4	C	2001	MES	1	0
2	D	1000	HEM	7	0
2	E	1000	HEM	10	0
4	E	2001	MES	1	0
2	F	1000	HEM	13	0
4	F	2001	MES	2	0
2	G	1000	HEM	10	0
2	H	1000	HEM	14	0
4	H	2001	MES	1	0
2	I	1000	HEM	8	0
2	J	1000	HEM	14	0
3	J	2000	NO2	1	0
2	K	1000	HEM	11	0
2	L	1000	HEM	12	0
2	M	1000	HEM	13	0
2	N	1000	HEM	11	0
4	N	2001	MES	1	0
2	O	1000	HEM	10	0
4	O	2001	MES	1	0
2	P	1000	HEM	10	0
4	P	2001	MES	1	0
2	Q	1000	HEM	10	0
2	R	1000	HEM	9	0
2	S	1000	HEM	15	0
4	S	2001	MES	1	0
2	T	1000	HEM	10	0
4	T	2001	MES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	241/248 (97%)	-0.84	0 100 100	6, 18, 44, 57	0
1	B	241/248 (97%)	-0.77	1 (0%) 92 81	8, 18, 42, 63	0
1	C	241/248 (97%)	-0.73	1 (0%) 92 81	6, 18, 45, 64	0
1	D	241/248 (97%)	-0.76	0 100 100	9, 21, 47, 71	0
1	E	241/248 (97%)	-0.83	0 100 100	4, 15, 39, 57	0
1	F	241/248 (97%)	-0.54	0 100 100	13, 36, 68, 94	0
1	G	241/248 (97%)	-0.77	0 100 100	12, 26, 51, 80	0
1	H	241/248 (97%)	-0.78	0 100 100	8, 21, 47, 68	0
1	I	241/248 (97%)	-0.69	0 100 100	8, 21, 54, 71	0
1	J	241/248 (97%)	-0.71	0 100 100	12, 27, 64, 83	0
1	K	241/248 (97%)	-0.69	0 100 100	11, 26, 56, 78	0
1	L	241/248 (97%)	-0.72	0 100 100	11, 23, 52, 72	0
1	M	241/248 (97%)	-0.70	2 (0%) 86 69	10, 23, 50, 74	0
1	N	241/248 (97%)	-0.59	1 (0%) 92 81	14, 28, 62, 74	0
1	O	241/248 (97%)	-0.61	0 100 100	14, 31, 61, 84	0
1	P	241/248 (97%)	-0.39	0 100 100	30, 52, 92, 117	0
1	Q	241/248 (97%)	-0.56	1 (0%) 92 81	17, 43, 87, 107	0
1	R	241/248 (97%)	-0.39	0 100 100	20, 44, 88, 110	0
1	S	241/248 (97%)	-0.34	2 (0%) 86 69	30, 57, 98, 118	0
1	T	241/248 (97%)	-0.41	0 100 100	27, 53, 98, 121	0
All	All	4820/4960 (97%)	-0.64	8 (0%) 94 88	4, 29, 74, 121	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	SER	4.6
1	M	132	SER	3.5
1	Q	132	SER	3.2
1	C	38	VAL	2.8
1	S	132	SER	2.6
1	S	8	LYS	2.5
1	M	8	LYS	2.1
1	N	38	VAL	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MES	Q	2001	12/12	0.84	0.57	8.77	68,71,72,73	0
4	MES	M	2001	12/12	0.84	0.63	8.73	56,60,62,62	0
5	CA	M	1001	1/1	0.96	0.18	7.42	21,21,21,21	0
4	MES	B	2001	12/12	0.81	0.60	7.39	52,55,57,57	0
4	MES	F	2001	12/12	0.86	0.53	5.97	72,76,77,78	0
3	NO2	B	2000	3/3	0.92	0.32	5.88	26,26,28,30	0
4	MES	N	2001	12/12	0.89	0.30	5.88	60,65,67,67	0
4	MES	G	2001	12/12	0.91	0.27	4.96	60,62,65,66	0
3	NO2	R	2000	3/3	0.95	0.29	4.71	36,36,37,37	0
4	MES	T	2001	12/12	0.91	0.53	4.61	80,83,85,85	0
3	NO2	M	2000	3/3	0.95	0.28	3.18	24,24,25,28	0
4	MES	S	2001	12/12	0.91	0.32	3.08	88,91,93,94	0
4	MES	A	2001	12/12	0.93	0.23	2.93	47,51,52,53	0
4	MES	O	2001	12/12	0.94	0.23	2.58	64,66,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MES	P	2001	12/12	0.91	0.30	2.54	76,79,82,82	0
3	NO2	K	2000	3/3	0.98	0.21	2.49	26,26,26,27	0
4	MES	H	2001	12/12	0.96	0.22	2.43	49,51,52,53	0
2	HEM	G	1000	43/43	0.95	0.18	2.30	14,19,27,32	0
3	NO2	A	2000	3/3	0.98	0.19	2.03	20,20,21,22	0
4	MES	E	2001	12/12	0.96	0.19	1.99	47,48,49,50	0
2	HEM	D	1000	43/43	0.95	0.20	1.74	10,16,25,30	0
2	HEM	I	1000	43/43	0.95	0.19	1.70	8,12,20,27	0
2	HEM	A	1000	43/43	0.96	0.19	1.64	8,13,20,30	0
4	MES	K	2001	12/12	0.96	0.21	1.54	54,56,58,59	0
2	HEM	K	1000	43/43	0.96	0.20	1.52	13,17,25,30	0
4	MES	I	2001	12/12	0.96	0.19	1.50	50,52,54,54	0
4	MES	C	2001	12/12	0.96	0.19	1.50	49,51,52,53	0
2	HEM	E	1000	43/43	0.96	0.17	1.46	5,10,17,22	0
2	HEM	B	1000	43/43	0.92	0.22	1.42	10,13,21,25	0
2	HEM	J	1000	43/43	0.95	0.19	1.42	12,16,24,32	0
2	HEM	M	1000	43/43	0.94	0.21	1.41	11,16,23,28	0
4	MES	L	2001	12/12	0.97	0.19	1.22	52,54,56,57	0
2	HEM	L	1000	43/43	0.96	0.18	1.05	11,15,23,27	0
2	HEM	O	1000	43/43	0.96	0.18	1.02	19,23,32,37	0
2	HEM	H	1000	43/43	0.96	0.18	0.99	8,12,20,25	0
3	NO2	T	2000	3/3	0.98	0.26	0.94	45,45,46,47	0
4	MES	R	2001	12/12	0.92	0.21	0.87	65,67,68,68	0
2	HEM	R	1000	43/43	0.94	0.21	0.78	20,26,31,44	0
2	HEM	F	1000	43/43	0.94	0.24	0.77	20,28,37,42	0
2	HEM	C	1000	43/43	0.96	0.16	0.64	8,11,20,26	0
2	HEM	Q	1000	43/43	0.95	0.18	0.60	22,24,30,34	0
5	CA	K	1001	1/1	0.96	0.16	0.47	20,20,20,20	0
4	MES	D	2001	12/12	0.94	0.19	0.46	54,56,58,59	0
3	NO2	P	2000	3/3	0.98	0.19	0.45	45,45,45,45	0
2	HEM	N	1000	43/43	0.96	0.17	0.41	16,23,29,39	0
5	CA	L	1001	1/1	0.94	0.14	0.37	20,20,20,20	0
5	CA	G	1001	1/1	0.95	0.14	0.30	18,18,18,18	0
3	NO2	O	2000	3/3	0.98	0.13	0.18	32,32,32,32	0
5	CA	A	1001	1/1	0.97	0.12	0.13	16,16,16,16	0
4	MES	J	2001	12/12	0.96	0.14	0.13	54,56,58,58	0
3	NO2	I	2000	3/3	0.99	0.15	0.07	21,21,21,21	0
2	HEM	P	1000	43/43	0.96	0.19	0.06	32,35,43,47	0
2	HEM	T	1000	43/43	0.95	0.20	0.02	30,36,43,50	0
2	HEM	S	1000	43/43	0.95	0.20	-0.02	36,43,52,59	0
5	CA	O	1001	1/1	0.97	0.14	-0.13	21,21,21,21	0
3	NO2	J	2000	3/3	0.99	0.14	-0.13	25,25,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	B	1001	1/1	0.98	0.13	-0.49	14,14,14,14	0
3	NO2	C	2000	3/3	0.99	0.12	-0.61	21,21,21,22	0
3	NO2	N	2000	3/3	0.98	0.14	-0.61	32,32,33,33	0
3	NO2	G	2000	3/3	0.98	0.13	-0.62	28,28,28,28	0
3	NO2	Q	2000	3/3	0.98	0.14	-0.69	37,37,38,38	0
5	CA	S	1001	1/1	0.93	0.15	-0.74	50,50,50,50	0
3	NO2	F	2000	3/3	0.99	0.14	-0.77	35,35,36,36	0
3	NO2	L	2000	3/3	0.99	0.12	-0.80	24,24,24,25	0
5	CA	R	1001	1/1	0.96	0.14	-0.93	39,39,39,39	0
5	CA	Q	1001	1/1	0.96	0.13	-0.96	36,36,36,36	0
5	CA	J	1001	1/1	0.98	0.13	-1.20	26,26,26,26	0
5	CA	H	1001	1/1	0.96	0.10	-1.29	17,17,17,17	0
5	CA	F	1001	1/1	0.97	0.12	-1.37	25,25,25,25	0
5	CA	P	1001	1/1	0.96	0.10	-1.41	44,44,44,44	0
5	CA	C	1001	1/1	0.97	0.09	-1.46	17,17,17,17	0
5	CA	N	1001	1/1	0.96	0.11	-1.57	28,28,28,28	0
3	NO2	D	2000	3/3	0.99	0.11	-1.64	24,24,24,25	0
3	NO2	E	2000	3/3	0.99	0.10	-2.15	15,15,15,16	0
5	CA	D	1001	1/1	0.96	0.09	-2.23	19,19,19,19	0
3	NO2	S	2000	3/3	0.99	0.12	-2.31	52,52,52,52	0
5	CA	T	1001	1/1	0.95	0.14	-2.40	44,44,44,44	0
3	NO2	H	2000	3/3	0.99	0.09	-2.89	21,21,21,21	0
5	CA	I	1001	1/1	0.94	0.08	-3.15	18,18,18,18	0
5	CA	E	1001	1/1	0.99	0.09	-4.06	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.