



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 04:20 PM EDT

PDB ID : 4U8U
Title : The Crystallographic structure of the giant hemoglobin from *Glossoscolex paulistus* at 3.2 Å resolution.
Authors : Bachega, J.F.R.; Maluf, F.V.; Andi, B.; D'Muniz Pereira, H.; Carazzollea, M.F.; Orville, A.; Tabak, M.; Garratt, R.C.; Horjales, E.
Deposited on : 2014-08-04
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

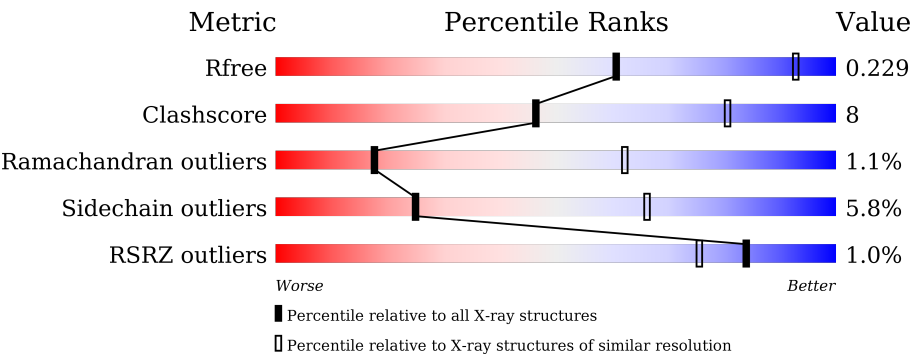
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	150	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>66%29% . .</div></div>
1	E	150	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>63%31%5% .</div></div>
1	I	150	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>63%30%5% .</div></div>
1	P	150	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>71%24% . .</div></div>
1	T	150	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>69%25% . .</div></div>
1	X	150	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%22% . .</div></div>


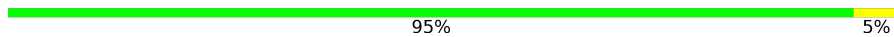
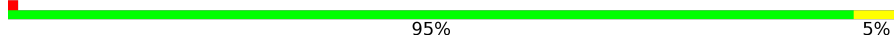
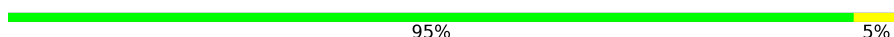
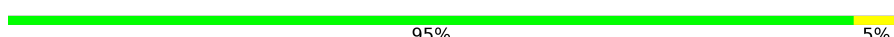









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Mol	Chain	Length	Quality of chain
1	e	150	
1	i	150	
1	m	150	
2	B	142	
2	F	142	
2	J	142	
2	Q	142	
2	U	142	
2	Y	142	
2	f	142	
2	j	142	
2	n	142	
3	C	151	
3	G	151	
3	K	151	
3	R	151	
3	V	151	
3	Z	151	
3	g	151	
3	k	151	
3	o	151	
4	D	141	
4	H	141	
4	L	141	
4	S	141	

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Mol	Chain	Length	Quality of chain
4	W	141	
4	a	141	
4	h	141	
4	l	141	
4	p	141	
5	M	224	
5	b	224	
5	q	224	
6	N	236	
6	c	236	
6	r	236	
7	O	218	
7	d	218	
7	s	218	

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
9	CYN	F	202	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 59163 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 Globin a chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	E	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	I	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	P	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	T	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	X	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	e	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	i	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	m	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			

- Molecule 2 is a protein called Globin b Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	F	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	J	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	Q	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	U	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	f	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	j	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	n	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			

- Molecule 3 is a protein called Globin c Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	G	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	K	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	R	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	V	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	Z	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	g	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	k	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	o	151	Total	C	N	O	S	0	0	0
			1189	755	208	220	6			

- Molecule 4 is a protein called Globin d Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	H	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	L	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	S	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	W	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	a	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	h	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	l	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	p	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			

- Molecule 5 is a protein called Linker L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	222	Total	C	N	O	S	0	0	0
			1754	1092	315	337	10			
5	b	222	Total	C	N	O	S	0	0	0
			1754	1092	315	337	10			
5	q	222	Total	C	N	O	S	0	0	0
			1754	1092	315	337	10			

- Molecule 6 is a protein called Linker L2.

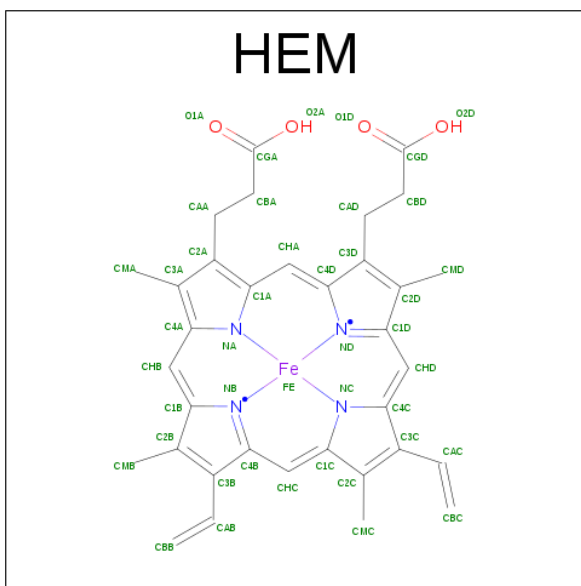
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	219	Total	C	N	O	S	0	0	0
			1713	1060	326	317	10			
6	c	219	Total	C	N	O	S	0	0	0
			1713	1060	326	317	10			
6	r	219	Total	C	N	O	S	0	0	0
			1713	1060	326	317	10			

- Molecule 7 is a protein called Linker L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	213	Total	C	N	O	S	0	0	0
			1686	1044	297	337	8			
7	d	213	Total	C	N	O	S	0	0	0
			1686	1044	297	337	8			
7	s	213	Total	C	N	O	S	0	0	0
			1686	1044	297	337	8			

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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

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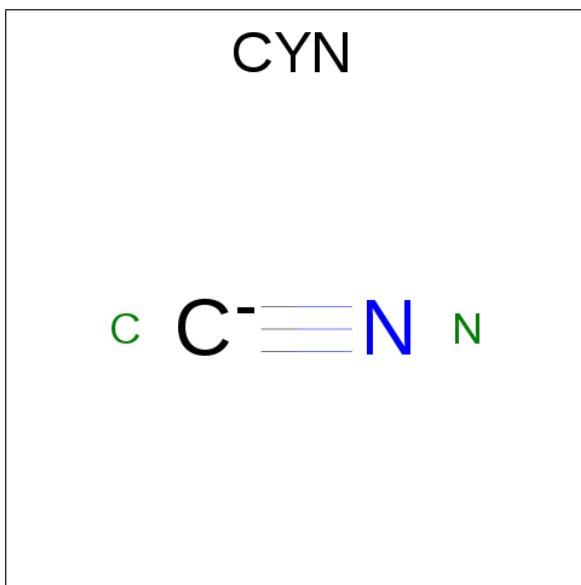
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	Y	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	Z	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	a	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	g	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	h	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	i	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	j	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	k	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	l	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	m	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	n	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	o	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
8	p	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 9 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			2	1	1		
9	B	1	Total	C	N	0	0
			2	1	1		
9	C	1	Total	C	N	0	0
			2	1	1		
9	D	1	Total	C	N	0	0
			2	1	1		
9	E	1	Total	C	N	0	0
			2	1	1		
9	F	1	Total	C	N	0	0
			2	1	1		
9	G	1	Total	C	N	0	0
			2	1	1		
9	H	1	Total	C	N	0	0
			2	1	1		
9	I	1	Total	C	N	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	J	1	Total	C	N	0	0
			2	1	1		
9	K	1	Total	C	N	0	0
			2	1	1		
9	L	1	Total	C	N	0	0
			2	1	1		
9	P	1	Total	C	N	0	0
			2	1	1		
9	Q	1	Total	C	N	0	0
			2	1	1		
9	R	1	Total	C	N	0	0
			2	1	1		
9	S	1	Total	C	N	0	0
			2	1	1		
9	T	1	Total	C	N	0	0
			2	1	1		
9	U	1	Total	C	N	0	0
			2	1	1		
9	V	1	Total	C	N	0	0
			2	1	1		
9	W	1	Total	C	N	0	0
			2	1	1		
9	X	1	Total	C	N	0	0
			2	1	1		
9	Y	1	Total	C	N	0	0
			2	1	1		
9	Z	1	Total	C	N	0	0
			2	1	1		
9	a	1	Total	C	N	0	0
			2	1	1		
9	e	1	Total	C	N	0	0
			2	1	1		
9	f	1	Total	C	N	0	0
			2	1	1		
9	g	1	Total	C	N	0	0
			2	1	1		
9	h	1	Total	C	N	0	0
			2	1	1		
9	i	1	Total	C	N	0	0
			2	1	1		
9	j	1	Total	C	N	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	k	1	Total	C	N	0	0
			2	1	1		
9	l	1	Total	C	N	0	0
			2	1	1		
9	m	1	Total	C	N	0	0
			2	1	1		
9	n	1	Total	C	N	0	0
			2	1	1		
9	o	1	Total	C	N	0	0
			2	1	1		
9	p	1	Total	C	N	0	0
			2	1	1		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	q	1	Total	Ca	0	0
			1	1		
10	d	1	Total	Ca	0	0
			1	1		
10	b	1	Total	Ca	0	0
			1	1		
10	c	1	Total	Ca	0	0
			1	1		
10	N	1	Total	Ca	0	0
			1	1		
10	O	1	Total	Ca	0	0
			1	1		
10	r	1	Total	Ca	0	0
			1	1		
10	s	1	Total	Ca	0	0
			1	1		
10	M	1	Total	Ca	0	0
			1	1		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

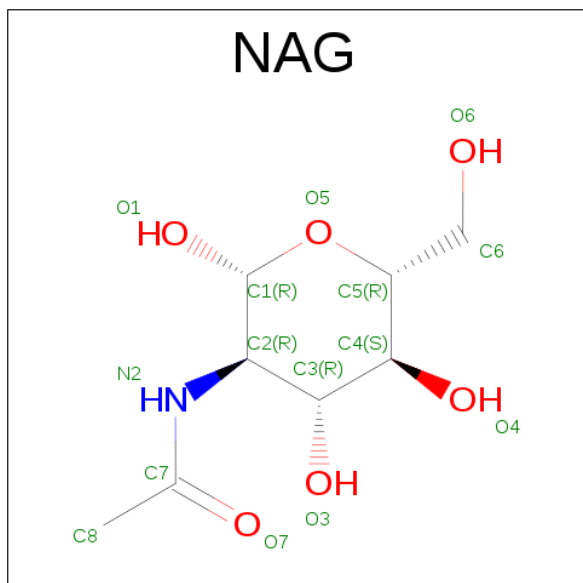
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	O	2	Total	Zn	0	0
			2	2		
11	d	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	c	1	Total	Zn	0	0
			1	1		
11	s	1	Total	Zn	0	0
			1	1		

- Molecule 12 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	O	1	Total	C	N	O	0	0
			14	8	1	5		
12	d	1	Total	C	N	O	0	0
			14	8	1	5		
12	s	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	O	1	Total	O	0	0
			1	1		
13	c	1	Total	O	0	0
			1	1		
13	d	2	Total	O	0	0
			2	2		
13	r	1	Total	O	0	0
			1	1		

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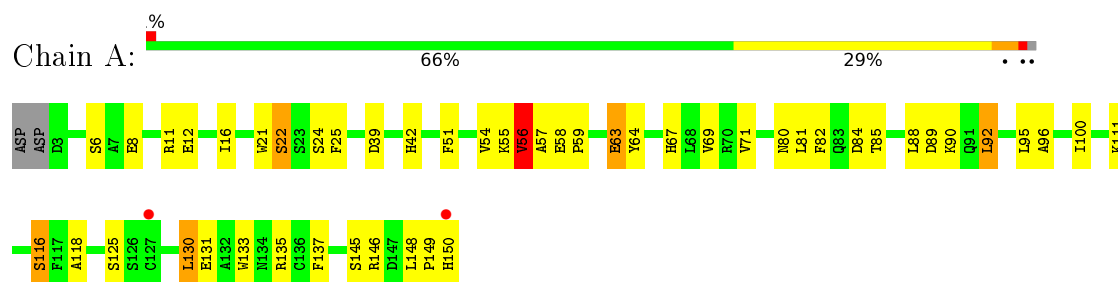
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	s	1	Total	O	0	0
			1	1		

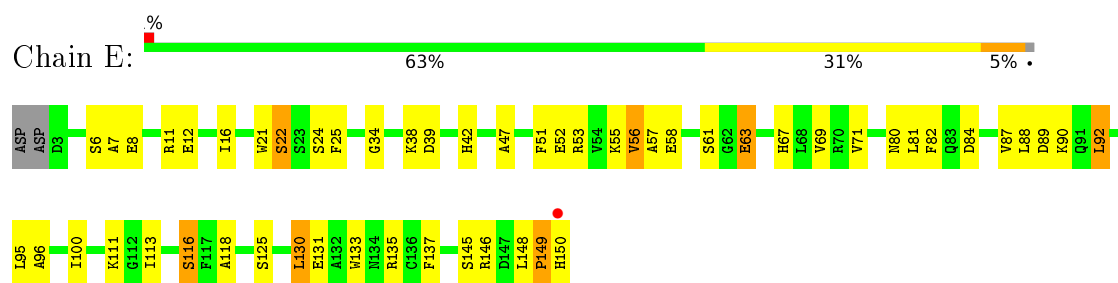
3 Residue-property plots [i](#)

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

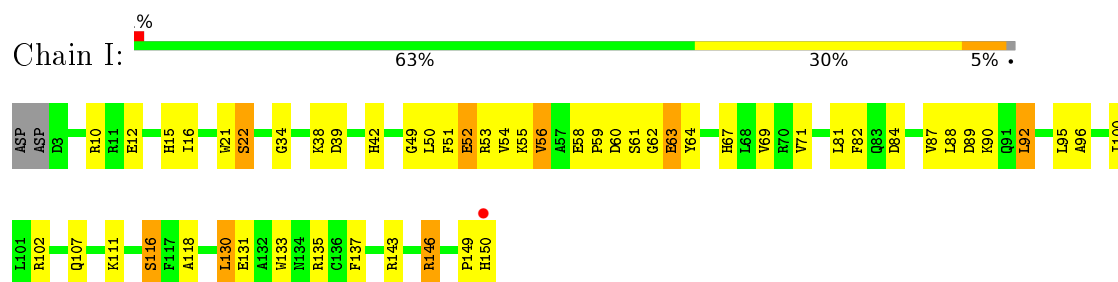
- Molecule 1: Globin a chain



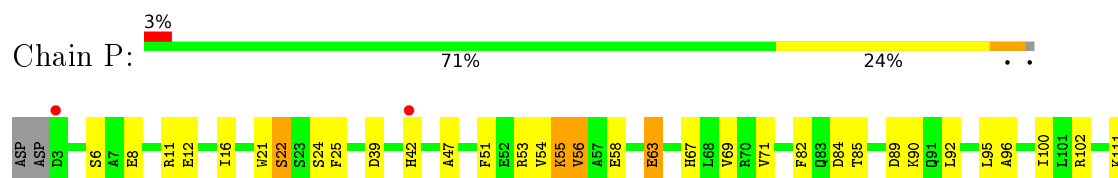
- Molecule 1: Globin a chain

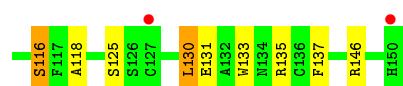


- Molecule 1: Globin a chain

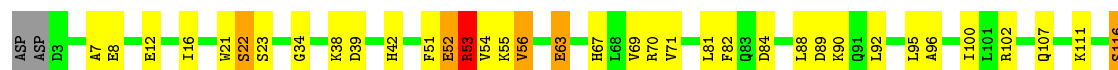


- Molecule 1: Globin a chain

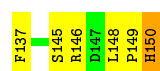




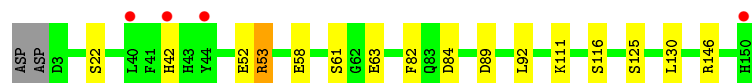
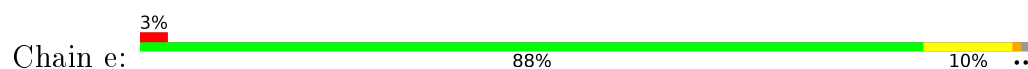
- Molecule 1: Globin a chain



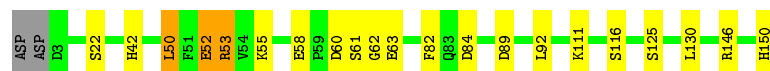
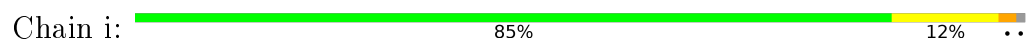
- Molecule 1: Globin a chain



- Molecule 1: Globin a chain



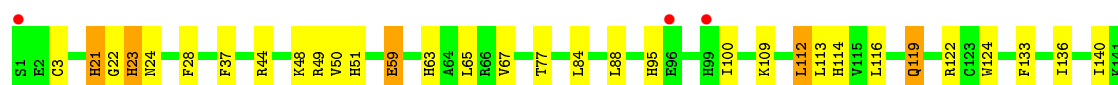
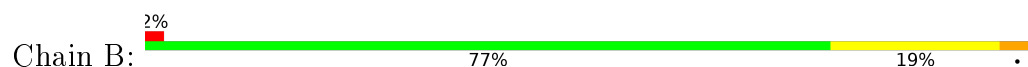
- Molecule 1: Globin a chain



- Molecule 1: Globin a chain

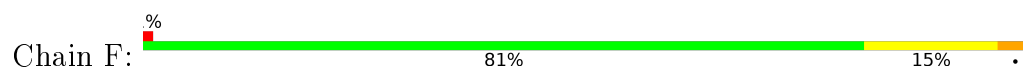


- Molecule 2: Globin b Chain

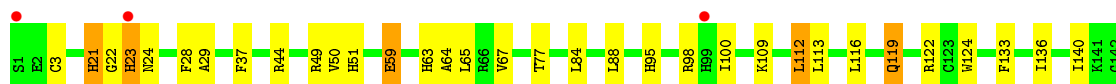
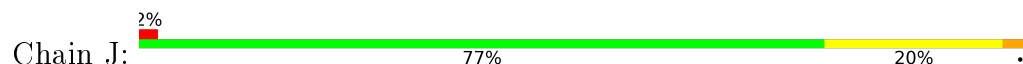


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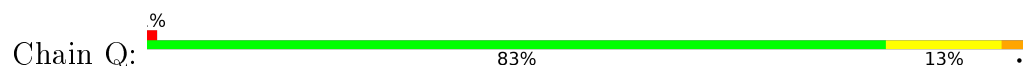
- Molecule 2: Globin b Chain



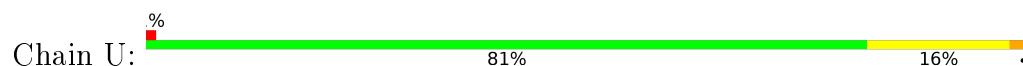
- Molecule 2: Globin b Chain



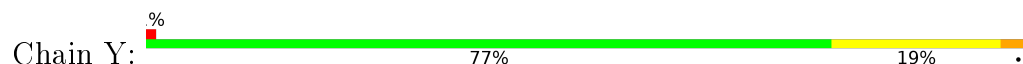
- Molecule 2: Globin b Chain



- Molecule 2: Globin b Chain



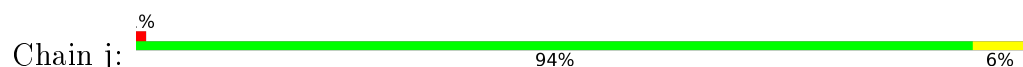
- Molecule 2: Globin b Chain

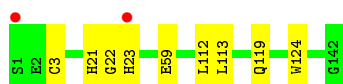


- Molecule 2: Globin b Chain

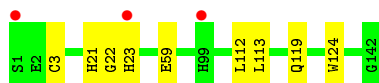


- Molecule 2: Globin b Chain

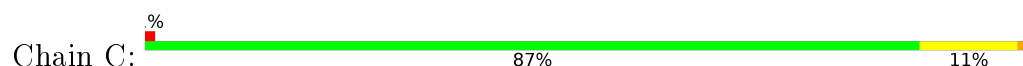




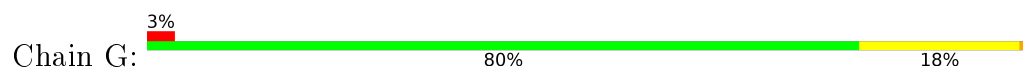
• Molecule 2: Globin b Chain



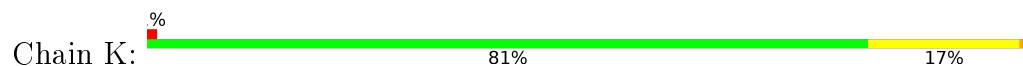
• Molecule 3: Globin c Chain



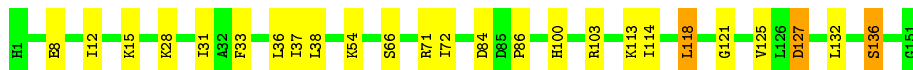
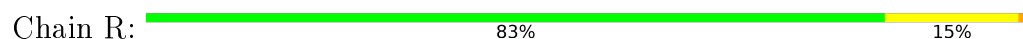
• Molecule 3: Globin c Chain



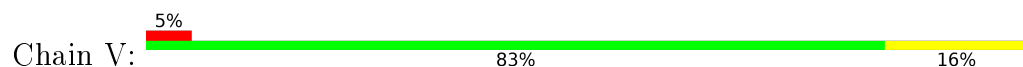
• Molecule 3: Globin c Chain



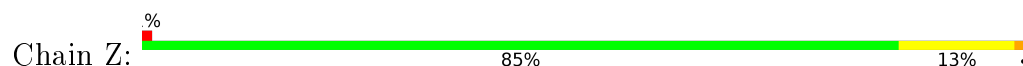
• Molecule 3: Globin c Chain



• Molecule 3: Globin c Chain



• Molecule 3: Globin c Chain





• Molecule 3: Globin c Chain



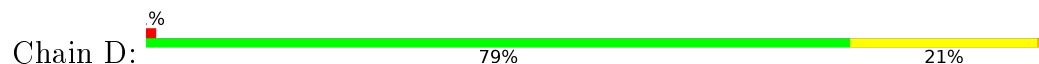
• Molecule 3: Globin c Chain



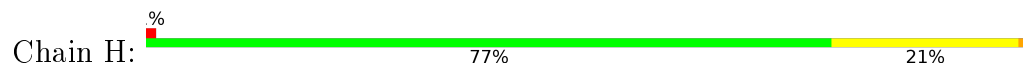
• Molecule 3: Globin c Chain



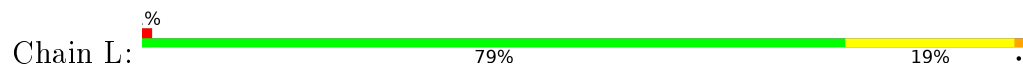
• Molecule 4: Globin d Chain



• Molecule 4: Globin d Chain

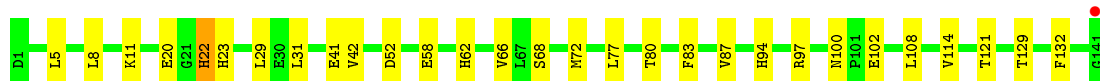
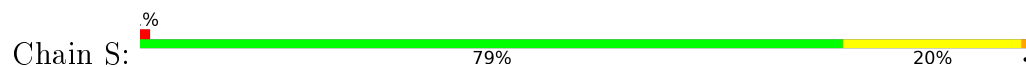


• Molecule 4: Globin d Chain

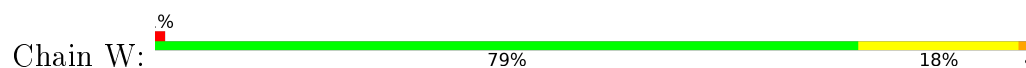




- Molecule 4: Globin d Chain



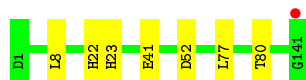
- Molecule 4: Globin d Chain



- Molecule 4: Globin d Chain



- Molecule 4: Globin d Chain



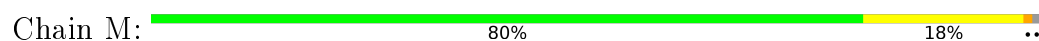
- Molecule 4: Globin d Chain



- Molecule 4: Globin d Chain



- Molecule 5: Linker L1





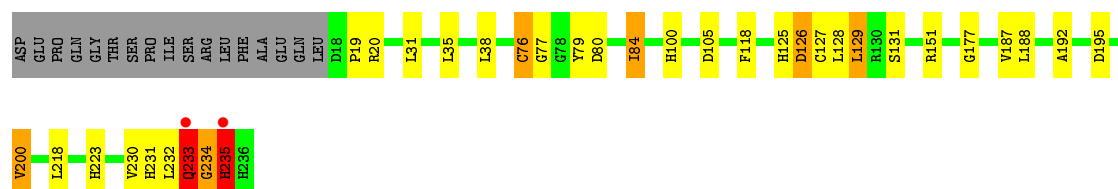
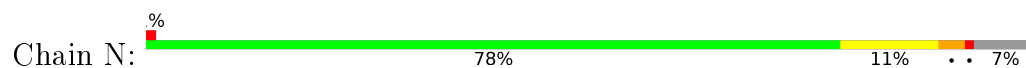
• Molecule 5: Linker L1



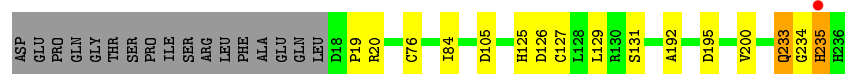
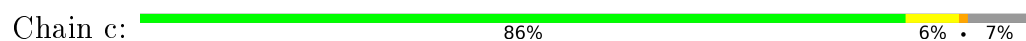
• Molecule 5: Linker L1



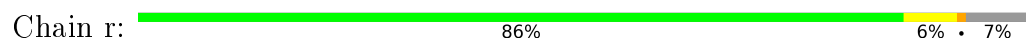
• Molecule 6: Linker L2



• Molecule 6: Linker L2



• Molecule 6: Linker L2



• Molecule 7: Linker L3

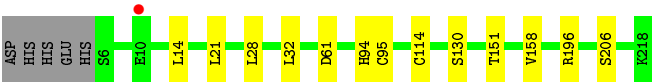
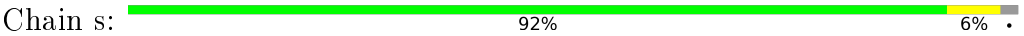




● Molecule 7: Linker L3



● Molecule 7: Linker L3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	272.68Å 319.90Å 333.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 3.20 49.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.66-3.20) 94.1 (49.91-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.235 0.208 , 0.229	Depositor DCC
R_{free} test set	11220 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	59163	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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, ZN, CA, NAG, CYN

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	0.45	0/1231	0.52	0/1665
1	E	0.34	0/1231	0.50	0/1665
1	I	0.37	0/1231	0.95	3/1665 (0.2%)
1	P	0.33	0/1231	0.49	0/1665
1	T	0.49	0/1231	0.52	0/1665
1	X	0.59	0/1231	0.59	0/1665
1	e	0.53	0/1231	0.57	1/1665 (0.1%)
1	i	0.56	0/1231	0.63	2/1665 (0.1%)
1	m	0.37	0/1231	0.50	0/1665
2	B	0.32	0/1181	0.50	0/1600
2	F	0.32	0/1181	0.50	0/1600
2	J	0.31	0/1181	0.49	0/1600
2	Q	0.32	0/1181	0.50	0/1600
2	U	0.32	0/1181	0.51	0/1600
2	Y	0.32	0/1181	0.50	0/1600
2	f	0.32	0/1181	0.50	0/1600
2	j	0.31	0/1181	0.50	0/1600
2	n	0.32	0/1181	0.49	0/1600
3	C	0.29	0/1203	0.44	0/1622
3	G	0.29	0/1203	0.43	0/1622
3	K	0.28	0/1203	0.43	0/1622
3	R	0.29	0/1203	0.44	0/1622
3	V	0.28	0/1203	0.43	0/1622
3	Z	0.28	0/1203	0.43	0/1622
3	g	0.28	0/1203	0.43	0/1622
3	k	0.27	0/1203	0.43	0/1622
3	o	0.29	0/1213	0.44	0/1635
4	D	0.29	0/1172	0.46	0/1584
4	H	0.31	0/1172	0.46	0/1584
4	L	0.30	0/1172	0.46	0/1584
4	S	0.29	0/1172	0.46	0/1584
4	W	0.30	0/1172	0.46	0/1584

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	a	0.30	0/1172	0.46	0/1584
4	h	0.30	0/1172	0.46	0/1584
4	l	0.29	0/1172	0.46	0/1584
4	p	0.29	0/1172	0.46	0/1584
5	M	0.40	2/1793 (0.1%)	0.51	0/2421
5	b	0.35	0/1793	0.51	0/2421
5	q	0.34	0/1793	0.51	0/2421
6	N	0.32	0/1748	0.51	0/2357
6	c	0.32	0/1748	0.51	0/2357
6	r	0.33	0/1748	0.51	0/2357
7	O	0.32	0/1723	0.49	0/2328
7	d	0.33	0/1723	0.49	0/2328
7	s	0.32	0/1723	0.49	0/2328
All	All	0.34	2/58885 (0.0%)	0.50	6/79570 (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
7	O	0	1
7	d	0	1
7	s	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	210	ASN	CG-ND2	-6.95	1.15	1.32
5	M	210	ASN	CG-OD1	-5.54	1.11	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	10	ARG	NE-CZ-NH1	-23.21	108.69	120.30
1	I	10	ARG	NE-CZ-NH2	21.13	130.87	120.30
1	I	10	ARG	CD-NE-CZ	10.18	137.85	123.60
1	i	50	LEU	CB-CG-CD2	-6.72	99.58	111.00
1	i	60	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	e	52	GLU	CB-CA-C	-5.38	99.65	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	O	94	HIS	Peptide
7	d	94	HIS	Peptide
7	s	94	HIS	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	1200	0	1155	52	0
1	E	1200	0	1155	63	0
1	I	1200	0	1155	67	0
1	P	1200	0	1155	35	1
1	T	1200	0	1155	51	0
1	X	1200	0	1153	33	0
1	e	1200	0	1150	0	0
1	i	1200	0	1155	0	1
1	m	1200	0	1155	0	0
2	B	1148	0	1103	37	0
2	F	1148	0	1103	30	0
2	J	1148	0	1103	27	0
2	Q	1148	0	1103	18	0
2	U	1148	0	1103	22	0
2	Y	1148	0	1103	22	0
2	f	1148	0	1103	0	0
2	j	1148	0	1103	0	0
2	n	1148	0	1103	0	0
3	C	1180	0	1182	13	0
3	G	1180	0	1182	25	1
3	K	1180	0	1182	25	0
3	R	1180	0	1182	18	0
3	V	1180	0	1182	19	0
3	Z	1180	0	1182	14	0
3	g	1180	0	1182	0	0
3	k	1180	0	1182	0	0
3	o	1189	0	1193	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1140	0	1105	21	0
4	H	1140	0	1105	27	0
4	L	1140	0	1105	23	0
4	S	1140	0	1105	20	0
4	W	1140	0	1105	20	1
4	a	1140	0	1105	0	0
4	h	1140	0	1105	0	0
4	l	1140	0	1105	0	0
4	p	1140	0	1105	0	0
5	M	1754	0	1631	35	0
5	b	1754	0	1631	0	0
5	q	1754	0	1631	0	0
6	N	1713	0	1628	19	0
6	c	1713	0	1628	0	0
6	r	1713	0	1628	0	0
7	O	1686	0	1565	19	0
7	d	1686	0	1565	0	0
7	s	1686	0	1565	0	0
8	A	43	0	30	1	0
8	B	43	0	30	8	0
8	C	43	0	30	1	0
8	D	43	0	30	2	0
8	E	43	0	30	6	0
8	F	43	0	30	8	0
8	G	43	0	30	1	0
8	H	43	0	30	4	0
8	I	43	0	30	6	0
8	J	43	0	30	8	0
8	K	43	0	30	2	0
8	L	43	0	30	3	0
8	P	43	0	30	3	0
8	Q	43	0	30	7	0
8	R	43	0	30	2	0
8	S	43	0	30	4	0
8	T	43	0	30	2	0
8	U	43	0	30	9	0
8	V	43	0	30	0	0
8	W	43	0	30	3	0
8	X	43	0	30	4	0
8	Y	43	0	30	6	0
8	Z	43	0	30	0	0
8	a	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	e	43	0	30	0	0
8	f	43	0	30	0	0
8	g	43	0	30	0	0
8	h	43	0	30	0	0
8	i	43	0	30	0	0
8	j	43	0	30	0	0
8	k	43	0	30	0	0
8	l	43	0	30	0	0
8	m	43	0	30	0	0
8	n	43	0	30	0	0
8	o	43	0	30	0	0
8	p	43	0	30	0	0
9	A	2	0	0	0	0
9	B	2	0	0	1	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	2	0	0	0	0
9	F	2	0	0	2	0
9	G	2	0	0	0	0
9	H	2	0	0	0	0
9	I	2	0	0	0	0
9	J	2	0	0	1	0
9	K	2	0	0	0	0
9	L	2	0	0	0	0
9	P	2	0	0	0	0
9	Q	2	0	0	1	0
9	R	2	0	0	0	0
9	S	2	0	0	0	0
9	T	2	0	0	0	0
9	U	2	0	0	1	0
9	V	2	0	0	0	0
9	W	2	0	0	0	0
9	X	2	0	0	0	0
9	Y	2	0	0	0	0
9	Z	2	0	0	0	0
9	a	2	0	0	0	0
9	e	2	0	0	0	0
9	f	2	0	0	0	0
9	g	2	0	0	0	0
9	h	2	0	0	0	0
9	i	2	0	0	0	0
9	j	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	k	2	0	0	0	0
9	l	2	0	0	0	0
9	m	2	0	0	0	0
9	n	2	0	0	0	0
9	o	2	0	0	0	0
9	p	2	0	0	0	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	b	1	0	0	0	0
10	c	1	0	0	0	0
10	d	1	0	0	0	0
10	q	1	0	0	0	0
10	r	1	0	0	0	0
10	s	1	0	0	0	0
11	O	2	0	0	0	0
11	c	1	0	0	0	0
11	d	2	0	0	0	0
11	s	1	0	0	0	0
12	O	14	0	13	0	0
12	d	14	0	13	0	0
12	s	14	0	13	0	0
13	O	1	0	0	0	0
13	c	1	0	0	0	0
13	d	2	0	0	0	0
13	r	1	0	0	0	0
13	s	1	0	0	0	0
All	All	59163	0	56500	660	2

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 8.

All (660) 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:T:55:LYS:CD	1:T:63:GLU:HG3	1.17	1.58
1:T:55:LYS:HD2	1:T:63:GLU:CG	1.09	1.52
1:T:55:LYS:NZ	1:T:63:GLU:CD	1.73	1.42
1:E:52:GLU:CG	1:E:53:ARG:N	4.63	1.35
1:T:55:LYS:HZ1	1:T:63:GLU:CD	1.33	1.20
1:T:55:LYS:NZ	1:T:63:GLU:OE2	1.67	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:55:LYS:HD2	1:T:63:GLU:HG2	1.18	1.18
1:T:55:LYS:CE	1:T:63:GLU:HG3	1.75	1.15
1:E:55:LYS:HG3	1:E:63:GLU:HG3	2.64	1.14
1:I:50:LEU:HD23	1:I:50:LEU:N	3.58	1.13
1:I:55:LYS:HD2	1:I:63:GLU:CG	1.79	1.12
1:E:55:LYS:HD2	1:E:63:GLU:CG	1.81	1.11
1:I:52:GLU:O	1:I:55:LYS:N	3.04	1.11
1:I:53:ARG:NH2	8:I:201:HEM:O2D	2.56	1.07
1:I:52:GLU:O	1:I:54:VAL:N	3.18	1.07
1:E:52:GLU:HG2	1:E:53:ARG:N	5.05	1.07
1:X:55:LYS:HG3	1:X:63:GLU:HG3	1.28	1.06
1:E:52:GLU:HG3	1:E:53:ARG:CA	6.19	1.04
1:T:55:LYS:CD	1:T:63:GLU:CG	1.93	1.04
1:I:55:LYS:CD	1:I:63:GLU:HG3	1.88	1.02
1:E:55:LYS:CD	1:E:63:GLU:HG3	1.90	1.01
1:E:55:LYS:HD2	1:E:63:GLU:HG3	0.99	0.99
1:P:55:LYS:HD2	1:P:63:GLU:HG3	1.43	0.98
1:P:55:LYS:CD	1:P:63:GLU:HG3	1.94	0.97
1:I:55:LYS:HD2	1:I:63:GLU:HG3	0.97	0.96
1:X:150:HIS:CD2	1:X:150:HIS:H	1.71	0.94
1:E:52:GLU:HG3	1:E:53:ARG:N	4.76	0.94
1:X:51:PHE:HB2	1:X:56:VAL:CG2	1.99	0.93
1:I:150:HIS:CD2	1:I:150:HIS:H	3.17	0.92
1:X:150:HIS:H	1:X:150:HIS:HD2	1.11	0.92
1:A:54:VAL:O	1:A:55:LYS:HB2	1.73	0.87
1:T:55:LYS:CE	1:T:63:GLU:CG	2.42	0.87
1:A:12:GLU:OE1	5:M:210:ASN:ND2	2.07	0.87
2:B:48:LYS:NZ	2:F:48:LYS:NZ	94.13	0.86
1:E:55:LYS:CG	1:E:63:GLU:HG3	2.65	0.86
1:I:61:SER:HB2	1:I:63:GLU:HG2	2.20	0.86
1:T:55:LYS:CE	1:T:63:GLU:CD	2.44	0.85
1:X:51:PHE:HB2	1:X:56:VAL:HG22	1.57	0.85
2:B:48:LYS:HZ1	2:F:48:LYS:HZ1	94.25	0.84
1:A:51:PHE:O	1:A:56:VAL:CG2	2.24	0.84
1:E:55:LYS:HG3	1:E:63:GLU:CG	3.56	0.83
1:I:150:HIS:HD2	1:I:150:HIS:H	3.13	0.83
1:A:55:LYS:HG3	1:A:63:GLU:HG3	1.60	0.83
1:I:61:SER:O	1:I:63:GLU:N	3.20	0.82
1:A:55:LYS:C	1:A:57:ALA:H	1.81	0.81
1:X:150:HIS:CD2	1:X:150:HIS:N	2.47	0.81
2:F:140:ILE:HD12	8:F:201:HEM:HBB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:51:PHE:O	1:T:56:VAL:CG2	2.29	0.80
5:M:72:ASP:OD1	7:O:196:ARG:NH1	2.16	0.79
1:P:8:GLU:OE2	3:V:6:SER:OG	2.01	0.78
1:A:51:PHE:HB2	1:A:56:VAL:HG21	1.65	0.77
1:I:52:GLU:C	1:I:54:VAL:N	3.07	0.77
1:A:51:PHE:O	1:A:56:VAL:HG23	1.84	0.77
2:Q:24:ASN:ND2	2:Q:119:GLN:OE1	2.18	0.76
2:F:24:ASN:ND2	2:F:119:GLN:OE1	2.23	0.76
2:B:48:LYS:NZ	2:F:48:LYS:HZ1	94.41	0.75
1:T:55:LYS:CG	1:T:63:GLU:HG3	2.14	0.75
5:M:79:ASP:HB3	5:M:144:ARG:HH22	1.48	0.75
6:N:151:ARG:HH11	6:N:151:ARG:HG3	1.51	0.75
2:U:140:ILE:HD12	8:U:201:HEM:HBB2	1.69	0.74
1:A:55:LYS:C	1:A:57:ALA:N	2.38	0.73
1:I:52:GLU:C	1:I:54:VAL:H	2.79	0.73
1:I:61:SER:O	1:I:62:GLY:C	2.91	0.73
1:A:54:VAL:O	1:A:55:LYS:CB	2.30	0.73
1:I:150:HIS:CD2	1:I:150:HIS:N	3.59	0.73
2:J:140:ILE:HD12	8:J:201:HEM:HBB2	1.87	0.73
2:U:24:ASN:ND2	2:U:119:GLN:OE1	2.21	0.73
2:B:24:ASN:ND2	2:B:119:GLN:OE1	2.20	0.72
1:E:61:SER:HB2	1:E:63:GLU:HG2	2.21	0.72
1:I:53:ARG:HH21	8:I:201:HEM:CGD	3.07	0.72
2:Y:24:ASN:ND2	2:Y:119:GLN:OE1	2.22	0.72
2:J:24:ASN:ND2	2:J:119:GLN:OE1	2.23	0.72
1:I:12:GLU:OE1	7:O:206:SER:OG	2.08	0.71
1:T:55:LYS:HZ2	1:T:63:GLU:CD	1.64	0.70
1:I:69:VAL:HG12	4:L:72:MET:HE3	1.72	0.70
7:O:201:ILE:HB	7:O:211:ALA:HB3	1.74	0.70
2:B:48:LYS:HZ1	2:F:48:LYS:NZ	93.98	0.70
2:J:122:ARG:HD3	7:O:207:LYS:NZ	2.07	0.70
1:X:51:PHE:HB2	1:X:56:VAL:HG21	1.73	0.70
2:B:140:ILE:HD12	8:B:201:HEM:HBB2	1.72	0.70
1:A:51:PHE:HB2	1:A:56:VAL:CG2	2.23	0.69
1:I:52:GLU:O	1:I:53:ARG:C	2.93	0.68
4:D:108:LEU:HD21	4:D:129:THR:HG22	1.76	0.68
4:H:108:LEU:HD21	4:H:129:THR:HG22	1.75	0.68
1:P:55:LYS:CG	1:P:63:GLU:HG3	2.23	0.67
3:K:86:PRO:HG3	6:N:129:LEU:HD13	1.77	0.67
1:P:11:ARG:NH1	3:V:8:GLU:HG3	2.10	0.67
4:L:108:LEU:HD21	4:L:129:THR:HG22	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:49:ARG:NH1	8:Y:201:HEM:O1D	2.28	0.67
1:A:69:VAL:HG12	4:D:72:MET:HE3	1.77	0.67
4:W:108:LEU:HD21	4:W:129:THR:HG22	1.77	0.67
1:I:49:GLY:C	1:I:50:LEU:HD23	4.30	0.67
1:T:55:LYS:NZ	1:T:63:GLU:CG	2.57	0.67
2:Q:51:HIS:CG	2:Q:59:GLU:HG3	2.30	0.66
2:Y:140:ILE:HD12	8:Y:201:HEM:HBB2	1.78	0.66
1:E:51:PHE:HB2	1:E:56:VAL:CG2	2.96	0.66
2:B:51:HIS:CG	2:B:59:GLU:HG3	2.31	0.66
4:S:108:LEU:HD21	4:S:129:THR:HG22	1.78	0.66
1:E:6:SER:HB3	3:K:3:PHE:HA	2.42	0.65
1:T:54:VAL:HG23	1:T:54:VAL:O	1.95	0.65
2:F:51:HIS:CG	2:F:59:GLU:HG3	2.31	0.65
3:G:22:GLY:HA3	4:H:15:ARG:NH1	2.12	0.65
1:T:51:PHE:O	1:T:56:VAL:HG23	1.97	0.65
1:A:55:LYS:O	1:A:57:ALA:N	2.29	0.64
1:T:51:PHE:HB2	1:T:56:VAL:HG21	1.79	0.64
1:T:52:GLU:O	1:T:54:VAL:N	2.30	0.64
1:E:51:PHE:CB	1:E:56:VAL:HG22	3.19	0.64
2:J:51:HIS:CG	2:J:59:GLU:HG3	2.33	0.64
1:X:51:PHE:CB	1:X:56:VAL:HG22	2.28	0.64
2:U:51:HIS:CG	2:U:59:GLU:HG3	2.32	0.64
1:E:52:GLU:HG3	1:E:53:ARG:HA	6.38	0.63
6:N:151:ARG:NH1	6:N:151:ARG:HG3	2.11	0.63
6:N:232:LEU:O	6:N:234:GLY:N	2.32	0.63
2:U:100:ILE:HG23	8:U:201:HEM:HAC	1.79	0.63
2:Y:51:HIS:CG	2:Y:59:GLU:HG3	2.32	0.63
1:E:69:VAL:HG12	4:H:72:MET:HE3	1.80	0.63
4:L:83:PHE:O	4:L:87:VAL:HG23	2.02	0.62
1:P:11:ARG:HH12	3:V:8:GLU:HG3	1.65	0.62
1:E:52:GLU:CG	1:E:53:ARG:CA	5.99	0.62
1:E:51:PHE:CB	1:E:56:VAL:CG2	3.72	0.62
1:P:69:VAL:HG12	4:S:72:MET:HE3	1.82	0.62
1:E:51:PHE:HB2	1:E:56:VAL:HG21	2.60	0.62
1:E:90:LYS:NZ	4:H:58:GLU:HG3	2.13	0.62
2:B:95:HIS:HE1	8:B:201:HEM:NA	1.97	0.62
4:W:83:PHE:O	4:W:87:VAL:HG23	2.00	0.62
1:E:90:LYS:HZ3	4:H:58:GLU:HG3	1.64	0.61
1:I:90:LYS:NZ	4:L:58:GLU:HG3	2.15	0.61
1:E:145:SER:O	1:E:148:LEU:HB2	2.00	0.61
1:I:54:VAL:O	1:I:55:LYS:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:69:VAL:HG12	4:W:72:MET:HE3	1.81	0.61
1:P:55:LYS:HG3	1:P:63:GLU:HG3	1.82	0.61
8:Q:201:HEM:C1D	9:Q:202:CYN:N	2.54	0.60
1:T:7:ALA:HB3	3:Z:8:GLU:HB3	1.82	0.60
2:J:21:HIS:O	2:J:23:HIS:N	2.33	0.60
1:A:6:SER:HB3	3:G:3:PHE:HA	1.82	0.60
1:P:6:SER:HB3	3:V:3:PHE:HA	1.83	0.60
1:I:51:PHE:CB	1:I:56:VAL:HG22	3.21	0.60
1:E:52:GLU:O	1:E:55:LYS:N	3.04	0.60
2:F:100:ILE:HG23	8:F:201:HEM:HAC	1.90	0.59
2:U:21:HIS:O	2:U:23:HIS:N	2.34	0.59
8:X:201:HEM:HBD1	8:X:201:HEM:HHA	1.83	0.59
4:D:83:PHE:O	4:D:87:VAL:HG23	2.02	0.59
4:H:83:PHE:O	4:H:87:VAL:HG23	2.02	0.59
1:I:90:LYS:HZ3	4:L:58:GLU:HG3	1.71	0.59
2:J:100:ILE:HG23	8:J:201:HEM:HAC	1.83	0.59
5:M:198:ARG:HG3	5:M:203:HIS:HB2	1.83	0.59
1:T:8:GLU:CD	3:Z:8:GLU:HB2	2.23	0.59
2:Q:21:HIS:O	2:Q:23:HIS:N	2.34	0.59
1:A:90:LYS:NZ	4:D:58:GLU:HG3	2.17	0.58
1:I:55:LYS:HG2	1:I:63:GLU:HG3	3.52	0.58
5:M:63:LYS:HE3	5:M:64:GLU:H	1.68	0.58
1:A:51:PHE:CB	1:A:56:VAL:CG2	2.81	0.58
1:I:52:GLU:HA	1:I:56:VAL:HG23	3.05	0.58
4:S:83:PHE:O	4:S:87:VAL:HG23	2.03	0.58
1:E:149:PRO:O	1:E:150:HIS:C	2.40	0.58
2:F:21:HIS:O	2:F:23:HIS:N	2.33	0.58
2:B:48:LYS:HZ2	2:F:48:LYS:NZ	94.55	0.57
2:Q:100:ILE:HG23	8:Q:201:HEM:HAC	1.84	0.57
2:Q:140:ILE:HD12	8:Q:201:HEM:HBB2	1.85	0.57
6:N:188:LEU:HB2	6:N:200:VAL:HG13	1.86	0.57
2:Y:21:HIS:O	2:Y:23:HIS:N	2.34	0.57
2:B:100:ILE:HG23	8:B:201:HEM:HAC	1.87	0.57
4:H:97:ARG:CZ	8:H:201:HEM:HAD2	2.35	0.57
5:M:90:LYS:NZ	1:P:58:GLU:HG3	100.49	0.57
2:Y:95:HIS:HE1	8:Y:201:HEM:C4A	2.21	0.57
2:J:95:HIS:HE1	8:J:201:HEM:NA	2.00	0.57
4:D:31:LEU:HA	4:D:114:VAL:HG21	1.87	0.57
1:P:53:ARG:NH2	8:P:201:HEM:O2D	2.38	0.57
2:U:95:HIS:HE1	8:U:201:HEM:NA	1.96	0.57
1:E:8:GLU:CD	3:K:8:GLU:HB2	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:C	1:A:56:VAL:CG2	2.73	0.56
5:M:168:ARG:NH1	5:M:184:ARG:HG3	2.20	0.56
1:A:12:GLU:CD	5:M:210:ASN:ND2	2.59	0.56
1:E:47:ALA:HB1	8:E:201:HEM:HBC1	2.02	0.56
1:T:107:GLN:OE1	1:T:150:HIS:ND1	2.37	0.56
4:L:31:LEU:HA	4:L:114:VAL:HG21	1.88	0.56
3:C:36:LEU:HD22	4:D:5:LEU:HD21	1.87	0.56
2:B:23:HIS:HD2	5:M:63:LYS:HG2	1.70	0.56
7:O:129:ILE:HG12	7:O:141:LEU:HD22	1.87	0.56
2:J:122:ARG:HD3	7:O:207:LYS:HZ3	1.70	0.56
4:H:31:LEU:HA	4:H:114:VAL:HG21	1.89	0.56
8:K:201:HEM:HHA	8:K:201:HEM:HBD2	2.06	0.55
2:Y:95:HIS:HE1	8:Y:201:HEM:NA	1.94	0.55
2:U:63:HIS:O	2:U:67:VAL:HG23	2.07	0.55
4:W:31:LEU:HA	4:W:114:VAL:HG21	1.88	0.55
8:F:201:HEM:C1D	9:F:202:CYN:N	3.18	0.55
2:J:95:HIS:HE1	8:J:201:HEM:C4A	2.25	0.55
2:Q:95:HIS:HE1	8:Q:201:HEM:NA	2.01	0.55
2:F:95:HIS:HE1	8:F:201:HEM:NA	2.00	0.55
2:U:50:VAL:HG21	2:U:63:HIS:HB2	1.89	0.55
1:A:55:LYS:CG	1:A:63:GLU:HG3	2.34	0.55
1:T:55:LYS:HE3	1:T:63:GLU:HG3	1.83	0.55
1:A:90:LYS:HZ3	4:D:58:GLU:HG3	1.71	0.54
2:F:50:VAL:HG21	2:F:63:HIS:HB2	1.91	0.54
8:B:201:HEM:C1D	9:B:202:CYN:N	2.76	0.54
5:M:198:ARG:HD2	6:N:79:TYR:CZ	2.42	0.54
2:B:49:ARG:NH1	8:B:201:HEM:O1D	2.41	0.54
1:I:51:PHE:HB2	1:I:56:VAL:CG2	2.97	0.54
2:Y:63:HIS:O	2:Y:67:VAL:HG23	2.08	0.54
2:F:63:HIS:O	2:F:67:VAL:HG23	2.08	0.54
1:X:145:SER:O	1:X:148:LEU:HB2	2.08	0.54
2:J:50:VAL:HG21	2:J:63:HIS:HB2	1.90	0.54
1:T:39:ASP:OD1	1:T:116:SER:HB3	2.08	0.54
2:Y:50:VAL:HG21	2:Y:63:HIS:HB2	1.90	0.54
1:X:150:HIS:N	1:X:150:HIS:HD2	1.93	0.53
2:J:63:HIS:O	2:J:67:VAL:HG23	2.08	0.53
2:Q:50:VAL:HG21	2:Q:63:HIS:HB2	1.90	0.53
6:N:31:LEU:HD23	7:O:21:LEU:HD13	1.90	0.53
2:Q:63:HIS:O	2:Q:67:VAL:HG23	2.09	0.53
5:M:195:HIS:CE1	5:M:197:ASP:HB3	2.44	0.53
3:R:127:ASP:N	3:R:127:ASP:OD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:31:LEU:HA	4:S:114:VAL:HG21	1.89	0.53
4:S:97:ARG:CZ	8:S:201:HEM:HAD2	2.38	0.53
2:B:63:HIS:O	2:B:67:VAL:HG23	2.08	0.53
1:I:51:PHE:CB	1:I:56:VAL:CG2	3.73	0.53
1:E:25:PHE:CE2	3:G:28:LYS:HG2	2.86	0.53
5:M:90:LYS:HZ3	1:P:58:GLU:HG3	101.03	0.53
2:B:21:HIS:O	2:B:23:HIS:N	2.34	0.53
1:E:137:PHE:CZ	8:E:201:HEM:HBB1	2.43	0.53
1:X:47:ALA:O	1:X:50:LEU:HD12	2.08	0.53
1:T:51:PHE:O	1:T:56:VAL:HG22	2.08	0.53
3:G:108:LYS:NZ	2:U:102:ASP:OD1	92.56	0.53
2:Y:76:SER:HB3	3:Z:27:SER:HB3	1.91	0.52
2:B:50:VAL:HG21	2:B:63:HIS:HB2	1.91	0.52
1:A:51:PHE:CB	1:A:56:VAL:HG22	2.40	0.52
1:X:54:VAL:HG23	1:X:54:VAL:O	2.09	0.52
6:N:77:GLY:H	6:N:80:ASP:HB3	1.74	0.52
3:R:36:LEU:HD22	4:S:5:LEU:HD21	1.91	0.52
4:H:108:LEU:HB2	4:H:132:PHE:CE2	2.46	0.52
1:I:39:ASP:OD1	1:I:116:SER:HB3	2.10	0.52
2:B:48:LYS:HZ2	2:F:48:LYS:HZ2	95.25	0.52
2:F:95:HIS:HE1	8:F:201:HEM:C4A	2.29	0.52
3:G:31:ILE:HD13	3:G:66:SER:HB3	1.94	0.51
5:M:111:PHE:HB3	5:M:222:ALA:HB1	1.92	0.51
1:X:51:PHE:CB	1:X:56:VAL:CG2	2.76	0.51
4:D:97:ARG:CZ	8:D:201:HEM:HAD2	2.40	0.51
2:Q:49:ARG:NH1	8:Q:201:HEM:O1D	2.42	0.51
5:M:87:LYS:HE3	5:M:92:GLY:HA3	1.92	0.51
1:X:51:PHE:HZ	8:X:201:HEM:HBC2	1.76	0.51
1:A:145:SER:O	1:A:148:LEU:HB2	2.09	0.51
3:G:114:ILE:O	3:G:118:LEU:HB2	2.11	0.51
1:T:118:ALA:HB1	1:T:130:LEU:HD21	1.93	0.51
3:Z:127:ASP:N	3:Z:127:ASP:OD1	2.37	0.51
1:E:11:ARG:NH1	3:K:8:GLU:HG3	2.72	0.51
6:N:177:GLY:HA3	6:N:187:VAL:O	2.10	0.51
1:X:145:SER:HA	1:X:148:LEU:HD12	1.92	0.51
2:Q:95:HIS:HE1	8:Q:201:HEM:C4A	2.27	0.51
4:S:108:LEU:HB2	4:S:132:PHE:CE2	2.46	0.51
2:U:28:PHE:CD1	2:U:119:GLN:HG3	2.46	0.51
2:B:23:HIS:CD2	5:M:63:LYS:HE2	2.45	0.51
4:D:108:LEU:HB2	4:D:132:PHE:CE2	2.45	0.51
1:I:61:SER:C	1:I:63:GLU:N	3.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:67:HIS:O	1:T:71:VAL:HG23	2.11	0.51
1:E:58:GLU:O	1:E:61:SER:OG	2.60	0.51
3:R:31:ILE:HD13	3:R:66:SER:HB3	1.93	0.51
3:V:31:ILE:HD13	3:V:66:SER:HB3	1.92	0.51
3:V:8:GLU:O	3:V:12:ILE:HG12	2.12	0.51
1:E:118:ALA:HB1	1:E:130:LEU:HD21	1.93	0.50
4:W:108:LEU:HB2	4:W:132:PHE:CE2	2.47	0.50
3:R:127:ASP:OD2	4:S:121:THR:HG21	2.12	0.50
3:C:114:ILE:O	3:C:118:LEU:HB2	2.11	0.50
1:E:95:LEU:HD21	8:E:201:HEM:HMB2	1.93	0.50
1:P:39:ASP:OD1	1:P:116:SER:HB3	2.11	0.50
4:W:42:VAL:HG13	8:W:201:HEM:HBC1	1.93	0.50
3:Z:114:ILE:O	3:Z:118:LEU:HB2	2.11	0.50
1:A:25:PHE:CE2	3:C:28:LYS:HG2	2.47	0.50
1:I:59:PRO:C	1:I:60:ASP:OD1	3.51	0.50
1:X:39:ASP:OD1	1:X:116:SER:HB3	2.11	0.50
1:I:59:PRO:O	1:I:60:ASP:OD1	3.66	0.50
1:I:55:LYS:O	1:I:58:GLU:O	2.90	0.50
5:M:198:ARG:HH21	5:M:205:ASP:HB2	1.76	0.50
3:R:114:ILE:O	3:R:118:LEU:HB2	2.11	0.50
1:T:95:LEU:HD21	8:T:201:HEM:HMB2	1.92	0.50
1:T:52:GLU:O	1:T:53:ARG:C	2.47	0.50
1:A:51:PHE:O	1:A:56:VAL:HG22	2.10	0.50
4:S:42:VAL:HG13	8:S:201:HEM:HBC1	1.94	0.50
3:V:114:ILE:O	3:V:118:LEU:HB2	2.12	0.50
1:X:149:PRO:O	1:X:150:HIS:O	2.30	0.50
2:B:28:PHE:CD1	2:B:119:GLN:HG3	2.47	0.50
4:L:108:LEU:HB2	4:L:132:PHE:CE2	2.49	0.50
4:H:100:ASN:OD1	4:H:102:GLU:HG2	2.12	0.50
2:B:48:LYS:NZ	2:F:48:LYS:HZ2	94.84	0.49
1:E:67:HIS:O	1:E:71:VAL:HG23	2.12	0.49
1:I:61:SER:O	1:I:64:TYR:N	3.29	0.49
3:K:8:GLU:O	3:K:12:ILE:HG12	2.14	0.49
2:F:28:PHE:CD1	2:F:119:GLN:HG3	2.47	0.49
4:H:62:HIS:O	4:H:66:VAL:HG23	2.12	0.49
2:J:49:ARG:NH1	8:J:201:HEM:O1D	2.45	0.49
3:Z:31:ILE:HD13	3:Z:66:SER:HB3	1.94	0.49
1:I:51:PHE:HB2	1:I:56:VAL:HG21	2.62	0.49
5:M:72:ASP:OD2	7:O:216:HIS:NE2	2.40	0.49
1:T:90:LYS:NZ	4:W:58:GLU:HG3	2.26	0.49
1:I:67:HIS:O	1:I:71:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:201:HEM:HBD2	8:R:201:HEM:HHA	1.93	0.49
3:K:114:ILE:O	3:K:118:LEU:HB2	2.11	0.49
1:T:55:LYS:CD	1:T:63:GLU:HG2	2.04	0.49
3:R:33:PHE:CE2	3:R:37:ILE:HD11	2.48	0.49
1:A:149:PRO:O	1:A:150:HIS:O	2.30	0.49
1:E:149:PRO:O	1:E:150:HIS:O	2.29	0.49
1:E:96:ALA:O	1:E:100:ILE:HG13	2.17	0.49
3:G:36:LEU:HD22	4:H:5:LEU:HD21	2.04	0.49
4:H:42:VAL:HG13	8:H:201:HEM:HBC1	1.95	0.49
1:T:137:PHE:CZ	8:T:201:HEM:HBB1	2.47	0.49
4:W:62:HIS:O	4:W:66:VAL:HG23	2.13	0.49
1:I:149:PRO:O	1:I:150:HIS:O	2.89	0.49
1:A:54:VAL:C	1:A:55:LYS:CG	2.75	0.49
3:K:31:ILE:HD13	3:K:66:SER:HB3	1.95	0.49
3:K:33:PHE:CE2	3:K:37:ILE:HD11	2.48	0.49
2:U:95:HIS:HE1	8:U:201:HEM:C4A	2.30	0.49
1:A:39:ASP:OD1	1:A:116:SER:HB3	2.13	0.48
3:C:31:ILE:HD13	3:C:66:SER:HB3	1.94	0.48
1:P:118:ALA:HB1	1:P:130:LEU:HD21	1.95	0.48
4:S:62:HIS:O	4:S:66:VAL:HG23	2.13	0.48
1:T:52:GLU:C	1:T:54:VAL:N	2.66	0.48
4:L:62:HIS:O	4:L:66:VAL:HG23	2.13	0.48
2:Y:100:ILE:HG23	8:Y:201:HEM:HAC	1.94	0.48
1:E:53:ARG:HE	1:E:53:ARG:HB3	2.77	0.48
4:H:94:HIS:HE1	8:H:201:HEM:C4A	2.39	0.48
5:M:134:ALA:HB3	5:M:148:ARG:HB2	1.95	0.48
7:O:107:GLY:HA2	7:O:215:PHE:HA	1.94	0.48
1:P:67:HIS:O	1:P:71:VAL:HG23	2.13	0.48
2:Y:77:THR:O	2:Y:84:LEU:HB2	2.14	0.48
1:T:53:ARG:O	1:T:53:ARG:HD2	2.13	0.48
1:E:39:ASP:OD1	1:E:116:SER:HB3	2.13	0.48
1:I:118:ALA:HB1	1:I:130:LEU:HD21	1.95	0.48
1:X:149:PRO:O	1:X:150:HIS:C	2.50	0.48
3:C:127:ASP:OD2	4:D:121:THR:HG21	2.14	0.48
2:J:122:ARG:HD3	7:O:207:LYS:HZ2	1.78	0.48
2:J:28:PHE:CD1	2:J:119:GLN:HG3	2.49	0.48
2:U:98:ARG:CZ	8:U:201:HEM:HAD2	2.43	0.48
6:N:126:ASP:O	6:N:128:LEU:N	2.46	0.48
2:Q:28:PHE:CD1	2:Q:119:GLN:HG3	2.48	0.48
1:E:51:PHE:HB3	1:E:56:VAL:HG22	3.15	0.48
2:F:49:ARG:NH1	8:F:201:HEM:O1D	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:31:ILE:HD12	6:N:35:LEU:HD22	1.96	0.48
1:T:51:PHE:CB	1:T:56:VAL:HG21	2.44	0.48
3:V:33:PHE:CE2	3:V:37:ILE:HD11	2.49	0.48
1:A:80:ASN:HB3	4:D:24:ARG:NH2	2.29	0.47
2:B:122:ARG:HG2	5:M:193:ARG:HH22	1.79	0.47
2:B:95:HIS:HE1	8:B:201:HEM:C4A	2.32	0.47
1:I:95:LEU:HD21	8:I:201:HEM:HMB2	2.12	0.47
1:E:7:ALA:HB3	3:K:8:GLU:HB3	1.97	0.47
1:T:90:LYS:HZ3	4:W:58:GLU:HG3	1.77	0.47
1:X:67:HIS:O	1:X:71:VAL:HG23	2.13	0.47
2:Y:28:PHE:CD1	2:Y:119:GLN:HG3	2.49	0.47
3:Z:8:GLU:O	3:Z:12:ILE:HG12	2.14	0.47
1:I:51:PHE:CZ	8:I:201:HEM:HBC2	2.55	0.47
4:L:42:VAL:HG13	8:L:201:HEM:HBC1	1.95	0.47
5:M:168:ARG:HH11	5:M:184:ARG:HG3	1.78	0.47
6:N:118:PHE:HB3	6:N:230:VAL:HB	1.95	0.47
3:G:8:GLU:O	3:G:12:ILE:HG12	2.13	0.47
4:L:97:ARG:CZ	8:L:201:HEM:HAD2	2.50	0.47
1:A:58:GLU:HG3	1:X:90:LYS:NZ	114.58	0.47
1:I:96:ALA:O	1:I:100:ILE:HG13	2.15	0.47
1:I:21:TRP:HD1	1:I:22:SER:H	1.63	0.47
3:K:127:ASP:OD1	3:K:127:ASP:N	2.37	0.47
3:G:108:LYS:NZ	2:U:102:ASP:OD2	94.52	0.47
1:X:12:GLU:O	1:X:16:ILE:HG13	2.14	0.47
1:A:67:HIS:O	1:A:71:VAL:HG23	2.15	0.47
2:B:23:HIS:HD2	5:M:63:LYS:CG	2.28	0.47
1:P:54:VAL:O	1:P:55:LYS:HB2	2.14	0.47
4:H:94:HIS:CE1	8:H:201:HEM:C4A	3.10	0.47
1:X:118:ALA:HB1	1:X:130:LEU:HD21	1.96	0.47
1:A:118:ALA:HB1	1:A:130:LEU:HD21	1.95	0.47
2:J:77:THR:O	2:J:84:LEU:HB2	2.14	0.47
1:A:55:LYS:HG3	1:A:63:GLU:CG	2.39	0.47
2:J:49:ARG:HD3	8:J:201:HEM:O2D	2.15	0.47
1:P:51:PHE:O	1:P:56:VAL:HG22	2.15	0.47
2:B:77:THR:O	2:B:84:LEU:HB2	2.15	0.47
1:E:51:PHE:O	1:E:56:VAL:HG22	2.15	0.47
3:G:33:PHE:CE2	3:G:37:ILE:HD11	2.50	0.47
5:M:63:LYS:HD2	5:M:63:LYS:HA	1.73	0.47
1:X:96:ALA:O	1:X:100:ILE:HG13	2.15	0.47
3:R:8:GLU:O	3:R:12:ILE:HG12	2.14	0.46
1:X:21:TRP:HD1	1:X:22:SER:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:PHE:CE2	3:C:37:ILE:HD11	2.50	0.46
1:I:51:PHE:HZ	8:I:201:HEM:HBC2	1.90	0.46
1:P:96:ALA:O	1:P:100:ILE:HG13	2.15	0.46
2:U:49:ARG:HD3	8:U:201:HEM:O2D	2.15	0.46
3:Z:33:PHE:CE2	3:Z:37:ILE:HD11	2.50	0.46
1:A:24:SER:O	4:D:11:LYS:HE3	2.15	0.46
1:I:12:GLU:O	1:I:16:ILE:HG13	2.15	0.46
1:X:55:LYS:HG3	1:X:63:GLU:CG	2.20	0.46
6:N:218:LEU:HD12	6:N:223:HIS:HB3	1.97	0.46
6:N:231:HIS:CE1	6:N:233:GLN:HG2	2.50	0.46
1:T:54:VAL:O	1:T:55:LYS:HB2	2.15	0.46
3:G:54:LYS:HD2	3:G:103:ARG:HH22	1.81	0.46
4:S:94:HIS:HE1	8:S:201:HEM:C4A	2.33	0.46
1:A:12:GLU:O	1:A:16:ILE:HG13	2.16	0.46
4:D:62:HIS:O	4:D:66:VAL:HG23	2.15	0.46
1:E:21:TRP:HD1	1:E:22:SER:H	1.62	0.46
1:P:12:GLU:O	1:P:16:ILE:HG13	2.16	0.46
4:D:72:MET:HB3	4:D:72:MET:HE2	1.78	0.46
3:C:8:GLU:O	3:C:12:ILE:HG12	2.15	0.46
1:E:131:GLU:HB3	1:E:135:ARG:NH1	2.31	0.46
5:M:178:LEU:HB3	5:M:194:CYS:HB2	1.97	0.46
6:N:38:LEU:HD23	7:O:28:LEU:HD13	1.96	0.46
1:P:131:GLU:HB3	1:P:135:ARG:NH1	2.31	0.46
2:Q:77:THR:O	2:Q:84:LEU:HB2	2.16	0.46
2:U:77:THR:O	2:U:84:LEU:HB2	2.15	0.46
1:I:137:PHE:CZ	8:I:201:HEM:HBB1	2.55	0.46
3:K:54:LYS:HD2	3:K:103:ARG:HH22	1.83	0.46
3:G:38:LEU:HD23	3:G:38:LEU:HA	1.73	0.45
1:I:51:PHE:O	1:I:56:VAL:HG22	2.16	0.45
1:T:21:TRP:HD1	1:T:22:SER:H	1.62	0.45
1:A:21:TRP:HD1	1:A:22:SER:H	1.63	0.45
1:A:57:ALA:C	1:A:58:GLU:HG3	2.36	0.45
1:E:51:PHE:HZ	8:E:201:HEM:HBC2	1.94	0.45
2:F:98:ARG:HG2	2:F:98:ARG:HH11	1.81	0.45
3:K:38:LEU:HA	3:K:38:LEU:HD23	1.73	0.45
1:A:58:GLU:HG3	1:X:90:LYS:HZ3	114.72	0.45
1:A:131:GLU:HB3	1:A:135:ARG:NH1	2.31	0.45
1:P:8:GLU:OE2	3:V:6:SER:CB	2.64	0.45
1:T:23:SER:OG	3:V:23:ASP:OD2	2.34	0.45
1:A:96:ALA:O	1:A:100:ILE:HG13	2.15	0.45
5:M:32:ASP:OD2	5:M:36:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:28:LYS:HB2	3:K:28:LYS:HE2	1.76	0.45
4:S:100:ASN:OD1	4:S:102:GLU:HG2	2.17	0.45
1:T:63:GLU:HA	4:W:85:ALA:HB1	1.99	0.45
3:V:132:LEU:O	3:V:136:SER:HB2	2.17	0.45
3:Z:54:LYS:HD2	3:Z:103:ARG:HH22	1.82	0.45
1:E:12:GLU:O	1:E:16:ILE:HG13	2.18	0.45
1:P:54:VAL:O	1:P:55:LYS:CB	2.64	0.45
1:I:58:GLU:O	1:I:61:SER:OG	2.61	0.45
3:R:28:LYS:HE2	3:R:28:LYS:HB2	1.75	0.45
1:P:25:PHE:CE2	3:R:28:LYS:HG2	2.52	0.45
1:I:60:ASP:N	1:I:60:ASP:OD1	3.08	0.45
1:E:25:PHE:CD2	3:G:28:LYS:HG2	2.85	0.45
3:G:132:LEU:O	3:G:136:SER:HB2	2.18	0.45
3:K:84:ASP:O	3:K:86:PRO:HD3	2.17	0.45
1:P:54:VAL:C	1:P:55:LYS:CG	2.83	0.45
3:V:15:LYS:HB2	3:V:15:LYS:HE3	1.84	0.45
8:F:201:HEM:C4D	9:F:202:CYN:N	2.85	0.45
3:R:132:LEU:O	3:R:136:SER:HB2	2.17	0.45
4:S:72:MET:HB3	4:S:72:MET:HE2	1.83	0.45
1:T:12:GLU:O	1:T:16:ILE:HG13	2.17	0.45
1:T:96:ALA:O	1:T:100:ILE:HG13	2.16	0.45
1:A:51:PHE:HB3	1:A:56:VAL:HG22	1.99	0.44
3:K:22:GLY:HA3	4:L:15:ARG:NH1	2.39	0.44
5:M:84:ASP:HB3	5:M:143:PRO:HG3	1.99	0.44
3:V:54:LYS:HD2	3:V:103:ARG:HH22	1.82	0.44
3:G:127:ASP:OD2	4:H:121:THR:HG21	2.41	0.44
3:Z:144:LYS:HE2	3:Z:144:LYS:HB2	1.73	0.44
1:A:133:TRP:CZ2	1:A:137:PHE:HD2	2.34	0.44
1:E:8:GLU:OE2	3:K:6:SER:OG	2.71	0.44
1:A:12:GLU:OE2	5:M:210:ASN:ND2	2.50	0.44
1:X:131:GLU:HB3	1:X:135:ARG:NH1	2.33	0.44
1:P:25:PHE:CD2	3:R:28:LYS:HG2	2.52	0.44
1:P:90:LYS:NZ	4:S:58:GLU:HG3	2.33	0.44
1:A:8:GLU:OE2	3:G:6:SER:OG	2.22	0.44
3:C:84:ASP:O	3:C:86:PRO:HD3	2.17	0.44
1:A:81:LEU:HD11	4:D:64:GLU:HG2	1.99	0.44
2:B:48:LYS:CE	2:F:48:LYS:HZ1	93.13	0.44
2:F:77:THR:O	2:F:84:LEU:HB2	2.18	0.44
3:G:15:LYS:HE3	3:G:15:LYS:HB2	1.84	0.44
1:A:11:ARG:NH1	3:G:8:GLU:HG3	2.31	0.44
5:M:28:LEU:HD21	7:O:24:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:76:SER:HB3	3:V:27:SER:HB3	2.00	0.44
2:U:98:ARG:HH11	2:U:98:ARG:HG2	1.83	0.44
3:V:121:GLY:O	3:V:125:VAL:HG22	2.18	0.44
1:A:55:LYS:O	1:A:56:VAL:C	2.56	0.44
3:C:28:LYS:HE2	3:C:28:LYS:HB2	1.76	0.44
1:E:133:TRP:CZ2	1:E:137:PHE:HD2	2.37	0.44
1:I:51:PHE:HB3	1:I:56:VAL:HG22	3.17	0.44
3:K:125:VAL:HG13	4:L:5:LEU:HD22	2.00	0.44
1:P:95:LEU:HD21	8:P:201:HEM:HMB2	2.00	0.44
4:W:100:ASN:OD1	4:W:102:GLU:HG2	2.18	0.44
4:H:29:LEU:HD12	4:H:29:LEU:HA	1.83	0.44
6:N:76:CYS:O	6:N:100:HIS:ND1	2.51	0.44
4:D:108:LEU:HB2	4:D:132:PHE:CD2	2.53	0.44
1:E:25:PHE:CE2	4:H:11:LYS:HE2	2.53	0.44
1:I:107:GLN:CD	1:I:150:HIS:HD1	2.20	0.44
3:R:54:LYS:HD2	3:R:103:ARG:HH22	1.82	0.44
1:E:51:PHE:CZ	8:E:201:HEM:HBC2	2.64	0.44
2:F:112:LEU:HD22	2:F:116:LEU:HG	2.00	0.44
4:H:108:LEU:HB2	4:H:132:PHE:CD2	2.53	0.44
1:I:150:HIS:HD2	1:I:150:HIS:N	3.74	0.44
4:D:100:ASN:OD1	4:D:102:GLU:HG2	2.17	0.43
4:D:42:VAL:HG13	8:D:201:HEM:HBC1	2.00	0.43
3:G:121:GLY:O	3:G:125:VAL:HG22	2.18	0.43
8:G:201:HEM:HBD2	8:G:201:HEM:HHA	2.13	0.43
3:G:28:LYS:HE2	3:G:28:LYS:HB2	1.76	0.43
1:I:133:TRP:CZ2	1:I:137:PHE:HD2	2.38	0.43
2:J:98:ARG:CZ	8:J:201:HEM:HAD2	2.48	0.43
1:P:85:THR:HG21	3:V:132:LEU:H	1.83	0.43
2:Y:112:LEU:HD22	2:Y:116:LEU:HG	2.00	0.43
2:B:48:LYS:HZ1	2:F:48:LYS:CE	93.22	0.43
1:P:24:SER:O	4:S:11:LYS:HE3	2.18	0.43
1:I:81:LEU:HD21	1:I:87:VAL:HG12	2.07	0.43
4:L:72:MET:HE2	4:L:72:MET:HB3	1.85	0.43
4:L:8:LEU:HD12	4:L:8:LEU:HA	1.86	0.43
1:T:102:ARG:HD3	1:T:102:ARG:HA	1.87	0.43
4:W:29:LEU:HA	4:W:29:LEU:HD12	1.86	0.43
3:Z:121:GLY:O	3:Z:125:VAL:HG22	2.18	0.43
1:A:59:PRO:HA	1:A:64:TYR:CD2	2.54	0.43
3:K:121:GLY:O	3:K:125:VAL:HG22	2.18	0.43
2:U:100:ILE:CG2	8:U:201:HEM:HAC	2.47	0.43
4:W:107:PHE:CE2	8:W:201:HEM:HAB	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:ILE:HA	2:F:101:PRO:HD2	1.91	0.43
4:H:72:MET:HB3	4:H:72:MET:HE2	1.70	0.43
4:L:100:ASN:OD1	4:L:102:GLU:HG2	2.20	0.43
4:L:29:LEU:HD12	4:L:29:LEU:HA	1.86	0.43
5:M:187:LYS:O	5:M:189:VAL:N	2.51	0.43
3:V:144:LYS:HB2	3:V:144:LYS:HE2	1.74	0.43
3:Z:28:LYS:HE2	3:Z:28:LYS:HB2	1.76	0.43
3:C:132:LEU:O	3:C:136:SER:HB2	2.18	0.43
8:C:201:HEM:HHA	8:C:201:HEM:HBD2	2.01	0.43
1:E:80:ASN:HB3	4:H:24:ARG:NH2	2.45	0.43
1:E:24:SER:O	4:H:11:LYS:HE3	2.35	0.43
3:K:132:LEU:O	3:K:136:SER:HB2	2.18	0.43
4:S:94:HIS:CE1	8:S:201:HEM:C4A	3.05	0.43
1:E:88:LEU:O	1:E:92:LEU:HB2	2.22	0.43
1:E:11:ARG:HH12	3:K:8:GLU:HG3	2.18	0.43
1:P:47:ALA:HB1	8:P:201:HEM:HBC1	2.01	0.43
4:D:29:LEU:HA	4:D:29:LEU:HD12	1.87	0.43
1:E:92:LEU:HD12	1:E:92:LEU:HA	1.92	0.43
3:G:84:ASP:O	3:G:86:PRO:HD3	2.20	0.43
4:L:108:LEU:HB2	4:L:132:PHE:CD2	2.58	0.43
1:T:131:GLU:HB3	1:T:135:ARG:NH1	2.33	0.43
4:W:108:LEU:HB2	4:W:132:PHE:CD2	2.54	0.43
3:K:144:LYS:HE2	3:K:144:LYS:HB2	1.74	0.43
8:U:201:HEM:C4D	9:U:202:CYN:N	2.86	0.43
2:B:49:ARG:HH11	8:B:201:HEM:CGD	2.31	0.43
1:E:113:ILE:HD13	8:E:201:HEM:HBB2	2.30	0.43
1:P:21:TRP:HD1	1:P:22:SER:H	1.62	0.43
3:Z:84:ASP:O	3:Z:86:PRO:HD3	2.19	0.43
2:B:88:LEU:HD21	2:B:136:ILE:HG23	2.01	0.42
3:C:54:LYS:HD2	3:C:103:ARG:HH22	1.83	0.42
1:E:131:GLU:HB3	1:E:135:ARG:HH12	1.83	0.42
1:T:34:GLY:O	1:T:38:LYS:HG3	2.19	0.42
1:X:51:PHE:CZ	8:X:201:HEM:HBC2	2.54	0.42
2:Y:49:ARG:HH11	8:Y:201:HEM:CGD	2.32	0.42
2:Y:65:LEU:HD23	2:Y:65:LEU:HA	1.90	0.42
1:E:81:LEU:HD11	4:H:64:GLU:HG2	2.03	0.42
5:M:187:LYS:O	5:M:189:VAL:HG23	2.20	0.42
1:P:133:TRP:CZ2	1:P:137:PHE:HD2	2.36	0.42
1:I:131:GLU:HB3	1:I:135:ARG:NH1	2.33	0.42
1:I:143:ARG:NH1	1:I:146:ARG:HH11	2.20	0.42
1:I:92:LEU:HD12	1:I:92:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:68:SER:O	4:L:72:MET:HG3	2.19	0.42
1:I:15:HIS:ND1	7:O:205:ALA:O	2.52	0.42
1:P:131:GLU:HB3	1:P:135:ARG:HH12	1.85	0.42
1:T:133:TRP:CZ2	1:T:137:PHE:HD2	2.37	0.42
1:I:58:GLU:HA	1:I:59:PRO:HD2	2.17	0.42
2:J:112:LEU:HD22	2:J:116:LEU:HG	2.02	0.42
4:L:20:GLU:HB3	4:L:22:HIS:CE1	2.55	0.42
7:O:28:LEU:HD22	7:O:32:LEU:HD22	2.02	0.42
3:R:121:GLY:O	3:R:125:VAL:HG22	2.20	0.42
1:A:88:LEU:O	1:A:92:LEU:HB2	2.20	0.42
3:R:38:LEU:HA	3:R:38:LEU:HD23	1.73	0.42
3:V:84:ASP:O	3:V:86:PRO:HD3	2.20	0.42
4:W:8:LEU:HA	4:W:8:LEU:HD12	1.87	0.42
3:G:127:ASP:OD1	3:G:127:ASP:N	2.35	0.42
3:K:36:LEU:HD22	4:L:5:LEU:HD21	2.19	0.42
1:I:15:HIS:CG	7:O:206:SER:HA	2.55	0.42
2:Q:73:ILE:HD11	3:R:71:ARG:HA	2.02	0.42
3:R:84:ASP:O	3:R:86:PRO:HD3	2.19	0.42
4:S:108:LEU:HB2	4:S:132:PHE:CD2	2.54	0.42
4:W:97:ARG:CZ	8:W:201:HEM:HAD2	2.49	0.42
2:B:122:ARG:HD3	5:M:214:LEU:HD21	2.02	0.42
1:E:51:PHE:HB2	1:E:56:VAL:HG22	2.64	0.42
3:G:144:LYS:HB2	3:G:144:LYS:HE2	1.73	0.42
1:I:102:ARG:HA	1:I:102:ARG:HD3	1.87	0.42
1:T:131:GLU:HB3	1:T:135:ARG:HH12	1.85	0.42
1:A:95:LEU:HD21	8:A:201:HEM:HMB2	2.01	0.42
3:G:70:LEU:HD23	3:G:70:LEU:HA	1.86	0.42
8:J:201:HEM:C4D	9:J:202:CYN:N	3.01	0.42
1:X:95:LEU:HD21	8:X:201:HEM:HMB2	2.01	0.42
2:F:88:LEU:HD21	2:F:136:ILE:HG23	2.02	0.41
2:J:88:LEU:HD21	2:J:136:ILE:HG23	2.02	0.41
3:K:125:VAL:CG1	4:L:5:LEU:HD22	2.50	0.41
2:F:50:VAL:CG2	2:F:63:HIS:HB2	2.50	0.41
4:H:77:LEU:HA	4:H:77:LEU:HD12	1.91	0.41
3:K:100:HIS:HE1	8:K:201:HEM:C4A	2.41	0.41
7:O:107:GLY:HA2	7:O:214:ILE:O	2.20	0.41
4:S:68:SER:O	4:S:72:MET:HG3	2.20	0.41
2:U:140:ILE:CD1	8:U:201:HEM:HBB2	2.46	0.41
3:Z:132:LEU:O	3:Z:136:SER:HB2	2.20	0.41
2:B:112:LEU:HD22	2:B:116:LEU:HG	2.02	0.41
1:E:34:GLY:O	1:E:38:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:LEU:HD23	1:E:88:LEU:HA	2.02	0.41
2:B:48:LYS:NZ	2:F:48:LYS:CE	93.37	0.41
2:B:65:LEU:HD23	2:B:65:LEU:HA	1.93	0.41
1:E:81:LEU:HD21	1:E:87:VAL:HG12	2.03	0.41
1:E:12:GLU:OE1	6:N:218:LEU:HD13	2.21	0.41
4:S:29:LEU:HD12	4:S:29:LEU:HA	1.87	0.41
1:T:51:PHE:C	1:T:56:VAL:CG2	2.89	0.41
2:U:50:VAL:CG2	2:U:63:HIS:HB2	2.49	0.41
1:X:133:TRP:CZ2	1:X:137:PHE:HD2	2.37	0.41
1:E:55:LYS:C	1:E:57:ALA:N	3.09	0.41
1:A:85:THR:HG21	3:G:132:LEU:H	1.85	0.41
1:I:81:LEU:HD23	1:I:88:LEU:HA	2.04	0.41
2:J:65:LEU:HA	2:J:65:LEU:HD23	1.94	0.41
1:X:34:GLY:O	1:X:38:LYS:HG3	2.21	0.41
4:D:68:SER:O	4:D:72:MET:HG3	2.21	0.41
2:B:48:LYS:CE	2:F:48:LYS:NZ	92.85	0.41
1:T:70:ARG:HD3	4:W:86:GLN:OE1	2.20	0.41
4:W:20:GLU:HB3	4:W:22:HIS:CE1	2.55	0.41
4:H:20:GLU:HB3	4:H:22:HIS:CE1	2.56	0.41
2:J:50:VAL:CG2	2:J:63:HIS:HB2	2.50	0.41
4:L:107:PHE:CE2	8:L:201:HEM:HAB	2.56	0.41
2:B:114:HIS:NE2	5:M:138:LYS:HG3	2.36	0.41
6:N:234:GLY:O	6:N:235:HIS:HB3	2.20	0.41
4:D:20:GLU:HB3	4:D:22:HIS:CE1	2.56	0.41
4:H:68:SER:O	4:H:72:MET:HG3	2.25	0.41
2:J:136:ILE:O	2:J:140:ILE:HG13	2.26	0.41
3:R:100:HIS:CD2	8:R:201:HEM:NC	2.89	0.41
4:S:20:GLU:HB3	4:S:22:HIS:CE1	2.56	0.41
1:T:51:PHE:CB	1:T:56:VAL:CG2	2.98	0.41
2:Y:29:ALA:HB1	2:Y:64:ALA:HB1	2.03	0.41
1:A:131:GLU:HB3	1:A:135:ARG:HH12	1.85	0.41
2:B:100:ILE:CG2	8:B:201:HEM:HAC	2.50	0.41
2:J:51:HIS:ND1	2:J:59:GLU:HG3	2.39	0.41
1:I:81:LEU:HD11	4:L:64:GLU:HG2	2.03	0.41
5:M:107:ILE:HA	5:M:132:ILE:HG22	2.02	0.41
6:N:84:ILE:HD13	6:N:84:ILE:HA	1.77	0.41
1:I:55:LYS:O	1:I:56:VAL:C	2.94	0.41
7:O:13:LYS:HA	7:O:13:LYS:HD2	1.79	0.41
1:P:21:TRP:CD1	1:P:22:SER:N	2.89	0.41
2:Q:98:ARG:HH11	2:Q:98:ARG:HG2	1.86	0.41
7:O:117:ARG:O	7:O:149:LYS:NZ	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:28:LYS:HB2	3:V:28:LYS:HE2	1.77	0.41
1:A:21:TRP:CD1	1:A:22:SER:N	2.89	0.40
2:B:37:PHE:HB3	2:B:44:ARG:NH1	2.36	0.40
1:I:53:ARG:O	1:I:53:ARG:HD2	2.21	0.40
2:J:98:ARG:HH11	2:J:98:ARG:HG2	1.87	0.40
5:M:142:LYS:N	5:M:143:PRO:HD3	2.36	0.40
1:I:16:ILE:HG12	7:O:205:ALA:HB1	2.02	0.40
1:P:102:ARG:HA	1:P:102:ARG:HD3	1.86	0.40
2:Q:50:VAL:CG2	2:Q:63:HIS:HB2	2.50	0.40
1:T:81:LEU:HD23	1:T:88:LEU:HA	2.03	0.40
2:Y:16:ARG:O	2:Y:20:SER:OG	2.38	0.40
2:Y:50:VAL:CG2	2:Y:63:HIS:HB2	2.51	0.40
1:A:25:PHE:CD2	3:C:28:LYS:HG2	2.56	0.40
2:J:29:ALA:HB1	2:J:64:ALA:HB1	2.02	0.40
3:K:70:LEU:HD23	3:K:70:LEU:HA	1.86	0.40
4:W:68:SER:O	4:W:72:MET:HG3	2.22	0.40
1:X:131:GLU:HB3	1:X:135:ARG:HH12	1.86	0.40
2:Y:109:LYS:HB2	2:Y:133:PHE:CE1	2.56	0.40
2:B:109:LYS:HB2	2:B:133:PHE:CE1	2.56	0.40
2:B:50:VAL:CG2	2:B:63:HIS:HB2	2.52	0.40
3:C:15:LYS:HE3	3:C:15:LYS:HB2	1.85	0.40
2:F:113:LEU:HD12	2:F:113:LEU:HA	1.88	0.40
2:F:98:ARG:CZ	8:F:201:HEM:HAD2	2.51	0.40
1:I:131:GLU:HB3	1:I:135:ARG:HH12	1.87	0.40
2:Q:2:GLU:HG2	2:Q:3:CYS:H	1.86	0.40
2:U:100:ILE:HA	2:U:101:PRO:HD2	1.89	0.40
2:U:29:ALA:HB1	2:U:64:ALA:HB1	2.03	0.40
1:X:95:LEU:HD12	1:X:95:LEU:HA	1.93	0.40
2:Y:100:ILE:HA	2:Y:101:PRO:HD2	1.90	0.40
1:I:34:GLY:O	1:I:38:LYS:HG3	2.23	0.40
2:J:109:LYS:HB2	2:J:133:PHE:CE1	2.58	0.40
5:M:27:ASP:O	5:M:31:ILE:HG13	2.21	0.40
2:Y:98:ARG:HH11	2:Y:98:ARG:HG2	1.87	0.40
4:H:8:LEU:HA	4:H:8:LEU:HD12	1.90	0.40
2:J:37:PHE:HB3	2:J:44:ARG:NH1	2.39	0.40
2:Q:49:ARG:HH11	8:Q:201:HEM:CGD	2.34	0.40
2:Q:51:HIS:ND1	2:Q:59:GLU:HG3	2.37	0.40
3:R:15:LYS:HE3	3:R:15:LYS:HB2	1.84	0.40
4:W:74:ILE:O	4:W:77:LEU:HB2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:107:LYS:NZ	1:P:58:GLU:OE2[2_555]	1.95	0.25
4:W:100:ASN:ND2	1:i:52:GLU:OE2[8_444]	2.19	0.01

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	146/150 (97%)	141 (97%)	3 (2%)	2 (1%)	14	57
1	E	146/150 (97%)	140 (96%)	4 (3%)	2 (1%)	14	57
1	I	146/150 (97%)	142 (97%)	3 (2%)	1 (1%)	26	72
1	P	146/150 (97%)	142 (97%)	3 (2%)	1 (1%)	26	72
1	T	146/150 (97%)	141 (97%)	3 (2%)	2 (1%)	14	57
1	X	146/150 (97%)	139 (95%)	6 (4%)	1 (1%)	26	72
1	e	146/150 (97%)	140 (96%)	4 (3%)	2 (1%)	14	57
1	i	146/150 (97%)	136 (93%)	7 (5%)	3 (2%)	9	46
1	m	146/150 (97%)	142 (97%)	3 (2%)	1 (1%)	26	72
2	B	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	46
2	F	140/142 (99%)	133 (95%)	4 (3%)	3 (2%)	9	46
2	J	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	46
2	Q	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	46
2	U	140/142 (99%)	133 (95%)	4 (3%)	3 (2%)	9	46
2	Y	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	46
2	f	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	46
2	j	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	46
2	n	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	46
3	C	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	G	149/151 (99%)	145 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	R	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	V	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	Z	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	g	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	o	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
4	D	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	H	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	L	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	S	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	W	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	a	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	h	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	l	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	p	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
5	M	220/224 (98%)	208 (94%)	10 (4%)	2 (1%)	21	67
5	b	220/224 (98%)	208 (94%)	10 (4%)	2 (1%)	21	67
5	q	220/224 (98%)	207 (94%)	11 (5%)	2 (1%)	21	67
6	N	217/236 (92%)	198 (91%)	11 (5%)	8 (4%)	4	29
6	c	217/236 (92%)	199 (92%)	10 (5%)	8 (4%)	4	29
6	r	217/236 (92%)	198 (91%)	11 (5%)	8 (4%)	4	29
7	O	211/218 (97%)	199 (94%)	10 (5%)	2 (1%)	21	67
7	d	211/218 (97%)	200 (95%)	9 (4%)	2 (1%)	21	67
7	s	211/218 (97%)	199 (94%)	10 (5%)	2 (1%)	21	67
All	All	7110/7290 (98%)	6781 (95%)	251 (4%)	78 (1%)	17	62

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	19	PRO
6	N	76	CYS
6	N	233	GLN

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Mol	Chain	Res	Type
6	N	235	HIS
6	c	19	PRO
6	c	76	CYS
6	c	233	GLN
6	c	235	HIS
1	e	53	ARG
1	i	53	ARG
6	r	19	PRO
6	r	76	CYS
6	r	233	GLN
6	r	235	HIS
2	B	21	HIS
2	B	22	GLY
2	F	21	HIS
2	F	22	GLY
2	J	21	HIS
2	J	22	GLY
7	O	95	CYS
2	Q	21	HIS
2	Q	22	GLY
1	T	53	ARG
2	U	21	HIS
2	U	22	GLY
2	Y	21	HIS
2	Y	22	GLY
2	f	21	HIS
2	f	22	GLY
1	i	62	GLY
2	j	21	HIS
2	j	22	GLY
2	n	21	HIS
2	n	22	GLY
7	s	95	CYS
5	M	188	PRO
6	N	192	ALA
6	N	195	ASP
6	N	234	GLY
5	b	188	PRO
6	c	192	ALA
6	c	195	ASP
6	c	234	GLY
7	d	95	CYS

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Mol	Chain	Res	Type
5	q	188	PRO
6	r	192	ALA
6	r	195	ASP
1	A	22	SER
1	E	22	SER
2	F	23	HIS
1	I	22	SER
6	N	127	CYS
1	P	22	SER
1	T	22	SER
2	U	23	HIS
1	X	22	SER
6	c	127	CYS
1	e	22	SER
2	f	23	HIS
1	i	22	SER
2	j	23	HIS
1	m	22	SER
6	r	127	CYS
6	r	234	GLY
2	B	23	HIS
2	J	23	HIS
2	Q	23	HIS
2	Y	23	HIS
2	n	23	HIS
7	s	114	CYS
1	A	56	VAL
1	E	149	PRO
5	M	187	LYS
7	O	114	CYS
5	b	187	LYS
7	d	114	CYS
5	q	187	LYS

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	129/131 (98%)	117 (91%)	12 (9%)	11	41
1	E	129/131 (98%)	117 (91%)	12 (9%)	11	41
1	I	129/131 (98%)	117 (91%)	12 (9%)	11	41
1	P	129/131 (98%)	116 (90%)	13 (10%)	9	36
1	T	129/131 (98%)	116 (90%)	13 (10%)	9	36
1	X	129/131 (98%)	118 (92%)	11 (8%)	13	47
1	e	129/131 (98%)	115 (89%)	14 (11%)	8	33
1	i	129/131 (98%)	111 (86%)	18 (14%)	4	20
1	m	129/131 (98%)	118 (92%)	11 (8%)	13	47
2	B	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	F	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	J	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	Q	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	U	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	Y	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	f	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	j	117/117 (100%)	111 (95%)	6 (5%)	29	70
2	n	117/117 (100%)	111 (95%)	6 (5%)	29	70
3	C	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	G	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	K	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	R	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	V	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	Z	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	g	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	k	128/130 (98%)	123 (96%)	5 (4%)	39	78
3	o	130/130 (100%)	122 (94%)	8 (6%)	23	64
4	D	120/120 (100%)	113 (94%)	7 (6%)	25	66
4	H	120/120 (100%)	113 (94%)	7 (6%)	25	66
4	L	120/120 (100%)	113 (94%)	7 (6%)	25	66
4	S	120/120 (100%)	113 (94%)	7 (6%)	25	66
4	W	120/120 (100%)	113 (94%)	7 (6%)	25	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	a	120/120 (100%)	113 (94%)	7 (6%)	25	66
4	h	120/120 (100%)	113 (94%)	7 (6%)	25	66
4	l	120/120 (100%)	113 (94%)	7 (6%)	25	66
4	p	120/120 (100%)	113 (94%)	7 (6%)	25	66
5	M	185/194 (95%)	181 (98%)	4 (2%)	60	87
5	b	185/194 (95%)	181 (98%)	4 (2%)	60	87
5	q	185/194 (95%)	181 (98%)	4 (2%)	60	87
6	N	181/205 (88%)	171 (94%)	10 (6%)	27	68
6	c	181/205 (88%)	171 (94%)	10 (6%)	27	68
6	r	181/205 (88%)	171 (94%)	10 (6%)	27	68
7	O	187/193 (97%)	177 (95%)	10 (5%)	28	69
7	d	187/193 (97%)	177 (95%)	10 (5%)	28	69
7	s	187/193 (97%)	177 (95%)	10 (5%)	28	69
All	All	6107/6258 (98%)	5754 (94%)	353 (6%)	25	66

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	56	VAL
1	A	63	GLU
1	A	82	PHE
1	A	84	ASP
1	A	89	ASP
1	A	92	LEU
1	A	111	LYS
1	A	116	SER
1	A	125	SER
1	A	130	LEU
1	A	146	ARG
2	B	3	CYS
2	B	59	GLU
2	B	112	LEU
2	B	113	LEU
2	B	119	GLN
2	B	124	TRP
3	C	72	ILE

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Mol	Chain	Res	Type
3	C	113	LYS
3	C	118	LEU
3	C	127	ASP
3	C	136	SER
4	D	8	LEU
4	D	22	HIS
4	D	23	HIS
4	D	41	GLU
4	D	52	ASP
4	D	77	LEU
4	D	80	THR
1	E	42	HIS
1	E	56	VAL
1	E	63	GLU
1	E	82	PHE
1	E	84	ASP
1	E	89	ASP
1	E	92	LEU
1	E	111	LYS
1	E	116	SER
1	E	125	SER
1	E	130	LEU
1	E	146	ARG
2	F	3	CYS
2	F	59	GLU
2	F	112	LEU
2	F	113	LEU
2	F	119	GLN
2	F	124	TRP
3	G	72	ILE
3	G	113	LYS
3	G	118	LEU
3	G	127	ASP
3	G	136	SER
4	H	8	LEU
4	H	22	HIS
4	H	23	HIS
4	H	41	GLU
4	H	52	ASP
4	H	77	LEU
4	H	80	THR
1	I	42	HIS

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Mol	Chain	Res	Type
1	I	52	GLU
1	I	56	VAL
1	I	63	GLU
1	I	82	PHE
1	I	84	ASP
1	I	89	ASP
1	I	92	LEU
1	I	111	LYS
1	I	116	SER
1	I	130	LEU
1	I	146	ARG
2	J	3	CYS
2	J	59	GLU
2	J	112	LEU
2	J	113	LEU
2	J	119	GLN
2	J	124	TRP
3	K	72	ILE
3	K	113	LYS
3	K	118	LEU
3	K	127	ASP
3	K	136	SER
4	L	8	LEU
4	L	22	HIS
4	L	23	HIS
4	L	41	GLU
4	L	52	ASP
4	L	77	LEU
4	L	80	THR
5	M	42	VAL
5	M	80	LEU
5	M	130	VAL
5	M	162	ILE
6	N	20	ARG
6	N	84	ILE
6	N	105	ASP
6	N	125	HIS
6	N	126	ASP
6	N	129	LEU
6	N	131	SER
6	N	200	VAL
6	N	233	GLN

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Mol	Chain	Res	Type
6	N	235	HIS
7	O	14	LEU
7	O	21	LEU
7	O	28	LEU
7	O	32	LEU
7	O	61	ASP
7	O	130	SER
7	O	151	THR
7	O	158	VAL
7	O	196	ARG
7	O	206	SER
1	P	42	HIS
1	P	55	LYS
1	P	56	VAL
1	P	63	GLU
1	P	82	PHE
1	P	84	ASP
1	P	89	ASP
1	P	92	LEU
1	P	111	LYS
1	P	116	SER
1	P	125	SER
1	P	130	LEU
1	P	146	ARG
2	Q	3	CYS
2	Q	59	GLU
2	Q	112	LEU
2	Q	113	LEU
2	Q	119	GLN
2	Q	124	TRP
3	R	72	ILE
3	R	113	LYS
3	R	118	LEU
3	R	127	ASP
3	R	136	SER
4	S	8	LEU
4	S	22	HIS
4	S	23	HIS
4	S	41	GLU
4	S	52	ASP
4	S	77	LEU
4	S	80	THR

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Mol	Chain	Res	Type
1	T	42	HIS
1	T	52	GLU
1	T	53	ARG
1	T	56	VAL
1	T	63	GLU
1	T	82	PHE
1	T	84	ASP
1	T	89	ASP
1	T	92	LEU
1	T	111	LYS
1	T	116	SER
1	T	130	LEU
1	T	146	ARG
2	U	3	CYS
2	U	59	GLU
2	U	112	LEU
2	U	113	LEU
2	U	119	GLN
2	U	124	TRP
3	V	72	ILE
3	V	113	LYS
3	V	118	LEU
3	V	127	ASP
3	V	136	SER
4	W	8	LEU
4	W	22	HIS
4	W	23	HIS
4	W	41	GLU
4	W	52	ASP
4	W	77	LEU
4	W	80	THR
1	X	42	HIS
1	X	63	GLU
1	X	82	PHE
1	X	84	ASP
1	X	89	ASP
1	X	92	LEU
1	X	111	LYS
1	X	116	SER
1	X	130	LEU
1	X	146	ARG
1	X	150	HIS

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Mol	Chain	Res	Type
2	Y	3	CYS
2	Y	59	GLU
2	Y	112	LEU
2	Y	113	LEU
2	Y	119	GLN
2	Y	124	TRP
3	Z	72	ILE
3	Z	113	LYS
3	Z	118	LEU
3	Z	127	ASP
3	Z	136	SER
4	a	8	LEU
4	a	22	HIS
4	a	23	HIS
4	a	41	GLU
4	a	52	ASP
4	a	77	LEU
4	a	80	THR
5	b	42	VAL
5	b	80	LEU
5	b	130	VAL
5	b	162	ILE
6	c	20	ARG
6	c	84	ILE
6	c	105	ASP
6	c	125	HIS
6	c	126	ASP
6	c	129	LEU
6	c	131	SER
6	c	200	VAL
6	c	233	GLN
6	c	235	HIS
7	d	14	LEU
7	d	21	LEU
7	d	28	LEU
7	d	32	LEU
7	d	61	ASP
7	d	130	SER
7	d	151	THR
7	d	158	VAL
7	d	196	ARG
7	d	206	SER

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Mol	Chain	Res	Type
1	e	42	HIS
1	e	53	ARG
1	e	58	GLU
1	e	61	SER
1	e	63	GLU
1	e	82	PHE
1	e	84	ASP
1	e	89	ASP
1	e	92	LEU
1	e	111	LYS
1	e	116	SER
1	e	125	SER
1	e	130	LEU
1	e	146	ARG
2	f	3	CYS
2	f	59	GLU
2	f	112	LEU
2	f	113	LEU
2	f	119	GLN
2	f	124	TRP
3	g	72	ILE
3	g	113	LYS
3	g	118	LEU
3	g	127	ASP
3	g	136	SER
4	h	8	LEU
4	h	22	HIS
4	h	23	HIS
4	h	41	GLU
4	h	52	ASP
4	h	77	LEU
4	h	80	THR
1	i	42	HIS
1	i	50	LEU
1	i	52	GLU
1	i	53	ARG
1	i	55	LYS
1	i	58	GLU
1	i	61	SER
1	i	63	GLU
1	i	82	PHE
1	i	84	ASP

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Mol	Chain	Res	Type
1	i	89	ASP
1	i	92	LEU
1	i	111	LYS
1	i	116	SER
1	i	125	SER
1	i	130	LEU
1	i	146	ARG
1	i	150	HIS
2	j	3	CYS
2	j	59	GLU
2	j	112	LEU
2	j	113	LEU
2	j	119	GLN
2	j	124	TRP
3	k	72	ILE
3	k	113	LYS
3	k	118	LEU
3	k	127	ASP
3	k	136	SER
4	l	8	LEU
4	l	22	HIS
4	l	23	HIS
4	l	41	GLU
4	l	52	ASP
4	l	77	LEU
4	l	80	THR
1	m	42	HIS
1	m	56	VAL
1	m	63	GLU
1	m	82	PHE
1	m	84	ASP
1	m	89	ASP
1	m	92	LEU
1	m	111	LYS
1	m	116	SER
1	m	130	LEU
1	m	146	ARG
2	n	3	CYS
2	n	59	GLU
2	n	112	LEU
2	n	113	LEU
2	n	119	GLN

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Mol	Chain	Res	Type
2	n	124	TRP
3	o	1	HIS
3	o	72	ILE
3	o	73	LEU
3	o	113	LYS
3	o	118	LEU
3	o	125	VAL
3	o	127	ASP
3	o	136	SER
4	p	8	LEU
4	p	22	HIS
4	p	23	HIS
4	p	41	GLU
4	p	52	ASP
4	p	77	LEU
4	p	80	THR
5	q	42	VAL
5	q	80	LEU
5	q	130	VAL
5	q	162	ILE
6	r	20	ARG
6	r	84	ILE
6	r	105	ASP
6	r	125	HIS
6	r	126	ASP
6	r	129	LEU
6	r	131	SER
6	r	200	VAL
6	r	233	GLN
6	r	235	HIS
7	s	14	LEU
7	s	21	LEU
7	s	28	LEU
7	s	32	LEU
7	s	61	ASP
7	s	130	SER
7	s	151	THR
7	s	158	VAL
7	s	196	ARG
7	s	206	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	HIS
5	M	195	HIS
6	N	231	HIS
2	Q	23	HIS
1	T	43	HIS
1	X	150	HIS
4	a	62	HIS
5	b	195	HIS
6	c	231	HIS
2	f	23	HIS
1	i	150	HIS
1	m	150	HIS
5	q	195	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 15 are monoatomic - leaving 75 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	HEM	A	201	1	24,50,50	2.69	11 (45%)	16,82,82	3.35	4 (25%)
9	CYN	A	202	-	0,1,1	0.00	-	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	HEM	B	201	9,2	24,50,50	2.61	10 (41%)	16,82,82	3.03	5 (31%)
9	CYN	B	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	C	201	3	24,50,50	2.61	11 (45%)	16,82,82	2.79	5 (31%)
9	CYN	C	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	D	201	4	24,50,50	2.60	11 (45%)	16,82,82	3.11	5 (31%)
9	CYN	D	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	E	201	1	24,50,50	2.66	11 (45%)	16,82,82	3.21	4 (25%)
9	CYN	E	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	F	201	9,2	24,50,50	2.65	11 (45%)	16,82,82	3.11	5 (31%)
9	CYN	F	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	G	201	9,3	24,50,50	2.57	11 (45%)	16,82,82	3.11	5 (31%)
9	CYN	G	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	H	201	4	24,50,50	2.63	11 (45%)	16,82,82	2.93	4 (25%)
9	CYN	H	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	I	201	1	24,50,50	2.68	12 (50%)	16,82,82	3.22	5 (31%)
9	CYN	I	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	J	201	9,2	24,50,50	2.69	12 (50%)	16,82,82	3.07	4 (25%)
9	CYN	J	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	K	201	3	24,50,50	2.64	12 (50%)	16,82,82	3.08	4 (25%)
9	CYN	K	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	L	201	4	24,50,50	2.67	11 (45%)	16,82,82	3.31	4 (25%)
9	CYN	L	202	-	0,1,1	0.00	-	0,0,0	0.00	-
12	NAG	O	304	7	14,14,15	0.39	0	15,19,21	1.94	4 (26%)
8	HEM	P	201	1	24,50,50	2.72	11 (45%)	16,82,82	3.15	4 (25%)
9	CYN	P	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	Q	201	2	24,50,50	2.64	10 (41%)	16,82,82	2.99	5 (31%)
9	CYN	Q	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	R	201	3	24,50,50	2.65	12 (50%)	16,82,82	2.90	5 (31%)
9	CYN	R	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	S	201	4	24,50,50	2.65	11 (45%)	16,82,82	3.17	5 (31%)
9	CYN	S	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	T	201	1	24,50,50	2.67	12 (50%)	16,82,82	3.19	4 (25%)
9	CYN	T	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	U	201	9,2	24,50,50	2.67	11 (45%)	16,82,82	2.89	4 (25%)
9	CYN	U	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	V	201	9,3	24,50,50	2.66	12 (50%)	16,82,82	3.18	4 (25%)
9	CYN	V	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	W	201	9,4	24,50,50	2.66	11 (45%)	16,82,82	3.24	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CYN	W	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	X	201	1	24,50,50	2.75	12 (50%)	16,82,82	3.31	6 (37%)
9	CYN	X	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	Y	201	9,2	24,50,50	2.65	11 (45%)	16,82,82	3.08	3 (18%)
9	CYN	Y	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	Z	201	3	24,50,50	2.65	12 (50%)	16,82,82	3.17	4 (25%)
9	CYN	Z	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	a	201	9,4	24,50,50	2.63	12 (50%)	16,82,82	3.38	5 (31%)
9	CYN	a	202	8	0,1,1	0.00	-	0,0,0	0.00	-
12	NAG	d	304	7	14,14,15	0.41	0	15,19,21	1.31	2 (13%)
8	HEM	e	201	1,9	24,50,50	2.66	11 (45%)	16,82,82	3.29	6 (37%)
9	CYN	e	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	f	201	9,2	24,50,50	2.61	10 (41%)	16,82,82	3.05	4 (25%)
9	CYN	f	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	g	201	3	24,50,50	2.69	12 (50%)	16,82,82	3.07	3 (18%)
9	CYN	g	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	h	201	4	24,50,50	2.64	12 (50%)	16,82,82	3.20	3 (18%)
9	CYN	h	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	i	201	1	24,50,50	2.68	12 (50%)	16,82,82	3.26	4 (25%)
9	CYN	i	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	j	201	9,2	24,50,50	2.64	11 (45%)	16,82,82	2.98	5 (31%)
9	CYN	j	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	k	201	9,3	24,50,50	2.67	12 (50%)	16,82,82	3.14	3 (18%)
9	CYN	k	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	l	201	4	24,50,50	2.68	11 (45%)	16,82,82	3.09	5 (31%)
9	CYN	l	202	-	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	m	201	1,9	24,50,50	2.73	12 (50%)	16,82,82	3.30	7 (43%)
9	CYN	m	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	n	201	9,2	24,50,50	2.66	11 (45%)	16,82,82	3.08	4 (25%)
9	CYN	n	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	o	201	9,3	24,50,50	2.62	12 (50%)	16,82,82	2.94	5 (31%)
9	CYN	o	202	8	0,1,1	0.00	-	0,0,0	0.00	-
8	HEM	p	201	9,4	24,50,50	2.67	12 (50%)	16,82,82	3.39	5 (31%)
9	CYN	p	202	8	0,1,1	0.00	-	0,0,0	0.00	-
12	NAG	s	303	7	14,14,15	0.46	0	15,19,21	1.43	2 (13%)

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. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	A	201	1	-	0/6/54/54	0/0/8/8
9	CYN	A	202	-	-	0/0/0/0	0/0/0/0
8	HEM	B	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	B	202	8	-	0/0/0/0	0/0/0/0
8	HEM	C	201	3	-	0/6/54/54	0/0/8/8
9	CYN	C	202	-	-	0/0/0/0	0/0/0/0
8	HEM	D	201	4	-	0/6/54/54	0/0/8/8
9	CYN	D	202	-	-	0/0/0/0	0/0/0/0
8	HEM	E	201	1	-	0/6/54/54	0/0/8/8
9	CYN	E	202	-	-	0/0/0/0	0/0/0/0
8	HEM	F	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	F	202	8	-	0/0/0/0	0/0/0/0
8	HEM	G	201	9,3	-	0/6/54/54	0/0/8/8
9	CYN	G	202	8	-	0/0/0/0	0/0/0/0
8	HEM	H	201	4	-	0/6/54/54	0/0/8/8
9	CYN	H	202	-	-	0/0/0/0	0/0/0/0
8	HEM	I	201	1	-	0/6/54/54	0/0/8/8
9	CYN	I	202	-	-	0/0/0/0	0/0/0/0
8	HEM	J	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	J	202	8	-	0/0/0/0	0/0/0/0
8	HEM	K	201	3	-	0/6/54/54	0/0/8/8
9	CYN	K	202	-	-	0/0/0/0	0/0/0/0
8	HEM	L	201	4	-	0/6/54/54	0/0/8/8
9	CYN	L	202	-	-	0/0/0/0	0/0/0/0
12	NAG	O	304	7	-	0/6/23/26	0/1/1/1
8	HEM	P	201	1	-	0/6/54/54	0/0/8/8
9	CYN	P	202	-	-	0/0/0/0	0/0/0/0
8	HEM	Q	201	2	-	0/6/54/54	0/0/8/8
9	CYN	Q	202	-	-	0/0/0/0	0/0/0/0
8	HEM	R	201	3	-	0/6/54/54	0/0/8/8
9	CYN	R	202	-	-	0/0/0/0	0/0/0/0
8	HEM	S	201	4	-	0/6/54/54	0/0/8/8
9	CYN	S	202	-	-	0/0/0/0	0/0/0/0
8	HEM	T	201	1	-	0/6/54/54	0/0/8/8
9	CYN	T	202	-	-	0/0/0/0	0/0/0/0
8	HEM	U	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	U	202	8	-	0/0/0/0	0/0/0/0
8	HEM	V	201	9,3	-	0/6/54/54	0/0/8/8
9	CYN	V	202	8	-	0/0/0/0	0/0/0/0
8	HEM	W	201	9,4	-	0/6/54/54	0/0/8/8
9	CYN	W	202	8	-	0/0/0/0	0/0/0/0
8	HEM	X	201	1	-	2/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CYN	X	202	-	-	0/0/0/0	0/0/0/0
8	HEM	Y	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	Y	202	8	-	0/0/0/0	0/0/0/0
8	HEM	Z	201	3	-	0/6/54/54	0/0/8/8
9	CYN	Z	202	-	-	0/0/0/0	0/0/0/0
8	HEM	a	201	9,4	-	0/6/54/54	0/0/8/8
9	CYN	a	202	8	-	0/0/0/0	0/0/0/0
12	NAG	d	304	7	-	0/6/23/26	0/1/1/1
8	HEM	e	201	1,9	-	0/6/54/54	0/0/8/8
9	CYN	e	202	8	-	0/0/0/0	0/0/0/0
8	HEM	f	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	f	202	8	-	0/0/0/0	0/0/0/0
8	HEM	g	201	3	-	0/6/54/54	0/0/8/8
9	CYN	g	202	-	-	0/0/0/0	0/0/0/0
8	HEM	h	201	4	-	0/6/54/54	0/0/8/8
9	CYN	h	202	-	-	0/0/0/0	0/0/0/0
8	HEM	i	201	1	-	0/6/54/54	0/0/8/8
9	CYN	i	202	-	-	0/0/0/0	0/0/0/0
8	HEM	j	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	j	202	8	-	0/0/0/0	0/0/0/0
8	HEM	k	201	9,3	-	0/6/54/54	0/0/8/8
9	CYN	k	202	8	-	0/0/0/0	0/0/0/0
8	HEM	l	201	4	-	0/6/54/54	0/0/8/8
9	CYN	l	202	-	-	0/0/0/0	0/0/0/0
8	HEM	m	201	1,9	-	0/6/54/54	0/0/8/8
9	CYN	m	202	8	-	0/0/0/0	0/0/0/0
8	HEM	n	201	9,2	-	0/6/54/54	0/0/8/8
9	CYN	n	202	8	-	0/0/0/0	0/0/0/0
8	HEM	o	201	9,3	-	0/6/54/54	0/0/8/8
9	CYN	o	202	8	-	0/0/0/0	0/0/0/0
8	HEM	p	201	9,4	-	0/6/54/54	0/0/8/8
9	CYN	p	202	8	-	0/0/0/0	0/0/0/0
12	NAG	s	303	7	-	0/6/23/26	0/1/1/1

All (409) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	201	HEM	C3C-C2C	-5.64	1.33	1.40
8	X	201	HEM	C3B-C2B	-5.53	1.33	1.40
8	Q	201	HEM	C3C-C2C	-5.52	1.33	1.40
8	V	201	HEM	C3B-C2B	-5.51	1.33	1.40
8	Z	201	HEM	C3B-C2B	-5.48	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	201	HEM	C3B-C2B	-5.47	1.33	1.40
8	a	201	HEM	C3C-C2C	-5.45	1.33	1.40
8	h	201	HEM	C3C-C2C	-5.44	1.33	1.40
8	A	201	HEM	C3B-C2B	-5.43	1.33	1.40
8	g	201	HEM	C3B-C2B	-5.42	1.33	1.40
8	I	201	HEM	C3B-C2B	-5.39	1.33	1.40
8	P	201	HEM	C3B-C2B	-5.36	1.33	1.40
8	J	201	HEM	C3C-C2C	-5.35	1.33	1.40
8	K	201	HEM	C3B-C2B	-5.34	1.33	1.40
8	F	201	HEM	C3C-C2C	-5.33	1.33	1.40
8	n	201	HEM	C3C-C2C	-5.30	1.33	1.40
8	D	201	HEM	C3C-C2C	-5.30	1.33	1.40
8	p	201	HEM	C3C-C2C	-5.27	1.33	1.40
8	g	201	HEM	C3C-C2C	-5.25	1.33	1.40
8	P	201	HEM	C3C-C2C	-5.25	1.33	1.40
8	S	201	HEM	C3C-C2C	-5.24	1.33	1.40
8	f	201	HEM	C3C-C2C	-5.23	1.33	1.40
8	A	201	HEM	C3C-C2C	-5.22	1.33	1.40
8	C	201	HEM	C3B-C2B	-5.21	1.33	1.40
8	U	201	HEM	C3C-C2C	-5.20	1.33	1.40
8	W	201	HEM	C3C-C2C	-5.18	1.33	1.40
8	o	201	HEM	C3B-C2B	-5.16	1.33	1.40
8	m	201	HEM	C3B-C2B	-5.15	1.33	1.40
8	e	201	HEM	C3B-C2B	-5.14	1.33	1.40
8	k	201	HEM	C3B-C2B	-5.13	1.33	1.40
8	m	201	HEM	C3C-C2C	-5.12	1.33	1.40
8	E	201	HEM	C3B-C2B	-5.09	1.33	1.40
8	i	201	HEM	C3B-C2B	-5.09	1.33	1.40
8	Y	201	HEM	C3C-C2C	-5.08	1.33	1.40
8	i	201	HEM	C3C-C2C	-5.07	1.33	1.40
8	e	201	HEM	C3C-C2C	-5.06	1.33	1.40
8	j	201	HEM	C3C-C2C	-5.02	1.34	1.40
8	E	201	HEM	C3C-C2C	-5.02	1.34	1.40
8	H	201	HEM	C3C-C2C	-5.01	1.34	1.40
8	B	201	HEM	C3C-C2C	-5.00	1.34	1.40
8	l	201	HEM	C3C-C2C	-4.94	1.34	1.40
8	G	201	HEM	C3B-C2B	-4.93	1.34	1.40
8	Z	201	HEM	C3C-C2C	-4.93	1.34	1.40
8	I	201	HEM	C3C-C2C	-4.86	1.34	1.40
8	X	201	HEM	C3C-C2C	-4.86	1.34	1.40
8	F	201	HEM	C3B-C2B	-4.86	1.34	1.40
8	L	201	HEM	C3B-C2B	-4.85	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	201	HEM	C3B-C2B	-4.82	1.34	1.40
8	W	201	HEM	C3B-C2B	-4.81	1.34	1.40
8	T	201	HEM	C3C-C2C	-4.77	1.34	1.40
8	C	201	HEM	C3C-C2C	-4.77	1.34	1.40
8	l	201	HEM	C3B-C2B	-4.76	1.34	1.40
8	K	201	HEM	C3C-C2C	-4.73	1.34	1.40
8	k	201	HEM	C3C-C2C	-4.72	1.34	1.40
8	B	201	HEM	C3B-C2B	-4.67	1.34	1.40
8	U	201	HEM	C3B-C2B	-4.67	1.34	1.40
8	R	201	HEM	C3C-C2C	-4.65	1.34	1.40
8	j	201	HEM	C3B-C2B	-4.63	1.34	1.40
8	a	201	HEM	C3B-C2B	-4.62	1.34	1.40
8	H	201	HEM	C3B-C2B	-4.60	1.34	1.40
8	Q	201	HEM	C3B-C2B	-4.58	1.34	1.40
8	S	201	HEM	C3B-C2B	-4.53	1.34	1.40
8	o	201	HEM	C3C-C2C	-4.51	1.34	1.40
8	f	201	HEM	C3B-C2B	-4.48	1.34	1.40
8	G	201	HEM	C3C-C2C	-4.46	1.34	1.40
8	V	201	HEM	C3C-C2C	-4.39	1.34	1.40
8	p	201	HEM	C3B-C2B	-4.36	1.34	1.40
8	n	201	HEM	C3B-C2B	-4.33	1.34	1.40
8	Y	201	HEM	C3B-C2B	-4.26	1.34	1.40
8	h	201	HEM	C3B-C2B	-4.26	1.34	1.40
8	D	201	HEM	C3B-C2B	-4.25	1.35	1.40
8	J	201	HEM	C3B-C2B	-4.18	1.35	1.40
8	i	201	HEM	CAA-C2A	2.01	1.55	1.52
8	C	201	HEM	C1B-NB	2.01	1.39	1.36
8	I	201	HEM	CAD-C3D	2.01	1.54	1.52
8	n	201	HEM	CAA-C2A	2.03	1.55	1.52
8	g	201	HEM	C1B-NB	2.04	1.39	1.36
8	Z	201	HEM	C4C-NC	2.04	1.39	1.36
8	p	201	HEM	CAD-C3D	2.07	1.54	1.52
8	F	201	HEM	C1B-NB	2.07	1.39	1.36
8	J	201	HEM	CAD-C3D	2.09	1.55	1.52
8	Z	201	HEM	C1B-NB	2.09	1.39	1.36
8	Y	201	HEM	CAD-C3D	2.10	1.55	1.52
8	h	201	HEM	CAD-C3D	2.10	1.55	1.52
8	R	201	HEM	C4C-NC	2.10	1.39	1.36
8	K	201	HEM	C4C-NC	2.10	1.39	1.36
8	K	201	HEM	CAD-C3D	2.11	1.55	1.52
8	K	201	HEM	C1B-NB	2.12	1.39	1.36
8	a	201	HEM	CAD-C3D	2.12	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	201	HEM	C1B-NB	2.12	1.39	1.36
8	J	201	HEM	C1B-NB	2.13	1.39	1.36
8	k	201	HEM	C4C-NC	2.15	1.39	1.36
8	D	201	HEM	C4C-NC	2.16	1.39	1.36
8	i	201	HEM	C1B-NB	2.17	1.39	1.36
8	Z	201	HEM	CAD-C3D	2.17	1.55	1.52
8	o	201	HEM	CAD-C3D	2.17	1.55	1.52
8	H	201	HEM	C1B-NB	2.18	1.39	1.36
8	a	201	HEM	C1B-NB	2.18	1.39	1.36
8	j	201	HEM	C1B-NB	2.19	1.39	1.36
8	h	201	HEM	C1B-NB	2.19	1.39	1.36
8	G	201	HEM	C1B-NB	2.20	1.39	1.36
8	h	201	HEM	C4C-NC	2.21	1.39	1.36
8	k	201	HEM	C1B-NB	2.21	1.39	1.36
8	E	201	HEM	C1B-NB	2.22	1.39	1.36
8	P	201	HEM	C4C-NC	2.22	1.39	1.36
8	W	201	HEM	C1B-NB	2.23	1.39	1.36
8	g	201	HEM	C4C-NC	2.24	1.39	1.36
8	e	201	HEM	C4C-NC	2.24	1.39	1.36
8	U	201	HEM	C1B-NB	2.24	1.39	1.36
8	V	201	HEM	C4C-NC	2.24	1.39	1.36
8	K	201	HEM	C1C-NC	2.26	1.39	1.36
8	a	201	HEM	C4C-NC	2.26	1.39	1.36
8	o	201	HEM	C1B-NB	2.26	1.39	1.36
8	p	201	HEM	C1B-NB	2.26	1.39	1.36
8	o	201	HEM	C4C-NC	2.26	1.39	1.36
8	V	201	HEM	CAD-C3D	2.27	1.55	1.52
8	G	201	HEM	C4C-NC	2.28	1.39	1.36
8	R	201	HEM	CAD-C3D	2.28	1.55	1.52
8	T	201	HEM	CAD-C3D	2.28	1.55	1.52
8	R	201	HEM	C1C-NC	2.29	1.39	1.36
8	C	201	HEM	C4C-NC	2.29	1.39	1.36
8	V	201	HEM	C1B-NB	2.34	1.39	1.36
8	g	201	HEM	C1C-NC	2.35	1.39	1.36
8	C	201	HEM	C1C-NC	2.36	1.39	1.36
8	D	201	HEM	C1B-NB	2.36	1.39	1.36
8	Z	201	HEM	C1C-NC	2.36	1.39	1.36
8	X	201	HEM	C4C-NC	2.38	1.39	1.36
8	I	201	HEM	C1B-NB	2.39	1.40	1.36
8	S	201	HEM	C4C-NC	2.39	1.40	1.36
8	A	201	HEM	C1B-NB	2.39	1.40	1.36
8	m	201	HEM	C1B-NB	2.39	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	201	HEM	C1B-NB	2.39	1.40	1.36
8	G	201	HEM	C1C-NC	2.40	1.40	1.36
8	F	201	HEM	C4C-NC	2.40	1.40	1.36
8	L	201	HEM	C1B-NB	2.41	1.40	1.36
8	f	201	HEM	C4C-NC	2.41	1.40	1.36
8	X	201	HEM	C1C-NC	2.42	1.40	1.36
8	H	201	HEM	C4C-NC	2.42	1.40	1.36
8	G	201	HEM	C4D-ND	2.44	1.40	1.36
8	A	201	HEM	C4C-NC	2.45	1.40	1.36
8	W	201	HEM	C4C-NC	2.45	1.40	1.36
8	L	201	HEM	C4C-NC	2.45	1.40	1.36
8	j	201	HEM	C4C-NC	2.45	1.40	1.36
8	H	201	HEM	C4D-ND	2.46	1.40	1.36
8	Q	201	HEM	C4C-NC	2.46	1.40	1.36
8	I	201	HEM	C4C-NC	2.46	1.40	1.36
8	D	201	HEM	C1C-NC	2.47	1.40	1.36
8	k	201	HEM	C1C-NC	2.48	1.40	1.36
8	B	201	HEM	C4C-NC	2.49	1.40	1.36
8	X	201	HEM	C1B-NB	2.51	1.40	1.36
8	l	201	HEM	C4C-NC	2.51	1.40	1.36
8	L	201	HEM	C4D-ND	2.52	1.40	1.36
8	n	201	HEM	C4C-NC	2.52	1.40	1.36
8	e	201	HEM	C1B-NB	2.54	1.40	1.36
8	p	201	HEM	C4C-NC	2.54	1.40	1.36
8	D	201	HEM	C4D-ND	2.55	1.40	1.36
8	a	201	HEM	C1C-NC	2.55	1.40	1.36
8	k	201	HEM	CAD-C3D	2.56	1.55	1.52
8	V	201	HEM	C1C-NC	2.56	1.40	1.36
8	o	201	HEM	C1C-NC	2.56	1.40	1.36
8	A	201	HEM	C1C-NC	2.56	1.40	1.36
8	o	201	HEM	C4D-ND	2.57	1.40	1.36
8	I	201	HEM	C1C-NC	2.59	1.40	1.36
8	S	201	HEM	C4D-ND	2.60	1.40	1.36
8	T	201	HEM	C1B-NB	2.62	1.40	1.36
8	U	201	HEM	C4D-ND	2.63	1.40	1.36
8	e	201	HEM	C1C-NC	2.63	1.40	1.36
8	E	201	HEM	C4C-NC	2.64	1.40	1.36
8	F	201	HEM	C1C-NC	2.65	1.40	1.36
8	C	201	HEM	C4D-ND	2.65	1.40	1.36
8	m	201	HEM	CAD-C3D	2.65	1.55	1.52
8	W	201	HEM	C1C-NC	2.66	1.40	1.36
8	i	201	HEM	C4C-NC	2.66	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	201	HEM	C1C-NC	2.67	1.40	1.36
8	K	201	HEM	C4D-ND	2.67	1.40	1.36
8	T	201	HEM	C1C-NC	2.67	1.40	1.36
8	g	201	HEM	CAD-C3D	2.67	1.55	1.52
8	l	201	HEM	C1C-NC	2.67	1.40	1.36
8	T	201	HEM	C4C-NC	2.68	1.40	1.36
8	U	201	HEM	C4C-NC	2.68	1.40	1.36
8	h	201	HEM	C4D-ND	2.68	1.40	1.36
8	S	201	HEM	C1C-NC	2.68	1.40	1.36
8	i	201	HEM	C1C-NC	2.69	1.40	1.36
8	m	201	HEM	C4C-NC	2.70	1.40	1.36
8	L	201	HEM	C1C-NC	2.70	1.40	1.36
8	Z	201	HEM	C4D-ND	2.70	1.40	1.36
8	g	201	HEM	C4D-ND	2.71	1.40	1.36
8	a	201	HEM	C4D-ND	2.73	1.40	1.36
8	h	201	HEM	C1C-NC	2.73	1.40	1.36
8	n	201	HEM	C1C-NC	2.75	1.40	1.36
8	F	201	HEM	C4D-ND	2.75	1.40	1.36
8	Y	201	HEM	C4C-NC	2.75	1.40	1.36
8	j	201	HEM	C4D-ND	2.76	1.40	1.36
8	H	201	HEM	C1C-NC	2.76	1.40	1.36
8	S	201	HEM	CAD-C3D	2.76	1.55	1.52
8	R	201	HEM	C4D-ND	2.76	1.40	1.36
8	f	201	HEM	C1C-NC	2.76	1.40	1.36
8	Q	201	HEM	C1C-NC	2.78	1.40	1.36
8	p	201	HEM	C1C-NC	2.78	1.40	1.36
8	E	201	HEM	C1C-NC	2.78	1.40	1.36
8	m	201	HEM	C1C-NC	2.81	1.40	1.36
8	J	201	HEM	C4C-NC	2.84	1.40	1.36
8	B	201	HEM	C1C-NC	2.84	1.40	1.36
8	l	201	HEM	C4D-ND	2.85	1.40	1.36
8	k	201	HEM	C4D-ND	2.86	1.40	1.36
8	l	201	HEM	CAD-C3D	2.87	1.56	1.52
8	Q	201	HEM	C4D-ND	2.87	1.40	1.36
8	W	201	HEM	C4D-ND	2.88	1.40	1.36
8	B	201	HEM	C4D-ND	2.89	1.40	1.36
8	U	201	HEM	C1C-NC	2.89	1.40	1.36
8	f	201	HEM	C4D-ND	2.90	1.40	1.36
8	h	201	HEM	C3C-CAC	2.92	1.53	1.47
8	X	201	HEM	CAD-C3D	2.93	1.56	1.52
8	Y	201	HEM	C1C-NC	2.94	1.40	1.36
8	J	201	HEM	C1C-NC	2.94	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	201	HEM	C4D-ND	2.95	1.40	1.36
8	Y	201	HEM	C4D-ND	2.95	1.40	1.36
8	T	201	HEM	C4D-ND	2.97	1.40	1.36
8	j	201	HEM	C1C-NC	2.98	1.40	1.36
8	a	201	HEM	C3C-CAC	2.98	1.53	1.47
8	L	201	HEM	C3C-CAC	2.99	1.54	1.47
8	V	201	HEM	C4D-ND	3.00	1.40	1.36
8	p	201	HEM	C4D-ND	3.02	1.40	1.36
8	i	201	HEM	C4D-ND	3.02	1.40	1.36
8	D	201	HEM	C3C-CAC	3.04	1.54	1.47
8	W	201	HEM	C3C-CAC	3.04	1.54	1.47
8	e	201	HEM	C4D-ND	3.05	1.40	1.36
8	p	201	HEM	C3C-CAC	3.06	1.54	1.47
8	F	201	HEM	C3C-CAC	3.08	1.54	1.47
8	J	201	HEM	C3C-CAC	3.10	1.54	1.47
8	Z	201	HEM	C3B-CAB	3.10	1.54	1.47
8	C	201	HEM	C3B-CAB	3.10	1.54	1.47
8	V	201	HEM	C3B-CAB	3.11	1.54	1.47
8	Q	201	HEM	C3C-CAC	3.11	1.54	1.47
8	J	201	HEM	C4D-ND	3.12	1.40	1.36
8	Y	201	HEM	C3C-CAC	3.12	1.54	1.47
8	I	201	HEM	C3B-CAB	3.13	1.54	1.47
8	P	201	HEM	C4D-ND	3.16	1.41	1.36
8	n	201	HEM	C3C-CAC	3.16	1.54	1.47
8	I	201	HEM	C4D-ND	3.16	1.41	1.36
8	A	201	HEM	C4D-ND	3.17	1.41	1.36
8	S	201	HEM	C3C-CAC	3.17	1.54	1.47
8	R	201	HEM	C3B-CAB	3.18	1.54	1.47
8	X	201	HEM	C4D-ND	3.18	1.41	1.36
8	n	201	HEM	C4D-ND	3.19	1.41	1.36
8	B	201	HEM	C3C-CAC	3.20	1.54	1.47
8	g	201	HEM	C3B-CAB	3.20	1.54	1.47
8	k	201	HEM	C3B-CAB	3.21	1.54	1.47
8	o	201	HEM	C3B-CAB	3.21	1.54	1.47
8	e	201	HEM	C3B-CAB	3.22	1.54	1.47
8	H	201	HEM	C3C-CAC	3.22	1.54	1.47
8	m	201	HEM	C3B-CAB	3.23	1.54	1.47
8	A	201	HEM	C3B-CAB	3.23	1.54	1.47
8	K	201	HEM	C3B-CAB	3.23	1.54	1.47
8	U	201	HEM	C3C-CAC	3.25	1.54	1.47
8	f	201	HEM	C3C-CAC	3.25	1.54	1.47
8	i	201	HEM	C3C-CAC	3.26	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	201	HEM	C3B-CAB	3.27	1.54	1.47
8	X	201	HEM	C3B-CAB	3.29	1.54	1.47
8	j	201	HEM	C3C-CAC	3.30	1.54	1.47
8	l	201	HEM	C3C-CAC	3.30	1.54	1.47
8	A	201	HEM	C3C-CAC	3.31	1.54	1.47
8	i	201	HEM	C3B-CAB	3.32	1.54	1.47
8	P	201	HEM	C3B-CAB	3.33	1.54	1.47
8	P	201	HEM	C3C-CAC	3.34	1.54	1.47
8	h	201	HEM	CBC-CAC	3.35	1.54	1.28
8	L	201	HEM	CBC-CAC	3.35	1.54	1.28
8	p	201	HEM	CBC-CAC	3.35	1.54	1.28
8	W	201	HEM	CBC-CAC	3.36	1.54	1.28
8	l	201	HEM	CBC-CAC	3.36	1.54	1.28
8	T	201	HEM	C3B-CAB	3.36	1.54	1.47
8	e	201	HEM	CBB-CAB	3.36	1.54	1.28
8	S	201	HEM	CBC-CAC	3.36	1.54	1.28
8	C	201	HEM	CBB-CAB	3.37	1.54	1.28
8	A	201	HEM	CBB-CAB	3.37	1.54	1.28
8	H	201	HEM	CBC-CAC	3.37	1.54	1.28
8	a	201	HEM	CBC-CAC	3.37	1.54	1.28
8	E	201	HEM	C3B-CAB	3.38	1.55	1.47
8	e	201	HEM	C3C-CAC	3.38	1.54	1.47
8	m	201	HEM	CBB-CAB	3.38	1.54	1.28
8	T	201	HEM	CBB-CAB	3.38	1.54	1.28
8	E	201	HEM	C3C-CAC	3.39	1.54	1.47
8	I	201	HEM	CBB-CAB	3.39	1.54	1.28
8	P	201	HEM	CBB-CAB	3.39	1.54	1.28
8	H	201	HEM	CBB-CAB	3.39	1.54	1.28
8	g	201	HEM	C3C-CAC	3.40	1.54	1.47
8	K	201	HEM	CBB-CAB	3.40	1.54	1.28
8	Y	201	HEM	CBC-CAC	3.40	1.54	1.28
8	Q	201	HEM	CBC-CAC	3.40	1.54	1.28
8	g	201	HEM	CBB-CAB	3.40	1.54	1.28
8	D	201	HEM	CBC-CAC	3.41	1.54	1.28
8	m	201	HEM	C3C-CAC	3.41	1.54	1.47
8	i	201	HEM	CBB-CAB	3.41	1.54	1.28
8	X	201	HEM	CBB-CAB	3.41	1.54	1.28
8	V	201	HEM	CBB-CAB	3.41	1.54	1.28
8	Z	201	HEM	CBB-CAB	3.41	1.54	1.28
8	B	201	HEM	C3B-CAB	3.41	1.55	1.47
8	f	201	HEM	CBB-CAB	3.41	1.54	1.28
8	I	201	HEM	C3C-CAC	3.41	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	201	HEM	CBC-CAC	3.42	1.54	1.28
8	f	201	HEM	CBC-CAC	3.42	1.54	1.28
8	G	201	HEM	CBB-CAB	3.42	1.54	1.28
8	U	201	HEM	CBB-CAB	3.42	1.54	1.28
8	B	201	HEM	CBC-CAC	3.42	1.54	1.28
8	W	201	HEM	CBB-CAB	3.42	1.54	1.28
8	R	201	HEM	CBB-CAB	3.42	1.54	1.28
8	T	201	HEM	CBC-CAC	3.42	1.54	1.28
8	W	201	HEM	C3B-CAB	3.43	1.55	1.47
8	P	201	HEM	CBC-CAC	3.43	1.54	1.28
8	k	201	HEM	CBB-CAB	3.43	1.54	1.28
8	Q	201	HEM	CBB-CAB	3.43	1.54	1.28
8	S	201	HEM	CBB-CAB	3.43	1.54	1.28
8	C	201	HEM	CBC-CAC	3.43	1.54	1.28
8	e	201	HEM	CBC-CAC	3.43	1.54	1.28
8	m	201	HEM	C4D-ND	3.43	1.41	1.36
8	X	201	HEM	CBC-CAC	3.43	1.54	1.28
8	o	201	HEM	CBB-CAB	3.43	1.54	1.28
8	j	201	HEM	CBB-CAB	3.44	1.54	1.28
8	L	201	HEM	CBB-CAB	3.44	1.54	1.28
8	B	201	HEM	CBB-CAB	3.44	1.54	1.28
8	m	201	HEM	CBC-CAC	3.44	1.54	1.28
8	R	201	HEM	CBC-CAC	3.44	1.54	1.28
8	D	201	HEM	CBB-CAB	3.44	1.54	1.28
8	A	201	HEM	CBC-CAC	3.44	1.54	1.28
8	l	201	HEM	CBB-CAB	3.44	1.54	1.28
8	X	201	HEM	C3C-CAC	3.44	1.54	1.47
8	E	201	HEM	CBC-CAC	3.44	1.54	1.28
8	I	201	HEM	CBC-CAC	3.44	1.54	1.28
8	n	201	HEM	CBB-CAB	3.44	1.54	1.28
8	E	201	HEM	CBB-CAB	3.45	1.54	1.28
8	Y	201	HEM	CBB-CAB	3.45	1.54	1.28
8	F	201	HEM	CBB-CAB	3.45	1.54	1.28
8	j	201	HEM	CBC-CAC	3.45	1.54	1.28
8	h	201	HEM	CBB-CAB	3.45	1.54	1.28
8	f	201	HEM	C3B-CAB	3.45	1.55	1.47
8	i	201	HEM	CBC-CAC	3.45	1.54	1.28
8	J	201	HEM	CBC-CAC	3.45	1.54	1.28
8	L	201	HEM	C3B-CAB	3.45	1.55	1.47
8	p	201	HEM	CBB-CAB	3.45	1.54	1.28
8	n	201	HEM	CBC-CAC	3.46	1.54	1.28
8	Z	201	HEM	C3C-CAC	3.46	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	j	201	HEM	C3B-CAB	3.46	1.55	1.47
8	J	201	HEM	CBB-CAB	3.46	1.54	1.28
8	F	201	HEM	CBC-CAC	3.46	1.54	1.28
8	a	201	HEM	CBB-CAB	3.46	1.54	1.28
8	g	201	HEM	CBC-CAC	3.47	1.54	1.28
8	o	201	HEM	CBC-CAC	3.48	1.55	1.28
8	S	201	HEM	C3B-CAB	3.49	1.55	1.47
8	D	201	HEM	C3B-CAB	3.49	1.55	1.47
8	Z	201	HEM	CBC-CAC	3.49	1.55	1.28
8	k	201	HEM	CBC-CAC	3.49	1.55	1.28
8	G	201	HEM	CBC-CAC	3.49	1.55	1.28
8	p	201	HEM	C3B-CAB	3.50	1.55	1.47
8	K	201	HEM	C3C-CAC	3.51	1.55	1.47
8	V	201	HEM	CBC-CAC	3.51	1.55	1.28
8	K	201	HEM	CBC-CAC	3.51	1.55	1.28
8	T	201	HEM	C3C-CAC	3.52	1.55	1.47
8	l	201	HEM	C3B-CAB	3.53	1.55	1.47
8	F	201	HEM	C3B-CAB	3.54	1.55	1.47
8	H	201	HEM	C3B-CAB	3.54	1.55	1.47
8	Y	201	HEM	C3B-CAB	3.54	1.55	1.47
8	o	201	HEM	C3C-CAC	3.54	1.55	1.47
8	V	201	HEM	C3C-CAC	3.55	1.55	1.47
8	a	201	HEM	C3B-CAB	3.59	1.55	1.47
8	U	201	HEM	C3B-CAB	3.59	1.55	1.47
8	G	201	HEM	C3C-CAC	3.59	1.55	1.47
8	k	201	HEM	C3C-CAC	3.60	1.55	1.47
8	J	201	HEM	C3B-CAB	3.61	1.55	1.47
8	n	201	HEM	C3B-CAB	3.62	1.55	1.47
8	C	201	HEM	C3C-CAC	3.62	1.55	1.47
8	h	201	HEM	C3B-CAB	3.62	1.55	1.47
8	Q	201	HEM	C3B-CAB	3.64	1.55	1.47
8	R	201	HEM	C3C-CAC	3.65	1.55	1.47
8	C	201	HEM	C3D-C2D	5.21	1.53	1.37
8	f	201	HEM	C3D-C2D	5.27	1.53	1.37
8	E	201	HEM	C3D-C2D	5.31	1.53	1.37
8	A	201	HEM	C3D-C2D	5.32	1.53	1.37
8	B	201	HEM	C3D-C2D	5.34	1.53	1.37
8	g	201	HEM	C3D-C2D	5.36	1.53	1.37
8	m	201	HEM	C3D-C2D	5.37	1.53	1.37
8	e	201	HEM	C3D-C2D	5.37	1.53	1.37
8	K	201	HEM	C3D-C2D	5.38	1.53	1.37
8	R	201	HEM	C3D-C2D	5.39	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	201	HEM	C3D-C2D	5.39	1.53	1.37
8	Q	201	HEM	C3D-C2D	5.40	1.53	1.37
8	o	201	HEM	C3D-C2D	5.40	1.53	1.37
8	I	201	HEM	C3D-C2D	5.40	1.53	1.37
8	V	201	HEM	C3D-C2D	5.42	1.53	1.37
8	Z	201	HEM	C3D-C2D	5.43	1.53	1.37
8	L	201	HEM	C3D-C2D	5.44	1.53	1.37
8	P	201	HEM	C3D-C2D	5.48	1.53	1.37
8	a	201	HEM	C3D-C2D	5.48	1.53	1.37
8	T	201	HEM	C3D-C2D	5.49	1.53	1.37
8	F	201	HEM	C3D-C2D	5.50	1.54	1.37
8	i	201	HEM	C3D-C2D	5.50	1.54	1.37
8	X	201	HEM	C3D-C2D	5.54	1.54	1.37
8	j	201	HEM	C3D-C2D	5.57	1.54	1.37
8	k	201	HEM	C3D-C2D	5.57	1.54	1.37
8	h	201	HEM	C3D-C2D	5.58	1.54	1.37
8	n	201	HEM	C3D-C2D	5.58	1.54	1.37
8	Y	201	HEM	C3D-C2D	5.60	1.54	1.37
8	H	201	HEM	C3D-C2D	5.60	1.54	1.37
8	S	201	HEM	C3D-C2D	5.61	1.54	1.37
8	U	201	HEM	C3D-C2D	5.62	1.54	1.37
8	D	201	HEM	C3D-C2D	5.63	1.54	1.37
8	W	201	HEM	C3D-C2D	5.63	1.54	1.37
8	p	201	HEM	C3D-C2D	5.69	1.54	1.37
8	J	201	HEM	C3D-C2D	5.70	1.54	1.37
8	l	201	HEM	C3D-C2D	5.72	1.54	1.37

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	201	HEM	C3C-CAC-CBC	-10.18	105.93	126.40
8	a	201	HEM	C3C-CAC-CBC	-10.06	106.17	126.40
8	h	201	HEM	C3C-CAC-CBC	-9.95	106.40	126.40
8	p	201	HEM	C3C-CAC-CBC	-9.75	106.79	126.40
8	F	201	HEM	C3C-CAC-CBC	-9.49	107.31	126.40
8	W	201	HEM	C3C-CAC-CBC	-9.48	107.34	126.40
8	Y	201	HEM	C3C-CAC-CBC	-9.29	107.72	126.40
8	D	201	HEM	C3C-CAC-CBC	-9.15	108.00	126.40
8	I	201	HEM	C3B-CAB-CBB	-9.06	108.17	126.40
8	n	201	HEM	C3C-CAC-CBC	-9.06	108.18	126.40
8	J	201	HEM	C3C-CAC-CBC	-9.04	108.21	126.40
8	H	201	HEM	C3C-CAC-CBC	-8.95	108.40	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	201	HEM	C3C-CAC-CBC	-8.94	108.43	126.40
8	m	201	HEM	C3B-CAB-CBB	-8.94	108.43	126.40
8	S	201	HEM	C3C-CAC-CBC	-8.87	108.56	126.40
8	A	201	HEM	C3B-CAB-CBB	-8.80	108.71	126.40
8	e	201	HEM	C3B-CAB-CBB	-8.79	108.72	126.40
8	Q	201	HEM	C3C-CAC-CBC	-8.72	108.87	126.40
8	Z	201	HEM	C3B-CAB-CBB	-8.69	108.93	126.40
8	T	201	HEM	C3B-CAB-CBB	-8.68	108.95	126.40
8	V	201	HEM	C3B-CAB-CBB	-8.66	108.98	126.40
8	A	201	HEM	C3C-CAC-CBC	-8.59	109.12	126.40
8	i	201	HEM	C3C-CAC-CBC	-8.55	109.21	126.40
8	B	201	HEM	C3C-CAC-CBC	-8.54	109.22	126.40
8	f	201	HEM	C3C-CAC-CBC	-8.53	109.24	126.40
8	X	201	HEM	C3C-CAC-CBC	-8.42	109.47	126.40
8	j	201	HEM	C3C-CAC-CBC	-8.36	109.58	126.40
8	i	201	HEM	C3B-CAB-CBB	-8.34	109.63	126.40
8	U	201	HEM	C3C-CAC-CBC	-8.34	109.64	126.40
8	X	201	HEM	C3B-CAB-CBB	-8.33	109.65	126.40
8	P	201	HEM	C3B-CAB-CBB	-8.31	109.69	126.40
8	E	201	HEM	C3B-CAB-CBB	-8.15	110.01	126.40
8	P	201	HEM	C3C-CAC-CBC	-8.13	110.05	126.40
8	K	201	HEM	C3B-CAB-CBB	-8.08	110.15	126.40
8	E	201	HEM	C3C-CAC-CBC	-8.07	110.16	126.40
8	k	201	HEM	C3B-CAB-CBB	-8.07	110.17	126.40
8	g	201	HEM	C3B-CAB-CBB	-8.03	110.26	126.40
8	o	201	HEM	C3B-CAB-CBB	-7.98	110.36	126.40
8	e	201	HEM	C3C-CAC-CBC	-7.96	110.39	126.40
8	Z	201	HEM	C3C-CAC-CBC	-7.93	110.45	126.40
8	V	201	HEM	C3C-CAC-CBC	-7.88	110.55	126.40
8	g	201	HEM	C3C-CAC-CBC	-7.87	110.57	126.40
8	k	201	HEM	C3C-CAC-CBC	-7.76	110.80	126.40
8	C	201	HEM	C3B-CAB-CBB	-7.72	110.88	126.40
8	I	201	HEM	C3C-CAC-CBC	-7.70	110.91	126.40
8	m	201	HEM	C3C-CAC-CBC	-7.63	111.06	126.40
8	T	201	HEM	C3C-CAC-CBC	-7.62	111.07	126.40
8	G	201	HEM	C3B-CAB-CBB	-7.60	111.11	126.40
8	K	201	HEM	C3C-CAC-CBC	-7.54	111.23	126.40
8	R	201	HEM	C3B-CAB-CBB	-7.49	111.33	126.40
8	G	201	HEM	C3C-CAC-CBC	-7.45	111.43	126.40
8	f	201	HEM	C3B-CAB-CBB	-7.09	112.15	126.40
8	o	201	HEM	C3C-CAC-CBC	-7.07	112.19	126.40
8	a	201	HEM	C3B-CAB-CBB	-7.04	112.24	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	201	HEM	C3B-CAB-CBB	-6.89	112.55	126.40
8	W	201	HEM	C3B-CAB-CBB	-6.85	112.62	126.40
8	B	201	HEM	C3B-CAB-CBB	-6.81	112.70	126.40
8	p	201	HEM	C3B-CAB-CBB	-6.80	112.73	126.40
8	n	201	HEM	C3B-CAB-CBB	-6.73	112.87	126.40
8	j	201	HEM	C3B-CAB-CBB	-6.71	112.91	126.40
8	S	201	HEM	C3B-CAB-CBB	-6.70	112.92	126.40
8	J	201	HEM	C3B-CAB-CBB	-6.64	113.05	126.40
8	D	201	HEM	C3B-CAB-CBB	-6.62	113.08	126.40
8	Y	201	HEM	C3B-CAB-CBB	-6.62	113.10	126.40
8	h	201	HEM	C3B-CAB-CBB	-6.60	113.13	126.40
8	R	201	HEM	C3C-CAC-CBC	-6.45	113.43	126.40
8	C	201	HEM	C3C-CAC-CBC	-6.30	113.72	126.40
8	l	201	HEM	C3B-CAB-CBB	-6.11	114.12	126.40
8	U	201	HEM	C3B-CAB-CBB	-6.08	114.16	126.40
8	Q	201	HEM	C3B-CAB-CBB	-6.03	114.27	126.40
8	F	201	HEM	C3B-CAB-CBB	-6.03	114.27	126.40
8	H	201	HEM	C3B-CAB-CBB	-6.01	114.31	126.40
12	s	303	NAG	C2-N2-C7	-4.20	117.64	123.11
8	G	201	HEM	CAA-CBA-CGA	-3.86	105.27	112.78
8	p	201	HEM	CAD-CBD-CGD	-3.84	105.30	112.78
12	O	304	NAG	C2-N2-C7	-3.65	118.36	123.11
8	R	201	HEM	CAA-CBA-CGA	-3.64	105.70	112.78
8	l	201	HEM	CBA-CAA-C2A	-3.44	106.44	112.49
8	W	201	HEM	CAD-CBD-CGD	-3.18	106.60	112.78
12	O	304	NAG	C4-C3-C2	-3.08	106.56	111.34
12	d	304	NAG	C2-N2-C7	-3.06	119.12	123.11
8	a	201	HEM	CBA-CAA-C2A	-3.05	107.13	112.49
8	G	201	HEM	CAD-CBD-CGD	-3.01	106.93	112.78
8	f	201	HEM	CAD-CBD-CGD	-2.92	107.09	112.78
8	k	201	HEM	CAA-CBA-CGA	-2.89	107.17	112.78
8	K	201	HEM	CAD-CBD-CGD	-2.84	107.26	112.78
8	j	201	HEM	CAD-CBD-CGD	-2.79	107.36	112.78
8	F	201	HEM	CBA-CAA-C2A	-2.76	107.63	112.49
8	m	201	HEM	CAD-C3D-C2D	-2.75	121.14	129.00
8	e	201	HEM	CAD-CBD-CGD	-2.73	107.46	112.78
8	K	201	HEM	CAA-CBA-CGA	-2.71	107.50	112.78
8	Q	201	HEM	CAA-CBA-CGA	-2.69	107.56	112.78
8	p	201	HEM	C3C-C4C-NC	-2.66	105.93	110.94
8	W	201	HEM	C3C-C4C-NC	-2.65	105.94	110.94
8	g	201	HEM	CAA-CBA-CGA	-2.65	107.63	112.78
8	E	201	HEM	CAD-CBD-CGD	-2.65	107.63	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	201	HEM	C3C-C4C-NC	-2.65	105.95	110.94
8	U	201	HEM	C3C-C4C-NC	-2.64	105.95	110.94
8	S	201	HEM	C3C-C4C-NC	-2.64	105.96	110.94
8	D	201	HEM	CBA-CAA-C2A	-2.62	107.89	112.49
8	Q	201	HEM	CAD-CBD-CGD	-2.60	107.73	112.78
8	L	201	HEM	C3C-C4C-NC	-2.60	106.04	110.94
8	e	201	HEM	CBA-CAA-C2A	-2.59	107.93	112.49
8	L	201	HEM	CAD-CBD-CGD	-2.58	107.76	112.78
8	B	201	HEM	CBA-CAA-C2A	-2.57	107.98	112.49
8	D	201	HEM	C3C-C4C-NC	-2.54	106.16	110.94
8	B	201	HEM	CAD-CBD-CGD	-2.52	107.88	112.78
8	A	201	HEM	CAD-CBD-CGD	-2.51	107.89	112.78
8	F	201	HEM	CAD-CBD-CGD	-2.51	107.89	112.78
8	a	201	HEM	CAD-CBD-CGD	-2.49	107.93	112.78
8	h	201	HEM	C3C-C4C-NC	-2.47	106.27	110.94
8	T	201	HEM	CAA-CBA-CGA	-2.47	107.98	112.78
8	J	201	HEM	C3C-C4C-NC	-2.47	106.29	110.94
8	C	201	HEM	CAD-CBD-CGD	-2.46	107.99	112.78
8	n	201	HEM	C3C-C4C-NC	-2.46	106.30	110.94
8	a	201	HEM	C3C-C4C-NC	-2.45	106.32	110.94
8	Q	201	HEM	C3C-C4C-NC	-2.43	106.36	110.94
8	H	201	HEM	C3C-C4C-NC	-2.40	106.42	110.94
8	X	201	HEM	CAD-C3D-C2D	-2.38	122.20	129.00
8	E	201	HEM	CBD-CAD-C3D	-2.38	108.29	112.47
8	n	201	HEM	CAD-CBD-CGD	-2.37	108.16	112.78
8	F	201	HEM	C3C-C4C-NC	-2.37	106.47	110.94
8	C	201	HEM	CAA-CBA-CGA	-2.36	108.18	112.78
8	R	201	HEM	CAD-CBD-CGD	-2.35	108.21	112.78
8	i	201	HEM	CAA-CBA-CGA	-2.34	108.24	112.78
8	B	201	HEM	C3C-C4C-NC	-2.32	106.56	110.94
8	j	201	HEM	C3C-C4C-NC	-2.32	106.57	110.94
8	o	201	HEM	C3C-C4C-NC	-2.32	106.57	110.94
8	U	201	HEM	CAD-CBD-CGD	-2.29	108.33	112.78
8	H	201	HEM	CAD-CBD-CGD	-2.28	108.35	112.78
8	S	201	HEM	CAD-CBD-CGD	-2.26	108.38	112.78
8	e	201	HEM	C3C-C4C-NC	-2.26	106.68	110.94
8	Y	201	HEM	C3C-C4C-NC	-2.25	106.70	110.94
8	P	201	HEM	C3C-C4C-NC	-2.25	106.70	110.94
8	X	201	HEM	CAD-CBD-CGD	-2.21	108.49	112.78
8	A	201	HEM	C3C-C4C-NC	-2.20	106.79	110.94
8	I	201	HEM	C3B-C4B-NB	-2.17	106.41	109.21
8	D	201	HEM	CAD-CBD-CGD	-2.16	108.57	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	o	201	HEM	CAA-CBA-CGA	-2.16	108.58	112.78
8	V	201	HEM	CAA-CBA-CGA	-2.14	108.61	112.78
8	i	201	HEM	C3C-C4C-NC	-2.13	106.92	110.94
8	f	201	HEM	C3C-C4C-NC	-2.12	106.94	110.94
8	e	201	HEM	C3B-C4B-NB	-2.12	106.47	109.21
8	T	201	HEM	C3C-C4C-NC	-2.12	106.94	110.94
8	J	201	HEM	CAD-CBD-CGD	-2.11	108.67	112.78
8	o	201	HEM	CBD-CAD-C3D	-2.09	108.81	112.47
8	I	201	HEM	CMA-C3A-C4A	-2.08	124.78	128.31
8	V	201	HEM	C3C-C4C-NC	-2.06	107.06	110.94
8	m	201	HEM	C3C-C4C-NC	-2.04	107.08	110.94
8	m	201	HEM	CBA-CAA-C2A	-2.04	108.90	112.49
8	G	201	HEM	C3C-C4C-NC	-2.04	107.09	110.94
8	R	201	HEM	CAA-C2A-C3A	-2.04	123.19	129.00
8	I	201	HEM	CAD-CBD-CGD	-2.03	108.83	112.78
8	P	201	HEM	C3B-C4B-NB	-2.03	106.59	109.21
8	m	201	HEM	CMA-C3A-C4A	-2.03	124.86	128.31
8	Z	201	HEM	C3C-C4C-NC	-2.03	107.12	110.94
8	j	201	HEM	CBA-CAA-C2A	-2.02	108.93	112.49
8	C	201	HEM	C3C-C4C-NC	-2.02	107.12	110.94
8	Z	201	HEM	CAD-CBD-CGD	-2.02	108.86	112.78
8	X	201	HEM	C3C-C4C-NC	-2.01	107.14	110.94
8	m	201	HEM	CBD-CAD-C3D	2.15	116.25	112.47
12	s	303	NAG	C1-O5-C5	2.32	115.55	112.14
8	p	201	HEM	CBD-CAD-C3D	2.34	116.58	112.47
8	l	201	HEM	CBD-CAD-C3D	2.39	116.66	112.47
12	O	304	NAG	O5-C5-C4	2.55	114.36	110.13
8	S	201	HEM	CBD-CAD-C3D	2.88	117.52	112.47
12	d	304	NAG	C1-O5-C5	3.03	116.60	112.14
8	X	201	HEM	CBD-CAD-C3D	3.13	117.97	112.47
12	O	304	NAG	C1-O5-C5	4.46	118.70	112.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	X	201	HEM	C2D-C3D-CAD-CBD
8	X	201	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

26 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	201	HEM	1	0
8	B	201	HEM	8	0
9	B	202	CYN	1	0
8	C	201	HEM	1	0
8	D	201	HEM	2	0
8	E	201	HEM	6	0
8	F	201	HEM	8	0
9	F	202	CYN	2	0
8	G	201	HEM	1	0
8	H	201	HEM	4	0
8	I	201	HEM	6	0
8	J	201	HEM	8	0
9	J	202	CYN	1	0
8	K	201	HEM	2	0
8	L	201	HEM	3	0
8	P	201	HEM	3	0
8	Q	201	HEM	7	0
9	Q	202	CYN	1	0
8	R	201	HEM	2	0
8	S	201	HEM	4	0
8	T	201	HEM	2	0
8	U	201	HEM	9	0
9	U	202	CYN	1	0
8	W	201	HEM	3	0
8	X	201	HEM	4	0
8	Y	201	HEM	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	148/150 (98%)	0.01	2 (1%) 78 65	11, 32, 58, 80	0
1	E	148/150 (98%)	0.02	1 (0%) 89 83	7, 28, 55, 74	0
1	I	148/150 (98%)	-0.16	1 (0%) 89 83	6, 24, 54, 70	0
1	P	148/150 (98%)	0.11	4 (2%) 58 44	8, 34, 63, 78	0
1	T	148/150 (98%)	-0.10	1 (0%) 89 83	8, 25, 50, 68	0
1	X	148/150 (98%)	-0.25	0 100 100	6, 26, 55, 67	0
1	e	148/150 (98%)	0.16	4 (2%) 58 44	13, 40, 69, 84	0
1	i	148/150 (98%)	-0.15	0 100 100	8, 30, 55, 70	0
1	m	148/150 (98%)	-0.05	0 100 100	8, 25, 52, 73	0
2	B	142/142 (100%)	-0.03	3 (2%) 67 52	9, 23, 59, 88	0
2	F	142/142 (100%)	-0.27	1 (0%) 89 83	7, 22, 54, 106	0
2	J	142/142 (100%)	-0.06	3 (2%) 67 52	6, 24, 62, 98	0
2	Q	142/142 (100%)	-0.07	1 (0%) 89 83	7, 22, 64, 86	0
2	U	142/142 (100%)	-0.35	1 (0%) 89 83	5, 23, 53, 94	0
2	Y	142/142 (100%)	-0.06	2 (1%) 78 65	10, 26, 58, 95	0
2	f	142/142 (100%)	-0.18	1 (0%) 89 83	5, 25, 63, 89	0
2	j	142/142 (100%)	-0.30	2 (1%) 78 65	6, 24, 53, 101	0
2	n	142/142 (100%)	-0.07	3 (2%) 67 52	6, 26, 58, 93	0
3	C	151/151 (100%)	-0.19	1 (0%) 89 83	8, 27, 59, 92	0
3	G	151/151 (100%)	-0.06	4 (2%) 59 45	9, 28, 66, 96	0
3	K	151/151 (100%)	-0.09	1 (0%) 89 83	8, 36, 62, 85	0
3	R	151/151 (100%)	-0.09	0 100 100	5, 27, 64, 88	0
3	V	151/151 (100%)	0.22	7 (4%) 36 23	8, 30, 71, 92	0
3	Z	151/151 (100%)	-0.13	2 (1%) 79 67	9, 35, 65, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	g	151/151 (100%)	-0.17	0 100 100	7, 28, 57, 88	0
3	k	151/151 (100%)	0.13	5 (3%) 50 35	11, 35, 72, 98	0
3	o	151/151 (100%)	0.00	2 (1%) 79 67	10, 37, 70, 82	0
4	D	141/141 (100%)	-0.07	2 (1%) 78 65	6, 30, 61, 80	0
4	H	141/141 (100%)	-0.26	1 (0%) 89 83	10, 24, 57, 81	0
4	L	141/141 (100%)	-0.17	1 (0%) 89 83	8, 26, 55, 83	0
4	S	141/141 (100%)	-0.06	1 (0%) 89 83	13, 32, 62, 79	0
4	W	141/141 (100%)	-0.24	1 (0%) 89 83	8, 30, 55, 79	0
4	a	141/141 (100%)	0.13	0 100 100	10, 33, 57, 82	0
4	h	141/141 (100%)	-0.12	1 (0%) 89 83	10, 35, 69, 89	0
4	l	141/141 (100%)	-0.17	0 100 100	10, 31, 61, 84	0
4	p	141/141 (100%)	-0.13	0 100 100	13, 29, 63, 77	0
5	M	222/224 (99%)	0.13	1 (0%) 91 87	6, 25, 65, 88	0
5	b	222/224 (99%)	0.10	1 (0%) 91 87	7, 25, 67, 89	0
5	q	222/224 (99%)	0.06	2 (0%) 85 78	7, 24, 70, 84	0
6	N	219/236 (92%)	0.08	2 (0%) 85 78	5, 23, 59, 88	0
6	c	219/236 (92%)	0.10	1 (0%) 91 87	5, 24, 56, 87	0
6	r	219/236 (92%)	0.01	1 (0%) 91 87	4, 24, 59, 90	0
7	O	213/218 (97%)	-0.01	1 (0%) 91 87	6, 24, 49, 84	0
7	d	213/218 (97%)	0.09	0 100 100	4, 25, 55, 89	0
7	s	213/218 (97%)	-0.07	1 (0%) 91 87	6, 23, 55, 85	0
All	All	7200/7290 (98%)	-0.05	69 (0%) 84 75	4, 27, 62, 106	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	1	HIS	6.7
3	G	1	HIS	5.7
3	V	2	GLN	5.4
1	e	150	HIS	5.4
2	Q	1	SER	4.6
4	S	141	GLY	4.5
3	k	2	GLN	4.4
3	V	3	PHE	4.4
2	Y	99	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
3	G	2	GLN	4.0
1	P	150	HIS	4.0
1	E	150	HIS	3.9
3	k	1	HIS	3.9
3	V	150	GLN	3.8
2	F	23	HIS	3.6
3	k	3	PHE	3.6
4	W	141	GLY	3.6
2	f	1	SER	3.5
3	G	3	PHE	3.5
1	T	150	HIS	3.4
4	H	141	GLY	3.3
2	B	1	SER	3.2
6	N	235	HIS	3.1
3	V	151	GLY	3.0
3	k	150	GLN	3.0
3	C	1	HIS	2.9
4	L	141	GLY	2.9
6	c	235	HIS	2.9
2	J	99	HIS	2.9
3	Z	151	GLY	2.8
2	j	23	HIS	2.8
5	M	7	ASP	2.8
5	b	7	ASP	2.8
1	e	44	TYR	2.7
5	q	4	THR	2.7
3	Z	150	GLN	2.6
1	A	150	HIS	2.6
2	n	23	HIS	2.6
2	j	1	SER	2.6
4	D	98	SER	2.5
3	k	53	ASN	2.5
2	J	23	HIS	2.5
1	A	127	CYS	2.4
1	P	127	CYS	2.4
4	D	141	GLY	2.4
1	e	42	HIS	2.4
6	r	194	ASP	2.3
5	q	7	ASP	2.3
1	P	3	ASP	2.3
1	P	42	HIS	2.2
2	B	99	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	Y	23	HIS	2.2
3	o	43	LYS	2.2
2	J	1	SER	2.2
4	h	141	GLY	2.2
2	U	23	HIS	2.2
3	o	150	GLN	2.2
7	s	10	GLU	2.2
1	e	40	LEU	2.1
2	n	1	SER	2.1
2	B	96	GLU	2.1
3	V	50	GLU	2.1
3	V	105	GLY	2.1
7	O	7	HIS	2.1
1	I	150	HIS	2.0
3	K	150	GLN	2.0
6	N	233	GLN	2.0
3	G	150	GLN	2.0
2	n	99	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	CYN	h	202	2/2	0.99	0.31	1.87	28,28,28,28	0
8	HEM	I	201	43/43	0.97	0.27	1.67	28,28,28,28	0
8	HEM	T	201	43/43	0.95	0.25	1.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	HEM	W	201	43/43	0.97	0.23	1.03	28,28,28,28	0
8	HEM	E	201	43/43	0.96	0.30	1.02	28,28,28,28	0
8	HEM	m	201	43/43	0.96	0.26	1.00	28,28,28,28	0
8	HEM	U	201	43/43	0.97	0.23	0.91	28,28,28,28	0
8	HEM	j	201	43/43	0.97	0.24	0.83	28,28,28,28	0
8	HEM	L	201	43/43	0.96	0.25	0.79	28,28,28,28	0
8	HEM	A	201	43/43	0.97	0.27	0.70	28,28,28,28	0
8	HEM	a	201	43/43	0.96	0.31	0.67	28,28,28,28	0
8	HEM	F	201	43/43	0.97	0.23	0.60	28,28,28,28	0
8	HEM	X	201	43/43	0.96	0.25	0.58	28,28,28,28	0
8	HEM	H	201	43/43	0.97	0.21	0.57	28,28,28,28	0
8	HEM	p	201	43/43	0.96	0.24	0.54	28,28,28,28	0
8	HEM	g	201	43/43	0.96	0.24	0.54	28,28,28,28	0
8	HEM	h	201	43/43	0.97	0.26	0.45	28,28,28,28	0
8	HEM	f	201	43/43	0.96	0.24	0.40	28,28,28,28	0
8	HEM	k	201	43/43	0.95	0.29	0.37	28,28,28,28	0
8	HEM	i	201	43/43	0.95	0.23	0.35	28,28,28,28	0
8	HEM	V	201	43/43	0.94	0.28	0.32	28,28,28,28	0
9	CYN	l	202	2/2	0.98	0.23	0.30	28,28,28,28	0
8	HEM	C	201	43/43	0.97	0.23	0.28	28,28,28,28	0
8	HEM	n	201	43/43	0.95	0.27	0.27	28,28,28,28	0
8	HEM	R	201	43/43	0.96	0.26	0.27	28,28,28,28	0
8	HEM	J	201	43/43	0.95	0.25	0.26	28,28,28,28	0
8	HEM	l	201	43/43	0.96	0.25	0.22	28,28,28,28	0
8	HEM	B	201	43/43	0.97	0.26	0.18	28,28,28,28	0
8	HEM	Q	201	43/43	0.96	0.24	0.09	28,28,28,28	0
8	HEM	S	201	43/43	0.96	0.25	0.08	28,28,28,28	0
8	HEM	e	201	43/43	0.90	0.27	0.07	28,28,28,28	0
8	HEM	Y	201	43/43	0.96	0.26	0.03	28,28,28,28	0
9	CYN	L	202	2/2	0.99	0.21	0.02	28,28,28,28	0
9	CYN	H	202	2/2	0.99	0.20	0.02	28,28,28,28	0
9	CYN	W	202	2/2	0.98	0.21	-0.08	28,28,28,28	0
8	HEM	K	201	43/43	0.96	0.21	-0.10	28,28,28,28	0
9	CYN	j	202	2/2	0.98	0.19	-0.11	28,28,28,28	0
8	HEM	D	201	43/43	0.97	0.26	-0.12	28,28,28,28	0
8	HEM	P	201	43/43	0.96	0.22	-0.17	28,28,28,28	0
8	HEM	G	201	43/43	0.97	0.21	-0.18	28,28,28,28	0
8	HEM	o	201	43/43	0.97	0.23	-0.20	28,28,28,28	0
8	HEM	Z	201	43/43	0.96	0.22	-0.24	28,28,28,28	0
9	CYN	F	202	2/2	0.98	0.20	-0.29	28,28,28,28	0
9	CYN	S	202	2/2	0.99	0.26	-0.60	28,28,28,28	0
9	CYN	U	202	2/2	0.98	0.17	-0.69	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	CYN	J	202	2/2	0.99	0.18	-0.88	28,28,28,28	0
9	CYN	n	202	2/2	0.99	0.16	-1.25	28,28,28,28	0
9	CYN	f	202	2/2	0.99	0.18	-1.35	28,28,28,28	0
9	CYN	D	202	2/2	0.99	0.18	-1.45	28,28,28,28	0
9	CYN	p	202	2/2	0.99	0.15	-1.56	28,28,28,28	0
10	CA	d	301	1/1	0.97	0.10	-1.62	28,28,28,28	0
9	CYN	Y	202	2/2	0.98	0.21	-1.62	28,28,28,28	0
10	CA	s	301	1/1	0.99	0.09	-1.86	28,28,28,28	0
10	CA	N	301	1/1	0.98	0.11	-2.07	28,28,28,28	0
10	CA	r	301	1/1	0.99	0.09	-2.22	28,28,28,28	0
9	CYN	a	202	2/2	0.99	0.14	-2.27	28,28,28,28	0
10	CA	q	301	1/1	0.98	0.07	-2.49	28,28,28,28	0
10	CA	M	301	1/1	0.98	0.08	-2.52	28,28,28,28	0
10	CA	c	301	1/1	0.99	0.08	-2.62	28,28,28,28	0
10	CA	b	301	1/1	0.98	0.08	-2.64	28,28,28,28	0
10	CA	O	301	1/1	0.98	0.06	-2.76	28,28,28,28	0
11	ZN	c	302	1/1	0.99	0.07	-2.87	28,28,28,28	0
11	ZN	d	303	1/1	0.98	0.05	-3.04	28,28,28,28	0
9	CYN	B	202	2/2	0.99	0.17	-3.11	28,28,28,28	0
11	ZN	O	303	1/1	0.99	0.08	-3.17	28,28,28,28	0
9	CYN	Q	202	2/2	1.00	0.12	-3.77	28,28,28,28	0
9	CYN	o	202	2/2	0.99	0.11	-	28,28,28,28	0
12	NAG	s	303	14/15	0.86	0.30	-	28,28,28,28	0
9	CYN	G	202	2/2	0.98	0.17	-	28,28,28,28	0
11	ZN	d	302	1/1	0.80	0.25	-	28,28,28,28	0
12	NAG	d	304	14/15	0.89	0.41	-	28,28,28,28	0
9	CYN	k	202	2/2	0.99	0.11	-	28,28,28,28	0
9	CYN	E	202	2/2	0.98	0.18	-	28,28,28,28	0
9	CYN	K	202	2/2	0.99	0.17	-	28,28,28,28	0
9	CYN	i	202	2/2	0.98	0.17	-	28,28,28,28	0
9	CYN	g	202	2/2	0.99	0.26	-	28,28,28,28	0
9	CYN	C	202	2/2	0.96	0.32	-	28,28,28,28	0
9	CYN	A	202	2/2	0.99	0.22	-	28,28,28,28	0
9	CYN	V	202	2/2	0.99	0.15	-	28,28,28,28	0
11	ZN	s	302	1/1	0.89	0.25	-	28,28,28,28	0
9	CYN	P	202	2/2	0.98	0.25	-	28,28,28,28	0
9	CYN	X	202	2/2	0.99	0.23	-	28,28,28,28	0
9	CYN	e	202	2/2	0.99	0.18	-	28,28,28,28	0
9	CYN	Z	202	2/2	0.98	0.18	-	28,28,28,28	0
9	CYN	I	202	2/2	0.99	0.19	-	28,28,28,28	0
11	ZN	O	302	1/1	0.91	0.30	-	28,28,28,28	0
12	NAG	O	304	14/15	0.88	0.34	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	CYN	T	202	2/2	0.98	0.18	-	28,28,28,28	0
9	CYN	R	202	2/2	0.97	0.32	-	28,28,28,28	0
9	CYN	m	202	2/2	0.99	0.18	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.