



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:51 AM UTC

PDB ID : 1N8J / pdb_00001n8j
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

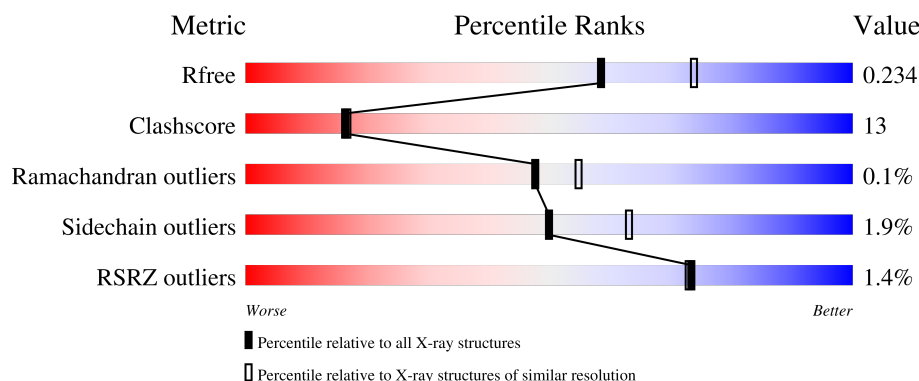
1 Overall quality at a glance

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.



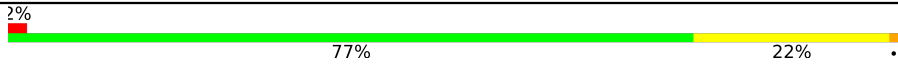
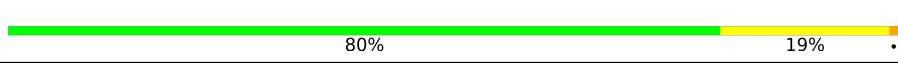
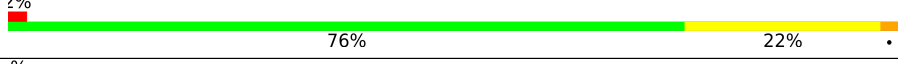
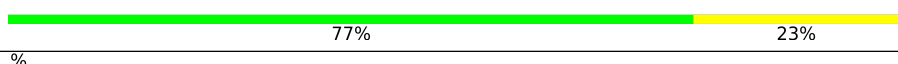
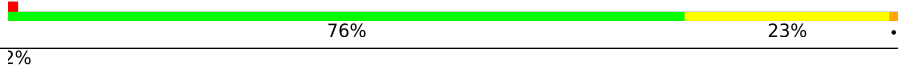
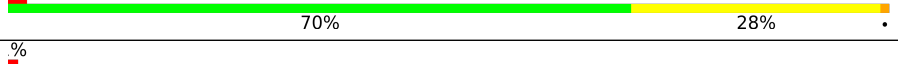
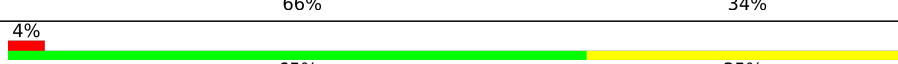
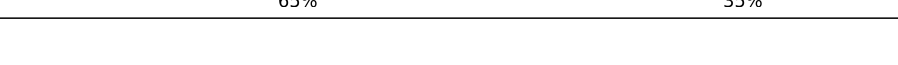
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	3% 71% 27% .
1	B	186	% 69% 30% .
1	C	186	2% 70% 28% .
1	D	186	2% 74% 24% .
1	E	186	74% 25% .

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Mol	Chain	Length	Quality of chain
1	F	186	
1	G	186	
1	H	186	
1	I	186	
1	J	186	
1	K	186	
1	L	186	
1	M	186	
1	N	186	
1	O	186	
1	P	186	
1	Q	186	
1	R	186	
1	S	186	
1	T	186	

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 mutation	UNP P0A251
B	46	SER	CYS	engineered mutation	UNP P0A251
C	46	SER	CYS	engineered mutation	UNP P0A251
D	46	SER	CYS	engineered mutation	UNP P0A251
E	46	SER	CYS	engineered mutation	UNP P0A251
F	46	SER	CYS	engineered mutation	UNP P0A251
G	46	SER	CYS	engineered mutation	UNP P0A251
H	46	SER	CYS	engineered mutation	UNP P0A251
I	46	SER	CYS	engineered mutation	UNP P0A251
J	46	SER	CYS	engineered mutation	UNP P0A251
K	46	SER	CYS	engineered mutation	UNP P0A251
L	46	SER	CYS	engineered mutation	UNP P0A251
M	46	SER	CYS	engineered mutation	UNP P0A251
N	46	SER	CYS	engineered mutation	UNP P0A251
O	46	SER	CYS	engineered mutation	UNP P0A251
P	46	SER	CYS	engineered mutation	UNP P0A251
Q	46	SER	CYS	engineered mutation	UNP P0A251
R	46	SER	CYS	engineered mutation	UNP P0A251
S	46	SER	CYS	engineered mutation	UNP P0A251
T	46	SER	CYS	engineered mutation	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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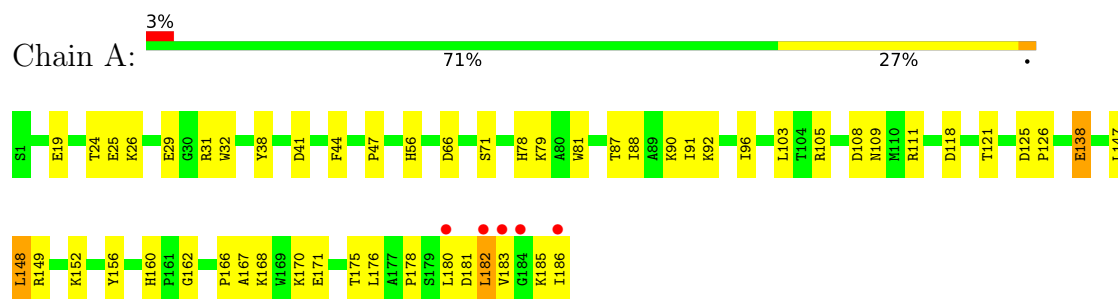
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	56	Total 56	O 56	0	0
2	E	77	Total 77	O 77	0	0
2	F	82	Total 82	O 82	0	0
2	G	94	Total 94	O 94	0	0
2	H	92	Total 92	O 92	0	0
2	I	72	Total 72	O 72	0	0
2	J	86	Total 86	O 86	0	0
2	K	106	Total 106	O 106	0	0
2	L	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

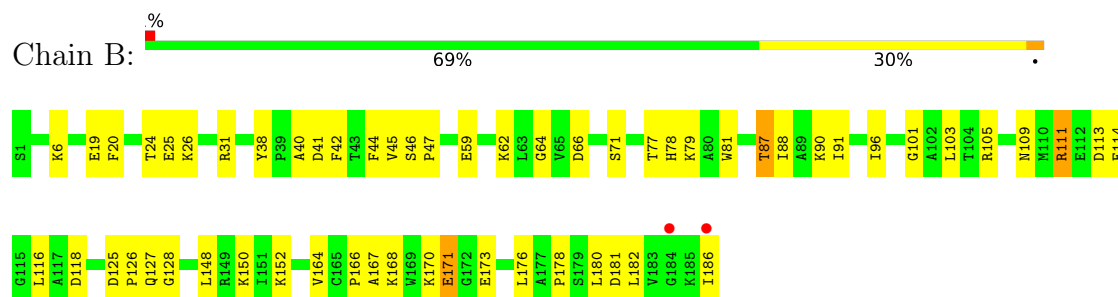
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

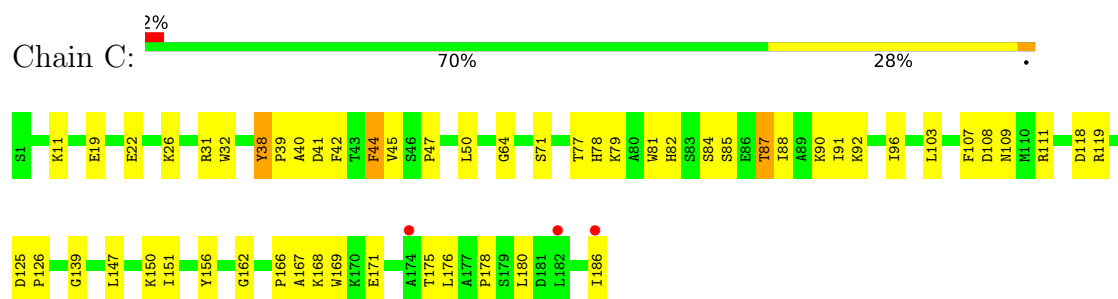
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



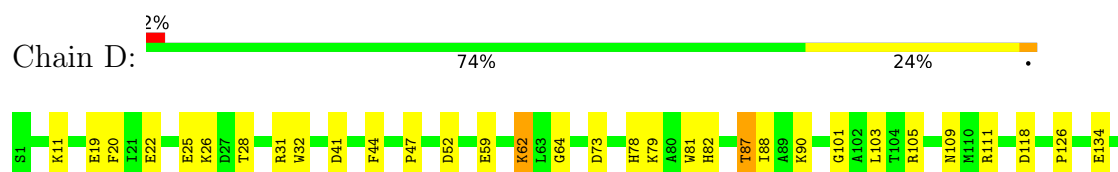
- Molecule 1: Alkyl hydroperoxide reductase C22 protein

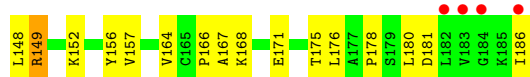


- Molecule 1: Alkyl hydroperoxide reductase C22 protein



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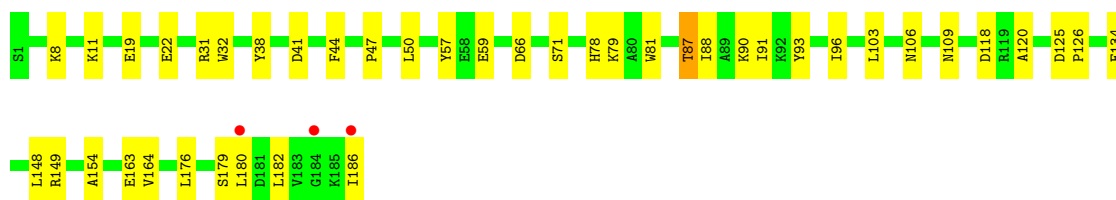
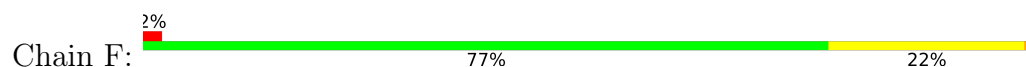




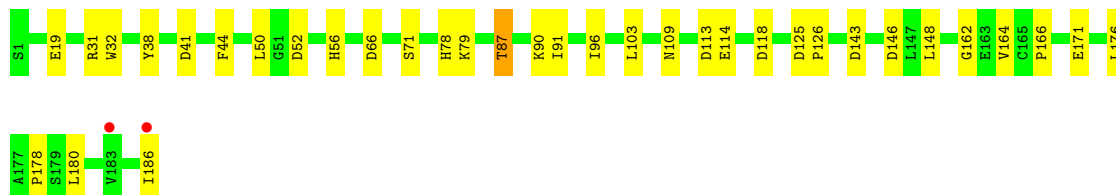
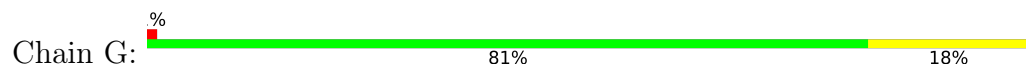
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



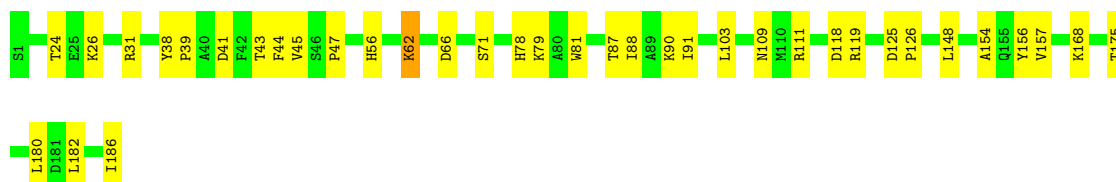
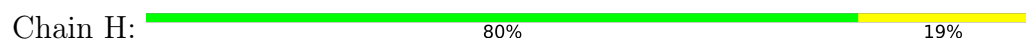
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- Molecule 1: Alkyl hydroperoxide reductase C22 protein

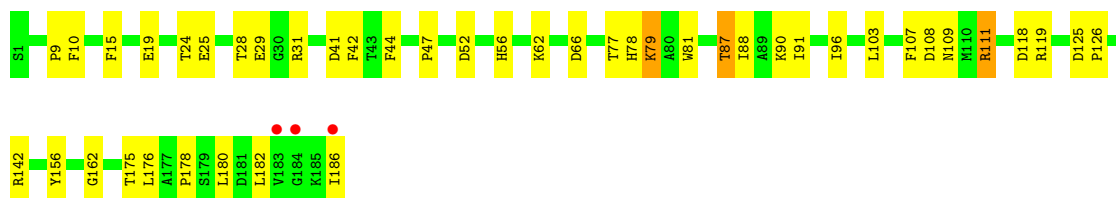


- Molecule 1: Alkyl hydroperoxide reductase C22 protein

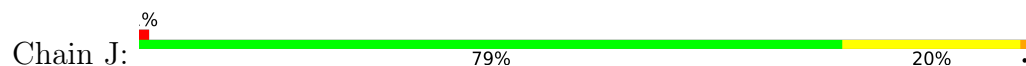


- Molecule 1: Alkyl hydroperoxide reductase C22 protein

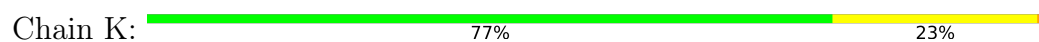




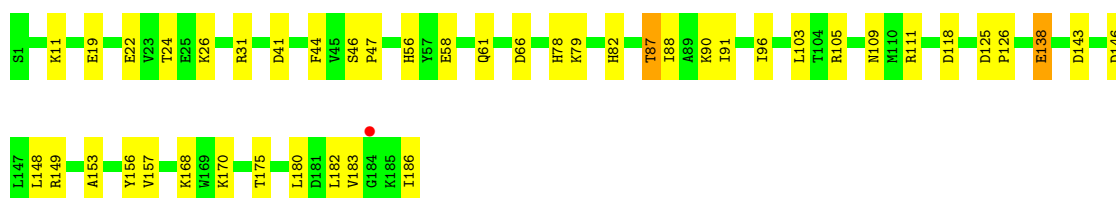
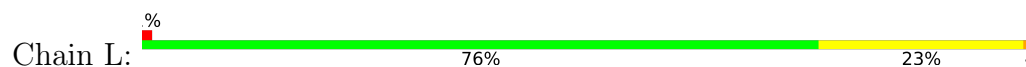
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



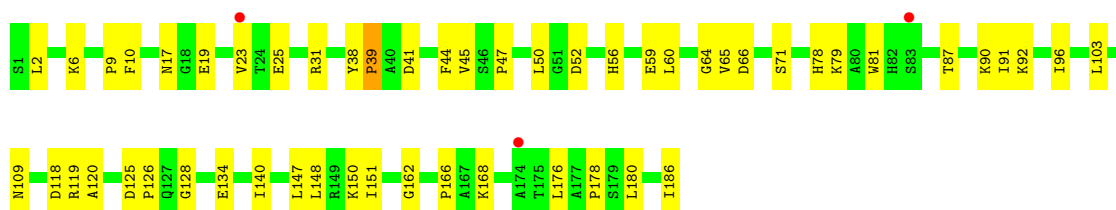
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



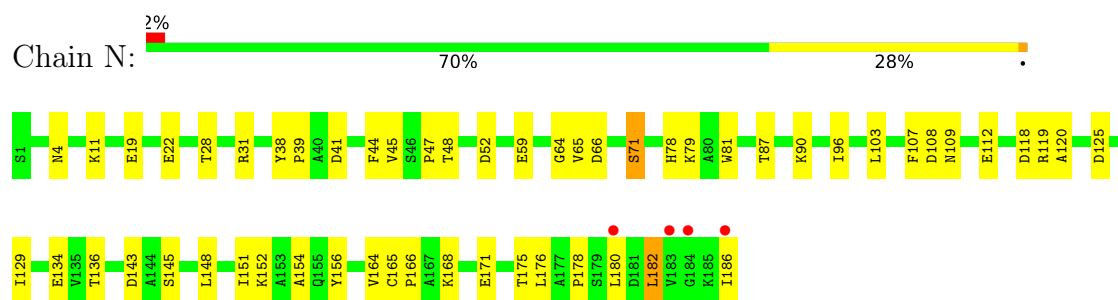
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



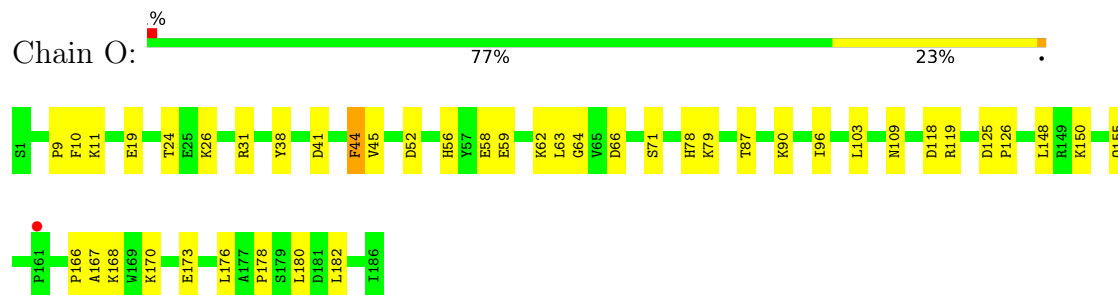
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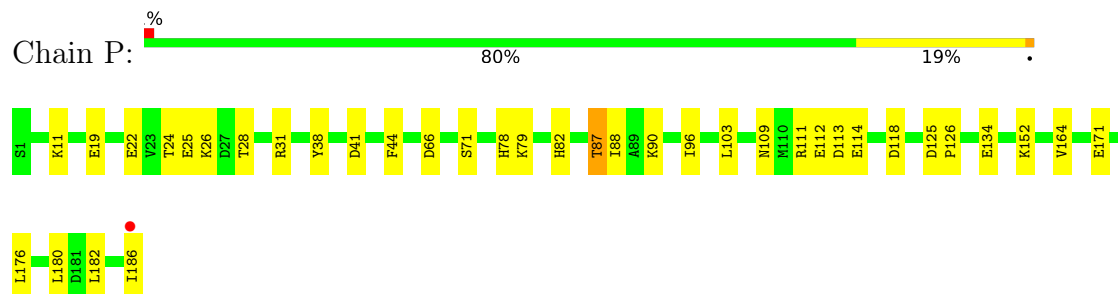
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



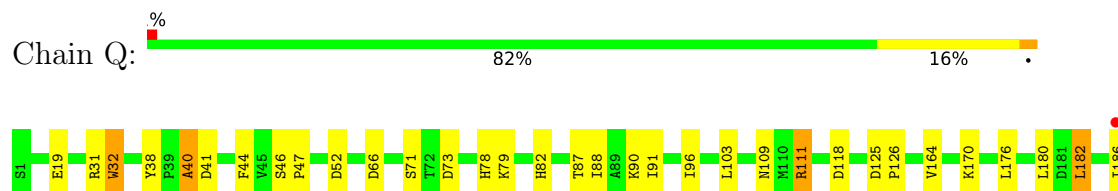
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



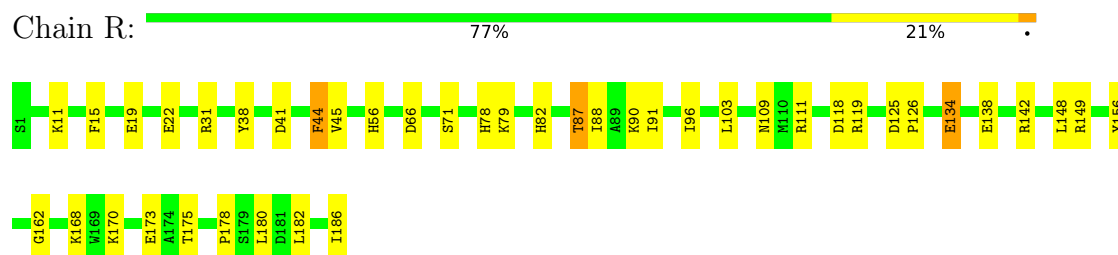
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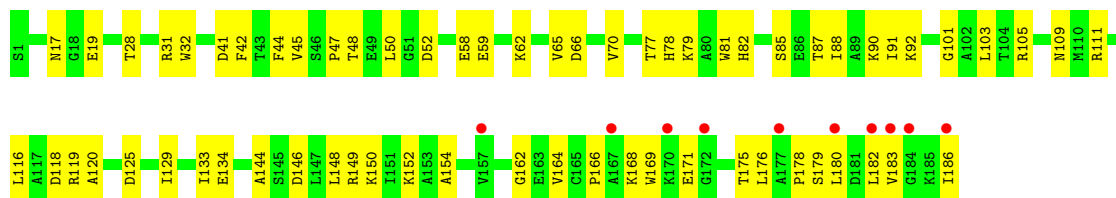
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



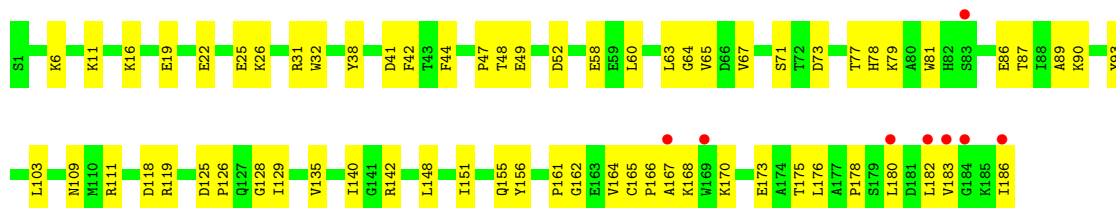
- Molecule 1: Alkyl hydroperoxide reductase C22 protein



- Molecule 1: Alkyl hydroperoxide reductase C22 protein



• Molecule 1: Alkyl hydroperoxide reductase C22 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	106.08Å 107.33Å 120.08Å 102.43° 116.22° 98.81°	Depositor
Resolution (Å)	19.99 – 2.17 19.99 – 2.17	Depositor EDS
% Data completeness (in resolution range)	89.3 (19.99-2.17) 89.2 (19.99-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.17Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.188 , 0.234 0.187 , 0.234	Depositor DCC
R_{free} test set	10527 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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 [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	0.46	0/1490	0.91	3/2019 (0.1%)
1	B	0.42	0/1490	0.89	2/2019 (0.1%)
1	C	0.40	0/1490	0.88	4/2019 (0.2%)
1	D	0.38	0/1490	0.88	2/2019 (0.1%)
1	E	0.43	0/1490	0.93	2/2019 (0.1%)
1	F	0.48	0/1490	0.92	1/2019 (0.0%)
1	G	0.52	0/1490	0.93	1/2019 (0.0%)
1	H	0.47	0/1490	0.93	2/2019 (0.1%)
1	I	0.45	0/1490	0.88	1/2019 (0.0%)
1	J	0.46	0/1490	0.88	1/2019 (0.0%)
1	K	0.50	0/1490	0.92	2/2019 (0.1%)
1	L	0.52	0/1490	0.91	0/2019
1	M	0.40	0/1490	0.88	0/2019
1	N	0.39	0/1490	0.86	1/2019 (0.0%)
1	O	0.47	0/1490	0.93	1/2019 (0.0%)
1	P	0.52	0/1490	0.95	1/2019 (0.0%)
1	Q	0.50	0/1490	0.92	4/2019 (0.2%)
1	R	0.49	0/1490	0.90	1/2019 (0.0%)
1	S	0.40	0/1490	0.86	1/2019 (0.0%)
1	T	0.38	0/1490	0.87	2/2019 (0.1%)
All	All	0.45	0/29800	0.90	32/40380 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	19	GLU	N-CA-C	6.56	119.39	109.41
1	A	32	TRP	N-CA-C	-6.42	100.05	110.20
1	C	44	PHE	N-CA-C	5.96	120.08	111.02
1	Q	111	ARG	N-CA-C	-5.87	97.66	107.99
1	S	70	VAL	N-CA-C	5.87	116.74	108.17
1	R	44	PHE	N-CA-C	5.81	120.08	112.13
1	B	111	ARG	N-CA-C	-5.79	97.81	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	112	GLU	N-CA-C	5.76	117.56	111.28
1	D	111	ARG	N-CA-C	-5.75	97.88	107.99
1	F	44	PHE	N-CA-C	5.70	119.94	112.13
1	K	32	TRP	N-CA-C	-5.65	100.47	109.96
1	Q	73	ASP	N-CA-C	-5.61	103.29	110.53
1	H	39	PRO	N-CA-C	5.59	121.46	113.47
1	O	44	PHE	N-CA-C	5.57	119.81	111.96
1	T	111	ARG	N-CA-C	-5.51	98.29	107.99
1	C	38	TYR	CA-C-N	5.46	126.66	119.84
1	C	38	TYR	C-N-CA	5.46	126.66	119.84
1	K	106	ASN	N-CA-C	-5.40	105.39	111.28
1	C	84	SER	N-CA-C	5.38	119.69	113.18
1	G	32	TRP	N-CA-C	-5.33	101.01	109.96
1	A	160	HIS	CA-C-N	5.31	125.23	119.76
1	A	160	HIS	C-N-CA	5.31	125.23	119.76
1	D	73	ASP	N-CA-C	-5.30	103.70	110.53
1	H	111	ARG	N-CA-C	-5.28	98.70	107.99
1	Q	32	TRP	N-CA-C	-5.23	101.93	110.20
1	Q	40	ALA	N-CA-C	5.23	117.02	108.76
1	B	40	ALA	N-CA-C	5.15	116.90	108.76
1	T	73	ASP	N-CA-C	-5.15	103.89	110.53
1	N	112	GLU	N-CA-C	5.13	117.54	111.33
1	I	111	ARG	N-CA-C	-5.13	98.96	107.99
1	J	96	ILE	N-CA-C	5.12	116.17	109.21
1	E	112	GLU	N-CA-C	5.09	117.49	111.33

There are no chirality outliers.

There are no planarity outliers.

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	1456	0	1418	45	0
1	B	1456	0	1418	53	0
1	C	1456	0	1418	52	0
1	D	1456	0	1418	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1456	0	1418	47	0
1	F	1456	0	1418	41	0
1	G	1456	0	1418	32	0
1	H	1456	0	1418	31	0
1	I	1456	0	1418	38	0
1	J	1456	0	1418	36	0
1	K	1456	0	1418	40	0
1	L	1456	0	1418	42	0
1	M	1456	0	1418	54	0
1	N	1456	0	1418	45	0
1	O	1456	0	1418	36	0
1	P	1456	0	1418	33	0
1	Q	1456	0	1418	37	0
1	R	1456	0	1418	37	0
1	S	1456	0	1418	70	0
1	T	1456	0	1418	71	0
2	A	77	0	0	3	0
2	B	71	0	0	4	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	745	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 (745) 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
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:B:79:LYS:HE2	1:F:180:LEU:O	1.85	0.76
1:C:41:ASP:OD2	1:C:78:HIS:HD2	1.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:109:ASN:HD21	1:P:118:ASP:HB2	1.49	0.75
1:A:180:LEU:O	1:E:79:LYS:HE2	1.86	0.75
1:E:24:THR:OG1	1:E:26:LYS:HD3	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:L:19:GLU:HA	1:P:180:LEU:HD13	1.70	0.73
1:N:41:ASP:OD2	1:N:78:HIS:HD2	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:11:LYS:HE3	1:T:22:GLU:CD	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:87:THR:O	1:I:90:LYS:HG2	1.91	0.70
1:I:109:ASN:ND2	1:I:118:ASP:HB2	2.05	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:S:79:LYS:HD3	1:S:79:LYS:C	2.17	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:D:41:ASP:OD2	1:D:78:HIS:HD2	1.75	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: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: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:HD23	1:S:182:LEU:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:P:182:LEU:O	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:44:PHE:C	1:D:47:PRO:HD2	2.26	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
1:R:88:ILE:HG23	1:R:91:ILE:HD12	1.85	0.58
1:B:109:ASN:HD21	1:B:118:ASP:HB2	1.69	0.58
1:B:111:ARG:HG3	1:B:116:LEU:O	2.03	0.58
1:G:44:PHE:HA	1:H:186:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:E:26:LYS:HD2	1.70	0.57
1:M:125:ASP:HB2	1:M:126:PRO:CD	2.34	0.57
1:I:44:PHE:C	1:I:47:PRO:HD2	2.30	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:J:44:PHE:C	1:J:47:PRO:HD2	2.29	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:B:44:PHE:C	1:B:47:PRO:HD2	2.31	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:G:52:ASP:CG	1:H:168:LYS:HD2	2.31	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: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:82:HIS:HD2	2:P:1011:HOH:O	1.88	0.55
1:P:111:ARG:HG2	1:P:118:ASP:OD2	2.07	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:HG22	1:J:186:ILE:OXT	2.08	0.54
1:O:44:PHE:CD1	1:P:182:LEU:HD22	2.40	0.53
1:P:125:ASP:HB2	1:P:126:PRO:CD	2.37	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
1:J:31:ARG:HD3	1:J:66:ASP:OD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:44:PHE:C	1:N:47:PRO:HD2	2.33	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:C:168:LYS:HD2	1:D:52:ASP:CG	2.33	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:Q:79:LYS:CE	1:T:183:VAL:HB	2.38	0.52
1:R:109:ASN:HD21	1:R:118:ASP:HB2	1.74	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: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:50:LEU:HB3	1:M:91:ILE:HD11	1.91	0.52
1:M:79:LYS:HD2	1:S:180:LEU:HD21	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:P:152:LYS:HD3	1:P:171:GLU:CD	2.35	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:H:180:LEU:HD23	1:H:180:LEU:C	2.35	0.51
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: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: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:A:181:ASP:C	1:A:183:VAL:H	2.18	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:19:GLU:HA	1:G:180:LEU:CD1	2.39	0.51
1:F:149:ARG:HD2	2:F:194:HOH:O	2.11	0.51
1:J:156:TYR:CE2	1:J:175:THR:HG21	2.46	0.51
1:M:31:ARG:HH11	1:M:66:ASP:CG	2.19	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: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:A:111:ARG:HH22	1:A:138:GLU:CD	2.20	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: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:R:125:ASP:OD1	1:R:125:ASP:C	2.54	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:78:HIS:HE1	1:B:96:ILE:O	1.94	0.49
1:B:125:ASP:HB2	1:B:126:PRO:HD2	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:25:GLU:HG2	1:T:26:LYS:N	2.27	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:I:180:LEU:C	1:I:180:LEU:HD23	2.38	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:Q:186:ILE:OXT	1:Q:186:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:19:GLU:HA	1:P:180:LEU:CD1	2.41	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:T:44:PHE:C	1:T:47:PRO:HD2	2.38	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:N:11:LYS:HZ2	1:N:22:GLU:CD	2.22	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:O	1:F:180:LEU:HD23	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:HD2	1:O:26:LYS:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HG23	1:B:91:ILE:HD12	1.97	0.47
1:L:79:LYS:HD2	1:P:180:LEU:HG	1.96	0.47
1:L:105:ARG:NH1	2:L:852:HOH:O	2.44	0.47
1:M:109:ASN:OD1	1:M:120:ALA:HB3	2.13	0.47
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: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:S:152:LYS:HD3	1:S:171:GLU:CD	2.39	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:HG22	1:F:186:ILE:OXT	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:NZ	1:C:92:LYS:HB3	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: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:168:LYS:HD2	1:N:52:ASP:CG	2.40	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:K:52:ASP:CG	1:L:168:LYS:HD2	2.41	0.46
1:M:39:PRO:C	2:M:1326:HOH:O	2.59	0.46
1:C:109:ASN:ND2	1:C:118:ASP:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:180:LEU:HD23	1:M:180:LEU:C	2.41	0.46
1:Q:38:TYR:CZ	1:Q:71:SER:HB3	2.50	0.46
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:A:181:ASP:HB3	1:A:185:LYS:HZ2	1.80	0.46
1:G:78:HIS:HE1	1:G:96:ILE:O	1.99	0.46
1:G:164:VAL:HG23	1:G:176:LEU:HB2	1.97	0.46
1:G:166:PRO:HG3	1:G:176:LEU:HG	1.98	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:E:111:ARG:HG2	1:E:118:ASP:OD2	2.17	0.45
1:L:125:ASP:OD1	1:L:125:ASP:C	2.58	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:32:TRP:HB2	1:S:65:VAL:HG22	1.98	0.45
1:S:176:LEU:HD13	1:T:44:PHE:HB3	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:A:185:LYS:O	1:A:186:ILE:C	2.60	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:F:180:LEU:HD23	1:F:180:LEU:C	2.42	0.45
1:G:38:TYR:CZ	1:G:71:SER:HB3	2.52	0.45
1:G:125:ASP:HB2	1:G:126:PRO:CD	2.47	0.45
1:A:38:TYR:CZ	1:A:71:SER:HB3	2.52	0.45
1:B:20:PHE:H	1:F:180:LEU:CD1	2.30	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:Q:44:PHE:C	1:Q:47:PRO:HD2	2.42	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:65:VAL:HG21	1:T:151:ILE:HG21	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:125:ASP:C	1:I:125:ASP:OD1	2.60	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:S:79:LYS:C	1:S:79:LYS:CD	2.90	0.45
1:C:85:SER:HB3	1:C:88:ILE:HB	1.99	0.44
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:44:PHE:C	1:S:47:PRO:HD2	2.41	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:Q:170:LYS:HE3	2:Q:806:HOH:O	2.17	0.44
1:C:11:LYS:HE3	1:C:22:GLU:CD	2.41	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:31:ARG:HH22	1:M:64:GLY:HA2	1.82	0.44
1:M:119:ARG:HG2	1:M:119:ARG:NH1	2.33	0.44
1:K:125:ASP:HB2	1:K:126:PRO:HD2	1.99	0.44
1:S:180:LEU:C	1:S:180:LEU:HD23	2.43	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:M:79:LYS:HE2	1:S:180:LEU:O	2.17	0.44
1:Q:87:THR:O	1:Q:90:LYS:HG2	2.18	0.44
1:F:81:TRP:CE2	1:F:88:ILE:HG13	2.53	0.43
1:L:11:LYS:HE3	1:L:22:GLU:CD	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:TYR:CZ	1:H:71:SER:HB3	2.53	0.43
1:H:44:PHE:C	1:H:47:PRO:HD2	2.43	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:C:44:PHE:C	1:C:47:PRO:HD2	2.44	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:K:44:PHE:C	1:K:47:PRO:HD2	2.43	0.43
1:O:63:LEU:HD22	1:O:155:GLN:HE22	1.82	0.43
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:Q:52:ASP:CG	1:R:168:LYS:HD2	2.43	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:N:107:PHE:O	1:N:108:ASP:C	2.61	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:D:11:LYS:NZ	1:D:22:GLU:OE2	2.49	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:19:GLU:CA	1:F:180:LEU:HD11	2.39	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:181:ASP:C	1:A:183:VAL:N	2.77	0.42
1:N:164:VAL:CG2	1:N:176:LEU:HB2	2.50	0.42
1:B:25:GLU:OE1	1:B:25:GLU:N	2.51	0.42
1:C:40:ALA:HB1	2:C:208:HOH:O	2.19	0.42
1:C:107:PHE:O	1:C:108:ASP:C	2.62	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:20:PHE:H	1:F:180:LEU:HD12	1.85	0.42
1:B:41:ASP:OD2	1:B:78:HIS:CD2	2.64	0.42
1:B:111:ARG:CD	1:B:118:ASP:OD2	2.64	0.42
1:I:107:PHE:O	1:I:108:ASP:C	2.62	0.42
1:J:119:ARG:HH11	1:J:119:ARG:HG2	1.83	0.42
1:L:24:THR:OG1	1:L:26:LYS:HB2	2.20	0.42
1:L:111:ARG:HH22	1:L:138:GLU:HB2	1.84	0.42
1:N:164:VAL:HG23	1:N:176:LEU:HB2	2.00	0.42
1:N:166:PRO:HG3	1:N:176:LEU:HG	2.01	0.42
1:M:52:ASP:CG	1:N:168:LYS:HD2	2.44	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:F:32:TRP:CE2	1:F:126:PRO:HD3	2.55	0.42
1:M:19:GLU:HA	1:S:180:LEU:HD11	2.00	0.42
1:M:147:LEU:O	1:M:151:ILE:HG13	2.19	0.42
1:N:182:LEU:HD22	1:N:186:ILE:HD11	2.02	0.42
1:S:168:LYS:HD2	1:T:52:ASP:CG	2.45	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:B:150:LYS:NZ	2:B:233:HOH:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:PRO:HA	1:M:25:GLU:HB3	2.02	0.42
1:M:120:ALA:HA	1:M:134:GLU:O	2.19	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:E:44:PHE:C	1:E:47:PRO:HD2	2.45	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:OXT	1:G:186:ILE:HG22	2.20	0.41
1:H:109:ASN:ND2	1:H:118:ASP:HB2	2.35	0.41
1:K:81:TRP:CD2	1:K:88:ILE:HG13	2.55	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:S:154:ALA:CA	1:T:140:ILE:HD11	2.45	0.41
1:T:6:LYS:HA	1:T:128:GLY:O	2.21	0.41
1:J:32:TRP:CE2	1:J:126:PRO:HD3	2.55	0.41
1:O:10:PHE:O	1:O:24:THR:HA	2.20	0.41
1:O:178:PRO:HB3	1:P:44:PHE:CE2	2.55	0.41
1:P:25:GLU:OE2	1:P:26:LYS:HD2	2.20	0.41
1:S:44:PHE:CE2	1:T:178:PRO:HB3	2.55	0.41
1:S:101:GLY:O	1:S:105:ARG:HG3	2.20	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:G:180:LEU:C	1:G:180:LEU:HD23	2.45	0.41
1:T:86:GLU:O	1:T:89:ALA:HB3	2.20	0.41
1:T:119:ARG:HG2	1:T:142:ARG:HH21	1.84	0.41
1:K:46:SER:HB2	1:K:47:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LYS:HD3	1:B:171:GLU:CD	2.46	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: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:K:42:PHE:O	1:L:183:VAL:HG13	2.20	0.41
1:L:125:ASP:HB2	1:L:126:PRO:CD	2.51	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:H:43:THR:O	1:H:47:PRO:HG2	2.21	0.41
1:I:41:ASP:OD2	1:I:77:THR:HG22	2.20	0.41
1:L:11:LYS:HE3	1:L:22:GLU:OE2	2.21	0.41
1:L:56:HIS:HB3	1:L:148:LEU:HD11	2.02	0.41
1:O:180:LEU:CD2	1:R:79:LYS:HD2	2.51	0.41
1:D:25:GLU:OE2	1:D:26:LYS:HD2	2.21	0.41
1:D:32:TRP:CE2	1:D:126:PRO:HD3	2.56	0.41
1:M:44:PHE:CE2	1:N:178:PRO:HB3	2.56	0.41
1:C:31:ARG:NH2	1:C:64:GLY:HA2	2.36	0.40
1:C:42:PHE:HE1	1:C:77:THR:HG23	1.86	0.40
1:C:111:ARG:HG2	1:C:118:ASP:CG	2.46	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:Q:79:LYS:CD	1:T:180:LEU:HG	2.46	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:B:45:VAL:C	1:B:47:PRO:HD2	2.47	0.40
1:B:180:LEU:HD12	1:D:20:PHE:CD2	2.57	0.40
1:C:180:LEU:C	1:C:180:LEU:HD23	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	184/186 (99%)	177 (96%)	6 (3%)	1 (0%)	24	25
1	B	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
1	C	184/186 (99%)	177 (96%)	6 (3%)	1 (0%)	24	25
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%)	11	9
1	N	184/186 (99%)	179 (97%)	4 (2%)	1 (0%)	24	25
1	O	184/186 (99%)	179 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48	55

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%)	34	43
1	B	154/154 (100%)	150 (97%)	4 (3%)	40	51
1	C	154/154 (100%)	152 (99%)	2 (1%)	61	74
1	D	154/154 (100%)	149 (97%)	5 (3%)	34	43
1	E	154/154 (100%)	151 (98%)	3 (2%)	50	63
1	F	154/154 (100%)	152 (99%)	2 (1%)	61	74
1	G	154/154 (100%)	151 (98%)	3 (2%)	50	63
1	H	154/154 (100%)	152 (99%)	2 (1%)	61	74
1	I	154/154 (100%)	151 (98%)	3 (2%)	50	63
1	J	154/154 (100%)	152 (99%)	2 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	154/154 (100%)	151 (98%)	3 (2%)	50	63
1	L	154/154 (100%)	150 (97%)	4 (3%)	40	51
1	M	154/154 (100%)	152 (99%)	2 (1%)	61	74
1	N	154/154 (100%)	150 (97%)	4 (3%)	40	51
1	O	154/154 (100%)	151 (98%)	3 (2%)	50	63
1	P	154/154 (100%)	152 (99%)	2 (1%)	61	74
1	Q	154/154 (100%)	152 (99%)	2 (1%)	61	74
1	R	154/154 (100%)	150 (97%)	4 (3%)	40	51
1	S	154/154 (100%)	152 (99%)	2 (1%)	61	74
1	T	154/154 (100%)	153 (99%)	1 (1%)	78	87
All	All	3080/3080 (100%)	3022 (98%)	58 (2%)	50	63

All (58) 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
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	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

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Mol	Chain	Res	Type
1	G	171	GLU
1	H	62	LYS
1	H	103	LEU
1	I	79	LYS
1	I	87	THR
1	I	103	LEU
1	J	11	LYS
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	92	LYS
1	M	103	LEU
1	N	4	ASN
1	N	71	SER
1	N	103	LEU
1	N	182	LEU
1	O	11	LYS
1	O	103	LEU
1	O	182	LEU
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	182	LEU
1	S	58	GLU
1	S	103	LEU
1	T	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	61	GLN
1	A	78	HIS

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Mol	Chain	Res	Type
1	A	82	HIS
1	A	109	ASN
1	A	155	GLN
1	B	4	ASN
1	B	75	HIS
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	56	HIS
1	D	78	HIS
1	D	109	ASN
1	D	155	GLN
1	D	160	HIS
1	E	17	ASN
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	61	GLN
1	F	78	HIS
1	F	82	HIS
1	F	109	ASN
1	F	127	GLN
1	F	155	GLN
1	G	61	GLN
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

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Mol	Chain	Res	Type
1	H	78	HIS
1	H	109	ASN
1	H	127	GLN
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	78	HIS
1	J	109	ASN
1	J	155	GLN
1	J	160	HIS
1	K	4	ASN
1	K	61	GLN
1	K	78	HIS
1	K	82	HIS
1	K	109	ASN
1	K	127	GLN
1	K	155	GLN
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	61	GLN
1	M	109	ASN
1	M	127	GLN
1	M	160	HIS
1	N	4	ASN
1	N	56	HIS
1	N	61	GLN
1	N	78	HIS
1	N	109	ASN
1	N	127	GLN
1	N	155	GLN
1	O	78	HIS
1	O	82	HIS

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Mol	Chain	Res	Type
1	O	109	ASN
1	O	155	GLN
1	O	160	HIS
1	P	61	GLN
1	P	78	HIS
1	P	82	HIS
1	P	109	ASN
1	P	127	GLN
1	P	155	GLN
1	P	160	HIS
1	Q	61	GLN
1	Q	78	HIS
1	Q	109	ASN
1	Q	127	GLN
1	Q	155	GLN
1	Q	160	HIS
1	R	61	GLN
1	R	78	HIS
1	R	82	HIS
1	R	109	ASN
1	R	127	GLN
1	S	4	ASN
1	S	17	ASN
1	S	109	ASN
1	S	155	GLN
1	T	78	HIS
1	T	109	ASN
1	T	155	GLN
1	T	160	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	186/186 (100%)	-0.24	5 (2%) 56 55	27, 41, 85, 124	0
1	B	186/186 (100%)	-0.19	2 (1%) 78 77	28, 47, 73, 92	0
1	C	186/186 (100%)	0.04	3 (1%) 70 70	32, 49, 85, 109	0
1	D	186/186 (100%)	0.08	4 (2%) 62 61	30, 53, 94, 116	0
1	E	186/186 (100%)	-0.21	0 100 100	27, 46, 68, 95	0
1	F	186/186 (100%)	-0.35	3 (1%) 70 70	23, 37, 83, 113	0
1	G	186/186 (100%)	-0.47	2 (1%) 78 77	24, 35, 63, 87	0
1	H	186/186 (100%)	-0.49	0 100 100	24, 36, 62, 82	0
1	I	186/186 (100%)	-0.20	3 (1%) 70 70	28, 43, 84, 106	0
1	J	186/186 (100%)	-0.34	2 (1%) 78 77	25, 39, 74, 100	0
1	K	186/186 (100%)	-0.47	0 100 100	22, 35, 60, 86	0
1	L	186/186 (100%)	-0.46	1 (0%) 87 86	23, 35, 66, 89	0
1	M	186/186 (100%)	0.35	3 (1%) 70 70	38, 58, 83, 95	0
1	N	186/186 (100%)	0.22	4 (2%) 62 61	35, 56, 87, 110	0
1	O	186/186 (100%)	-0.32	1 (0%) 87 86	22, 40, 67, 80	0
1	P	186/186 (100%)	-0.56	1 (0%) 87 86	21, 33, 64, 92	0
1	Q	186/186 (100%)	-0.47	1 (0%) 87 86	23, 35, 64, 87	0
1	R	186/186 (100%)	-0.42	0 100 100	24, 38, 63, 85	0
1	S	186/186 (100%)	0.29	10 (5%) 31 30	33, 51, 109, 121	0
1	T	186/186 (100%)	0.51	8 (4%) 40 39	40, 60, 96, 123	0
All	All	3720/3720 (100%)	-0.18	53 (1%) 73 73	21, 44, 79, 124	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	4.3
1	S	186	ILE	4.3
1	T	186	ILE	4.0
1	T	183	VAL	3.9
1	S	184	GLY	3.9
1	D	186	ILE	3.9
1	T	184	GLY	3.7
1	A	184	GLY	3.5
1	N	180	LEU	3.5
1	A	186	ILE	3.4
1	D	183	VAL	3.4
1	A	182	LEU	3.4
1	D	184	GLY	3.2
1	N	183	VAL	3.2
1	N	184	GLY	3.1
1	S	183	VAL	3.1
1	N	186	ILE	3.1
1	C	186	ILE	3.0
1	J	186	ILE	3.0
1	Q	186	ILE	3.0
1	S	177	ALA	2.9
1	I	183	VAL	2.7
1	T	180	LEU	2.6
1	S	167	ALA	2.6
1	S	182	LEU	2.6
1	A	180	LEU	2.6
1	I	184	GLY	2.5
1	L	184	GLY	2.5
1	I	186	ILE	2.5
1	F	184	GLY	2.4
1	C	174	ALA	2.3
1	F	186	ILE	2.3
1	T	182	LEU	2.3
1	B	186	ILE	2.3
1	P	186	ILE	2.2
1	T	83	SER	2.2
1	S	172	GLY	2.2
1	F	180	LEU	2.2
1	S	180	LEU	2.2
1	M	174	ALA	2.1
1	G	183	VAL	2.1
1	T	167	ALA	2.1
1	C	182	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	184	GLY	2.1
1	J	182	LEU	2.1
1	M	83	SER	2.1
1	O	161	PRO	2.1
1	M	23	VAL	2.1
1	S	157	VAL	2.1
1	D	182	LEU	2.0
1	S	170	LYS	2.0
1	G	186	ILE	2.0
1	T	169	TRP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.