



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:28 am GMT

PDB ID : 1N8J  
Title : Crystal Structure of AhpC with Active Site Cysteine mutated to Serine (C46S)  
Authors : Wood, Z.A.; Poole, L.B.; Karplus, P.A.  
Deposited on : 2002-11-20  
Resolution : 2.17 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

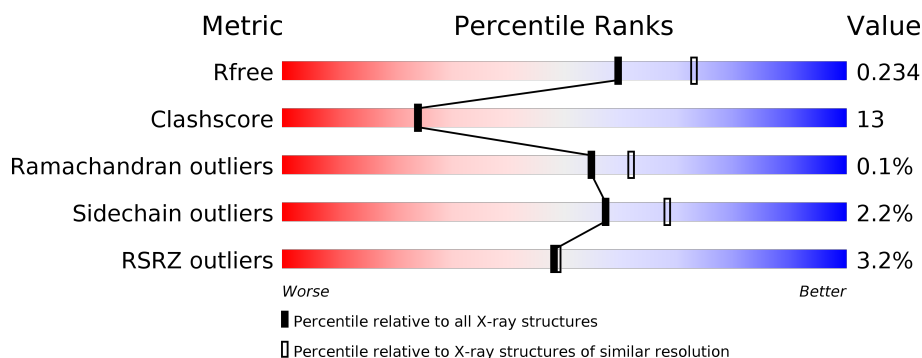
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	186	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div> </div>
1	B	186	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>28%</div> <div>.</div> </div> </div>
1	C	186	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>27%</div> <div>.</div> </div> </div>
1	D	186	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>
1	E	186	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
1	F	186	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>22%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	186	 3% 82% 18% •
1	H	186	 % 81% 18% •
1	I	186	 4% 77% 20% •
1	J	186	 3% 79% 21% •
1	K	186	 78% 22% •
1	L	186	 2% 76% 23% •
1	M	186	 4% 71% 28% •
1	N	186	 5% 73% 26% •
1	O	186	 % 78% 22% •
1	P	186	 2% 81% 18% •
1	Q	186	 % 83% 16% •
1	R	186	 % 78% 20% •
1	S	186	 8% 67% 33% •
1	T	186	 7% 66% 33% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30710 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 Alkyl hydroperoxide reductase C22 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	B	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	C	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	D	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	E	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	F	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	G	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	H	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	I	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	J	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	K	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	L	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	M	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	N	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	O	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	P	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	R	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	S	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			
1	T	186	Total	C	N	O	S	0	0	0
			1456	928	241	284	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	SER	CYS	ENGINEERED	UNP P0A251
B	46	SER	CYS	ENGINEERED	UNP P0A251
C	46	SER	CYS	ENGINEERED	UNP P0A251
D	46	SER	CYS	ENGINEERED	UNP P0A251
E	46	SER	CYS	ENGINEERED	UNP P0A251
F	46	SER	CYS	ENGINEERED	UNP P0A251
G	46	SER	CYS	ENGINEERED	UNP P0A251
H	46	SER	CYS	ENGINEERED	UNP P0A251
I	46	SER	CYS	ENGINEERED	UNP P0A251
J	46	SER	CYS	ENGINEERED	UNP P0A251
K	46	SER	CYS	ENGINEERED	UNP P0A251
L	46	SER	CYS	ENGINEERED	UNP P0A251
M	46	SER	CYS	ENGINEERED	UNP P0A251
N	46	SER	CYS	ENGINEERED	UNP P0A251
O	46	SER	CYS	ENGINEERED	UNP P0A251
P	46	SER	CYS	ENGINEERED	UNP P0A251
Q	46	SER	CYS	ENGINEERED	UNP P0A251
R	46	SER	CYS	ENGINEERED	UNP P0A251
S	46	SER	CYS	ENGINEERED	UNP P0A251
T	46	SER	CYS	ENGINEERED	UNP P0A251

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	77	Total	O	0	0
			77	77		
2	B	71	Total	O	0	0
			71	71		
2	C	58	Total	O	0	0
			58	58		

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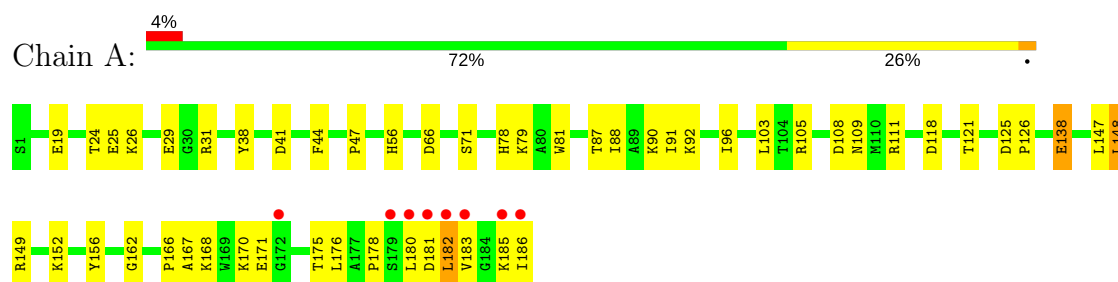
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	56	Total 56	O 56	0	0
2	E	77	Total 77	O 77	0	0
2	F	82	Total 82	O 82	0	0
2	G	94	Total 94	O 94	0	0
2	H	92	Total 92	O 92	0	0
2	I	72	Total 72	O 72	0	0
2	J	86	Total 86	O 86	0	0
2	K	106	Total 106	O 106	0	0
2	L	105	Total 105	O 105	0	0
2	M	49	Total 49	O 49	0	0
2	N	58	Total 58	O 58	0	0
2	O	95	Total 95	O 95	0	0
2	P	116	Total 116	O 116	0	0
2	Q	104	Total 104	O 104	0	0
2	R	93	Total 93	O 93	0	0
2	S	52	Total 52	O 52	0	0
2	T	47	Total 47	O 47	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

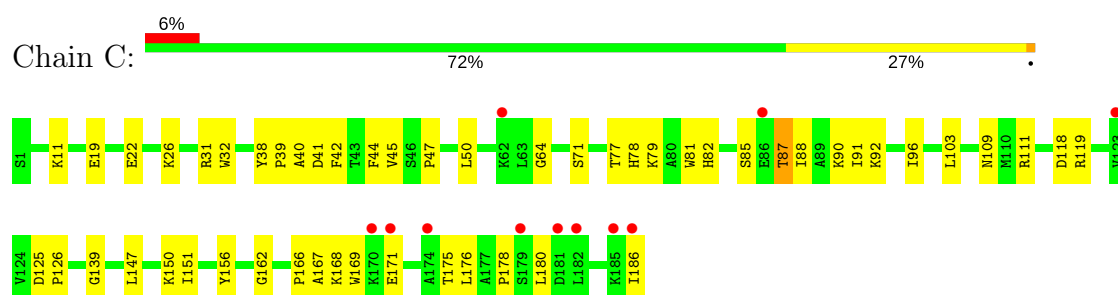
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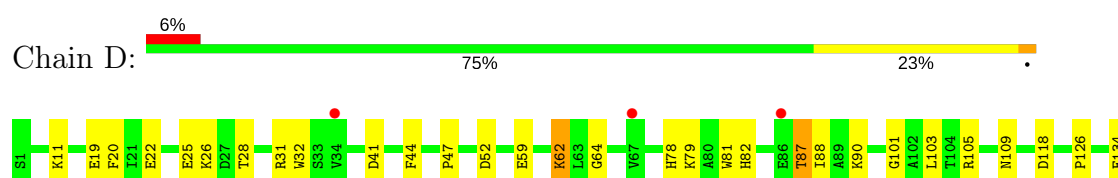
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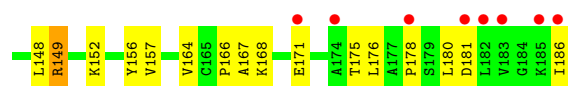


- Molecule 1: Alkyl hydroperoxide reductase C22 protein

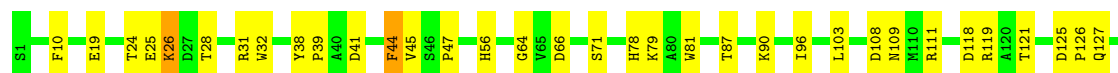
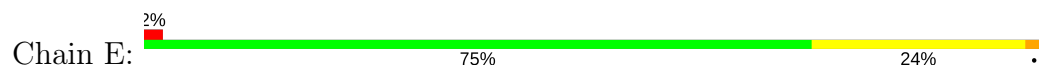


- Molecule 1: Alkyl hydroperoxide reductase C22 protein

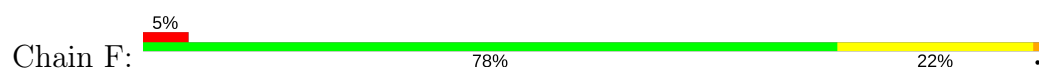




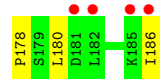
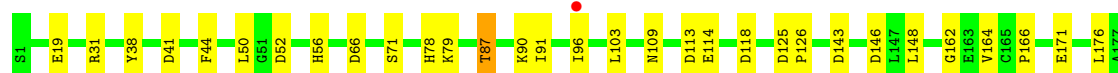
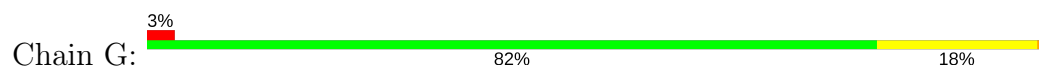
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



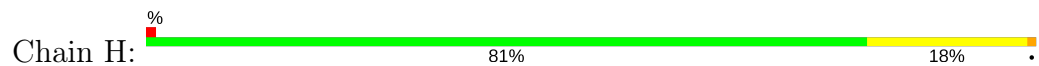
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



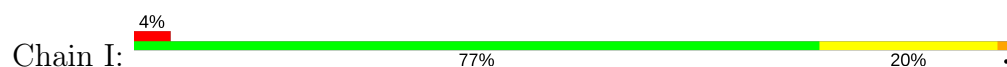
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



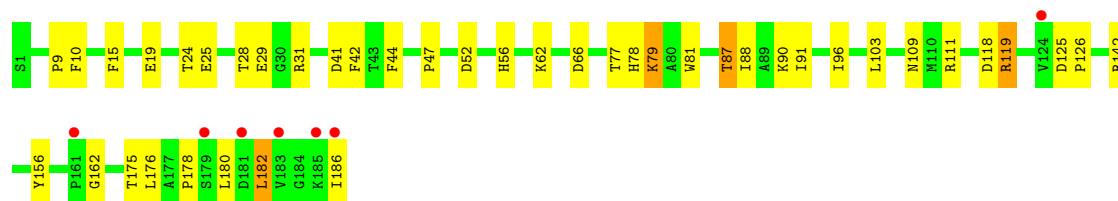
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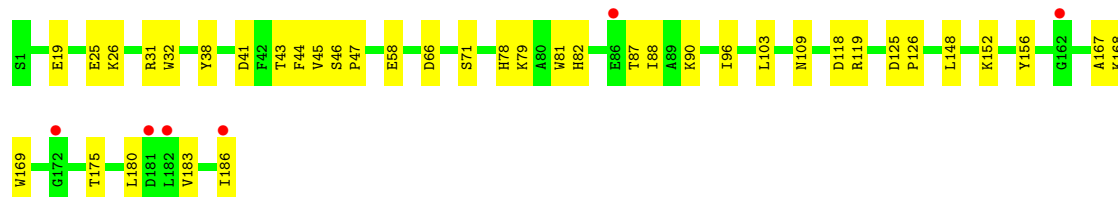
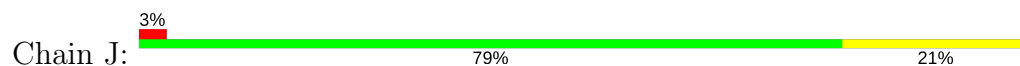
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



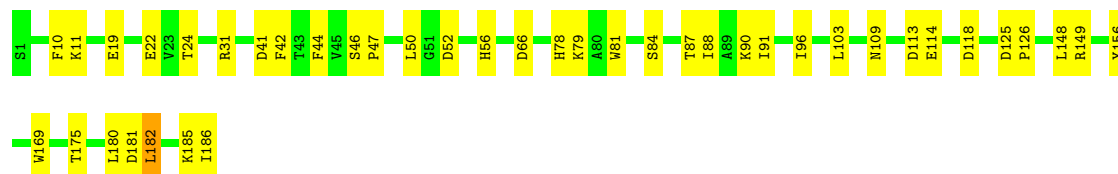
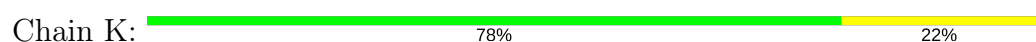




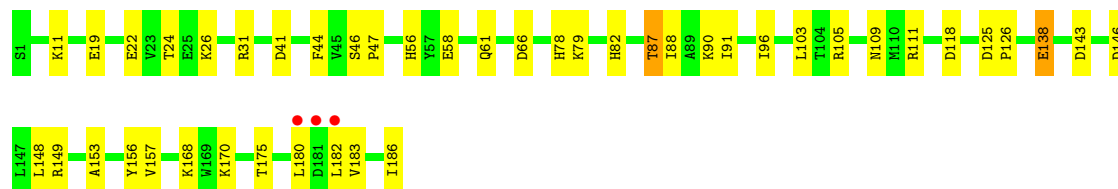
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



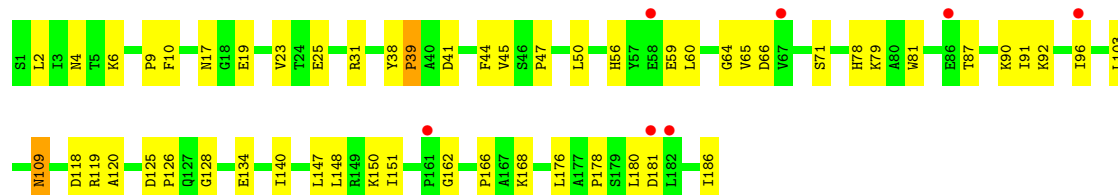
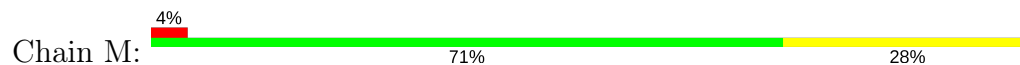
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



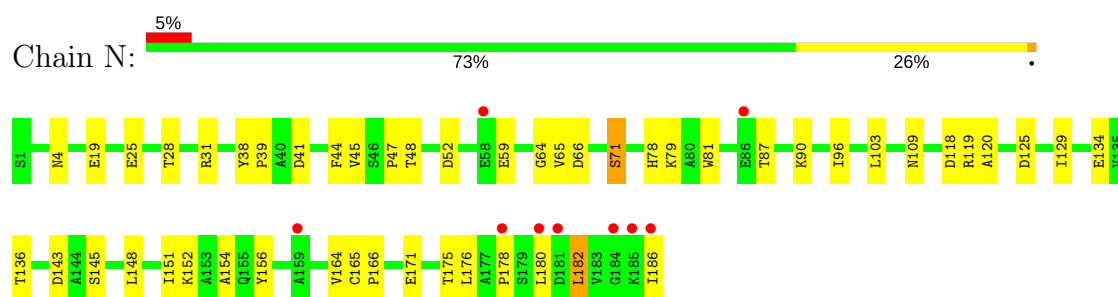
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



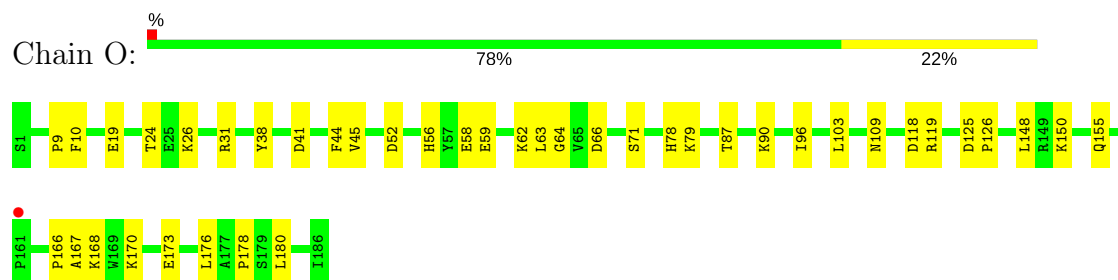
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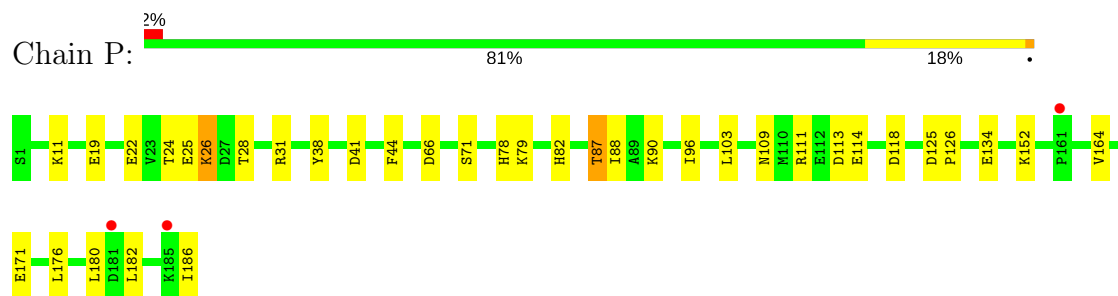
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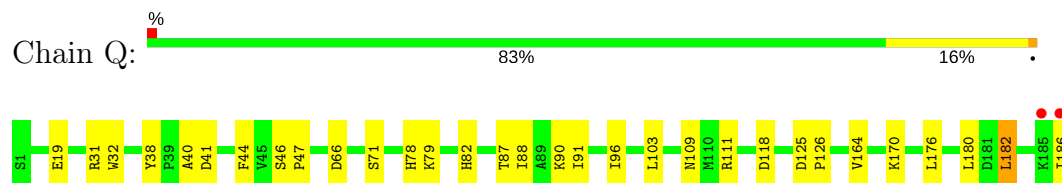
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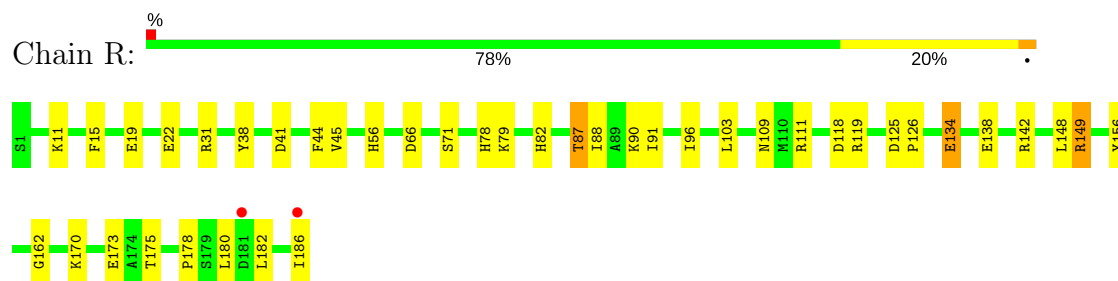
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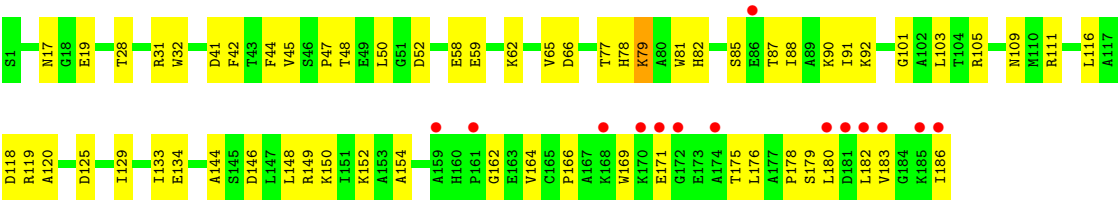


- Molecule 1: Alkyl hydroperoxide reductase C22 protein

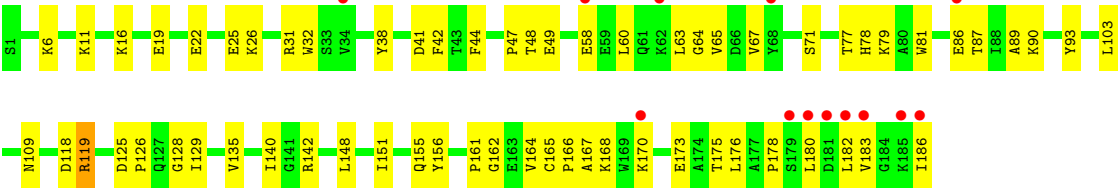


- Molecule 1: Alkyl hydroperoxide reductase C22 protein





● Molecule 1: Alkyl hydroperoxide reductase C22 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.08Å 107.33Å 120.08Å 102.43° 116.22° 98.81°	Depositor
Resolution (Å)	19.99 – 2.17 20.40 – 2.16	Depositor EDS
% Data completeness (in resolution range)	89.3 (19.99-2.17) 82.0 (20.40-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.17Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.188 , 0.234 0.187 , 0.234	Depositor DCC
$R_{free}$ test set	9671 reflections (4.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	30710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/1490	0.61	0/2019
1	B	0.38	0/1490	0.60	0/2019
1	C	0.35	0/1490	0.57	0/2019
1	D	0.34	0/1490	0.58	0/2019
1	E	0.38	0/1490	0.62	0/2019
1	F	0.40	0/1490	0.63	0/2019
1	G	0.43	0/1490	0.64	0/2019
1	H	0.40	0/1490	0.64	0/2019
1	I	0.40	0/1490	0.60	0/2019
1	J	0.38	0/1490	0.60	0/2019
1	K	0.42	0/1490	0.63	0/2019
1	L	0.43	0/1490	0.63	0/2019
1	M	0.35	0/1490	0.57	0/2019
1	N	0.35	0/1490	0.57	0/2019
1	O	0.42	0/1490	0.63	0/2019
1	P	0.43	0/1490	0.64	0/2019
1	Q	0.41	0/1490	0.63	0/2019
1	R	0.42	0/1490	0.63	0/2019
1	S	0.36	0/1490	0.57	0/2019
1	T	0.34	0/1490	0.56	0/2019
All	All	0.39	0/29800	0.61	0/40380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1456	0	1418	43	0
1	B	1456	0	1418	50	0
1	C	1456	0	1418	47	0
1	D	1456	0	1418	37	0
1	E	1456	0	1418	46	0
1	F	1456	0	1418	40	0
1	G	1456	0	1418	31	0
1	H	1456	0	1418	30	0
1	I	1456	0	1418	36	0
1	J	1456	0	1418	36	0
1	K	1456	0	1418	39	0
1	L	1456	0	1418	42	0
1	M	1456	0	1418	53	0
1	N	1456	0	1418	42	0
1	O	1456	0	1418	36	0
1	P	1456	0	1418	33	0
1	Q	1456	0	1418	36	0
1	R	1456	0	1418	36	0
1	S	1456	0	1418	66	0
1	T	1456	0	1418	70	0
2	A	77	0	0	3	0
2	B	71	0	0	3	0
2	C	58	0	0	4	0
2	D	56	0	0	2	0
2	E	77	0	0	4	0
2	F	82	0	0	2	0
2	G	94	0	0	0	0
2	H	92	0	0	0	0
2	I	72	0	0	2	0
2	J	86	0	0	0	0
2	K	106	0	0	0	0
2	L	105	0	0	6	0
2	M	49	0	0	2	0
2	N	58	0	0	2	0
2	O	95	0	0	1	0
2	P	116	0	0	3	0
2	Q	104	0	0	2	0
2	R	93	0	0	4	0
2	S	52	0	0	4	0
2	T	47	0	0	2	0
All	All	30710	0	28360	720	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (720) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:O	1:J:79:LYS:HE3	1.66	0.96
1:S:109:ASN:HD21	1:S:118:ASP:HB2	1.32	0.94
1:B:180:LEU:O	1:D:79:LYS:HE2	1.69	0.92
1:Q:79:LYS:HE2	1:T:180:LEU:O	1.71	0.91
1:T:109:ASN:HD21	1:T:118:ASP:HB2	1.38	0.89
1:K:79:LYS:HE2	1:M:180:LEU:O	1.74	0.88
1:B:19:GLU:HA	1:F:180:LEU:HD11	1.56	0.86
1:D:87:THR:O	1:D:90:LYS:HG2	1.77	0.84
1:L:149:ARG:HD2	2:L:704:HOH:O	1.77	0.84
1:A:47:PRO:HG3	1:A:81:TRP:HZ2	1.43	0.84
1:A:79:LYS:HE2	1:C:180:LEU:O	1.79	0.83
1:M:47:PRO:HG3	1:M:81:TRP:CZ2	2.13	0.83
1:L:79:LYS:HE2	1:P:180:LEU:O	1.78	0.83
1:T:109:ASN:ND2	1:T:118:ASP:HB2	1.92	0.83
1:L:180:LEU:O	1:N:79:LYS:HE2	1.79	0.82
1:T:151:ILE:O	1:T:155:GLN:HG3	1.79	0.81
1:N:47:PRO:HG3	1:N:81:TRP:HZ2	1.45	0.81
1:M:47:PRO:HG3	1:M:81:TRP:HZ2	1.45	0.80
1:L:41:ASP:OD2	1:L:78:HIS:HD2	1.65	0.80
1:H:41:ASP:OD2	1:H:78:HIS:HD2	1.65	0.79
1:M:71:SER:HB2	2:M:1326:HOH:O	1.81	0.79
1:S:166:PRO:HB3	1:T:48:THR:HG21	1.63	0.79
1:M:109:ASN:HD21	1:M:118:ASP:HB2	1.48	0.79
1:B:180:LEU:HD13	1:D:19:GLU:HA	1.64	0.79
1:I:41:ASP:OD2	1:I:78:HIS:HD2	1.64	0.79
1:D:44:PHE:O	1:D:47:PRO:HD2	1.83	0.78
1:A:108:ASP:HB2	2:A:238:HOH:O	1.83	0.78
1:C:79:LYS:HE3	1:I:180:LEU:O	1.83	0.78
1:C:171:GLU:HG3	2:C:223:HOH:O	1.83	0.78
1:E:183:VAL:HB	1:H:79:LYS:HE3	1.66	0.78
1:S:109:ASN:ND2	1:S:118:ASP:HB2	1.99	0.78
1:S:87:THR:O	1:S:90:LYS:HG2	1.85	0.77
1:B:19:GLU:HA	1:F:180:LEU:CD1	2.14	0.77
1:P:109:ASN:ND2	1:P:118:ASP:HB2	1.99	0.77
1:F:109:ASN:HD21	1:F:118:ASP:HB2	1.50	0.77
1:K:47:PRO:HG3	1:K:81:TRP:HZ2	1.50	0.77
1:A:180:LEU:CD1	1:E:19:GLU:HA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASP:OD2	1:F:78:HIS:HD2	1.68	0.76
1:J:41:ASP:OD2	1:J:78:HIS:HD2	1.68	0.76
1:D:109:ASN:HD21	1:D:118:ASP:HB2	1.51	0.76
1:C:41:ASP:OD2	1:C:78:HIS:HD2	1.69	0.76
1:B:79:LYS:HE2	1:F:180:LEU:O	1.85	0.76
1:P:109:ASN:HD21	1:P:118:ASP:HB2	1.49	0.75
1:E:24:THR:OG1	1:E:26:LYS:HD3	1.86	0.75
1:A:180:LEU:O	1:E:79:LYS:HE2	1.86	0.75
1:E:180:LEU:O	1:H:79:LYS:HE2	1.87	0.75
1:R:41:ASP:OD2	1:R:78:HIS:HD2	1.70	0.75
1:M:45:VAL:HB	1:M:119:ARG:NH2	2.02	0.75
1:S:182:LEU:HD22	1:T:44:PHE:HD1	1.52	0.75
1:S:162:GLY:O	1:S:178:PRO:HD2	1.86	0.75
1:G:41:ASP:OD2	1:G:78:HIS:HD2	1.70	0.75
1:F:109:ASN:ND2	1:F:118:ASP:HB2	2.02	0.74
1:L:180:LEU:HD13	1:N:19:GLU:HA	1.69	0.74
1:K:19:GLU:HA	1:M:180:LEU:HD13	1.70	0.74
1:N:180:LEU:HD13	1:T:19:GLU:HA	1.69	0.74
1:A:87:THR:O	1:A:90:LYS:HG2	1.87	0.74
1:A:41:ASP:OD2	1:A:78:HIS:HD2	1.70	0.74
1:B:62:LYS:HD2	2:B:202:HOH:O	1.88	0.74
1:O:44:PHE:HD1	1:P:182:LEU:HD22	1.52	0.74
1:I:109:ASN:HD21	1:I:118:ASP:HB2	1.53	0.73
1:N:41:ASP:OD2	1:N:78:HIS:HD2	1.70	0.73
1:L:19:GLU:HA	1:P:180:LEU:HD13	1.70	0.73
1:C:162:GLY:O	1:C:178:PRO:HD2	1.88	0.73
1:P:41:ASP:OD2	1:P:78:HIS:HD2	1.72	0.73
1:Q:79:LYS:HD2	1:T:180:LEU:HG	1.71	0.73
1:L:143:ASP:HB3	1:L:146:ASP:OD2	1.89	0.73
1:T:31:ARG:NH2	1:T:64:GLY:HA2	2.03	0.73
1:E:47:PRO:HG3	1:E:81:TRP:HZ2	1.54	0.72
1:R:180:LEU:HD13	1:S:19:GLU:HA	1.71	0.72
1:A:47:PRO:HG3	1:A:81:TRP:CZ2	2.24	0.72
1:R:15:PHE:CE1	1:R:79:LYS:HG3	2.24	0.72
1:C:44:PHE:O	1:C:47:PRO:HD2	1.89	0.72
1:S:44:PHE:O	1:S:47:PRO:HD2	1.90	0.72
1:C:11:LYS:HE3	1:C:22:GLU:OE2	1.90	0.72
1:O:41:ASP:OD2	1:O:78:HIS:HD2	1.73	0.72
1:C:111:ARG:HD3	1:C:118:ASP:OD2	1.90	0.71
1:K:180:LEU:HD13	1:O:19:GLU:HA	1.72	0.71
1:A:44:PHE:O	1:A:47:PRO:HD2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:PHE:O	1:H:47:PRO:HD2	1.91	0.71
1:A:31:ARG:HD3	1:A:66:ASP:OD2	1.91	0.71
1:H:47:PRO:HG3	1:H:81:TRP:HZ2	1.54	0.71
1:Q:41:ASP:OD2	1:Q:78:HIS:HD2	1.74	0.71
1:M:44:PHE:HA	1:N:186:ILE:HD12	1.73	0.71
1:I:31:ARG:HD3	1:I:66:ASP:OD2	1.91	0.71
1:Q:19:GLU:HA	1:T:180:LEU:HD13	1.73	0.71
1:S:154:ALA:HA	1:T:140:ILE:HD11	1.73	0.70
1:I:109:ASN:ND2	1:I:118:ASP:HB2	2.05	0.70
1:I:87:THR:O	1:I:90:LYS:HG2	1.91	0.70
1:C:45:VAL:HB	1:C:119:ARG:NH2	2.06	0.70
1:K:109:ASN:ND2	1:K:118:ASP:HB2	2.06	0.70
1:M:19:GLU:HA	1:S:180:LEU:CD1	2.21	0.70
1:B:182:LEU:HD22	1:B:186:ILE:HG13	1.73	0.69
1:C:47:PRO:HG3	1:C:81:TRP:HZ2	1.56	0.69
1:F:47:PRO:HG3	1:F:81:TRP:HZ2	1.56	0.69
1:Q:31:ARG:HD3	1:Q:66:ASP:OD2	1.91	0.69
1:G:19:GLU:HA	1:J:180:LEU:HD13	1.75	0.69
1:S:47:PRO:HG3	1:S:81:TRP:HZ2	1.56	0.69
1:D:41:ASP:OD2	1:D:78:HIS:HD2	1.75	0.69
1:E:166:PRO:HG3	1:E:176:LEU:HG	1.75	0.69
1:M:19:GLU:HA	1:S:180:LEU:HD13	1.75	0.69
1:D:166:PRO:HG3	1:D:176:LEU:HG	1.73	0.68
1:S:82:HIS:HA	1:S:88:ILE:HG22	1.75	0.68
1:T:11:LYS:HE3	1:T:22:GLU:CD	2.14	0.68
1:E:41:ASP:OD2	1:E:78:HIS:HD2	1.75	0.68
1:T:44:PHE:O	1:T:47:PRO:HD2	1.93	0.68
1:F:79:LYS:HE2	1:G:180:LEU:O	1.94	0.68
1:G:31:ARG:HD3	1:G:66:ASP:OD2	1.92	0.68
1:M:109:ASN:ND2	1:M:118:ASP:HB2	2.09	0.68
1:B:41:ASP:OD2	1:B:78:HIS:HD2	1.76	0.68
1:K:31:ARG:HD3	1:K:66:ASP:OD2	1.93	0.68
1:G:109:ASN:ND2	1:G:118:ASP:HB2	2.09	0.68
1:I:119:ARG:HG2	1:I:142:ARG:NH2	2.09	0.68
1:P:19:GLU:HA	1:Q:180:LEU:HD13	1.75	0.67
1:S:182:LEU:O	1:S:182:LEU:HD23	1.94	0.67
1:E:87:THR:O	1:E:90:LYS:HG2	1.95	0.66
1:A:171:GLU:HG3	2:A:209:HOH:O	1.95	0.66
1:K:11:LYS:HE3	1:K:22:GLU:OE2	1.96	0.66
1:A:24:THR:OG1	1:A:26:LYS:HD3	1.96	0.66
1:G:79:LYS:HE3	1:J:180:LEU:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:GLU:HA	1:G:180:LEU:HD13	1.76	0.66
1:B:111:ARG:HD3	1:B:118:ASP:OD2	1.96	0.65
1:S:182:LEU:HD21	1:S:186:ILE:CD1	2.26	0.65
1:F:31:ARG:HD3	1:F:66:ASP:OD2	1.97	0.65
1:E:47:PRO:HG3	1:E:81:TRP:CZ2	2.30	0.65
1:F:87:THR:O	1:F:90:LYS:HG2	1.96	0.65
1:H:41:ASP:OD2	1:H:78:HIS:CD2	2.48	0.65
1:K:109:ASN:HD21	1:K:118:ASP:HB2	1.62	0.65
1:K:41:ASP:OD2	1:K:78:HIS:HD2	1.80	0.65
1:E:44:PHE:HD1	1:F:182:LEU:HD22	1.62	0.65
1:E:183:VAL:HB	1:H:79:LYS:CE	2.27	0.65
1:R:87:THR:O	1:R:90:LYS:HG2	1.95	0.65
1:H:180:LEU:HD13	1:I:19:GLU:HA	1.79	0.64
1:M:87:THR:O	1:M:90:LYS:HG2	1.97	0.64
1:P:182:LEU:O	1:P:182:LEU:HD23	1.97	0.64
1:S:79:LYS:HD3	1:S:79:LYS:C	2.17	0.64
1:D:180:LEU:HD13	1:J:19:GLU:HA	1.80	0.64
1:Q:87:THR:HG23	1:R:186:ILE:OXT	1.97	0.64
1:B:87:THR:O	1:B:90:LYS:HG2	1.98	0.64
1:C:19:GLU:HA	1:I:180:LEU:CD1	2.28	0.64
1:A:19:GLU:HA	1:C:180:LEU:HD13	1.80	0.64
1:B:31:ARG:NH2	1:B:64:GLY:HA2	2.13	0.63
1:D:109:ASN:ND2	1:D:118:ASP:HB2	2.12	0.63
1:I:162:GLY:O	1:I:178:PRO:HD2	1.98	0.63
1:P:31:ARG:HD3	1:P:66:ASP:OD2	1.97	0.63
1:R:11:LYS:HE3	1:R:22:GLU:OE1	1.98	0.63
1:E:56:HIS:ND1	1:E:148:LEU:HD11	2.13	0.63
1:K:44:PHE:HA	1:L:186:ILE:HD12	1.80	0.63
1:C:47:PRO:HG3	1:C:81:TRP:CZ2	2.32	0.63
1:J:109:ASN:HD21	1:J:118:ASP:HB2	1.64	0.63
1:D:156:TYR:CE2	1:D:175:THR:HG21	2.34	0.63
1:O:180:LEU:HD13	1:R:19:GLU:HA	1.81	0.62
1:Q:79:LYS:HE3	1:T:183:VAL:HB	1.81	0.62
1:K:113:ASP:OD1	1:K:114:GLU:HG3	1.98	0.62
1:C:166:PRO:HG3	1:C:176:LEU:HG	1.82	0.62
1:I:156:TYR:CE2	1:I:175:THR:HG21	2.35	0.62
1:L:109:ASN:HD21	1:L:118:ASP:HB2	1.64	0.62
1:T:166:PRO:HG3	1:T:176:LEU:HG	1.82	0.62
1:J:44:PHE:O	1:J:47:PRO:HD2	1.98	0.62
1:S:164:VAL:CG2	1:S:176:LEU:HB2	2.30	0.61
1:L:78:HIS:HE1	1:L:96:ILE:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:GLU:HA	1:M:180:LEU:CD1	2.30	0.61
1:O:109:ASN:HD21	1:O:118:ASP:HB2	1.65	0.61
1:S:169:TRP:NE1	1:S:175:THR:HG22	2.15	0.61
1:T:47:PRO:HG3	1:T:81:TRP:HZ2	1.66	0.61
1:O:109:ASN:ND2	1:O:118:ASP:HB2	2.16	0.61
1:A:180:LEU:HD13	1:E:19:GLU:HA	1.82	0.61
1:T:11:LYS:HE3	1:T:22:GLU:OE2	2.00	0.61
1:A:166:PRO:HG3	1:A:176:LEU:HG	1.83	0.61
1:T:164:VAL:HG23	1:T:176:LEU:HB2	1.82	0.61
1:C:82:HIS:HA	1:C:88:ILE:HG22	1.84	0.60
1:H:87:THR:O	1:H:90:LYS:HG2	2.00	0.60
1:J:109:ASN:ND2	1:J:118:ASP:HB2	2.16	0.60
1:A:170:LYS:HE3	2:B:215:HOH:O	2.01	0.60
1:K:50:LEU:HB3	1:K:91:ILE:HD11	1.83	0.60
1:A:156:TYR:CE2	1:A:175:THR:HG21	2.37	0.60
1:M:41:ASP:OD2	1:M:78:HIS:HD2	1.84	0.60
1:C:44:PHE:HA	1:D:186:ILE:HD12	1.84	0.60
1:N:31:ARG:NH2	1:N:64:GLY:HA2	2.16	0.60
1:G:109:ASN:HD21	1:G:118:ASP:HB2	1.66	0.60
1:J:78:HIS:HE1	1:J:96:ILE:O	1.85	0.60
1:O:31:ARG:NH2	1:O:64:GLY:HA2	2.16	0.59
1:A:180:LEU:HD11	1:E:19:GLU:HA	1.84	0.59
1:L:31:ARG:HD3	1:L:66:ASP:OD2	2.01	0.59
1:E:26:LYS:CD	1:E:26:LYS:H	2.15	0.59
1:D:47:PRO:HG3	1:D:81:TRP:HZ2	1.67	0.59
1:F:41:ASP:OD2	1:F:78:HIS:CD2	2.54	0.59
1:S:41:ASP:OD2	1:S:78:HIS:ND1	2.32	0.59
1:S:182:LEU:HD22	1:T:44:PHE:CD1	2.37	0.59
1:B:31:ARG:HD3	1:B:66:ASP:OD2	2.02	0.59
1:N:47:PRO:HG3	1:N:81:TRP:CZ2	2.33	0.59
1:T:63:LEU:HB3	1:T:155:GLN:HE22	1.68	0.59
1:H:125:ASP:HB2	1:H:126:PRO:CD	2.33	0.58
1:J:47:PRO:HG3	1:J:81:TRP:HZ2	1.68	0.58
2:Q:959:HOH:O	1:R:170:LYS:HE3	2.03	0.58
1:C:41:ASP:OD2	1:C:78:HIS:CD2	2.55	0.58
1:G:87:THR:O	1:G:90:LYS:HG2	2.03	0.58
1:M:44:PHE:O	1:M:47:PRO:HD2	2.03	0.58
1:R:31:ARG:HD3	1:R:66:ASP:OD2	2.02	0.58
1:B:166:PRO:HG3	1:B:176:LEU:HG	1.85	0.58
1:I:78:HIS:HE1	1:I:96:ILE:O	1.85	0.58
1:K:156:TYR:CE2	1:K:175:THR:HG21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:88:ILE:HG23	1:R:91:ILE:HD12	1.85	0.58
1:B:111:ARG:HG3	1:B:116:LEU:O	2.03	0.58
1:B:109:ASN:HD21	1:B:118:ASP:HB2	1.69	0.58
1:G:44:PHE:HA	1:H:186:ILE:HD12	1.86	0.58
1:I:44:PHE:O	1:I:47:PRO:HD2	2.03	0.58
1:P:19:GLU:HA	1:Q:180:LEU:CD1	2.34	0.58
1:C:87:THR:O	1:C:90:LYS:HG2	2.04	0.57
1:T:156:TYR:CE2	1:T:175:THR:HG21	2.39	0.57
1:O:87:THR:O	1:O:90:LYS:HG2	2.04	0.57
1:P:78:HIS:HE1	1:P:96:ILE:O	1.86	0.57
1:E:121:THR:HG21	1:E:147:LEU:HD13	1.85	0.57
1:C:150:LYS:HD2	2:C:227:HOH:O	2.05	0.57
1:E:26:LYS:HD2	1:E:26:LYS:H	1.70	0.57
1:M:125:ASP:HB2	1:M:126:PRO:CD	2.34	0.57
1:K:182:LEU:HB3	1:L:44:PHE:CE1	2.40	0.57
1:N:31:ARG:HD3	1:N:66:ASP:OD2	2.04	0.57
1:R:41:ASP:OD2	1:R:78:HIS:CD2	2.54	0.57
1:M:166:PRO:HG3	1:M:176:LEU:HG	1.85	0.57
1:S:31:ARG:HD3	1:S:66:ASP:OD2	2.05	0.57
1:A:105:ARG:HD2	2:A:220:HOH:O	2.04	0.57
1:B:31:ARG:HH22	1:B:64:GLY:HA2	1.69	0.57
1:K:47:PRO:HG3	1:K:81:TRP:CZ2	2.35	0.57
1:R:56:HIS:ND1	1:R:148:LEU:HD12	2.19	0.57
1:C:156:TYR:CE2	1:C:175:THR:HG21	2.40	0.56
1:E:31:ARG:HD3	1:E:66:ASP:OD2	2.05	0.56
1:Q:182:LEU:HD22	1:Q:186:ILE:HG13	1.87	0.56
1:M:125:ASP:HB2	1:M:126:PRO:HD2	1.86	0.56
1:N:180:LEU:O	1:T:79:LYS:HE2	2.06	0.56
1:T:170:LYS:O	1:T:173:GLU:HG3	2.04	0.56
1:E:186:ILE:OXT	1:F:87:THR:HG23	2.06	0.56
1:F:47:PRO:HG3	1:F:81:TRP:CZ2	2.40	0.56
1:E:44:PHE:O	1:E:47:PRO:HD2	2.06	0.56
1:N:78:HIS:HE1	1:N:96:ILE:O	1.88	0.56
1:S:44:PHE:HA	1:T:186:ILE:HD12	1.87	0.56
1:T:16:LYS:O	1:T:19:GLU:HG2	2.05	0.56
1:I:52:ASP:O	1:I:56:HIS:HD2	1.89	0.56
1:S:42:PHE:O	1:T:183:VAL:HG13	2.06	0.56
1:B:180:LEU:CD1	1:D:19:GLU:HA	2.34	0.56
1:L:109:ASN:ND2	1:L:118:ASP:HB2	2.20	0.56
1:L:111:ARG:HG2	1:L:118:ASP:OD2	2.06	0.56
1:R:111:ARG:HH22	1:R:138:GLU:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LYS:HB3	1:S:31:ARG:NH1	2.20	0.55
1:T:31:ARG:HH21	1:T:64:GLY:HA2	1.69	0.55
1:A:78:HIS:HE1	1:A:96:ILE:O	1.90	0.55
1:F:50:LEU:HB3	1:F:91:ILE:HD11	1.87	0.55
1:N:44:PHE:O	1:N:47:PRO:HD2	2.06	0.55
1:R:56:HIS:ND1	1:R:148:LEU:CD1	2.69	0.55
1:I:119:ARG:HG2	1:I:142:ARG:HH21	1.71	0.55
1:Q:40:ALA:HB1	2:S:207:HOH:O	2.04	0.55
1:D:44:PHE:C	1:D:47:PRO:HD2	2.26	0.55
1:H:24:THR:OG1	1:H:26:LYS:HD3	2.06	0.55
1:H:56:HIS:ND1	1:H:148:LEU:CD1	2.70	0.55
1:I:186:ILE:HD12	1:J:44:PHE:HA	1.89	0.55
1:N:186:ILE:HG22	1:N:186:ILE:OXT	2.07	0.55
1:I:44:PHE:HA	1:J:186:ILE:HD12	1.89	0.55
1:T:87:THR:O	1:T:90:LYS:HG2	2.07	0.55
1:H:47:PRO:HG3	1:H:81:TRP:CZ2	2.40	0.55
1:P:111:ARG:HG2	1:P:118:ASP:OD2	2.07	0.55
1:P:82:HIS:HD2	2:P:1011:HOH:O	1.88	0.55
1:D:152:LYS:HD3	1:D:171:GLU:OE2	2.07	0.55
1:D:62:LYS:HG3	2:D:208:HOH:O	2.05	0.54
1:G:113:ASP:OD1	1:G:114:GLU:HG3	2.07	0.54
1:G:143:ASP:HB3	1:G:146:ASP:OD2	2.07	0.54
1:K:125:ASP:HB2	1:K:126:PRO:CD	2.37	0.54
1:R:109:ASN:ND2	1:R:118:ASP:HB2	2.22	0.54
1:B:109:ASN:ND2	1:B:118:ASP:HB2	2.21	0.54
1:O:59:GLU:OE2	1:O:148:LEU:HD13	2.07	0.54
1:Q:164:VAL:CG2	1:Q:176:LEU:HB2	2.38	0.54
1:S:59:GLU:OE2	1:S:148:LEU:HD13	2.07	0.54
1:B:47:PRO:HG3	1:B:81:TRP:HZ2	1.72	0.54
1:K:149:ARG:HH21	1:K:169:TRP:N	2.05	0.54
1:S:47:PRO:HG3	1:S:81:TRP:CZ2	2.40	0.54
1:H:31:ARG:HD3	1:H:66:ASP:OD2	2.06	0.54
1:E:108:ASP:HB2	2:E:259:HOH:O	2.08	0.54
1:N:109:ASN:ND2	1:N:118:ASP:HB2	2.23	0.54
1:S:182:LEU:HD21	1:S:186:ILE:HG13	1.90	0.54
1:P:171:GLU:HG3	2:P:899:HOH:O	2.07	0.54
1:J:186:ILE:OXT	1:J:186:ILE:HG22	2.08	0.54
1:P:125:ASP:HB2	1:P:126:PRO:CD	2.37	0.53
1:O:44:PHE:CD1	1:P:182:LEU:HD22	2.40	0.53
1:T:125:ASP:OD2	1:T:129:ILE:HB	2.08	0.53
1:A:25:GLU:O	1:A:29:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:ARG:HD3	1:J:66:ASP:OD2	2.08	0.53
1:O:31:ARG:HD3	1:O:66:ASP:OD2	2.08	0.53
1:O:45:VAL:HB	1:O:119:ARG:NH2	2.23	0.53
1:D:28:THR:HA	2:D:229:HOH:O	2.08	0.53
1:M:79:LYS:CE	1:S:183:VAL:HB	2.39	0.53
1:D:180:LEU:CD1	1:J:19:GLU:HA	2.38	0.53
1:J:38:TYR:CZ	1:J:71:SER:HB3	2.44	0.53
1:Q:78:HIS:HE1	1:Q:96:ILE:O	1.90	0.53
1:S:182:LEU:HD21	1:S:186:ILE:HD11	1.90	0.53
1:A:181:ASP:HB3	1:A:185:LYS:NZ	2.23	0.53
1:T:162:GLY:O	1:T:178:PRO:HD2	2.09	0.53
1:Q:186:ILE:OXT	1:R:87:THR:CG2	2.57	0.53
1:S:50:LEU:HB3	1:S:91:ILE:HD11	1.90	0.53
1:T:161:PRO:HB2	2:T:712:HOH:O	2.08	0.53
1:I:111:ARG:HG2	1:I:118:ASP:OD2	2.08	0.53
1:K:180:LEU:O	1:O:79:LYS:HE2	2.09	0.53
1:L:58:GLU:HB2	2:L:1033:HOH:O	2.08	0.53
1:N:152:LYS:HD3	1:N:171:GLU:OE2	2.09	0.53
1:B:42:PHE:HE1	1:B:77:THR:HG23	1.74	0.53
1:I:42:PHE:O	1:J:183:VAL:HG13	2.09	0.52
1:D:31:ARG:NH2	1:D:64:GLY:HA2	2.25	0.52
1:O:170:LYS:H	1:O:173:GLU:HG3	1.74	0.52
1:L:87:THR:O	1:L:90:LYS:HG2	2.08	0.52
1:R:109:ASN:HD21	1:R:118:ASP:HB2	1.74	0.52
1:Q:79:LYS:CE	1:T:183:VAL:HB	2.38	0.52
1:I:44:PHE:C	1:I:47:PRO:HD2	2.30	0.52
1:P:11:LYS:HE3	1:P:22:GLU:OE2	2.09	0.52
1:B:113:ASP:OD1	1:B:114:GLU:HG3	2.08	0.52
1:B:125:ASP:HB2	1:B:126:PRO:CD	2.40	0.52
1:M:78:HIS:HE1	1:M:96:ILE:O	1.92	0.52
1:F:38:TYR:CZ	1:F:71:SER:HB3	2.45	0.52
1:J:44:PHE:C	1:J:47:PRO:HD2	2.29	0.52
1:A:56:HIS:HB3	1:A:148:LEU:HD11	1.92	0.52
1:R:38:TYR:CZ	1:R:71:SER:HB3	2.44	0.52
1:A:111:ARG:HD2	1:A:118:ASP:OD2	2.09	0.52
1:M:79:LYS:HD2	1:S:180:LEU:HD21	1.91	0.52
1:M:50:LEU:HB3	1:M:91:ILE:HD11	1.91	0.52
1:J:41:ASP:OD2	1:J:78:HIS:CD2	2.58	0.52
1:K:78:HIS:HE1	1:K:96:ILE:O	1.93	0.52
1:C:31:ARG:HH21	1:C:64:GLY:HA2	1.75	0.52
1:C:109:ASN:HD21	1:C:118:ASP:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:HIS:HA	1:J:88:ILE:HG22	1.92	0.51
1:K:186:ILE:HD12	1:L:44:PHE:HA	1.91	0.51
1:N:38:TYR:CZ	1:N:71:SER:HB3	2.45	0.51
1:S:82:HIS:HA	1:S:88:ILE:CG2	2.40	0.51
1:M:140:ILE:HD11	1:N:154:ALA:HA	1.92	0.51
1:N:45:VAL:HB	1:N:119:ARG:NH2	2.25	0.51
1:O:38:TYR:CZ	1:O:71:SER:HB3	2.46	0.51
1:T:119:ARG:HG2	1:T:142:ARG:NH2	2.24	0.51
1:D:59:GLU:OE1	1:D:148:LEU:HD13	2.10	0.51
1:B:44:PHE:C	1:B:47:PRO:HD2	2.31	0.51
1:R:170:LYS:HB2	1:R:173:GLU:OE2	2.11	0.51
1:E:31:ARG:NH2	1:E:64:GLY:HA2	2.25	0.51
1:M:119:ARG:HG2	1:M:119:ARG:HH11	1.74	0.51
1:S:150:LYS:HA	2:S:235:HOH:O	2.09	0.51
1:C:50:LEU:HB3	1:C:91:ILE:HD11	1.92	0.51
1:O:170:LYS:HB2	1:O:173:GLU:HG3	1.92	0.51
1:G:52:ASP:CG	1:H:168:LYS:HD2	2.31	0.51
1:R:111:ARG:NH2	1:R:138:GLU:HB2	2.26	0.51
1:S:28:THR:HA	2:S:238:HOH:O	2.11	0.51
1:B:126:PRO:HB2	1:B:127:GLN:HE22	1.76	0.51
1:B:176:LEU:O	1:B:178:PRO:HD3	2.11	0.51
1:C:38:TYR:CZ	1:C:71:SER:HB3	2.46	0.51
1:F:149:ARG:HD2	2:F:194:HOH:O	2.11	0.51
1:F:19:GLU:HA	1:G:180:LEU:CD1	2.39	0.51
1:J:156:TYR:CE2	1:J:175:THR:HG21	2.46	0.51
1:M:162:GLY:O	1:M:178:PRO:HD2	2.11	0.51
1:O:26:LYS:H	1:O:26:LYS:HD2	1.75	0.51
1:E:78:HIS:HE1	1:E:96:ILE:O	1.94	0.51
1:C:125:ASP:HB2	1:C:126:PRO:CD	2.41	0.50
1:N:109:ASN:HD21	1:N:118:ASP:HB2	1.75	0.50
1:I:182:LEU:HD22	1:I:186:ILE:HG13	1.93	0.50
1:S:152:LYS:HD3	1:S:171:GLU:OE2	2.11	0.50
1:A:125:ASP:HB2	1:A:126:PRO:CD	2.42	0.50
1:B:44:PHE:O	1:B:47:PRO:HD2	2.11	0.50
1:Q:186:ILE:OXT	1:Q:186:ILE:HG22	2.11	0.50
1:S:111:ARG:HG2	1:S:118:ASP:OD2	2.11	0.50
1:O:56:HIS:ND1	1:O:148:LEU:CD1	2.75	0.50
1:Q:109:ASN:ND2	1:Q:118:ASP:HB2	2.26	0.50
1:J:125:ASP:HB2	1:J:126:PRO:CD	2.41	0.50
1:M:38:TYR:CZ	1:M:71:SER:HB3	2.46	0.50
1:S:42:PHE:HE1	1:S:77:THR:HG23	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PRO:HB2	1:B:127:GLN:NE2	2.27	0.50
1:B:182:LEU:HD22	1:B:186:ILE:CG1	2.39	0.50
1:E:109:ASN:ND2	1:E:118:ASP:HB2	2.27	0.50
1:E:170:LYS:HE3	2:E:232:HOH:O	2.11	0.50
1:K:87:THR:O	1:K:90:LYS:HG2	2.12	0.50
1:L:41:ASP:OD2	1:L:78:HIS:CD2	2.56	0.50
1:K:180:LEU:CD1	1:O:19:GLU:HA	2.39	0.50
1:Q:109:ASN:HD21	1:Q:118:ASP:HB2	1.76	0.50
1:S:169:TRP:HE1	1:S:175:THR:HG22	1.77	0.50
1:T:60:LEU:HD23	1:T:148:LEU:HD21	1.94	0.50
1:T:25:GLU:HG2	1:T:26:LYS:N	2.27	0.50
1:E:38:TYR:CZ	1:E:71:SER:HB3	2.47	0.49
1:Q:125:ASP:HB2	1:Q:126:PRO:CD	2.41	0.49
1:A:162:GLY:O	1:A:178:PRO:HD2	2.12	0.49
2:C:224:HOH:O	1:D:149:ARG:HD2	2.11	0.49
1:N:65:VAL:HG21	1:N:151:ILE:HG21	1.94	0.49
1:B:170:LYS:HE3	2:B:213:HOH:O	2.12	0.49
1:K:79:LYS:HD2	1:M:180:LEU:HG	1.92	0.49
1:G:50:LEU:HB3	1:G:91:ILE:HD11	1.93	0.49
1:L:170:LYS:HG2	2:L:704:HOH:O	2.11	0.49
1:B:125:ASP:HB2	1:B:126:PRO:HD2	1.94	0.49
1:B:78:HIS:HE1	1:B:96:ILE:O	1.94	0.49
1:D:31:ARG:HH22	1:D:64:GLY:HA2	1.77	0.49
1:E:156:TYR:O	1:E:160:HIS:HD2	1.95	0.49
1:M:31:ARG:HD3	1:M:66:ASP:OD2	2.12	0.49
1:O:166:PRO:HG3	1:O:176:LEU:HG	1.94	0.49
1:T:42:PHE:HE1	1:T:77:THR:HG23	1.77	0.49
1:F:59:GLU:OE1	1:F:148:LEU:HD13	2.12	0.49
1:M:166:PRO:HB3	1:N:48:THR:HG21	1.94	0.49
1:S:164:VAL:HG23	1:S:176:LEU:HB2	1.93	0.49
1:T:164:VAL:CG2	1:T:176:LEU:HB2	2.43	0.49
1:T:60:LEU:HD13	1:T:67:VAL:HG21	1.95	0.49
1:G:162:GLY:O	1:G:178:PRO:HD2	2.12	0.49
1:J:87:THR:O	1:J:90:LYS:HG2	2.12	0.49
1:L:156:TYR:CE2	1:L:175:THR:HG21	2.48	0.49
1:M:59:GLU:OE2	1:M:148:LEU:HD13	2.12	0.49
1:Q:164:VAL:HG23	1:Q:176:LEU:HB2	1.93	0.49
1:C:168:LYS:HD2	1:D:52:ASP:CG	2.33	0.49
1:T:38:TYR:CZ	1:T:71:SER:HB3	2.48	0.49
1:K:41:ASP:OD2	1:K:78:HIS:CD2	2.63	0.49
1:S:120:ALA:HA	1:S:134:GLU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:GLU:HA	1:P:180:LEU:CD1	2.41	0.48
1:N:44:PHE:C	1:N:47:PRO:HD2	2.33	0.48
1:Q:186:ILE:OXT	1:R:87:THR:HG23	2.13	0.48
1:R:180:LEU:O	1:S:79:LYS:NZ	2.46	0.48
1:F:164:VAL:HG23	1:F:176:LEU:HB2	1.94	0.48
1:O:56:HIS:ND1	1:O:148:LEU:HD11	2.28	0.48
1:P:87:THR:O	1:P:90:LYS:HG2	2.13	0.48
1:E:25:GLU:HG2	1:E:26:LYS:N	2.28	0.48
1:G:164:VAL:CG2	1:G:176:LEU:HB2	2.43	0.48
1:M:10:PHE:HE1	1:M:23:VAL:HG12	1.77	0.48
1:D:41:ASP:OD2	1:D:78:HIS:CD2	2.61	0.48
1:I:176:LEU:O	1:I:178:PRO:HD3	2.13	0.48
1:B:167:ALA:O	1:B:168:LYS:HB2	2.14	0.48
1:L:88:ILE:HG23	1:L:91:ILE:HD12	1.94	0.48
1:M:6:LYS:HA	1:M:128:GLY:O	2.12	0.48
1:R:156:TYR:CE2	1:R:175:THR:HG21	2.48	0.48
1:S:125:ASP:OD2	1:S:129:ILE:HB	2.14	0.48
1:S:183:VAL:HG13	1:T:42:PHE:O	2.13	0.48
1:F:180:LEU:HD23	1:F:180:LEU:O	2.14	0.48
1:T:49:GLU:OE2	1:T:142:ARG:N	2.44	0.48
1:F:164:VAL:CG2	1:F:176:LEU:HB2	2.44	0.48
1:L:180:LEU:CD1	1:N:19:GLU:HA	2.43	0.48
1:B:170:LYS:O	1:B:173:GLU:HG3	2.14	0.47
1:I:47:PRO:HG3	1:I:81:TRP:HZ2	1.78	0.47
1:N:156:TYR:HA	2:N:812:HOH:O	2.11	0.47
1:O:26:LYS:N	1:O:26:LYS:HD2	2.29	0.47
1:N:87:THR:O	1:N:90:LYS:HG3	2.14	0.47
1:C:150:LYS:NZ	1:D:134:GLU:OE2	2.44	0.47
1:G:186:ILE:HD12	1:H:44:PHE:HA	1.96	0.47
1:M:60:LEU:HD22	1:M:65:VAL:HG11	1.96	0.47
1:O:78:HIS:HE1	1:O:96:ILE:O	1.97	0.47
1:I:15:PHE:CE1	1:I:79:LYS:HG3	2.49	0.47
1:T:58:GLU:HA	2:T:1003:HOH:O	2.14	0.47
1:T:67:VAL:O	1:T:93:TYR:HB2	2.14	0.47
1:B:164:VAL:HG23	1:B:176:LEU:HB2	1.96	0.47
1:N:125:ASP:OD2	1:N:129:ILE:HB	2.14	0.47
1:T:25:GLU:HG2	1:T:26:LYS:HD2	1.96	0.47
1:B:88:ILE:HG23	1:B:91:ILE:HD12	1.97	0.47
1:L:105:ARG:NH1	2:L:852:HOH:O	2.44	0.47
1:L:79:LYS:HD2	1:P:180:LEU:HG	1.96	0.47
1:M:109:ASN:OD1	1:M:120:ALA:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:150:LYS:NZ	1:P:134:GLU:OE2	2.41	0.47
1:P:182:LEU:HD21	1:P:186:ILE:HG13	1.95	0.47
1:E:10:PHE:O	1:E:24:THR:HA	2.14	0.47
1:P:152:LYS:HD3	1:P:171:GLU:CD	2.35	0.47
1:F:78:HIS:HE1	1:F:96:ILE:O	1.97	0.47
1:H:45:VAL:HB	1:H:119:ARG:NH2	2.30	0.47
1:N:143:ASP:OD1	1:N:145:SER:HB2	2.14	0.47
1:S:182:LEU:HD21	1:S:186:ILE:CG1	2.45	0.47
1:A:19:GLU:HA	1:C:180:LEU:CD1	2.44	0.47
1:E:32:TRP:CE2	1:E:126:PRO:HD3	2.50	0.47
1:H:180:LEU:HD23	1:H:180:LEU:C	2.35	0.47
1:E:31:ARG:NH1	1:E:66:ASP:OD1	2.48	0.47
1:I:9:PRO:HG2	2:I:228:HOH:O	2.14	0.47
1:L:61:GLN:HG3	2:L:915:HOH:O	2.15	0.47
1:P:11:LYS:HG3	1:P:24:THR:HG22	1.97	0.47
1:P:79:LYS:HE3	1:Q:180:LEU:O	2.14	0.47
1:T:41:ASP:OD2	1:T:78:HIS:HD2	1.98	0.47
1:B:38:TYR:CZ	1:B:71:SER:HB3	2.50	0.47
1:Q:182:LEU:HD22	1:Q:186:ILE:CG1	2.45	0.47
1:F:186:ILE:OXT	1:F:186:ILE:HG22	2.15	0.46
1:L:153:ALA:O	1:L:157:VAL:HG22	2.15	0.46
1:B:59:GLU:OE2	1:B:148:LEU:HD22	2.16	0.46
1:I:41:ASP:OD2	1:I:78:HIS:CD2	2.56	0.46
1:O:9:PRO:HG2	2:O:262:HOH:O	2.15	0.46
1:C:92:LYS:HB3	1:C:92:LYS:NZ	2.31	0.46
1:J:25:GLU:OE2	1:J:26:LYS:HD2	2.16	0.46
1:Q:125:ASP:HB2	1:Q:126:PRO:HD2	1.97	0.46
1:A:181:ASP:C	1:A:183:VAL:H	2.18	0.46
1:F:182:LEU:HD23	1:F:182:LEU:O	2.16	0.46
1:Q:41:ASP:OD2	1:Q:78:HIS:CD2	2.62	0.46
1:C:78:HIS:HE1	1:C:96:ILE:O	1.99	0.46
1:M:31:ARG:HH11	1:M:66:ASP:CG	2.19	0.46
1:R:125:ASP:OD1	1:R:125:ASP:C	2.54	0.46
1:J:45:VAL:HB	1:J:119:ARG:NH2	2.30	0.46
1:K:44:PHE:O	1:K:47:PRO:HD2	2.16	0.46
1:R:149:ARG:NH2	2:R:1058:HOH:O	2.49	0.46
1:H:154:ALA:O	1:H:157:VAL:HG22	2.16	0.46
1:C:109:ASN:ND2	1:C:118:ASP:HB2	2.31	0.46
1:F:8:LYS:HE3	1:F:106:ASN:OD1	2.16	0.46
1:M:39:PRO:HD2	1:M:119:ARG:NH1	2.31	0.46
1:Q:38:TYR:CZ	1:Q:71:SER:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:125:ASP:HB2	1:R:126:PRO:CD	2.46	0.46
1:T:32:TRP:CE2	1:T:126:PRO:HD3	2.50	0.46
1:G:166:PRO:HG3	1:G:176:LEU:HG	1.98	0.46
1:G:164:VAL:HG23	1:G:176:LEU:HB2	1.97	0.46
1:G:78:HIS:HE1	1:G:96:ILE:O	1.99	0.46
1:L:170:LYS:HE2	2:L:704:HOH:O	2.14	0.46
1:P:125:ASP:HB2	1:P:126:PRO:HD2	1.97	0.46
1:C:44:PHE:CE2	1:D:178:PRO:HB3	2.51	0.45
1:A:111:ARG:HH22	1:A:138:GLU:CD	2.20	0.45
1:E:111:ARG:HG2	1:E:118:ASP:OD2	2.17	0.45
1:R:45:VAL:HB	1:R:119:ARG:NH2	2.32	0.45
1:A:41:ASP:OD2	1:A:78:HIS:CD2	2.60	0.45
1:S:176:LEU:HD13	1:T:44:PHE:HB3	1.98	0.45
1:S:32:TRP:HB2	1:S:65:VAL:HG22	1.98	0.45
1:A:109:ASN:ND2	1:A:118:ASP:HB2	2.31	0.45
1:I:125:ASP:HB2	1:I:126:PRO:CD	2.46	0.45
1:O:52:ASP:O	1:O:56:HIS:HD2	1.99	0.45
1:B:24:THR:OG1	1:B:26:LYS:HB2	2.17	0.45
1:C:147:LEU:O	1:C:151:ILE:HG13	2.15	0.45
1:S:166:PRO:HG3	1:S:176:LEU:HG	1.99	0.45
1:A:152:LYS:HD3	1:A:171:GLU:CG	2.47	0.45
1:G:125:ASP:HB2	1:G:126:PRO:CD	2.47	0.45
1:G:38:TYR:CZ	1:G:71:SER:HB3	2.52	0.45
1:A:38:TYR:CZ	1:A:71:SER:HB3	2.52	0.45
1:C:186:ILE:HG22	1:C:186:ILE:OXT	2.16	0.45
1:E:39:PRO:HD2	2:E:244:HOH:O	2.17	0.45
1:B:20:PHE:H	1:F:180:LEU:CD1	2.30	0.45
1:Q:82:HIS:HA	1:Q:88:ILE:HG22	1.99	0.45
1:R:78:HIS:HE1	1:R:96:ILE:O	2.00	0.45
1:S:17:ASN:HD21	1:S:92:LYS:HA	1.81	0.45
1:T:125:ASP:HB2	1:T:126:PRO:CD	2.47	0.45
1:T:125:ASP:HB2	1:T:126:PRO:HD2	1.99	0.45
1:T:65:VAL:HG21	1:T:151:ILE:HG21	1.99	0.45
1:E:125:ASP:HB2	1:E:126:PRO:HD2	1.98	0.45
1:T:60:LEU:CD2	1:T:148:LEU:HD21	2.46	0.45
1:G:19:GLU:HA	1:J:180:LEU:CD1	2.44	0.45
1:M:186:ILE:HG22	1:M:186:ILE:OXT	2.17	0.45
1:R:134:GLU:OE2	1:R:142:ARG:HG2	2.17	0.45
1:A:186:ILE:HD12	1:B:44:PHE:HA	1.98	0.45
1:G:79:LYS:HE2	1:J:180:LEU:HD21	1.99	0.45
1:C:85:SER:HB3	1:C:88:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:PHE:O	1:I:24:THR:HA	2.17	0.44
1:R:82:HIS:HD2	2:R:552:HOH:O	2.00	0.44
1:S:48:THR:HG21	1:T:166:PRO:HB3	1.97	0.44
1:S:82:HIS:HD2	2:S:198:HOH:O	2.00	0.44
1:I:180:LEU:C	1:I:180:LEU:HD23	2.38	0.44
1:Q:170:LYS:HE3	2:Q:806:HOH:O	2.17	0.44
1:P:82:HIS:HA	1:P:88:ILE:HG22	1.99	0.44
1:S:179:SER:O	1:S:183:VAL:HG23	2.18	0.44
1:T:47:PRO:HG3	1:T:81:TRP:CZ2	2.49	0.44
1:J:82:HIS:HA	1:J:88:ILE:CG2	2.48	0.44
1:K:56:HIS:ND1	1:K:148:LEU:HD12	2.33	0.44
1:O:180:LEU:HD21	1:R:79:LYS:HD2	2.00	0.44
1:K:182:LEU:HB3	1:L:44:PHE:HE1	1.80	0.44
1:M:119:ARG:HG2	1:M:119:ARG:NH1	2.33	0.44
1:M:31:ARG:HH22	1:M:64:GLY:HA2	1.82	0.44
1:K:125:ASP:HB2	1:K:126:PRO:HD2	1.99	0.44
1:T:44:PHE:C	1:T:47:PRO:HD2	2.38	0.44
1:A:111:ARG:HD2	1:A:118:ASP:HA	2.00	0.44
1:H:56:HIS:ND1	1:H:148:LEU:HD12	2.33	0.44
1:P:113:ASP:OD1	1:P:114:GLU:HG3	2.17	0.44
1:P:164:VAL:HG23	1:P:176:LEU:HB2	1.99	0.44
1:B:101:GLY:O	1:B:105:ARG:HG3	2.18	0.44
1:Q:87:THR:O	1:Q:90:LYS:HG2	2.18	0.44
1:M:79:LYS:HE2	1:S:180:LEU:O	2.17	0.44
1:F:81:TRP:CE2	1:F:88:ILE:HG13	2.53	0.43
1:E:126:PRO:HB2	1:E:127:GLN:NE2	2.33	0.43
1:H:62:LYS:HB2	1:H:62:LYS:HE3	1.55	0.43
1:I:28:THR:HA	2:I:227:HOH:O	2.17	0.43
1:D:47:PRO:HG3	1:D:81:TRP:CZ2	2.51	0.43
1:H:38:TYR:CZ	1:H:71:SER:HB3	2.53	0.43
1:S:146:ASP:O	1:S:149:ARG:HB3	2.17	0.43
1:T:31:ARG:HH21	1:T:64:GLY:CA	2.31	0.43
1:K:186:ILE:OXT	1:L:87:THR:HG23	2.18	0.43
1:R:109:ASN:HA	2:R:1251:HOH:O	2.18	0.43
1:S:111:ARG:HG3	1:S:116:LEU:O	2.18	0.43
1:T:186:ILE:HG22	1:T:186:ILE:OXT	2.18	0.43
1:A:152:LYS:HD3	1:A:171:GLU:HG3	2.01	0.43
1:C:19:GLU:HA	1:I:180:LEU:HD13	1.97	0.43
1:D:167:ALA:O	1:D:168:LYS:HB2	2.18	0.43
1:E:164:VAL:CG2	1:E:176:LEU:HB2	2.49	0.43
1:O:63:LEU:HD22	1:O:155:GLN:HE22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HG2	2:R:1411:HOH:O	2.18	0.43
1:A:88:ILE:HG23	1:A:91:ILE:HD12	2.00	0.43
1:H:182:LEU:HD22	1:H:186:ILE:HG13	2.01	0.43
1:N:120:ALA:HA	1:N:134:GLU:O	2.19	0.43
1:S:45:VAL:HB	1:S:119:ARG:NH2	2.33	0.43
1:C:32:TRP:CE2	1:C:126:PRO:HD3	2.54	0.43
1:J:46:SER:HB2	1:J:47:PRO:HD3	2.01	0.43
1:K:181:ASP:O	1:K:185:LYS:HG3	2.18	0.43
1:L:82:HIS:HE1	1:L:91:ILE:O	2.02	0.43
1:N:31:ARG:HH22	1:N:64:GLY:HA2	1.81	0.43
1:Q:46:SER:N	1:Q:47:PRO:HD2	2.34	0.43
1:O:180:LEU:O	1:R:79:LYS:HE2	2.18	0.43
1:P:38:TYR:CZ	1:P:71:SER:HB3	2.54	0.43
1:T:31:ARG:NH2	1:T:64:GLY:CA	2.79	0.43
1:E:125:ASP:HB2	1:E:126:PRO:CD	2.49	0.43
1:S:59:GLU:O	1:S:62:LYS:HB3	2.19	0.43
1:T:41:ASP:OD2	1:T:78:HIS:CD2	2.72	0.43
1:D:82:HIS:HA	1:D:88:ILE:HG22	2.01	0.43
1:K:78:HIS:CE1	1:K:96:ILE:O	2.72	0.43
1:Q:111:ARG:HG2	1:Q:118:ASP:OD2	2.19	0.43
1:B:46:SER:N	1:B:47:PRO:CD	2.82	0.42
1:C:139:GLY:O	1:D:157:VAL:HG11	2.19	0.42
1:B:19:GLU:CA	1:F:180:LEU:HD11	2.39	0.42
1:G:56:HIS:HB3	1:G:148:LEU:HD11	2.00	0.42
1:J:167:ALA:O	1:J:168:LYS:HB2	2.19	0.42
1:O:41:ASP:OD2	1:O:78:HIS:CD2	2.63	0.42
1:E:28:THR:HA	2:E:235:HOH:O	2.20	0.42
1:J:43:THR:HB	1:J:44:PHE:H	1.69	0.42
1:N:164:VAL:CG2	1:N:176:LEU:HB2	2.50	0.42
1:B:25:GLU:N	1:B:25:GLU:OE1	2.51	0.42
1:C:40:ALA:HB1	2:C:208:HOH:O	2.19	0.42
1:F:179:SER:OG	1:F:182:LEU:HB2	2.19	0.42
1:M:150:LYS:HE3	1:N:136:THR:HG21	2.02	0.42
1:O:125:ASP:HB2	1:O:126:PRO:CD	2.49	0.42
1:B:111:ARG:CD	1:B:118:ASP:OD2	2.64	0.42
1:B:41:ASP:OD2	1:B:78:HIS:CD2	2.64	0.42
1:B:20:PHE:H	1:F:180:LEU:HD12	1.85	0.42
1:J:119:ARG:HH11	1:J:119:ARG:HG2	1.83	0.42
1:L:111:ARG:HH22	1:L:138:GLU:HB2	1.84	0.42
1:L:24:THR:OG1	1:L:26:LYS:HB2	2.20	0.42
1:N:166:PRO:HG3	1:N:176:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:164:VAL:HG23	1:N:176:LEU:HB2	2.00	0.42
1:T:182:LEU:HD22	1:T:186:ILE:HD11	2.01	0.42
1:C:125:ASP:HB2	1:C:126:PRO:HD2	2.00	0.42
1:D:164:VAL:HG23	1:D:176:LEU:HB2	2.01	0.42
1:F:163:GLU:HA	1:F:176:LEU:O	2.20	0.42
1:K:56:HIS:ND1	1:K:148:LEU:CD1	2.82	0.42
1:K:186:ILE:OXT	1:L:87:THR:CG2	2.68	0.42
1:O:167:ALA:O	1:O:168:LYS:HB2	2.20	0.42
1:S:152:LYS:HD3	1:S:171:GLU:CD	2.39	0.42
1:F:32:TRP:CE2	1:F:126:PRO:HD3	2.55	0.42
1:M:147:LEU:O	1:M:151:ILE:HG13	2.19	0.42
1:M:19:GLU:HA	1:S:180:LEU:HD11	2.00	0.42
1:N:182:LEU:HD22	1:N:186:ILE:HD11	2.02	0.42
1:A:167:ALA:O	1:A:168:LYS:HB2	2.20	0.42
1:N:59:GLU:OE2	1:N:148:LEU:HD13	2.20	0.42
1:A:25:GLU:OE2	1:A:26:LYS:HD2	2.20	0.42
1:D:11:LYS:NZ	1:D:22:GLU:OE2	2.49	0.42
1:I:62:LYS:HB3	1:I:62:LYS:HE3	1.76	0.42
1:J:169:TRP:NE1	1:J:175:THR:HG22	2.35	0.42
1:M:120:ALA:HA	1:M:134:GLU:O	2.19	0.42
1:M:9:PRO:HA	1:M:25:GLU:HB3	2.02	0.42
1:N:165:CYS:HA	1:N:166:PRO:HD3	1.93	0.42
1:S:44:PHE:CD1	1:T:182:LEU:HB3	2.54	0.42
1:C:19:GLU:HA	1:I:180:LEU:HD11	2.01	0.41
1:H:156:TYR:CE2	1:H:175:THR:HG21	2.54	0.41
1:N:28:THR:HA	2:N:1120:HOH:O	2.19	0.41
1:Q:88:ILE:HG23	1:Q:91:ILE:HD12	2.02	0.41
1:S:133:ILE:HB	1:T:135:VAL:HB	2.02	0.41
1:F:120:ALA:HA	1:F:134:GLU:O	2.21	0.41
1:I:25:GLU:O	1:I:29:GLU:HG3	2.20	0.41
1:M:2:LEU:HD23	1:M:2:LEU:HA	1.92	0.41
1:M:56:HIS:HB3	1:M:148:LEU:HD11	2.00	0.41
1:S:178:PRO:HB3	1:T:44:PHE:CE2	2.55	0.41
1:C:167:ALA:O	1:C:168:LYS:HB2	2.20	0.41
1:E:45:VAL:HB	1:E:119:ARG:NH2	2.35	0.41
1:E:156:TYR:O	1:E:160:HIS:CD2	2.72	0.41
1:E:164:VAL:HG23	1:E:176:LEU:HB2	2.01	0.41
1:F:59:GLU:HG3	2:F:261:HOH:O	2.19	0.41
1:G:125:ASP:HB2	1:G:126:PRO:HD2	2.03	0.41
1:G:186:ILE:HG22	1:G:186:ILE:OXT	2.20	0.41
1:H:109:ASN:ND2	1:H:118:ASP:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:ASP:CG	1:L:168:LYS:HD2	2.41	0.41
1:K:81:TRP:CD2	1:K:88:ILE:HG13	2.55	0.41
1:M:168:LYS:HD2	1:N:52:ASP:CG	2.40	0.41
1:O:58:GLU:O	1:O:62:LYS:HD3	2.20	0.41
1:P:28:THR:HA	2:P:1125:HOH:O	2.20	0.41
1:T:6:LYS:HA	1:T:128:GLY:O	2.21	0.41
1:S:154:ALA:CA	1:T:140:ILE:HD11	2.45	0.41
1:J:32:TRP:CE2	1:J:126:PRO:HD3	2.55	0.41
1:O:178:PRO:HB3	1:P:44:PHE:CE2	2.55	0.41
1:O:10:PHE:O	1:O:24:THR:HA	2.20	0.41
1:P:25:GLU:OE2	1:P:26:LYS:HD2	2.20	0.41
1:S:101:GLY:O	1:S:105:ARG:HG3	2.20	0.41
1:S:44:PHE:CE2	1:T:178:PRO:HB3	2.55	0.41
1:A:182:LEU:HB3	1:B:44:PHE:HD1	1.84	0.41
1:C:169:TRP:NE1	1:C:175:THR:HG22	2.35	0.41
1:F:11:LYS:NZ	1:F:22:GLU:OE2	2.50	0.41
1:T:119:ARG:HG2	1:T:142:ARG:HH21	1.84	0.41
1:T:86:GLU:O	1:T:89:ALA:HB3	2.20	0.41
1:K:46:SER:HB2	1:K:47:PRO:HD3	2.03	0.41
1:E:140:ILE:HD11	1:F:154:ALA:HA	2.03	0.41
1:G:87:THR:HG23	1:H:186:ILE:OXT	2.21	0.41
1:M:180:LEU:HD23	1:M:180:LEU:C	2.41	0.41
1:T:167:ALA:O	1:T:168:LYS:HB2	2.21	0.41
1:A:121:THR:HG21	1:A:147:LEU:HD13	2.03	0.41
1:E:56:HIS:ND1	1:E:148:LEU:CD1	2.82	0.41
1:L:125:ASP:HB2	1:L:126:PRO:CD	2.51	0.41
1:K:42:PHE:O	1:L:183:VAL:HG13	2.20	0.41
1:M:87:THR:CG2	1:N:186:ILE:OXT	2.69	0.41
1:N:156:TYR:CE2	1:N:175:THR:HG21	2.56	0.41
1:Q:32:TRP:CE2	1:Q:126:PRO:HD3	2.55	0.41
1:R:162:GLY:O	1:R:178:PRO:HD2	2.20	0.41
1:F:57:TYR:CE1	1:F:93:TYR:HB3	2.56	0.41
1:I:41:ASP:OD2	1:I:77:THR:HG22	2.20	0.41
1:L:125:ASP:C	1:L:125:ASP:OD1	2.58	0.41
1:L:56:HIS:HB3	1:L:148:LEU:HD11	2.02	0.41
1:H:43:THR:O	1:H:47:PRO:HG2	2.21	0.41
1:L:11:LYS:HE3	1:L:22:GLU:OE2	2.21	0.41
1:O:180:LEU:CD2	1:R:79:LYS:HD2	2.51	0.41
1:Q:44:PHE:C	1:Q:47:PRO:HD2	2.42	0.41
1:D:32:TRP:CE2	1:D:126:PRO:HD3	2.56	0.41
1:D:25:GLU:OE2	1:D:26:LYS:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:44:PHE:CE2	1:N:178:PRO:HB3	2.56	0.41
1:C:42:PHE:HE1	1:C:77:THR:HG23	1.86	0.40
1:C:31:ARG:NH2	1:C:64:GLY:HA2	2.36	0.40
1:F:125:ASP:HB2	1:F:126:PRO:CD	2.51	0.40
1:H:109:ASN:HD21	1:H:118:ASP:HB2	1.86	0.40
1:M:39:PRO:C	2:M:1326:HOH:O	2.59	0.40
1:S:85:SER:HB3	1:S:88:ILE:HB	2.03	0.40
1:T:165:CYS:HA	1:T:166:PRO:HD3	1.97	0.40
1:Q:79:LYS:CD	1:T:180:LEU:HG	2.46	0.40
1:A:185:LYS:O	1:A:186:ILE:C	2.60	0.40
1:B:180:LEU:HD12	1:D:20:PHE:CD2	2.57	0.40
1:E:109:ASN:HD21	1:E:118:ASP:HB2	1.85	0.40
1:I:88:ILE:HG23	1:I:91:ILE:HD12	2.02	0.40
1:Q:186:ILE:HD12	1:R:44:PHE:HA	2.02	0.40
1:C:31:ARG:HH21	1:C:64:GLY:CA	2.33	0.40
1:J:148:LEU:O	1:J:152:LYS:HG3	2.22	0.40
1:K:10:PHE:O	1:K:24:THR:HA	2.21	0.40
1:L:11:LYS:HE3	1:L:22:GLU:CD	2.42	0.40
1:D:101:GLY:O	1:D:105:ARG:HG3	2.21	0.40
1:E:24:THR:CB	1:E:26:LYS:HD3	2.52	0.40
1:G:41:ASP:OD2	1:G:78:HIS:CD2	2.62	0.40
1:L:46:SER:N	1:L:47:PRO:HD2	2.37	0.40
1:M:140:ILE:HD11	1:N:154:ALA:CA	2.51	0.40
1:B:6:LYS:HA	1:B:128:GLY:O	2.22	0.40
1:G:79:LYS:HE2	1:J:180:LEU:CD2	2.50	0.40
1:H:88:ILE:HG23	1:H:91:ILE:HD12	2.03	0.40
1:S:52:ASP:OD2	1:S:144:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/186 (99%)	177 (96%)	6 (3%)	1 (0%)	32	32
1	B	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
1	C	184/186 (99%)	177 (96%)	6 (3%)	1 (0%)	32	32
1	D	184/186 (99%)	178 (97%)	6 (3%)	0	100	100
1	E	184/186 (99%)	178 (97%)	6 (3%)	0	100	100
1	F	184/186 (99%)	182 (99%)	2 (1%)	0	100	100
1	G	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	H	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	I	184/186 (99%)	177 (96%)	7 (4%)	0	100	100
1	J	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
1	K	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	L	184/186 (99%)	181 (98%)	3 (2%)	0	100	100
1	M	184/186 (99%)	178 (97%)	4 (2%)	2 (1%)	17	12
1	N	184/186 (99%)	179 (97%)	4 (2%)	1 (0%)	32	32
1	O	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
1	P	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	Q	184/186 (99%)	181 (98%)	3 (2%)	0	100	100
1	R	184/186 (99%)	178 (97%)	6 (3%)	0	100	100
1	S	184/186 (99%)	178 (97%)	6 (3%)	0	100	100
1	T	184/186 (99%)	176 (96%)	8 (4%)	0	100	100
All	All	3680/3720 (99%)	3577 (97%)	98 (3%)	5 (0%)	55	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	LEU
1	M	17	ASN
1	C	39	PRO
1	M	39	PRO
1	N	39	PRO

### 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	154/154 (100%)	149 (97%)	5 (3%)	44	53
1	B	154/154 (100%)	150 (97%)	4 (3%)	51	61
1	C	154/154 (100%)	152 (99%)	2 (1%)	73	84
1	D	154/154 (100%)	149 (97%)	5 (3%)	44	53
1	E	154/154 (100%)	149 (97%)	5 (3%)	44	53
1	F	154/154 (100%)	152 (99%)	2 (1%)	73	84
1	G	154/154 (100%)	151 (98%)	3 (2%)	62	73
1	H	154/154 (100%)	151 (98%)	3 (2%)	62	73
1	I	154/154 (100%)	149 (97%)	5 (3%)	44	53
1	J	154/154 (100%)	152 (99%)	2 (1%)	73	84
1	K	154/154 (100%)	151 (98%)	3 (2%)	62	73
1	L	154/154 (100%)	150 (97%)	4 (3%)	51	61
1	M	154/154 (100%)	149 (97%)	5 (3%)	44	53
1	N	154/154 (100%)	149 (97%)	5 (3%)	44	53
1	O	154/154 (100%)	153 (99%)	1 (1%)	89	94
1	P	154/154 (100%)	151 (98%)	3 (2%)	62	73
1	Q	154/154 (100%)	152 (99%)	2 (1%)	73	84
1	R	154/154 (100%)	149 (97%)	5 (3%)	44	53
1	S	154/154 (100%)	151 (98%)	3 (2%)	62	73
1	T	154/154 (100%)	152 (99%)	2 (1%)	73	84
All	All	3080/3080 (100%)	3011 (98%)	69 (2%)	57	68

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	103	LEU
1	A	138	GLU
1	A	148	LEU
1	A	149	ARG
1	B	87	THR
1	B	103	LEU
1	B	171	GLU

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Mol	Chain	Res	Type
1	B	181	ASP
1	C	87	THR
1	C	103	LEU
1	D	62	LYS
1	D	87	THR
1	D	103	LEU
1	D	149	ARG
1	D	181	ASP
1	E	26	LYS
1	E	44	PHE
1	E	103	LEU
1	E	171	GLU
1	E	180	LEU
1	F	87	THR
1	F	103	LEU
1	G	87	THR
1	G	103	LEU
1	G	171	GLU
1	H	26	LYS
1	H	62	LYS
1	H	103	LEU
1	I	79	LYS
1	I	87	THR
1	I	103	LEU
1	I	119	ARG
1	I	182	LEU
1	J	58	GLU
1	J	103	LEU
1	K	84	SER
1	K	103	LEU
1	K	182	LEU
1	L	87	THR
1	L	103	LEU
1	L	138	GLU
1	L	182	LEU
1	M	4	ASN
1	M	92	LYS
1	M	103	LEU
1	M	109	ASN
1	M	181	ASP
1	N	4	ASN
1	N	25	GLU

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Mol	Chain	Res	Type
1	N	71	SER
1	N	103	LEU
1	N	182	LEU
1	O	103	LEU
1	P	26	LYS
1	P	87	THR
1	P	103	LEU
1	Q	103	LEU
1	Q	182	LEU
1	R	87	THR
1	R	103	LEU
1	R	134	GLU
1	R	149	ARG
1	R	182	LEU
1	S	58	GLU
1	S	79	LYS
1	S	103	LEU
1	T	103	LEU
1	T	119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	78	HIS
1	A	109	ASN
1	A	155	GLN
1	B	4	ASN
1	B	78	HIS
1	B	82	HIS
1	B	109	ASN
1	B	127	GLN
1	B	155	GLN
1	B	160	HIS
1	C	4	ASN
1	C	78	HIS
1	C	109	ASN
1	C	155	GLN
1	C	160	HIS
1	D	4	ASN
1	D	56	HIS
1	D	78	HIS

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Mol	Chain	Res	Type
1	D	82	HIS
1	D	109	ASN
1	D	155	GLN
1	D	160	HIS
1	E	78	HIS
1	E	109	ASN
1	E	127	GLN
1	E	155	GLN
1	E	160	HIS
1	F	56	HIS
1	F	78	HIS
1	F	82	HIS
1	F	109	ASN
1	F	155	GLN
1	F	160	HIS
1	G	78	HIS
1	G	82	HIS
1	G	109	ASN
1	G	127	GLN
1	G	155	GLN
1	G	160	HIS
1	H	4	ASN
1	H	78	HIS
1	H	109	ASN
1	H	155	GLN
1	H	160	HIS
1	I	56	HIS
1	I	78	HIS
1	I	82	HIS
1	I	109	ASN
1	I	155	GLN
1	I	160	HIS
1	J	4	ASN
1	J	78	HIS
1	J	109	ASN
1	J	155	GLN
1	J	160	HIS
1	K	4	ASN
1	K	78	HIS
1	K	82	HIS
1	K	109	ASN
1	K	155	GLN

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Mol	Chain	Res	Type
1	K	160	HIS
1	L	4	ASN
1	L	78	HIS
1	L	82	HIS
1	L	109	ASN
1	L	127	GLN
1	L	155	GLN
1	M	4	ASN
1	M	78	HIS
1	M	109	ASN
1	M	127	GLN
1	M	160	HIS
1	N	4	ASN
1	N	78	HIS
1	N	82	HIS
1	N	109	ASN
1	N	127	GLN
1	N	155	GLN
1	N	160	HIS
1	O	78	HIS
1	O	82	HIS
1	O	109	ASN
1	O	155	GLN
1	O	160	HIS
1	P	4	ASN
1	P	78	HIS
1	P	82	HIS
1	P	109	ASN
1	P	155	GLN
1	P	160	HIS
1	Q	4	ASN
1	Q	78	HIS
1	Q	109	ASN
1	Q	155	GLN
1	Q	160	HIS
1	R	4	ASN
1	R	78	HIS
1	R	82	HIS
1	R	109	ASN
1	R	127	GLN
1	R	155	GLN
1	S	4	ASN

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Mol	Chain	Res	Type
1	S	17	ASN
1	S	82	HIS
1	S	109	ASN
1	S	155	GLN
1	S	160	HIS
1	T	4	ASN
1	T	109	ASN
1	T	155	GLN
1	T	160	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	186/186 (100%)	-0.10	8 (4%)	36 36	27, 41, 85, 124	0
1	B	186/186 (100%)	-0.10	3 (1%)	72 72	28, 47, 73, 92	0
1	C	186/186 (100%)	0.13	11 (5%)	23 24	32, 49, 85, 109	0
1	D	186/186 (100%)	0.13	11 (5%)	23 24	30, 53, 94, 116	0
1	E	186/186 (100%)	-0.08	3 (1%)	72 72	27, 46, 68, 95	0
1	F	186/186 (100%)	-0.14	9 (4%)	31 32	23, 37, 83, 113	0
1	G	186/186 (100%)	-0.28	5 (2%)	55 55	24, 35, 63, 87	0
1	H	186/186 (100%)	-0.36	1 (0%)	90 90	24, 36, 62, 82	0
1	I	186/186 (100%)	-0.04	7 (3%)	41 41	28, 43, 84, 106	0
1	J	186/186 (100%)	-0.21	6 (3%)	48 49	25, 39, 74, 100	0
1	K	186/186 (100%)	-0.31	0	100 100	22, 35, 60, 86	0
1	L	186/186 (100%)	-0.31	3 (1%)	72 72	23, 35, 66, 89	0
1	M	186/186 (100%)	0.25	7 (3%)	41 41	38, 58, 83, 95	0
1	N	186/186 (100%)	0.17	9 (4%)	31 32	35, 56, 87, 110	0
1	O	186/186 (100%)	-0.18	1 (0%)	90 90	22, 40, 67, 80	0
1	P	186/186 (100%)	-0.33	3 (1%)	72 72	21, 33, 64, 92	0
1	Q	186/186 (100%)	-0.31	2 (1%)	80 81	23, 35, 64, 87	0
1	R	186/186 (100%)	-0.31	2 (1%)	80 81	24, 38, 63, 85	0
1	S	186/186 (100%)	0.30	14 (7%)	15 15	33, 51, 109, 121	0
1	T	186/186 (100%)	0.36	13 (6%)	17 18	40, 60, 96, 123	0
All	All	3720/3720 (100%)	-0.09	118 (3%)	48 49	21, 44, 79, 124	0

All (118) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	S	186	ILE	6.4
1	D	186	ILE	6.1
1	N	180	LEU	5.8
1	A	182	LEU	5.7
1	A	181	ASP	5.3
1	N	184	GLY	5.3
1	F	182	LEU	5.1
1	D	174	ALA	5.1
1	A	183	VAL	4.9
1	D	185	LYS	4.8
1	S	182	LEU	4.6
1	F	180	LEU	4.6
1	S	171	GLU	4.2
1	T	181	ASP	4.2
1	Q	186	ILE	4.1
1	C	174	ALA	3.9
1	T	183	VAL	3.9
1	D	86	GLU	3.7
1	S	161	PRO	3.7
1	T	185	LYS	3.7
1	N	185	LYS	3.6
1	T	186	ILE	3.6
1	C	182	LEU	3.6
1	F	186	ILE	3.6
1	S	159	ALA	3.5
1	I	181	ASP	3.4
1	N	181	ASP	3.4
1	A	185	LYS	3.4
1	T	86	GLU	3.4
1	S	172	GLY	3.4
1	C	185	LYS	3.2
1	A	180	LEU	3.2
1	C	181	ASP	3.2
1	S	174	ALA	3.2
1	J	181	ASP	3.1
1	M	58	GLU	3.1
1	D	183	VAL	3.1
1	D	171	GLU	3.1
1	D	67	VAL	3.0
1	F	181	ASP	3.0
1	D	182	LEU	3.0
1	P	161	PRO	2.9
1	I	185	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	Q	185	LYS	2.9
1	S	185	LYS	2.9
1	A	179	SER	2.9
1	I	186	ILE	2.8
1	S	181	ASP	2.8
1	M	67	VAL	2.8
1	A	186	ILE	2.8
1	A	172	GLY	2.7
1	T	179	SER	2.7
1	T	62	LYS	2.7
1	T	180	LEU	2.7
1	F	179	SER	2.6
1	J	182	LEU	2.6
1	J	172	GLY	2.6
1	N	186	ILE	2.6
1	T	182	LEU	2.6
1	F	174	ALA	2.6
1	C	186	ILE	2.6
1	N	159	ALA	2.6
1	C	170	LYS	2.5
1	I	183	VAL	2.5
1	J	86	GLU	2.5
1	M	161	PRO	2.5
1	D	181	ASP	2.5
1	P	181	ASP	2.5
1	R	181	ASP	2.4
1	O	161	PRO	2.4
1	N	86	GLU	2.4
1	G	185	LYS	2.4
1	L	180	LEU	2.4
1	S	180	LEU	2.4
1	F	172	GLY	2.4
1	L	182	LEU	2.4
1	M	86	GLU	2.3
1	M	182	LEU	2.3
1	C	86	GLU	2.3
1	G	182	LEU	2.3
1	C	123	VAL	2.3
1	P	185	LYS	2.3
1	G	186	ILE	2.3
1	I	124	VAL	2.3
1	C	62	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	179	SER	2.2
1	F	185	LYS	2.2
1	J	162	GLY	2.2
1	T	68	TYR	2.2
1	S	183	VAL	2.2
1	C	171	GLU	2.2
1	D	178	PRO	2.2
1	S	170	LYS	2.2
1	G	181	ASP	2.2
1	N	58	GLU	2.2
1	S	86	GLU	2.2
1	C	179	SER	2.2
1	N	178	PRO	2.2
1	B	181	ASP	2.1
1	E	180	LEU	2.1
1	H	161	PRO	2.1
1	L	181	ASP	2.1
1	J	186	ILE	2.1
1	T	170	LYS	2.1
1	I	161	PRO	2.1
1	M	181	ASP	2.1
1	B	172	GLY	2.1
1	M	96	ILE	2.1
1	B	161	PRO	2.1
1	R	186	ILE	2.0
1	T	34	VAL	2.0
1	E	162	GLY	2.0
1	S	168	LYS	2.0
1	F	96	ILE	2.0
1	G	96	ILE	2.0
1	D	34	VAL	2.0
1	T	58	GLU	2.0
1	E	170	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.