Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 10:17 AM EDT

PDB ID	:	3IWP
Title	:	Crystal structure of human copper homeostasis protein CutC
Authors	:	Li, Y.; Du, J.; Zhang, P.; Ding, J.
Deposited on	:	2009-09-03
Resolution	:	2.50 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:

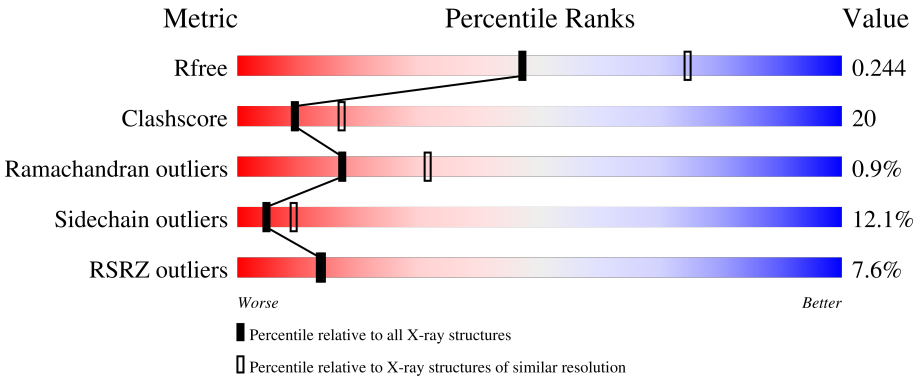
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	287	3% 47% 32% 8% 13%
1	B	287	% 57% 23% 6% 15%
1	C	287	% 58% 23% • 14%
1	D	287	% 48% 28% 9% 15%
1	E	287	6% 55% 25% 5% 16%

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Mol	Chain	Length	Quality of chain
1	F	287	4% 47% 31% 5% 16%
1	G	287	10% 53% 25% 5% 17%
1	H	287	10% 51% 27% 18%
1	I	287	5% 56% 27% 16%
1	J	287	7% 55% 24% 17%
1	K	287	10% 52% 27% 17%
1	L	287	18% 54% 28% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22740 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 Copper homeostasis protein cutC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1870	1166	329	357	18			
1	B	244	Total	C	N	O	S	0	0	0
			1837	1145	324	350	18			
1	C	247	Total	C	N	O	S	0	0	0
			1856	1157	327	354	18			
1	D	245	Total	C	N	O	S	0	0	0
			1843	1150	324	351	18			
1	E	242	Total	C	N	O	S	0	0	0
			1825	1138	322	348	17			
1	F	241	Total	C	N	O	S	0	0	0
			1817	1135	320	345	17			
1	G	237	Total	C	N	O	S	0	0	0
			1792	1119	317	340	16			
1	H	236	Total	C	N	O	S	0	0	0
			1779	1111	315	337	16			
1	I	241	Total	C	N	O	S	0	0	0
			1822	1138	321	347	16			
1	J	239	Total	C	N	O	S	0	0	0
			1807	1129	318	344	16			
1	K	238	Total	C	N	O	S	0	0	0
			1800	1127	317	340	16			
1	L	239	Total	C	N	O	S	0	0	0
			1804	1129	318	341	16			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q9NTM9
A	-12	ARG	-	expression tag	UNP Q9NTM9
A	-11	GLY	-	expression tag	UNP Q9NTM9
A	-10	SER	-	expression tag	UNP Q9NTM9
A	-9	HIS	-	expression tag	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP Q9NTM9
A	-7	HIS	-	expression tag	UNP Q9NTM9
A	-6	HIS	-	expression tag	UNP Q9NTM9
A	-5	HIS	-	expression tag	UNP Q9NTM9
A	-4	HIS	-	expression tag	UNP Q9NTM9
A	-3	GLY	-	expression tag	UNP Q9NTM9
A	-2	SER	-	expression tag	UNP Q9NTM9
A	-1	ALA	-	expression tag	UNP Q9NTM9
A	0	CYS	-	expression tag	UNP Q9NTM9
B	-13	MET	-	expression tag	UNP Q9NTM9
B	-12	ARG	-	expression tag	UNP Q9NTM9
B	-11	GLY	-	expression tag	UNP Q9NTM9
B	-10	SER	-	expression tag	UNP Q9NTM9
B	-9	HIS	-	expression tag	UNP Q9NTM9
B	-8	HIS	-	expression tag	UNP Q9NTM9
B	-7	HIS	-	expression tag	UNP Q9NTM9
B	-6	HIS	-	expression tag	UNP Q9NTM9
B	-5	HIS	-	expression tag	UNP Q9NTM9
B	-4	HIS	-	expression tag	UNP Q9NTM9
B	-3	GLY	-	expression tag	UNP Q9NTM9
B	-2	SER	-	expression tag	UNP Q9NTM9
B	-1	ALA	-	expression tag	UNP Q9NTM9
B	0	CYS	-	expression tag	UNP Q9NTM9
C	-13	MET	-	expression tag	UNP Q9NTM9
C	-12	ARG	-	expression tag	UNP Q9NTM9
C	-11	GLY	-	expression tag	UNP Q9NTM9
C	-10	SER	-	expression tag	UNP Q9NTM9
C	-9	HIS	-	expression tag	UNP Q9NTM9
C	-8	HIS	-	expression tag	UNP Q9NTM9
C	-7	HIS	-	expression tag	UNP Q9NTM9
C	-6	HIS	-	expression tag	UNP Q9NTM9
C	-5	HIS	-	expression tag	UNP Q9NTM9
C	-4	HIS	-	expression tag	UNP Q9NTM9
C	-3	GLY	-	expression tag	UNP Q9NTM9
C	-2	SER	-	expression tag	UNP Q9NTM9
C	-1	ALA	-	expression tag	UNP Q9NTM9
C	0	CYS	-	expression tag	UNP Q9NTM9
D	-13	MET	-	expression tag	UNP Q9NTM9
D	-12	ARG	-	expression tag	UNP Q9NTM9
D	-11	GLY	-	expression tag	UNP Q9NTM9
D	-10	SER	-	expression tag	UNP Q9NTM9
D	-9	HIS	-	expression tag	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP Q9NTM9
D	-7	HIS	-	expression tag	UNP Q9NTM9
D	-6	HIS	-	expression tag	UNP Q9NTM9
D	-5	HIS	-	expression tag	UNP Q9NTM9
D	-4	HIS	-	expression tag	UNP Q9NTM9
D	-3	GLY	-	expression tag	UNP Q9NTM9
D	-2	SER	-	expression tag	UNP Q9NTM9
D	-1	ALA	-	expression tag	UNP Q9NTM9
D	0	CYS	-	expression tag	UNP Q9NTM9
E	-13	MET	-	expression tag	UNP Q9NTM9
E	-12	ARG	-	expression tag	UNP Q9NTM9
E	-11	GLY	-	expression tag	UNP Q9NTM9
E	-10	SER	-	expression tag	UNP Q9NTM9
E	-9	HIS	-	expression tag	UNP Q9NTM9
E	-8	HIS	-	expression tag	UNP Q9NTM9
E	-7	HIS	-	expression tag	UNP Q9NTM9
E	-6	HIS	-	expression tag	UNP Q9NTM9
E	-5	HIS	-	expression tag	UNP Q9NTM9
E	-4	HIS	-	expression tag	UNP Q9NTM9
E	-3	GLY	-	expression tag	UNP Q9NTM9
E	-2	SER	-	expression tag	UNP Q9NTM9
E	-1	ALA	-	expression tag	UNP Q9NTM9
E	0	CYS	-	expression tag	UNP Q9NTM9
F	-13	MET	-	expression tag	UNP Q9NTM9
F	-12	ARG	-	expression tag	UNP Q9NTM9
F	-11	GLY	-	expression tag	UNP Q9NTM9
F	-10	SER	-	expression tag	UNP Q9NTM9
F	-9	HIS	-	expression tag	UNP Q9NTM9
F	-8	HIS	-	expression tag	UNP Q9NTM9
F	-7	HIS	-	expression tag	UNP Q9NTM9
F	-6	HIS	-	expression tag	UNP Q9NTM9
F	-5	HIS	-	expression tag	UNP Q9NTM9
F	-4	HIS	-	expression tag	UNP Q9NTM9
F	-3	GLY	-	expression tag	UNP Q9NTM9
F	-2	SER	-	expression tag	UNP Q9NTM9
F	-1	ALA	-	expression tag	UNP Q9NTM9
F	0	CYS	-	expression tag	UNP Q9NTM9
G	-13	MET	-	expression tag	UNP Q9NTM9
G	-12	ARG	-	expression tag	UNP Q9NTM9
G	-11	GLY	-	expression tag	UNP Q9NTM9
G	-10	SER	-	expression tag	UNP Q9NTM9
G	-9	HIS	-	expression tag	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	HIS	-	expression tag	UNP Q9NTM9
G	-7	HIS	-	expression tag	UNP Q9NTM9
G	-6	HIS	-	expression tag	UNP Q9NTM9
G	-5	HIS	-	expression tag	UNP Q9NTM9
G	-4	HIS	-	expression tag	UNP Q9NTM9
G	-3	GLY	-	expression tag	UNP Q9NTM9
G	-2	SER	-	expression tag	UNP Q9NTM9
G	-1	ALA	-	expression tag	UNP Q9NTM9
G	0	CYS	-	expression tag	UNP Q9NTM9
H	-13	MET	-	expression tag	UNP Q9NTM9
H	-12	ARG	-	expression tag	UNP Q9NTM9
H	-11	GLY	-	expression tag	UNP Q9NTM9
H	-10	SER	-	expression tag	UNP Q9NTM9
H	-9	HIS	-	expression tag	UNP Q9NTM9
H	-8	HIS	-	expression tag	UNP Q9NTM9
H	-7	HIS	-	expression tag	UNP Q9NTM9
H	-6	HIS	-	expression tag	UNP Q9NTM9
H	-5	HIS	-	expression tag	UNP Q9NTM9
H	-4	HIS	-	expression tag	UNP Q9NTM9
H	-3	GLY	-	expression tag	UNP Q9NTM9
H	-2	SER	-	expression tag	UNP Q9NTM9
H	-1	ALA	-	expression tag	UNP Q9NTM9
H	0	CYS	-	expression tag	UNP Q9NTM9
I	-13	MET	-	expression tag	UNP Q9NTM9
I	-12	ARG	-	expression tag	UNP Q9NTM9
I	-11	GLY	-	expression tag	UNP Q9NTM9
I	-10	SER	-	expression tag	UNP Q9NTM9
I	-9	HIS	-	expression tag	UNP Q9NTM9
I	-8	HIS	-	expression tag	UNP Q9NTM9
I	-7	HIS	-	expression tag	UNP Q9NTM9
I	-6	HIS	-	expression tag	UNP Q9NTM9
I	-5	HIS	-	expression tag	UNP Q9NTM9
I	-4	HIS	-	expression tag	UNP Q9NTM9
I	-3	GLY	-	expression tag	UNP Q9NTM9
I	-2	SER	-	expression tag	UNP Q9NTM9
I	-1	ALA	-	expression tag	UNP Q9NTM9
I	0	CYS	-	expression tag	UNP Q9NTM9
J	-13	MET	-	expression tag	UNP Q9NTM9
J	-12	ARG	-	expression tag	UNP Q9NTM9
J	-11	GLY	-	expression tag	UNP Q9NTM9
J	-10	SER	-	expression tag	UNP Q9NTM9
J	-9	HIS	-	expression tag	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	HIS	-	expression tag	UNP Q9NTM9
J	-7	HIS	-	expression tag	UNP Q9NTM9
J	-6	HIS	-	expression tag	UNP Q9NTM9
J	-5	HIS	-	expression tag	UNP Q9NTM9
J	-4	HIS	-	expression tag	UNP Q9NTM9
J	-3	GLY	-	expression tag	UNP Q9NTM9
J	-2	SER	-	expression tag	UNP Q9NTM9
J	-1	ALA	-	expression tag	UNP Q9NTM9
J	0	CYS	-	expression tag	UNP Q9NTM9
K	-13	MET	-	expression tag	UNP Q9NTM9
K	-12	ARG	-	expression tag	UNP Q9NTM9
K	-11	GLY	-	expression tag	UNP Q9NTM9
K	-10	SER	-	expression tag	UNP Q9NTM9
K	-9	HIS	-	expression tag	UNP Q9NTM9
K	-8	HIS	-	expression tag	UNP Q9NTM9
K	-7	HIS	-	expression tag	UNP Q9NTM9
K	-6	HIS	-	expression tag	UNP Q9NTM9
K	-5	HIS	-	expression tag	UNP Q9NTM9
K	-4	HIS	-	expression tag	UNP Q9NTM9
K	-3	GLY	-	expression tag	UNP Q9NTM9
K	-2	SER	-	expression tag	UNP Q9NTM9
K	-1	ALA	-	expression tag	UNP Q9NTM9
K	0	CYS	-	expression tag	UNP Q9NTM9
L	-13	MET	-	expression tag	UNP Q9NTM9
L	-12	ARG	-	expression tag	UNP Q9NTM9
L	-11	GLY	-	expression tag	UNP Q9NTM9
L	-10	SER	-	expression tag	UNP Q9NTM9
L	-9	HIS	-	expression tag	UNP Q9NTM9
L	-8	HIS	-	expression tag	UNP Q9NTM9
L	-7	HIS	-	expression tag	UNP Q9NTM9
L	-6	HIS	-	expression tag	UNP Q9NTM9
L	-5	HIS	-	expression tag	UNP Q9NTM9
L	-4	HIS	-	expression tag	UNP Q9NTM9
L	-3	GLY	-	expression tag	UNP Q9NTM9
L	-2	SER	-	expression tag	UNP Q9NTM9
L	-1	ALA	-	expression tag	UNP Q9NTM9
L	0	CYS	-	expression tag	UNP Q9NTM9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	145	Total	O	0	0
			145	145		

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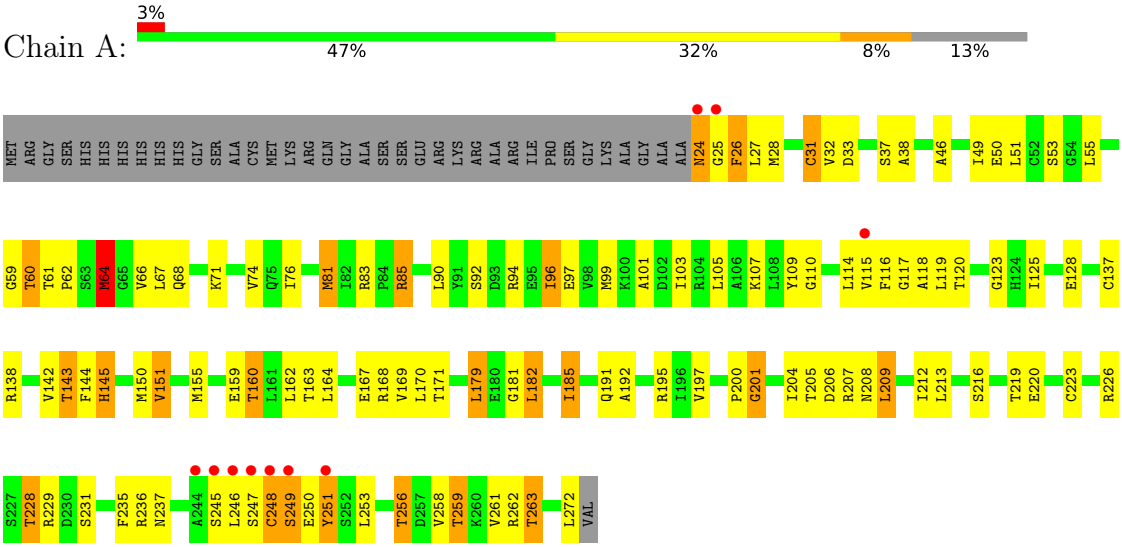
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	134	Total O 134 134	0	0
2	C	137	Total O 137 137	0	0
2	D	157	Total O 157 157	0	0
2	E	58	Total O 58 58	0	0
2	F	47	Total O 47 47	0	0
2	G	25	Total O 25 25	0	0
2	H	33	Total O 33 33	0	0
2	I	56	Total O 56 56	0	0
2	J	43	Total O 43 43	0	0
2	K	26	Total O 26 26	0	0
2	L	27	Total O 27 27	0	0

3 Residue-property plots (i)

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.

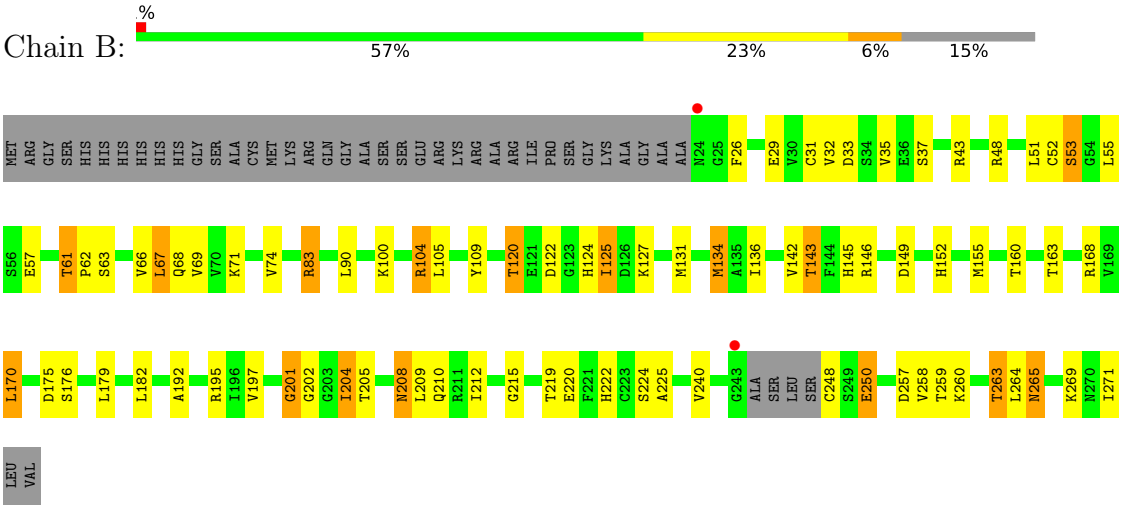
• Molecule 1: Copper homeostasis protein cutC homolog

Chain A:



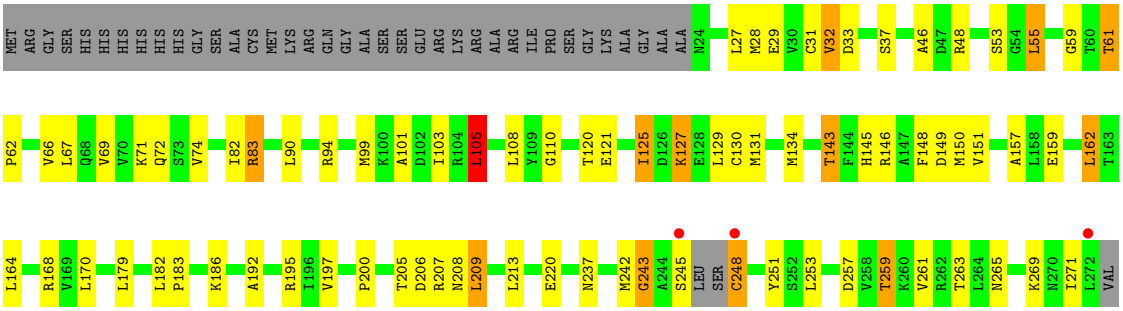
• Molecule 1: Copper homeostasis protein cutC homolog

Chain B:



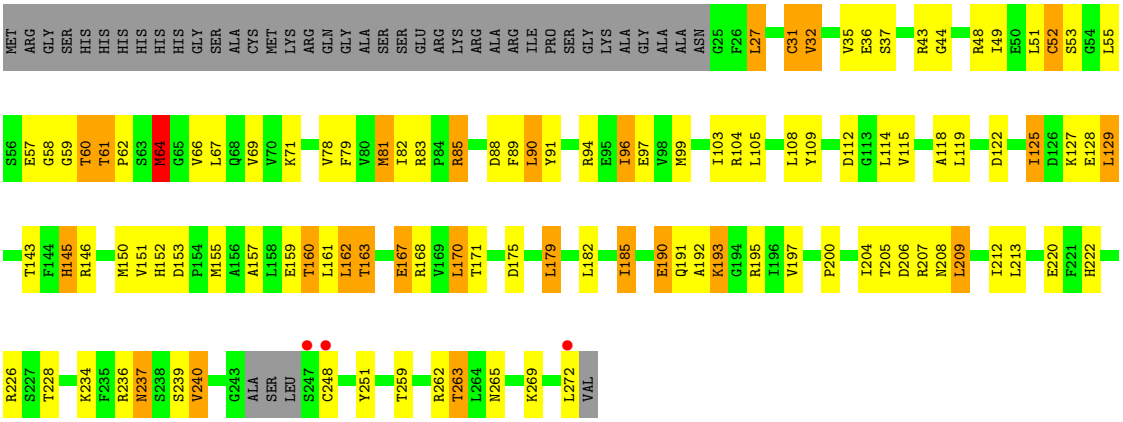
• Molecule 1: Copper homeostasis protein cutC homolog

Chain C:



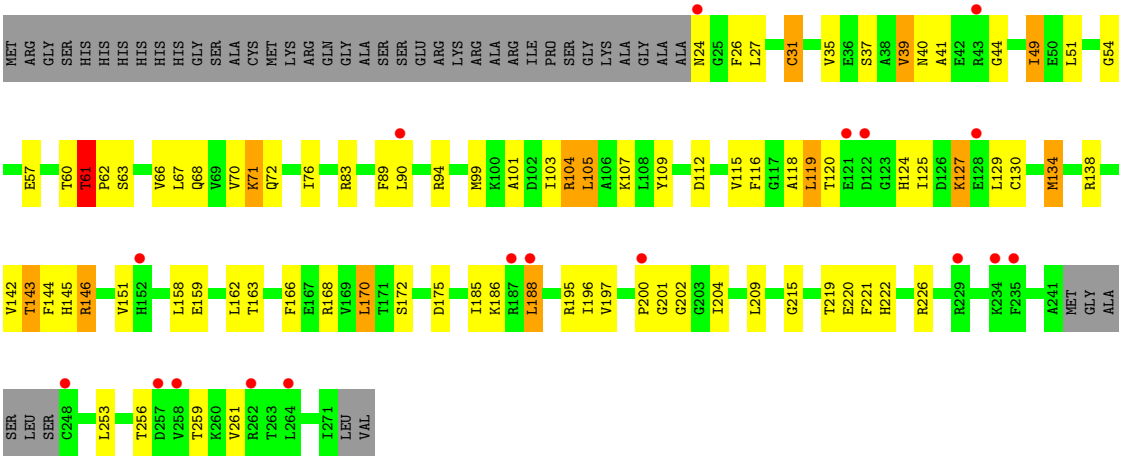
• Molecule 1: Copper homeostasis protein cutC homolog

Chain D:



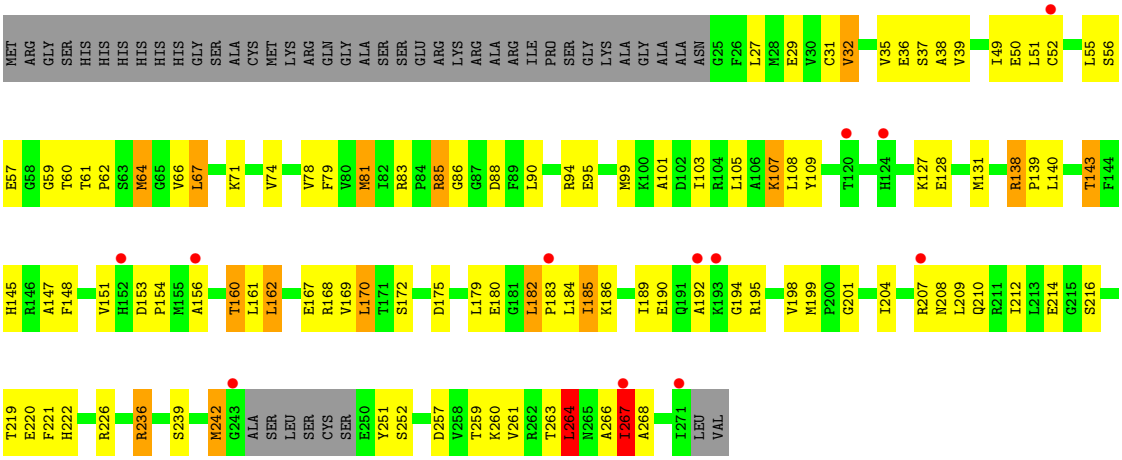
• Molecule 1: Copper homeostasis protein cutC homolog

Chain E:



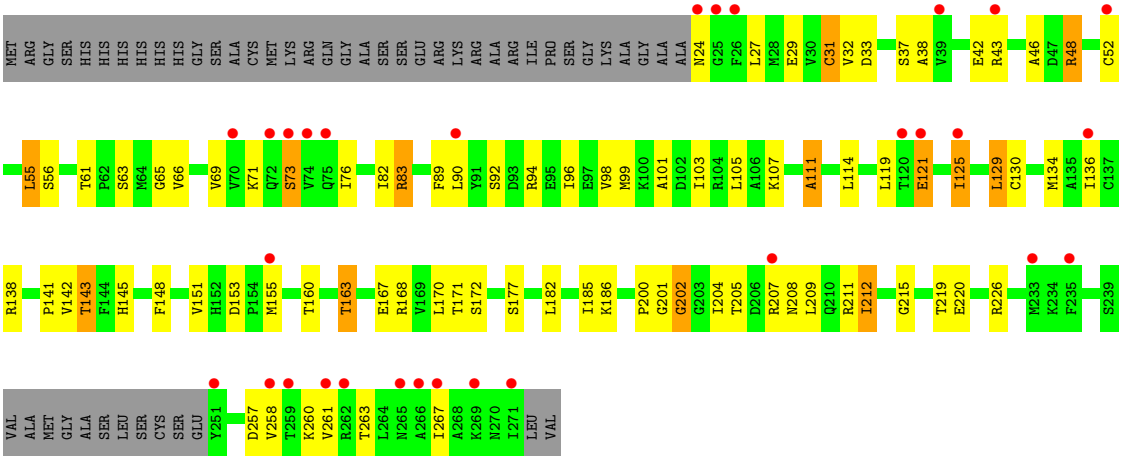
• Molecule 1: Copper homeostasis protein cutC homolog

Chain F:



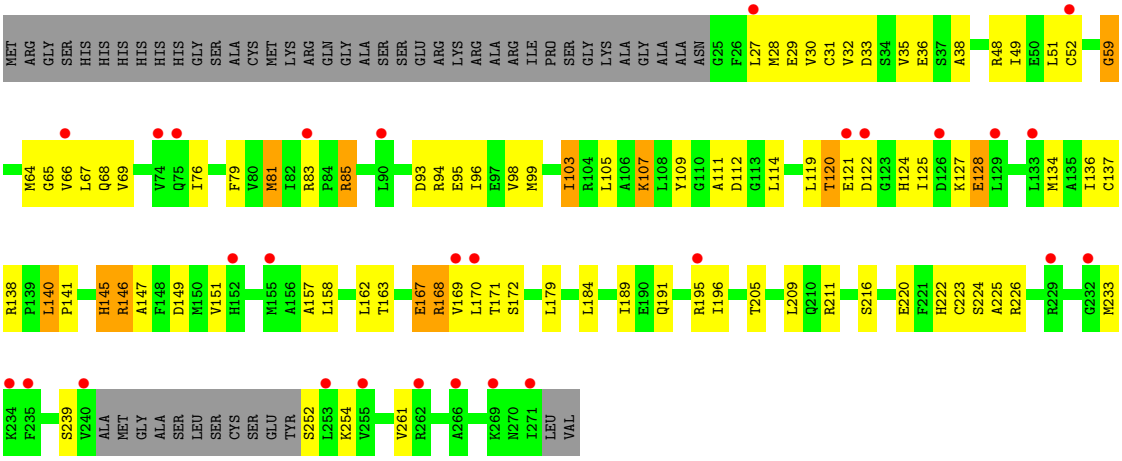
• Molecule 1: Copper homeostasis protein cutC homolog

Chain G:



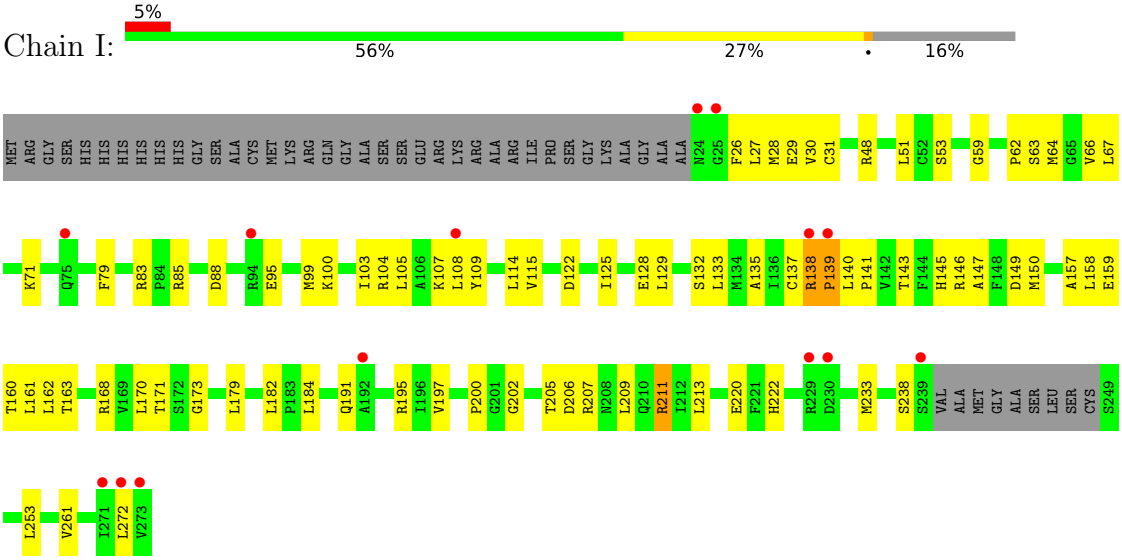
• Molecule 1: Copper homeostasis protein cutC homolog

Chain H:



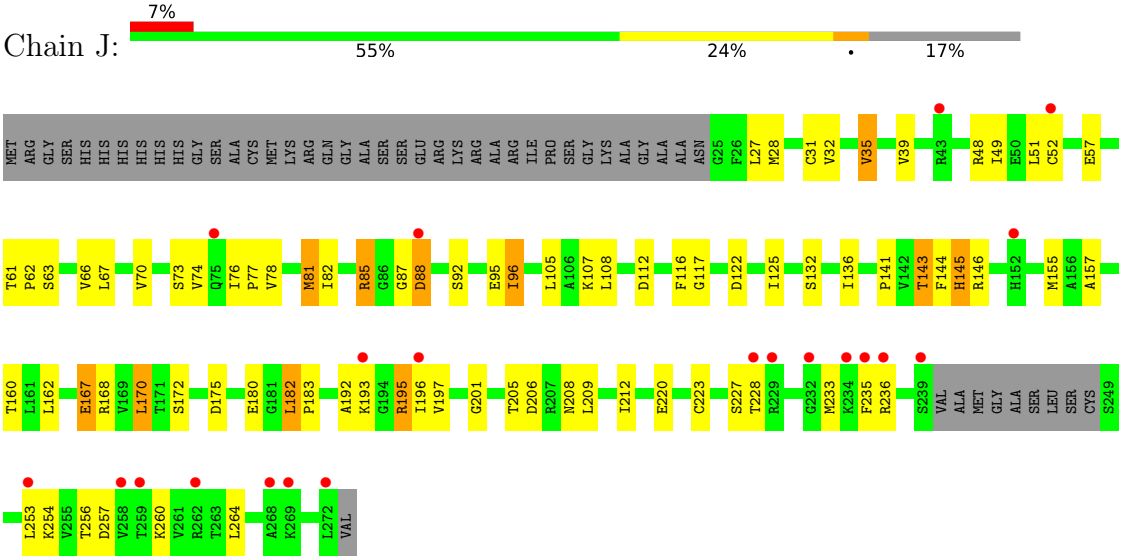
• Molecule 1: Copper homeostasis protein cutC homolog

Chain I:



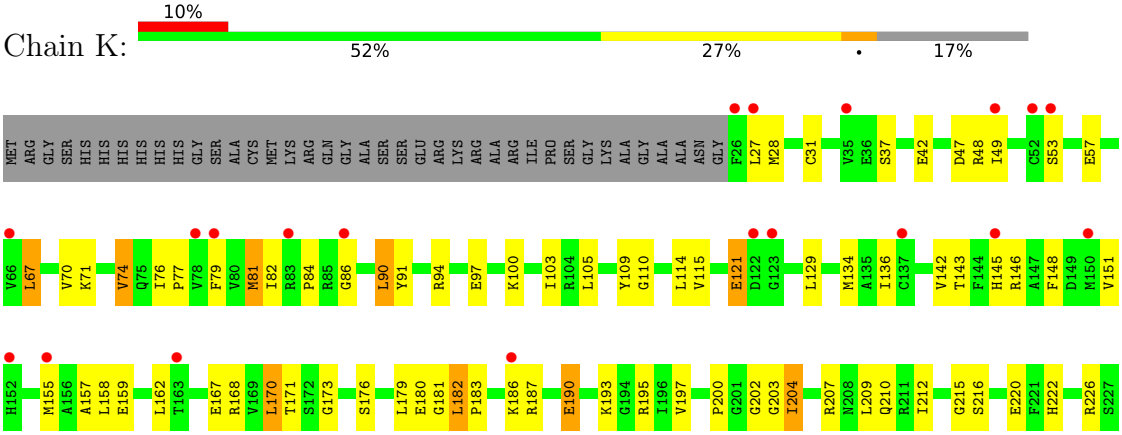
• Molecule 1: Copper homeostasis protein cutC homolog

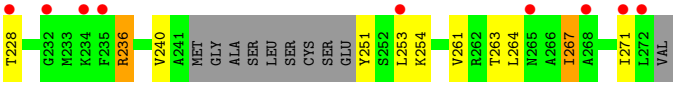
Chain J:



• Molecule 1: Copper homeostasis protein cutC homolog

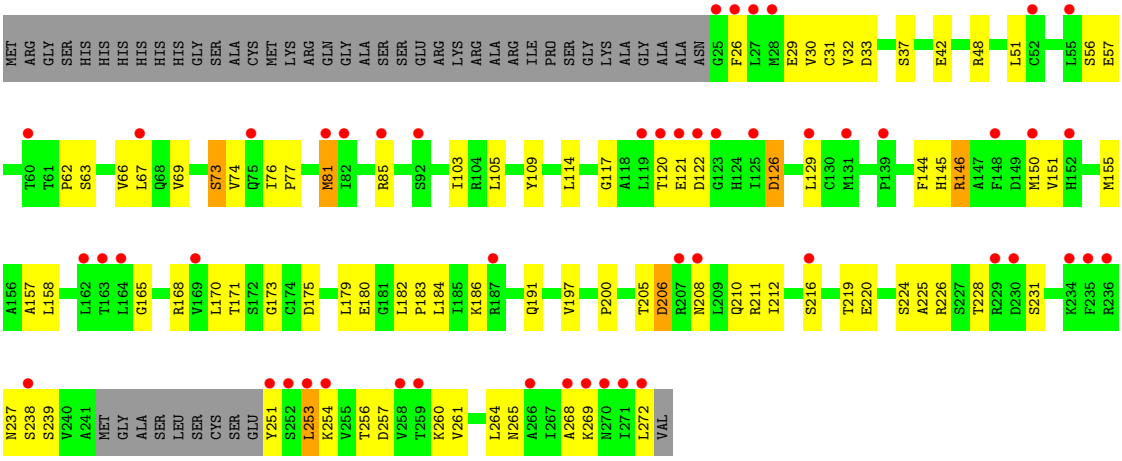
Chain K:





• Molecule 1: Copper homeostasis protein cutC homolog

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.16Å 78.41Å 170.35Å 76.84° 87.88° 71.86°	Depositor
Resolution (Å)	50.00 – 2.50 40.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.50) 98.5 (40.13-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 2.51Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.283 0.241 , 0.244	Depositor DCC
R_{free} test set	6413 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,-k+l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22740	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.64	0/1893	0.82	2/2549 (0.1%)
1	B	0.67	0/1859	0.78	0/2501
1	C	0.69	0/1878	0.84	1/2527 (0.0%)
1	D	0.69	1/1865 (0.1%)	0.83	3/2509 (0.1%)
1	E	0.46	0/1847	0.63	0/2486
1	F	0.49	0/1839	0.67	2/2474 (0.1%)
1	G	0.39	0/1814	0.58	0/2441
1	H	0.36	0/1800	0.58	0/2422
1	I	0.44	0/1844	0.61	0/2482
1	J	0.44	0/1829	0.61	0/2461
1	K	0.36	0/1822	0.57	0/2453
1	L	0.37	0/1826	0.55	0/2458
All	All	0.52	1/22116 (0.0%)	0.68	8/29763 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	CYS	CB-SG	6.06	1.92	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	27	LEU	CA-CB-CG	6.59	130.46	115.30
1	F	264	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	85	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	C	105	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	64	MET	CG-SD-CE	5.46	108.94	100.20
1	F	162	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	64	MET	CG-SD-CE	5.39	108.83	100.20
1	D	90	LEU	CA-CB-CG	5.23	127.33	115.30

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	1870	0	1905	125	0
1	B	1837	0	1867	70	0
1	C	1856	0	1888	70	0
1	D	1843	0	1877	107	0
1	E	1825	0	1855	67	0
1	F	1817	0	1851	73	0
1	G	1792	0	1825	74	0
1	H	1779	0	1819	69	0
1	I	1822	0	1856	63	0
1	J	1807	0	1841	61	0
1	K	1800	0	1841	75	0
1	L	1804	0	1844	50	0
2	A	145	0	0	14	0
2	B	134	0	0	9	0
2	C	137	0	0	12	0
2	D	157	0	0	17	0
2	E	58	0	0	8	0
2	F	47	0	0	4	0
2	G	25	0	0	4	0
2	H	33	0	0	3	0
2	I	56	0	0	9	0
2	J	43	0	0	4	0
2	K	26	0	0	6	0
2	L	27	0	0	5	0
All	All	22740	0	22269	863	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 20.

All (863) 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:B:61:THR:HG21	2:B:280:HOH:O	1.38	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:SER:CB	1:A:250:GLU:HA	1.68	1.18
1:J:88:ASP:HB2	2:J:294:HOH:O	1.50	1.08
1:I:138:ARG:HB3	1:I:139:PRO:HD2	1.38	1.04
1:C:61:THR:HG21	2:C:276:HOH:O	1.57	1.02
1:A:249:SER:HB3	1:A:250:GLU:HA	1.40	1.01
1:A:231:SER:HB2	1:A:251:TYR:O	1.61	1.00
1:C:143:THR:HG21	2:C:274:HOH:O	1.61	0.98
1:I:107:LYS:NZ	1:I:138:ARG:HB2	1.79	0.97
1:D:31:CYS:HB2	2:D:792:HOH:O	1.63	0.97
1:G:55:LEU:HD13	1:G:55:LEU:H	1.30	0.96
1:A:27:LEU:HB3	1:A:220:GLU:HG2	1.49	0.95
1:G:125:ILE:HD13	1:G:125:ILE:H	1.30	0.94
1:I:145:HIS:HD2	1:I:147:ALA:H	1.15	0.94
1:D:61:THR:HG21	2:D:275:HOH:O	1.67	0.94
1:K:48:ARG:NH2	1:K:168:ARG:HH12	1.65	0.94
1:G:48:ARG:HH11	1:G:48:ARG:HB3	1.33	0.93
1:D:185:ILE:HG21	2:D:277:HOH:O	1.66	0.93
1:F:101:ALA:O	1:F:105:LEU:HD23	1.67	0.93
1:J:175:ASP:OD2	1:J:180:GLU:HB3	1.69	0.91
1:A:231:SER:HB3	1:A:251:TYR:HB3	1.51	0.90
1:I:27:LEU:HB2	1:I:220:GLU:HG2	1.53	0.90
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.36	0.89
1:L:171:THR:HG22	1:L:173:GLY:H	1.35	0.89
1:D:48:ARG:NH1	1:D:168:ARG:HH12	1.71	0.89
1:A:250:GLU:HB3	2:A:363:HOH:O	1.72	0.89
1:D:159:GLU:HG2	2:D:332:HOH:O	1.72	0.87
1:I:138:ARG:HA	2:I:755:HOH:O	1.74	0.87
1:A:249:SER:OG	1:A:250:GLU:HA	1.75	0.87
1:G:55:LEU:CB	1:G:226:ARG:HH22	1.88	0.86
1:I:128:GLU:HG2	2:I:737:HOH:O	1.76	0.86
1:A:37:SER:HB3	1:A:256:THR:HG23	1.58	0.86
1:I:108:LEU:HB3	2:I:811:HOH:O	1.75	0.85
1:A:249:SER:CB	1:A:250:GLU:CA	2.54	0.85
1:F:143:THR:HG22	2:F:276:HOH:O	1.76	0.85
1:A:143:THR:HG22	2:A:331:HOH:O	1.76	0.85
1:C:206:ASP:HB2	2:C:782:HOH:O	1.76	0.84
1:J:205:THR:H	1:J:208:ASN:HB2	1.40	0.84
1:C:143:THR:HB	1:C:168:ARG:HB2	1.60	0.84
1:B:143:THR:HG21	2:B:292:HOH:O	1.75	0.84
1:G:55:LEU:HB2	1:G:226:ARG:HH22	1.43	0.84
1:A:115:VAL:HG13	1:A:143:THR:O	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:THR:HG22	1:K:173:GLY:H	1.39	0.84
1:I:107:LYS:HZ2	1:I:138:ARG:HB2	1.43	0.83
1:B:63:SER:OG	1:B:66:VAL:HG23	1.78	0.83
1:D:162:LEU:HD21	1:D:195:ARG:HB2	1.60	0.83
1:E:94:ARG:HH11	1:E:94:ARG:HB2	1.41	0.83
1:K:162:LEU:HD13	1:K:195:ARG:HD2	1.59	0.83
1:H:85:ARG:HG3	1:H:85:ARG:HH11	1.44	0.83
1:A:61:THR:HG21	2:A:277:HOH:O	1.77	0.82
1:B:248:CYS:N	1:C:248:CYS:SG	2.53	0.82
1:A:24:ASN:N	1:A:219:THR:HG1	1.76	0.82
1:G:27:LEU:HB2	1:G:220:GLU:HG2	1.62	0.82
1:C:251:TYR:OH	1:D:150:MET:HE2	1.81	0.81
1:E:195:ARG:HD2	2:E:281:HOH:O	1.81	0.81
1:I:105:LEU:O	1:I:109:TYR:HD1	1.62	0.81
1:B:182:LEU:O	1:B:182:LEU:HD23	1.81	0.81
1:C:55:LEU:CD2	1:C:55:LEU:H	1.94	0.80
1:I:114:LEU:HB2	2:I:282:HOH:O	1.79	0.80
1:L:42:GLU:HG3	1:L:76:ILE:HD12	1.63	0.80
1:A:118:ALA:O	1:A:119:LEU:HD23	1.80	0.80
1:J:63:SER:OG	1:J:66:VAL:HG23	1.81	0.80
1:A:249:SER:OG	1:A:250:GLU:CA	2.30	0.80
1:E:31:CYS:HB2	2:E:453:HOH:O	1.82	0.80
1:G:143:THR:HG21	2:G:275:HOH:O	1.82	0.80
1:K:115:VAL:HG13	1:K:145:HIS:CD2	2.17	0.80
1:A:31:CYS:SG	1:A:55:LEU:HD21	2.22	0.79
1:F:31:CYS:SG	1:F:55:LEU:HD21	2.22	0.79
1:J:208:ASN:HB3	1:J:212:ILE:HD12	1.64	0.79
1:F:192:ALA:HA	1:F:195:ARG:HH11	1.47	0.79
1:A:231:SER:CB	1:A:251:TYR:HB3	2.13	0.79
1:I:122:ASP:HA	1:J:235:PHE:CD1	2.18	0.79
1:A:116:PHE:O	1:A:145:HIS:CD2	2.36	0.78
1:H:27:LEU:HB3	1:H:220:GLU:HG2	1.64	0.78
1:A:28:MET:HE3	1:A:261:VAL:HG13	1.65	0.78
1:A:168:ARG:HG2	1:A:197:VAL:HB	1.65	0.78
1:K:263:THR:O	1:K:267:ILE:HG22	1.84	0.78
1:B:248:CYS:N	1:C:248:CYS:HG	1.82	0.78
1:E:27:LEU:HB2	1:E:220:GLU:HG2	1.66	0.77
1:E:61:THR:HG21	2:E:449:HOH:O	1.84	0.77
1:J:27:LEU:HB3	1:J:220:GLU:HG2	1.66	0.77
1:D:82:ILE:HD13	1:D:103:ILE:CG1	2.14	0.77
1:E:101:ALA:HA	1:E:104:ARG:HH11	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:OE2	1:B:222:HIS:HD2	1.65	0.77
1:A:143:THR:HG21	2:A:275:HOH:O	1.83	0.76
1:A:250:GLU:CB	2:A:363:HOH:O	2.32	0.76
1:B:205:THR:H	1:B:208:ASN:HD21	1.34	0.76
1:D:48:ARG:NH1	1:D:168:ARG:NH1	2.33	0.76
1:A:101:ALA:O	1:A:105:LEU:HD23	1.86	0.75
1:E:99:MET:O	1:E:103:ILE:HG12	1.86	0.75
1:G:141:PRO:HA	1:G:167:GLU:OE2	1.86	0.75
1:G:99:MET:O	1:G:103:ILE:HG12	1.86	0.75
1:I:138:ARG:O	1:I:140:LEU:N	2.20	0.75
1:D:59:GLY:O	1:D:83:ARG:HD3	1.86	0.75
1:A:116:PHE:HD1	1:A:117:GLY:H	1.32	0.74
2:A:342:HOH:O	1:B:250:GLU:HG3	1.87	0.74
1:I:171:THR:HG22	1:I:173:GLY:H	1.51	0.74
1:A:226:ARG:HH11	1:A:256:THR:HG22	1.51	0.74
1:D:152:HIS:CD2	2:D:645:HOH:O	2.41	0.74
1:I:145:HIS:CD2	1:I:147:ALA:H	2.05	0.73
1:A:231:SER:CB	1:A:251:TYR:O	2.35	0.73
1:B:143:THR:HB	1:B:168:ARG:HB2	1.71	0.72
1:D:82:ILE:HD13	1:D:103:ILE:HG13	1.71	0.72
1:E:105:LEU:HD23	2:F:784:HOH:O	1.90	0.72
1:K:42:GLU:OE2	1:K:76:ILE:HG12	1.90	0.72
1:B:143:THR:HG22	2:B:302:HOH:O	1.88	0.71
1:D:81:MET:CE	1:D:145:HIS:HD2	2.03	0.71
1:D:185:ILE:CG2	2:D:277:HOH:O	2.28	0.71
1:D:82:ILE:CD1	1:D:114:LEU:HD22	2.19	0.71
1:F:145:HIS:HD2	1:F:147:ALA:H	1.36	0.71
1:D:143:THR:HG22	2:D:328:HOH:O	1.88	0.71
1:E:130:CYS:O	1:E:134:MET:HB2	1.91	0.71
1:C:28:MET:HE1	1:C:261:VAL:HG13	1.72	0.70
1:H:81:MET:HB3	2:H:402:HOH:O	1.89	0.70
1:A:114:LEU:CD1	1:A:137:CYS:SG	2.79	0.70
1:A:250:GLU:O	1:A:250:GLU:HG3	1.92	0.70
1:K:228:THR:HG22	2:K:666:HOH:O	1.89	0.70
1:L:105:LEU:O	1:L:109:TYR:HD1	1.73	0.70
1:F:175:ASP:OD2	1:F:180:GLU:HB3	1.90	0.70
1:C:251:TYR:OH	1:D:150:MET:CE	2.40	0.70
1:K:168:ARG:HG2	1:K:197:VAL:HB	1.73	0.70
1:A:32:VAL:HG13	1:A:37:SER:HB2	1.74	0.70
1:D:32:VAL:HG22	1:D:37:SER:HB3	1.74	0.70
1:B:104:ARG:HH11	1:B:104:ARG:CG	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ILE:H	1:G:125:ILE:CD1	2.05	0.69
1:I:53:SER:HB2	1:I:62:PRO:HA	1.75	0.69
1:A:53:SER:HB3	1:A:60:THR:HG22	1.71	0.69
1:B:155:MET:SD	2:B:492:HOH:O	2.51	0.69
1:F:59:GLY:O	1:F:83:ARG:HD3	1.93	0.69
1:H:169:VAL:HG23	1:H:196:ILE:HG21	1.75	0.69
1:A:32:VAL:HG22	1:A:256:THR:HG21	1.74	0.69
1:D:209:LEU:HD22	1:D:213:LEU:HG	1.75	0.69
1:A:96:ILE:HA	1:A:99:MET:HE3	1.74	0.69
1:D:81:MET:HE3	1:D:145:HIS:HD2	1.58	0.69
1:K:204:ILE:CG2	1:K:212:ILE:HD13	2.23	0.69
1:A:259:THR:O	1:A:263:THR:HG23	1.93	0.69
1:E:158:LEU:HD13	1:E:188:LEU:CD1	2.24	0.68
1:D:143:THR:HG21	2:D:647:HOH:O	1.93	0.68
1:C:146:ARG:HD2	1:C:149:ASP:OD2	1.94	0.68
1:A:114:LEU:HD13	1:A:137:CYS:SG	2.33	0.68
1:G:55:LEU:H	1:G:55:LEU:CD1	2.01	0.68
1:A:207:ARG:HH22	1:D:239:SER:HB3	1.59	0.68
1:K:42:GLU:HG3	2:K:458:HOH:O	1.93	0.68
1:G:208:ASN:ND2	1:G:211:ARG:HH21	1.91	0.68
1:H:162:LEU:HD21	1:H:195:ARG:HB3	1.76	0.68
1:I:26:PHE:HE1	1:I:272:LEU:HD21	1.59	0.67
1:D:185:ILE:HD12	1:D:200:PRO:HB3	1.75	0.67
1:G:48:ARG:HB3	1:G:48:ARG:NH1	2.08	0.67
1:J:162:LEU:HD23	1:J:196:ILE:HG23	1.76	0.67
1:J:208:ASN:HB3	1:J:212:ILE:CD1	2.24	0.67
1:F:27:LEU:HB2	1:F:220:GLU:HG2	1.75	0.67
1:K:48:ARG:HH22	1:K:168:ARG:HH12	1.42	0.67
1:H:99:MET:O	1:H:103:ILE:HG22	1.94	0.67
1:C:55:LEU:H	1:C:55:LEU:HD23	1.57	0.67
1:A:114:LEU:HD12	1:A:137:CYS:CB	2.25	0.66
1:A:160:THR:O	1:A:163:THR:HG22	1.96	0.66
1:B:265:ASN:HD21	1:B:269:LYS:HE3	1.59	0.66
1:C:143:THR:HG22	2:C:302:HOH:O	1.94	0.66
1:H:103:ILE:O	1:H:107:LYS:HG2	1.94	0.66
1:F:192:ALA:HA	1:F:195:ARG:HD3	1.78	0.66
1:F:266:ALA:O	1:F:267:ILE:HG12	1.96	0.66
1:H:85:ARG:HH11	1:H:85:ARG:CG	2.09	0.66
1:L:269:LYS:H	1:L:272:LEU:HD12	1.61	0.66
1:J:85:ARG:HG2	1:J:87:GLY:H	1.60	0.66
1:B:104:ARG:NH1	2:B:345:HOH:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:THR:H	1:B:208:ASN:ND2	1.92	0.65
1:F:260:LYS:O	1:F:264:LEU:HD22	1.96	0.65
1:A:28:MET:CE	1:A:261:VAL:HG13	2.25	0.65
1:H:27:LEU:HB3	1:H:220:GLU:CG	2.27	0.65
1:I:28:MET:CE	1:I:261:VAL:HG13	2.26	0.65
1:B:204:ILE:HB	1:B:212:ILE:CD1	2.26	0.65
1:K:48:ARG:HD3	1:K:79:PHE:CD2	2.31	0.65
1:E:170:LEU:HD21	1:E:222:HIS:HB3	1.79	0.65
1:J:257:ASP:OD2	1:J:260:LYS:HG2	1.96	0.65
1:E:143:THR:HB	1:E:168:ARG:HB2	1.77	0.65
1:H:134:MET:HG2	1:H:138:ARG:NH2	2.10	0.65
1:B:48:ARG:NH2	1:B:220:GLU:OE1	2.28	0.65
1:A:53:SER:HB2	1:A:62:PRO:HA	1.79	0.65
1:D:82:ILE:HD13	1:D:103:ILE:HG12	1.79	0.65
1:E:172:SER:HB3	1:E:201:GLY:O	1.97	0.65
1:G:151:VAL:HG12	1:G:153:ASP:H	1.60	0.65
1:G:107:LYS:NZ	1:G:136:ILE:O	2.25	0.64
1:E:115:VAL:HG22	1:E:143:THR:HG23	1.79	0.64
1:H:83:ARG:HE	1:H:145:HIS:CE1	2.16	0.64
1:C:206:ASP:CB	2:C:782:HOH:O	2.39	0.64
1:E:118:ALA:HB1	1:E:129:LEU:HD13	1.80	0.64
1:L:165:GLY:N	2:L:783:HOH:O	2.29	0.64
1:K:28:MET:CE	1:K:261:VAL:HG13	2.28	0.64
1:H:103:ILE:CD1	1:H:137:CYS:SG	2.86	0.64
1:L:197:VAL:HG11	1:L:220:GLU:OE1	1.98	0.64
1:K:42:GLU:OE2	1:K:74:VAL:HG13	1.97	0.64
1:C:27:LEU:HB2	1:C:220:GLU:HG2	1.80	0.63
1:G:148:PHE:O	1:G:151:VAL:HG23	1.99	0.63
1:E:49:ILE:HD12	1:E:76:ILE:HD11	1.79	0.63
1:H:107:LYS:HE3	1:H:136:ILE:O	1.99	0.63
1:K:27:LEU:HB2	1:K:220:GLU:HG3	1.81	0.63
1:B:29:GLU:OE1	1:B:48:ARG:NH1	2.27	0.63
1:C:265:ASN:O	1:C:269:LYS:HG2	1.99	0.63
1:K:48:ARG:CZ	1:K:168:ARG:HH12	2.11	0.63
1:D:192:ALA:O	1:D:195:ARG:HG3	1.99	0.62
1:E:60:THR:O	1:E:61:THR:C	2.37	0.62
1:B:125:ILE:HD12	1:B:160:THR:CG2	2.30	0.62
1:F:185:ILE:HG13	1:F:186:LYS:N	2.14	0.62
1:G:32:VAL:HG13	1:G:37:SER:HB2	1.81	0.62
1:I:205:THR:HG22	1:I:206:ASP:H	1.65	0.62
1:A:114:LEU:HD12	1:A:137:CYS:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:PHE:O	1:F:151:VAL:HG22	2.00	0.62
1:A:179:LEU:HD13	1:C:179:LEU:HG	1.82	0.62
1:J:28:MET:CE	1:J:223:CYS:SG	2.88	0.62
1:K:209:LEU:HD12	1:K:264:LEU:HD23	1.81	0.62
1:A:116:PHE:CD1	1:A:117:GLY:N	2.58	0.62
1:D:53:SER:HB2	1:D:62:PRO:HA	1.81	0.62
1:I:138:ARG:CB	1:I:139:PRO:HD2	2.20	0.62
1:E:101:ALA:HA	1:E:104:ARG:NH1	2.14	0.62
1:F:64:MET:HG2	1:F:109:TYR:CD1	2.35	0.61
1:G:105:LEU:HD21	1:H:68:GLN:HE22	1.65	0.61
1:A:94:ARG:HA	1:A:97:GLU:HG2	1.81	0.61
1:B:204:ILE:HB	1:B:212:ILE:HD12	1.80	0.61
1:I:28:MET:HE3	1:I:261:VAL:HG13	1.83	0.61
1:A:231:SER:HB3	1:A:251:TYR:CB	2.26	0.61
1:C:32:VAL:HG22	1:C:37:SER:CB	2.30	0.61
1:C:150:MET:SD	1:D:240:VAL:HG22	2.40	0.61
1:F:32:VAL:CG2	1:F:37:SER:HB3	2.31	0.61
1:K:253:LEU:HD12	1:L:85:ARG:HD3	1.82	0.61
1:L:51:LEU:HB3	1:L:62:PRO:HG3	1.81	0.61
1:A:185:ILE:HD13	1:A:200:PRO:HB3	1.81	0.61
1:A:205:THR:HG22	1:A:208:ASN:ND2	2.15	0.61
1:B:225:ALA:N	2:B:308:HOH:O	2.34	0.61
1:D:61:THR:HG22	1:D:83:ARG:H	1.65	0.61
1:D:82:ILE:HD12	1:D:114:LEU:HD22	1.81	0.61
1:E:94:ARG:HB2	1:E:94:ARG:NH1	2.15	0.61
1:K:143:THR:HG23	1:K:168:ARG:HB2	1.83	0.61
1:A:116:PHE:O	1:A:145:HIS:NE2	2.33	0.61
1:I:205:THR:HG22	1:I:206:ASP:N	2.15	0.61
1:C:33:ASP:OD1	1:C:55:LEU:HD21	2.01	0.60
1:A:114:LEU:HD12	1:A:137:CYS:SG	2.40	0.60
1:E:120:THR:HG22	1:E:124:HIS:H	1.66	0.60
1:G:145:HIS:HA	1:G:170:LEU:HB2	1.84	0.60
1:L:117:GLY:HA2	1:L:144:PHE:CE1	2.36	0.60
1:B:61:THR:HG22	1:B:83:ARG:O	2.01	0.60
1:A:59:GLY:O	1:A:83:ARG:HD3	2.02	0.60
1:H:103:ILE:HD11	1:H:137:CYS:SG	2.42	0.60
1:L:126:ASP:OD2	1:L:129:LEU:HB2	2.02	0.60
1:G:31:CYS:HB2	2:G:544:HOH:O	2.01	0.60
1:G:55:LEU:HB3	1:G:226:ARG:HH22	1.65	0.60
1:H:179:LEU:HD11	1:H:211:ARG:HH21	1.67	0.60
1:J:162:LEU:HD21	1:J:195:ARG:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:GLU:HA	1:K:159:GLU:OE1	2.01	0.60
1:G:182:LEU:HA	1:G:185:ILE:HG12	1.83	0.60
1:H:225:ALA:HB3	1:H:261:VAL:HG23	1.82	0.60
1:D:182:LEU:HA	1:D:185:ILE:CG2	2.32	0.60
1:E:105:LEU:HD13	1:E:109:TYR:HE2	1.67	0.60
1:J:132:SER:O	1:J:136:ILE:HD12	2.02	0.60
1:D:143:THR:HG22	1:D:168:ARG:HB2	1.82	0.60
1:K:236:ARG:HH22	1:K:251:TYR:HB2	1.67	0.59
1:G:63:SER:OG	1:G:66:VAL:HG23	2.01	0.59
1:J:162:LEU:CD2	1:J:195:ARG:HB3	2.33	0.59
1:B:168:ARG:HG2	1:B:197:VAL:HB	1.85	0.59
1:J:143:THR:HG21	2:J:457:HOH:O	2.01	0.59
1:C:207:ARG:NH2	2:C:808:HOH:O	2.35	0.59
1:K:182:LEU:HB3	1:K:186:LYS:HE3	1.84	0.59
1:F:204:ILE:HA	1:F:208:ASN:HD21	1.68	0.59
1:G:257:ASP:O	1:G:261:VAL:HG23	2.02	0.59
1:H:151:VAL:HG11	1:H:157:ALA:HB2	1.85	0.59
1:D:61:THR:HG22	1:D:83:ARG:O	2.02	0.59
1:G:29:GLU:HA	1:G:48:ARG:O	2.03	0.59
1:G:55:LEU:HD22	1:G:56:SER:H	1.68	0.59
1:H:49:ILE:HG12	1:H:76:ILE:HD11	1.84	0.59
1:B:204:ILE:HD13	1:B:209:LEU:HD13	1.85	0.59
1:D:190:GLU:O	1:D:193:LYS:HD2	2.02	0.59
1:J:92:SER:O	1:J:96:ILE:HG23	2.02	0.59
1:F:143:THR:HG21	2:F:275:HOH:O	2.03	0.59
1:J:146:ARG:HH12	1:J:172:SER:HB3	1.68	0.58
2:E:446:HOH:O	1:G:205:THR:HG21	2.02	0.58
1:G:257:ASP:HB3	1:G:260:LYS:HB2	1.85	0.58
1:H:140:LEU:HD23	1:H:140:LEU:H	1.68	0.58
1:A:249:SER:H	1:A:250:GLU:HB2	1.69	0.58
1:B:127:LYS:O	1:B:131:MET:HG3	2.04	0.58
1:K:204:ILE:HG22	1:K:212:ILE:CD1	2.34	0.58
1:C:150:MET:SD	1:D:240:VAL:CG2	2.91	0.58
1:G:186:LYS:HA	2:G:781:HOH:O	2.02	0.58
1:K:134:MET:HG3	1:K:142:VAL:HG21	1.86	0.58
1:I:132:SER:O	1:I:135:ALA:HB3	2.03	0.58
1:C:61:THR:HG22	1:C:83:ARG:O	2.04	0.58
1:F:261:VAL:HA	1:F:264:LEU:CD2	2.34	0.58
1:K:182:LEU:O	1:K:186:LYS:HG3	2.04	0.58
1:A:103:ILE:HG23	1:A:114:LEU:HD11	1.85	0.58
1:B:125:ILE:HD12	1:B:160:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ARG:CZ	1:D:168:ARG:NH1	2.67	0.57
1:E:63:SER:OG	1:E:66:VAL:HG23	2.03	0.57
1:A:237:ASN:N	1:A:251:TYR:OH	2.36	0.57
1:C:28:MET:CE	1:C:261:VAL:HG13	2.34	0.57
1:D:226:ARG:NE	2:D:573:HOH:O	2.37	0.57
1:I:105:LEU:O	1:I:109:TYR:CD1	2.52	0.57
1:J:85:ARG:CG	1:J:87:GLY:H	2.18	0.57
1:E:107:LYS:NZ	2:E:793:HOH:O	2.37	0.57
1:A:31:CYS:HB2	1:A:50:GLU:HB3	1.86	0.57
1:A:192:ALA:O	1:A:195:ARG:HD3	2.05	0.57
1:B:83:ARG:HG2	2:B:282:HOH:O	2.04	0.57
1:I:146:ARG:NH2	1:I:202:GLY:HA2	2.19	0.57
1:F:167:GLU:HG3	2:F:509:HOH:O	2.04	0.57
1:F:168:ARG:NH1	1:F:220:GLU:OE1	2.38	0.57
1:A:32:VAL:HG13	1:A:37:SER:CB	2.35	0.57
1:B:29:GLU:OE2	1:B:222:HIS:CD2	2.54	0.57
1:G:204:ILE:HG13	1:G:212:ILE:HD12	1.86	0.57
1:C:28:MET:HE2	1:C:46:ALA:HA	1.86	0.56
1:H:103:ILE:HD12	1:H:137:CYS:SG	2.45	0.56
1:D:82:ILE:HD11	1:D:114:LEU:HD22	1.86	0.56
1:I:64:MET:HE3	2:I:481:HOH:O	2.04	0.56
1:J:182:LEU:HB3	1:J:183:PRO:HD3	1.86	0.56
1:A:114:LEU:O	1:A:142:VAL:HA	2.05	0.56
1:E:158:LEU:HD13	1:E:188:LEU:HD11	1.88	0.56
1:H:189:ILE:HD12	1:H:216:SER:HB2	1.87	0.56
1:L:48:ARG:HB3	1:L:77:PRO:HG2	1.87	0.56
1:A:37:SER:CB	1:A:256:THR:HG23	2.30	0.56
1:A:64:MET:HA	1:A:64:MET:CE	2.36	0.56
1:G:143:THR:HB	1:G:168:ARG:HB2	1.88	0.56
1:J:51:LEU:HB3	1:J:62:PRO:HG3	1.88	0.56
1:A:206:ASP:HB3	2:A:322:HOH:O	2.04	0.56
1:H:226:ARG:HH21	1:H:254:LYS:HD3	1.70	0.56
1:C:32:VAL:HG22	1:C:37:SER:HB3	1.88	0.56
1:D:64:MET:HG2	1:D:109:TYR:CD1	2.41	0.56
1:L:257:ASP:O	1:L:261:VAL:HG23	2.05	0.56
1:C:237:ASN:HB3	1:D:150:MET:HE3	1.88	0.56
1:E:57:GLU:O	1:E:83:ARG:NH2	2.39	0.56
1:F:85:ARG:HD2	1:F:86:GLY:O	2.05	0.56
1:G:182:LEU:CD1	1:G:212:ILE:HA	2.36	0.56
1:K:145:HIS:HB2	2:K:274:HOH:O	2.06	0.56
1:A:245:SER:O	1:A:246:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:THR:HG22	1:J:206:ASP:H	1.71	0.56
1:A:245:SER:O	1:C:245:SER:HB2	2.06	0.56
1:F:259:THR:O	1:F:263:THR:HG23	2.06	0.56
1:K:28:MET:HE3	1:K:261:VAL:HG13	1.87	0.56
1:A:116:PHE:O	1:A:145:HIS:CE1	2.59	0.55
1:G:92:SER:O	1:G:96:ILE:HG23	2.06	0.55
1:D:151:VAL:HG11	1:D:157:ALA:HB2	1.87	0.55
1:I:99:MET:O	1:I:103:ILE:HG13	2.06	0.55
1:L:105:LEU:O	1:L:109:TYR:CD1	2.58	0.55
1:L:205:THR:HG22	1:L:206:ASP:H	1.71	0.55
1:H:107:LYS:HD2	1:H:140:LEU:HD11	1.88	0.55
1:A:25:GLY:HA3	2:A:305:HOH:O	2.06	0.55
1:L:74:VAL:HG12	1:L:76:ILE:H	1.71	0.55
1:C:29:GLU:OE1	1:C:48:ARG:NH1	2.35	0.55
1:C:206:ASP:CG	2:C:782:HOH:O	2.44	0.55
1:E:134:MET:HE1	1:E:138:ARG:HG2	1.89	0.55
1:A:68:GLN:OE1	1:B:105:LEU:HD21	2.07	0.55
1:C:53:SER:O	1:C:59:GLY:HA2	2.06	0.55
1:C:168:ARG:HG2	1:C:197:VAL:HB	1.88	0.55
1:J:28:MET:HE2	1:J:223:CYS:SG	2.47	0.55
1:D:64:MET:HA	1:D:64:MET:CE	2.37	0.55
1:E:159:GLU:O	1:E:163:THR:HG22	2.07	0.55
1:H:179:LEU:HD11	1:H:211:ARG:NH2	2.22	0.55
1:I:29:GLU:OE2	1:I:222:HIS:HD2	1.89	0.55
1:J:85:ARG:NH1	1:J:95:GLU:OE1	2.39	0.55
1:K:90:LEU:HD11	1:K:121:GLU:HG2	1.89	0.55
1:H:30:VAL:HG13	1:H:224:SER:HA	1.88	0.54
1:B:146:ARG:HD2	1:B:149:ASP:OD1	2.07	0.54
1:G:200:PRO:HD2	1:G:220:GLU:O	2.07	0.54
1:G:204:ILE:HG13	1:G:212:ILE:CD1	2.37	0.54
1:H:134:MET:HG2	1:H:138:ARG:HH21	1.71	0.54
1:B:182:LEU:HD23	1:B:182:LEU:C	2.28	0.54
1:C:127:LYS:HD2	2:C:475:HOH:O	2.07	0.54
1:F:210:GLN:O	1:F:214:GLU:HG2	2.08	0.54
1:A:26:PHE:HA	1:A:219:THR:O	2.08	0.54
1:E:158:LEU:CD1	1:E:196:ILE:HD11	2.38	0.54
1:F:192:ALA:CA	1:F:195:ARG:HH11	2.20	0.54
1:I:128:GLU:HG3	2:I:281:HOH:O	2.07	0.54
1:J:125:ILE:HD11	1:J:157:ALA:HB1	1.88	0.54
1:D:152:HIS:HD2	2:D:645:HOH:O	1.86	0.54
1:D:269:LYS:C	2:D:407:HOH:O	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HG22	1:B:37:SER:HB3	1.90	0.53
1:J:35:VAL:O	1:J:39:VAL:HG23	2.09	0.53
1:A:205:THR:HG23	1:A:207:ARG:H	1.73	0.53
1:C:71:LYS:HE2	1:C:110:GLY:O	2.08	0.53
1:E:61:THR:HG22	1:E:83:ARG:O	2.09	0.53
1:E:51:LEU:HB3	1:E:62:PRO:HG3	1.91	0.53
1:E:67:LEU:O	1:E:71:LYS:HB2	2.08	0.53
1:G:177:SER:HB2	1:G:202:GLY:O	2.09	0.53
1:H:105:LEU:O	1:H:109:TYR:HD1	1.91	0.53
1:H:122:ASP:HB2	1:H:124:HIS:CE1	2.44	0.53
1:I:162:LEU:HD11	1:I:195:ARG:HB2	1.90	0.53
1:A:128:GLU:HB2	2:A:552:HOH:O	2.09	0.53
1:D:182:LEU:HA	1:D:185:ILE:HG23	1.90	0.53
1:F:127:LYS:O	1:F:131:MET:HG3	2.08	0.53
1:H:94:ARG:O	1:H:98:VAL:HG23	2.08	0.53
1:F:143:THR:HB	1:F:168:ARG:CB	2.39	0.53
1:I:103:ILE:HG23	1:I:114:LEU:HD13	1.90	0.53
1:K:204:ILE:HG21	1:K:212:ILE:HD13	1.90	0.53
1:A:209:LEU:HD22	1:A:213:LEU:HG	1.91	0.53
1:C:192:ALA:O	1:C:195:ARG:HD3	2.09	0.53
1:G:151:VAL:HG12	1:G:153:ASP:N	2.24	0.53
1:K:210:GLN:HB2	1:K:267:ILE:HD11	1.90	0.53
1:D:155:MET:SD	1:D:191:GLN:OE1	2.67	0.53
1:K:48:ARG:NH2	1:K:168:ARG:NH1	2.47	0.53
1:B:208:ASN:C	1:B:208:ASN:HD22	2.12	0.53
1:D:160:THR:HA	1:D:163:THR:CG2	2.39	0.53
1:I:141:PRO:HA	2:I:279:HOH:O	2.09	0.53
1:G:260:LYS:HA	1:G:263:THR:HG22	1.91	0.52
1:B:175:ASP:OD1	1:D:207:ARG:NH2	2.42	0.52
1:C:143:THR:CG2	2:C:274:HOH:O	2.35	0.52
1:I:125:ILE:HD13	1:I:161:LEU:HD21	1.91	0.52
1:J:183:PRO:HG2	1:L:211:ARG:NH1	2.24	0.52
1:A:208:ASN:C	1:A:208:ASN:OD1	2.48	0.52
1:C:53:SER:HB2	1:C:62:PRO:HA	1.90	0.52
1:I:107:LYS:HG2	1:I:140:LEU:CD1	2.39	0.52
1:J:27:LEU:CB	1:J:220:GLU:HG2	2.36	0.52
1:J:233:MET:O	1:J:236:ARG:HD3	2.09	0.52
1:F:50:GLU:OE1	1:F:81:MET:HG2	2.10	0.52
1:F:266:ALA:C	1:F:268:ALA:H	2.13	0.52
1:I:59:GLY:O	1:I:83:ARG:HD3	2.10	0.52
1:K:28:MET:HE1	1:K:261:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:HIS:CG	1:L:146:ARG:H	2.28	0.52
1:D:61:THR:HB	1:D:81:MET:O	2.09	0.52
1:K:167:GLU:HB2	2:K:621:HOH:O	2.08	0.52
1:B:134:MET:HE3	1:B:142:VAL:HG21	1.91	0.52
1:E:166:PHE:O	1:E:196:ILE:HG22	2.08	0.52
1:I:129:LEU:O	1:I:133:LEU:HG	2.09	0.52
1:I:149:ASP:OD1	1:I:171:THR:HG23	2.09	0.52
1:G:94:ARG:HH11	1:H:36:GLU:HG3	1.75	0.52
1:K:82:ILE:HD12	1:K:114:LEU:HD22	1.91	0.52
1:L:120:THR:O	1:L:122:ASP:N	2.43	0.52
1:B:192:ALA:O	1:B:195:ARG:HD3	2.10	0.52
1:H:127:LYS:HB2	1:H:128:GLU:OE1	2.10	0.52
1:K:204:ILE:CG2	1:K:212:ILE:CD1	2.88	0.52
1:K:267:ILE:O	1:K:267:ILE:HG13	2.10	0.52
1:C:55:LEU:H	1:C:55:LEU:HD22	1.74	0.51
1:D:162:LEU:HD11	1:D:195:ARG:HE	1.74	0.51
1:A:117:GLY:HA2	1:A:144:PHE:CE1	2.46	0.51
1:F:32:VAL:HG23	1:F:37:SER:HB3	1.90	0.51
1:G:42:GLU:HG3	1:G:76:ILE:HD12	1.92	0.51
1:H:138:ARG:HD3	2:H:796:HOH:O	2.11	0.51
1:C:32:VAL:HG22	1:C:37:SER:HB2	1.91	0.51
1:C:99:MET:O	1:C:103:ILE:HG12	2.10	0.51
1:C:127:LYS:HD2	1:C:127:LYS:H	1.76	0.51
1:K:148:PHE:O	1:K:151:VAL:HG23	2.10	0.51
1:L:155:MET:HG2	1:L:191:GLN:HE22	1.75	0.51
1:D:94:ARG:HA	1:D:97:GLU:HG2	1.92	0.51
1:F:161:LEU:HD13	1:F:169:VAL:CG2	2.41	0.51
1:H:28:MET:HE1	1:H:261:VAL:HG13	1.91	0.51
1:J:175:ASP:OD2	1:J:180:GLU:CB	2.50	0.51
1:A:81:MET:CE	1:A:145:HIS:HD2	2.24	0.51
1:I:107:LYS:HG2	1:I:140:LEU:HD12	1.93	0.51
1:I:138:ARG:C	1:I:140:LEU:H	2.12	0.51
1:K:151:VAL:HG11	1:K:157:ALA:HB2	1.91	0.51
1:G:61:THR:HG22	1:G:83:ARG:O	2.11	0.51
1:G:101:ALA:O	1:G:105:LEU:HD23	2.11	0.51
1:E:35:VAL:HG22	1:E:70:VAL:HG23	1.93	0.51
1:G:43:ARG:HH11	1:G:258:VAL:HG21	1.75	0.51
1:K:186:LYS:O	1:K:190:GLU:HG2	2.10	0.51
1:A:115:VAL:HG13	1:A:143:THR:C	2.31	0.51
1:C:32:VAL:CG2	1:C:37:SER:HB3	2.41	0.51
1:G:46:ALA:O	1:G:76:ILE:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:LEU:O	1:L:81:MET:HB2	2.11	0.51
1:D:170:LEU:HD21	1:D:222:HIS:HB3	1.93	0.50
1:E:146:ARG:NH2	1:E:172:SER:HB3	2.26	0.50
1:G:55:LEU:HD13	1:G:55:LEU:N	2.13	0.50
1:K:186:LYS:HG2	1:K:216:SER:HA	1.93	0.50
1:L:30:VAL:HG13	1:L:224:SER:HA	1.93	0.50
1:A:258:VAL:CG1	1:A:262:ARG:HH21	2.24	0.50
1:C:143:THR:HB	1:C:168:ARG:CB	2.37	0.50
1:G:182:LEU:HD11	1:G:215:GLY:HA3	1.93	0.50
1:K:71:LYS:HG3	1:K:110:GLY:O	2.11	0.50
1:A:71:LYS:HE2	1:A:110:GLY:O	2.11	0.50
1:A:223:CYS:HA	2:A:312:HOH:O	2.10	0.50
1:E:89:PHE:HB2	1:E:119:LEU:HB2	1.93	0.50
1:F:145:HIS:CD2	1:F:147:ALA:H	2.24	0.50
1:J:32:VAL:HG12	1:J:256:THR:HG21	1.92	0.50
1:L:26:PHE:HB2	1:L:269:LYS:HE2	1.92	0.50
1:B:53:SER:HB3	1:B:62:PRO:HA	1.94	0.50
1:B:210:GLN:HA	1:B:271:ILE:HD11	1.93	0.50
1:C:257:ASP:OD2	1:C:259:THR:HG23	2.12	0.50
1:F:67:LEU:O	1:F:71:LYS:HB2	2.11	0.50
1:A:115:VAL:CG1	1:A:143:THR:OG1	2.60	0.50
1:J:61:THR:HA	1:J:81:MET:O	2.12	0.50
1:J:107:LYS:NZ	1:J:136:ILE:O	2.37	0.50
1:D:81:MET:HE2	1:D:115:VAL:O	2.12	0.50
1:G:125:ILE:HD13	1:G:125:ILE:N	2.12	0.50
1:I:125:ILE:HD11	1:I:157:ALA:HB1	1.93	0.50
1:G:209:LEU:HD22	1:G:267:ILE:HG13	1.94	0.50
1:C:82:ILE:HG13	1:C:103:ILE:HD13	1.94	0.50
1:D:44:GLY:HA2	1:D:262:ARG:HG3	1.93	0.50
1:D:272:LEU:HB2	2:D:885:HOH:O	2.12	0.50
1:E:94:ARG:NH1	1:F:36:GLU:HB2	2.27	0.50
1:A:115:VAL:HG22	1:A:143:THR:HG23	1.92	0.49
1:E:204:ILE:HD11	1:E:221:PHE:HD2	1.77	0.49
1:J:49:ILE:HG22	1:J:78:VAL:HG13	1.93	0.49
1:L:151:VAL:HG11	1:L:157:ALA:HB2	1.94	0.49
1:A:205:THR:OG1	1:A:206:ASP:N	2.45	0.49
1:F:257:ASP:O	1:F:261:VAL:HG23	2.11	0.49
1:G:73:SER:HB2	2:G:579:HOH:O	2.11	0.49
1:K:197:VAL:HG11	1:K:220:GLU:OE1	2.12	0.49
1:B:209:LEU:HD22	1:B:264:LEU:CD2	2.43	0.49
1:E:168:ARG:HG2	1:E:197:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:THR:HG22	1:F:83:ARG:O	2.12	0.49
1:L:182:LEU:N	1:L:183:PRO:HD2	2.28	0.49
1:C:209:LEU:HD22	1:C:213:LEU:HG	1.94	0.49
1:J:27:LEU:HD13	1:J:220:GLU:OE2	2.13	0.49
1:A:123:GLY:O	1:A:151:VAL:HG22	2.13	0.49
1:D:127:LYS:NZ	2:D:561:HOH:O	2.45	0.49
1:F:172:SER:HB3	1:F:201:GLY:O	2.12	0.49
1:B:125:ILE:C	1:B:125:ILE:HD13	2.32	0.49
1:B:259:THR:HG22	2:B:310:HOH:O	2.13	0.49
1:G:182:LEU:O	1:G:185:ILE:HG12	2.12	0.49
1:J:116:PHE:O	1:J:144:PHE:HA	2.11	0.49
1:L:182:LEU:HD11	1:L:212:ILE:HA	1.95	0.49
1:A:114:LEU:O	1:A:115:VAL:HG22	2.13	0.49
1:A:115:VAL:HG13	1:A:143:THR:OG1	2.12	0.49
1:D:48:ARG:HH12	1:D:168:ARG:HH12	1.56	0.49
1:E:24:ASN:HB2	2:E:700:HOH:O	2.13	0.49
1:J:205:THR:HB	1:J:208:ASN:HD22	1.78	0.49
1:L:206:ASP:HB2	2:L:745:HOH:O	2.12	0.49
1:A:103:ILE:HG23	1:A:114:LEU:CD1	2.42	0.49
1:J:146:ARG:HG3	1:J:170:LEU:HD13	1.95	0.49
1:K:115:VAL:HG13	1:K:145:HIS:NE2	2.27	0.49
1:E:226:ARG:HA	1:E:256:THR:HA	1.94	0.49
1:F:236:ARG:HH21	1:F:251:TYR:HB3	1.77	0.49
1:A:247:SER:O	1:A:248:CYS:O	2.30	0.48
1:A:251:TYR:N	1:A:251:TYR:CD1	2.81	0.48
1:C:55:LEU:HD23	1:C:55:LEU:N	2.27	0.48
1:E:146:ARG:HH21	1:E:202:GLY:CA	2.26	0.48
1:J:192:ALA:O	1:J:195:ARG:HD2	2.12	0.48
1:L:208:ASN:OD1	1:L:211:ARG:NE	2.45	0.48
1:A:105:LEU:HD21	1:B:68:GLN:OE1	2.13	0.48
1:I:85:ARG:HH21	1:I:88:ASP:CG	2.15	0.48
1:L:56:SER:HB3	1:L:254:LYS:NZ	2.27	0.48
1:L:210:GLN:NE2	2:L:777:HOH:O	2.46	0.48
1:A:171:THR:O	1:A:200:PRO:HA	2.13	0.48
1:C:127:LYS:O	1:C:131:MET:HG3	2.12	0.48
1:J:48:ARG:NH2	1:J:168:ARG:HH11	2.11	0.48
1:K:105:LEU:O	1:K:109:TYR:HD1	1.95	0.48
1:L:205:THR:HG22	1:L:206:ASP:N	2.28	0.48
1:B:204:ILE:CD1	1:B:209:LEU:HD13	2.42	0.48
1:G:208:ASN:HD21	1:G:211:ARG:HH21	1.59	0.48
1:A:116:PHE:O	1:A:145:HIS:CG	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HG	1:D:179:LEU:HD13	1.96	0.48
1:H:32:VAL:HG11	1:H:38:ALA:HB2	1.94	0.48
1:H:114:LEU:HD13	1:H:137:CYS:SG	2.53	0.48
1:I:160:THR:HA	1:I:163:THR:HG22	1.95	0.48
1:E:26:PHE:HA	1:E:219:THR:O	2.14	0.48
1:I:211:ARG:H	1:I:211:ARG:HD2	1.78	0.48
1:K:155:MET:SD	1:K:187:ARG:NH2	2.83	0.48
1:B:26:PHE:HA	1:B:219:THR:O	2.13	0.48
1:B:105:LEU:HD12	1:B:109:TYR:HE1	1.78	0.48
1:K:103:ILE:HG23	1:K:114:LEU:HD13	1.95	0.48
1:A:236:ARG:HB3	1:A:251:TYR:CZ	2.48	0.48
1:D:205:THR:OG1	1:D:206:ASP:N	2.47	0.48
1:E:71:LYS:NZ	1:E:112:ASP:OD2	2.46	0.48
1:K:81:MET:HA	1:K:115:VAL:HB	1.95	0.48
1:K:82:ILE:CD1	1:K:114:LEU:HD22	2.44	0.48
1:B:51:LEU:HB3	1:B:62:PRO:HG3	1.95	0.48
1:C:69:VAL:HA	1:C:72:GLN:HG2	1.94	0.48
1:A:219:THR:HG21	2:A:541:HOH:O	2.13	0.48
1:D:234:LYS:HG2	2:D:661:HOH:O	2.14	0.48
1:G:71:LYS:HD2	1:G:111:ALA:H	1.79	0.48
1:K:200:PRO:HD2	1:K:220:GLU:O	2.14	0.48
1:A:229:ARG:O	1:A:253:LEU:HD23	2.14	0.47
1:B:209:LEU:HD22	1:B:264:LEU:HD23	1.96	0.47
1:F:239:SER:OG	1:G:207:ARG:NH2	2.47	0.47
1:J:81:MET:HE1	1:J:145:HIS:CD2	2.49	0.47
1:K:100:LYS:HG2	1:K:136:ILE:HD13	1.96	0.47
1:A:200:PRO:HD2	1:A:220:GLU:O	2.15	0.47
1:E:68:GLN:O	1:E:72:GLN:HG2	2.14	0.47
1:K:42:GLU:OE1	2:K:458:HOH:O	2.20	0.47
1:K:145:HIS:ND1	1:K:170:LEU:HD12	2.28	0.47
1:L:186:LYS:HG2	1:L:216:SER:HA	1.95	0.47
1:H:95:GLU:O	1:H:99:MET:HG3	2.13	0.47
1:C:101:ALA:O	1:C:105:LEU:HD22	2.14	0.47
1:C:182:LEU:O	1:C:183:PRO:C	2.51	0.47
1:C:243:GLY:HA2	1:D:57:GLU:C	2.35	0.47
1:D:160:THR:HA	1:D:163:THR:HG22	1.96	0.47
1:F:208:ASN:O	1:F:212:ILE:HG23	2.14	0.47
1:H:167:GLU:C	1:H:168:ARG:HG2	2.35	0.47
1:J:167:GLU:HG2	2:J:660:HOH:O	2.14	0.47
1:A:185:ILE:HD11	1:A:216:SER:CB	2.44	0.47
1:A:201:GLY:O	2:A:312:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:VAL:CG1	1:D:145:HIS:HB3	2.45	0.47
1:E:105:LEU:HD13	1:E:109:TYR:CE2	2.48	0.47
1:E:127:LYS:H	1:E:127:LYS:HD2	1.80	0.47
1:J:27:LEU:O	1:J:220:GLU:HA	2.15	0.47
1:L:251:TYR:N	2:L:277:HOH:O	2.47	0.47
1:B:100:LYS:HG2	1:B:136:ILE:HD12	1.97	0.47
1:F:99:MET:O	1:F:103:ILE:HG12	2.14	0.47
1:H:85:ARG:CG	1:H:85:ARG:NH1	2.74	0.47
1:K:94:ARG:O	1:K:97:GLU:HB2	2.14	0.47
1:C:243:GLY:HA2	1:D:58:GLY:N	2.30	0.47
1:D:168:ARG:HG2	1:D:197:VAL:HB	1.96	0.47
1:D:193:LYS:HB2	1:D:195:ARG:HH11	1.80	0.47
1:F:161:LEU:HD13	1:F:169:VAL:HG21	1.97	0.47
1:G:130:CYS:O	1:G:134:MET:HB2	2.14	0.47
1:B:259:THR:O	1:B:263:THR:HG22	2.15	0.47
1:D:151:VAL:HG12	1:D:153:ASP:H	1.80	0.47
1:I:85:ARG:NH1	1:I:95:GLU:OE1	2.48	0.47
1:A:81:MET:CE	1:A:145:HIS:CD2	2.98	0.46
1:A:150:MET:SD	1:B:240:VAL:HB	2.55	0.46
1:A:207:ARG:HH22	1:D:239:SER:CB	2.27	0.46
1:E:68:GLN:HE22	1:F:105:LEU:HD21	1.80	0.46
1:H:49:ILE:HG12	1:H:76:ILE:CD1	2.45	0.46
1:J:81:MET:CE	1:J:145:HIS:HD2	2.28	0.46
1:D:125:ILE:HD13	1:D:161:LEU:HD23	1.97	0.46
1:H:162:LEU:CD2	1:H:195:ARG:HB3	2.45	0.46
1:A:226:ARG:NH1	1:A:256:THR:HG22	2.26	0.46
1:D:48:ARG:HD2	1:D:79:PHE:CD2	2.51	0.46
1:F:49:ILE:HD11	1:F:78:VAL:HG22	1.97	0.46
1:I:205:THR:HG21	1:I:207:ARG:NH1	2.31	0.46
1:F:257:ASP:HB3	1:F:260:LYS:HB2	1.97	0.46
1:A:155:MET:SD	1:A:191:GLN:NE2	2.89	0.46
1:C:205:THR:H	1:C:208:ASN:HB2	1.80	0.46
1:D:115:VAL:HG12	1:D:145:HIS:HB3	1.97	0.46
1:H:51:LEU:O	1:H:81:MET:HB2	2.16	0.46
1:K:27:LEU:HA	1:K:47:ASP:OD2	2.16	0.46
1:E:60:THR:O	1:E:61:THR:O	2.34	0.46
1:E:158:LEU:HD13	1:E:188:LEU:HD13	1.97	0.46
1:K:253:LEU:HD23	1:K:253:LEU:H	1.80	0.46
1:A:31:CYS:HA	1:A:50:GLU:O	2.15	0.46
1:C:259:THR:HG22	2:C:420:HOH:O	2.15	0.46
1:D:96:ILE:HG21	1:D:129:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:ILE:HG23	1:G:114:LEU:HD13	1.97	0.46
1:H:168:ARG:HG3	1:H:168:ARG:HH11	1.80	0.46
1:A:37:SER:HB3	1:A:256:THR:CG2	2.39	0.46
1:B:125:ILE:HD12	1:B:160:THR:HG22	1.97	0.46
1:D:204:ILE:HG12	1:D:212:ILE:HD13	1.98	0.46
1:E:94:ARG:HH11	1:E:94:ARG:CB	2.20	0.46
1:F:182:LEU:HB3	1:F:183:PRO:HD3	1.98	0.46
1:D:159:GLU:O	1:D:163:THR:HG22	2.16	0.46
1:G:65:GLY:O	1:G:69:VAL:HG23	2.16	0.46
1:L:200:PRO:HD2	1:L:220:GLU:O	2.15	0.46
1:A:49:ILE:HG23	1:A:76:ILE:HD11	1.98	0.45
1:A:92:SER:O	1:A:96:ILE:HG23	2.16	0.45
1:D:104:ARG:NE	2:D:343:HOH:O	2.40	0.45
1:E:253:LEU:HD21	1:F:88:ASP:HB3	1.98	0.45
1:F:185:ILE:HD11	1:F:216:SER:CB	2.47	0.45
1:H:167:GLU:H	1:H:167:GLU:HG2	1.53	0.45
1:I:138:ARG:HB3	1:I:139:PRO:CD	2.28	0.45
1:J:193:LYS:HA	2:J:858:HOH:O	2.15	0.45
1:B:120:THR:HB	1:B:124:HIS:O	2.17	0.45
1:C:120:THR:HG22	1:C:121:GLU:H	1.81	0.45
1:D:35:VAL:HG21	1:D:69:VAL:CG1	2.47	0.45
1:D:48:ARG:CZ	1:D:168:ARG:HH11	2.29	0.45
1:D:269:LYS:HA	2:D:407:HOH:O	2.16	0.45
1:F:32:VAL:HG21	1:F:38:ALA:N	2.31	0.45
1:G:98:VAL:HG11	1:H:66:VAL:HG22	1.97	0.45
1:K:182:LEU:HD11	1:K:212:ILE:HA	1.98	0.45
1:L:145:HIS:CG	1:L:146:ARG:N	2.84	0.45
1:F:35:VAL:O	1:F:39:VAL:HG23	2.15	0.45
1:F:156:ALA:O	1:F:160:THR:HG22	2.17	0.45
1:A:64:MET:HG2	1:A:109:TYR:CD1	2.51	0.45
1:D:259:THR:O	1:D:263:THR:HG23	2.17	0.45
1:D:55:LEU:HD13	1:D:226:ARG:CZ	2.47	0.45
1:H:111:ALA:O	1:H:140:LEU:HD13	2.17	0.45
1:H:112:ASP:O	1:H:141:PRO:HD2	2.17	0.45
1:L:225:ALA:HB1	1:L:260:LYS:HB3	1.98	0.45
1:I:159:GLU:OE2	1:I:191:GLN:NE2	2.50	0.45
1:J:28:MET:HE3	1:J:223:CYS:SG	2.57	0.45
1:K:170:LEU:HD21	1:K:222:HIS:HB3	1.99	0.45
1:B:134:MET:CE	1:B:142:VAL:HG21	2.47	0.45
1:E:94:ARG:NE	2:E:739:HOH:O	2.34	0.45
1:J:66:VAL:O	1:J:70:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:197:VAL:HG11	1:J:220:GLU:OE1	2.16	0.45
1:C:146:ARG:C	1:C:148:PHE:N	2.70	0.45
1:I:149:ASP:OD1	1:I:171:THR:CG2	2.64	0.45
1:I:205:THR:HG22	1:I:206:ASP:OD1	2.17	0.45
1:A:107:LYS:NZ	1:A:138:ARG:O	2.50	0.45
1:A:181:GLY:O	1:A:185:ILE:HG23	2.17	0.44
1:B:257:ASP:HB3	1:B:260:LYS:HB2	1.99	0.44
1:C:55:LEU:HD23	2:C:315:HOH:O	2.17	0.44
1:D:237:ASN:ND2	1:D:239:SER:H	2.15	0.44
1:G:82:ILE:HG13	1:G:103:ILE:HD13	1.99	0.44
1:H:28:MET:CE	1:H:261:VAL:HG13	2.47	0.44
1:A:114:LEU:C	1:A:115:VAL:CG2	2.85	0.44
1:D:146:ARG:HG2	1:D:170:LEU:HD13	2.00	0.44
1:D:168:ARG:NH1	1:D:220:GLU:OE1	2.50	0.44
1:F:128:GLU:HA	1:F:131:MET:HE2	1.98	0.44
1:H:105:LEU:O	1:H:109:TYR:CD1	2.71	0.44
1:D:71:LYS:NZ	1:D:112:ASP:OD2	2.51	0.44
1:F:85:ARG:NH1	1:F:95:GLU:OE1	2.51	0.44
1:K:226:ARG:HH21	1:K:254:LYS:HB2	1.81	0.44
1:D:49:ILE:HD11	1:D:78:VAL:HG22	1.99	0.44
1:F:51:LEU:HB3	1:F:62:PRO:HG3	2.00	0.44
1:F:143:THR:HB	1:F:168:ARG:HB2	2.00	0.44
1:H:134:MET:SD	1:H:138:ARG:NH2	2.90	0.44
1:K:204:ILE:HD11	1:K:222:HIS:O	2.18	0.44
1:C:242:MET:SD	1:D:89:PHE:HZ	2.41	0.44
1:E:185:ILE:CD1	1:E:200:PRO:HB3	2.47	0.44
1:K:173:GLY:HA3	1:K:181:GLY:HA3	2.00	0.44
1:C:237:ASN:HB3	1:D:150:MET:CE	2.48	0.44
1:D:171:THR:O	1:D:200:PRO:HA	2.18	0.44
1:I:100:LYS:O	1:I:104:ARG:HG3	2.17	0.44
1:K:84:PRO:HD2	1:K:91:TYR:CE2	2.53	0.44
1:L:237:ASN:O	1:L:239:SER:N	2.49	0.44
1:D:170:LEU:HD21	1:D:222:HIS:CB	2.47	0.44
1:E:44:GLY:HA3	1:E:261:VAL:HG23	1.99	0.44
1:L:103:ILE:HG23	1:L:114:LEU:HD13	1.99	0.44
1:A:207:ARG:HE	1:A:207:ARG:HB2	1.67	0.44
1:C:159:GLU:O	1:C:162:LEU:HD12	2.17	0.43
1:C:200:PRO:HD2	1:C:220:GLU:O	2.18	0.43
1:F:143:THR:HB	1:F:168:ARG:HB3	2.00	0.43
1:K:49:ILE:HG13	1:K:76:ILE:HD11	1.98	0.43
1:C:55:LEU:CD2	1:C:55:LEU:N	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:PRO:HD2	1:E:220:GLU:O	2.17	0.43
1:G:55:LEU:CD2	1:G:56:SER:H	2.29	0.43
1:K:240:VAL:HG11	1:L:150:MET:HG3	1.99	0.43
1:E:116:PHE:CE2	1:E:142:VAL:HG11	2.54	0.43
1:F:103:ILE:O	1:F:107:LYS:HG2	2.19	0.43
1:F:138:ARG:HG2	1:F:139:PRO:HA	1.99	0.43
1:L:69:VAL:O	1:L:73:SER:OG	2.37	0.43
1:C:125:ILE:HD12	1:C:130:CYS:SG	2.59	0.43
1:I:168:ARG:HG2	1:I:197:VAL:HB	2.00	0.43
1:K:180:GLU:HG2	2:K:469:HOH:O	2.18	0.43
1:A:116:PHE:CE2	1:A:142:VAL:HG11	2.53	0.43
1:D:265:ASN:OD1	1:D:269:LYS:HE3	2.19	0.43
1:F:29:GLU:HG2	1:F:222:HIS:HD1	1.84	0.43
1:G:105:LEU:HD21	1:H:68:GLN:NE2	2.33	0.43
1:J:146:ARG:NH1	1:J:172:SER:HB3	2.32	0.43
1:J:260:LYS:O	1:J:264:LEU:HD23	2.18	0.43
1:L:268:ALA:O	1:L:269:LYS:HB2	2.18	0.43
1:A:114:LEU:C	1:A:115:VAL:HG23	2.39	0.43
1:A:228:THR:HG22	2:A:320:HOH:O	2.18	0.43
1:C:130:CYS:O	1:C:134:MET:HG3	2.18	0.43
1:I:28:MET:HE1	1:I:261:VAL:HG13	1.97	0.43
1:I:200:PRO:HD2	1:I:220:GLU:O	2.18	0.43
1:L:63:SER:OG	1:L:66:VAL:HG23	2.18	0.43
1:A:116:PHE:CG	1:A:117:GLY:N	2.85	0.43
1:D:182:LEU:HD23	1:D:182:LEU:O	2.19	0.43
1:H:93:ASP:HA	1:H:96:ILE:HD12	2.00	0.43
1:J:85:ARG:HH11	1:J:95:GLU:CD	2.21	0.43
1:L:208:ASN:HB2	2:L:473:HOH:O	2.19	0.43
1:B:122:ASP:OD2	1:B:124:HIS:ND1	2.52	0.43
1:D:205:THR:HG22	1:D:208:ASN:ND2	2.34	0.43
1:F:60:THR:CG2	1:F:61:THR:N	2.82	0.43
1:G:153:ASP:OD1	1:G:155:MET:HB2	2.18	0.43
1:G:172:SER:HB3	1:G:202:GLY:H	1.83	0.43
1:A:114:LEU:O	1:A:115:VAL:CG2	2.66	0.43
1:D:118:ALA:O	1:D:119:LEU:HD23	2.19	0.43
1:G:138:ARG:HE	1:G:142:VAL:HG23	1.83	0.43
1:I:115:VAL:HG22	1:I:143:THR:HB	2.00	0.43
1:J:117:GLY:HA2	1:J:144:PHE:CE1	2.54	0.43
1:A:81:MET:HE1	1:A:145:HIS:CD2	2.53	0.43
1:A:235:PHE:CE1	1:B:152:HIS:ND1	2.86	0.43
1:E:146:ARG:HH11	1:E:146:ARG:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLU:O	1:F:99:MET:HG3	2.19	0.43
1:H:59:GLY:O	1:H:83:ARG:HD2	2.19	0.43
1:J:205:THR:HG22	1:J:206:ASP:OD1	2.19	0.43
1:D:91:TYR:CG	1:D:99:MET:HE1	2.54	0.42
1:D:151:VAL:HG12	1:D:153:ASP:N	2.33	0.42
1:G:90:LEU:HD21	1:G:121:GLU:N	2.34	0.42
1:I:85:ARG:NH2	1:I:88:ASP:OD2	2.52	0.42
1:J:81:MET:HE2	1:J:82:ILE:N	2.34	0.42
1:K:70:VAL:O	1:K:74:VAL:HB	2.19	0.42
1:D:85:ARG:NH2	1:D:88:ASP:OD2	2.50	0.42
1:K:121:GLU:H	1:K:121:GLU:HG3	1.57	0.42
1:A:249:SER:OG	1:A:250:GLU:N	2.50	0.42
1:E:158:LEU:HD11	1:E:196:ILE:HD11	2.01	0.42
1:G:89:PHE:HB2	1:G:119:LEU:HD23	2.01	0.42
1:G:170:LEU:HD23	1:G:170:LEU:HA	1.91	0.42
1:I:63:SER:OG	1:I:66:VAL:HG23	2.19	0.42
1:K:48:ARG:HA	1:K:76:ILE:HD12	2.01	0.42
1:A:258:VAL:HG12	1:A:262:ARG:HH21	1.84	0.42
1:B:170:LEU:HD21	1:B:222:HIS:HB3	2.00	0.42
1:F:209:LEU:HD21	1:F:221:PHE:CE2	2.54	0.42
1:H:120:THR:HG22	1:H:121:GLU:H	1.83	0.42
1:J:235:PHE:C	1:J:236:ARG:HG2	2.40	0.42
1:B:210:GLN:HE21	1:B:210:GLN:HB2	1.57	0.42
1:F:182:LEU:HD11	1:F:212:ILE:HA	2.02	0.42
1:H:107:LYS:HD3	1:H:114:LEU:HD11	2.00	0.42
1:H:146:ARG:H	1:H:146:ARG:HG2	1.68	0.42
1:H:252:SER:N	2:H:289:HOH:O	2.52	0.42
1:K:186:LYS:HG2	1:K:215:GLY:O	2.18	0.42
1:E:116:PHE:O	1:E:144:PHE:HA	2.19	0.42
1:G:182:LEU:HD12	1:G:212:ILE:HA	2.01	0.42
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.83	0.42
1:C:94:ARG:NH1	1:D:36:GLU:HG3	2.34	0.42
1:D:61:THR:CG2	2:D:275:HOH:O	2.45	0.42
1:G:55:LEU:HB3	1:G:226:ARG:NH2	2.34	0.42
1:K:37:SER:HG	1:L:85:ARG:HH22	1.68	0.42
1:B:182:LEU:HD21	1:B:215:GLY:O	2.18	0.42
1:E:37:SER:HB3	1:E:256:THR:HG23	2.01	0.42
1:I:26:PHE:CE2	1:I:213:LEU:HD13	2.55	0.42
1:L:103:ILE:HG23	1:L:114:LEU:CD1	2.50	0.42
1:H:48:ARG:HD2	1:H:79:PHE:CE1	2.55	0.42
1:I:79:PHE:HE2	2:I:284:HOH:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:ASP:O	1:J:141:PRO:HD2	2.19	0.42
1:D:48:ARG:HD2	1:D:79:PHE:CE2	2.55	0.42
1:L:226:ARG:HA	1:L:256:THR:HA	2.00	0.42
1:A:160:THR:O	1:A:164:LEU:HG	2.20	0.41
1:C:150:MET:SD	1:D:240:VAL:HG21	2.59	0.41
1:H:29:GLU:OE2	1:H:222:HIS:CD2	2.73	0.41
1:H:137:CYS:O	1:H:140:LEU:HG	2.20	0.41
1:A:60:THR:CG2	1:A:61:THR:N	2.83	0.41
1:C:127:LYS:CD	2:C:475:HOH:O	2.67	0.41
1:F:199:MET:HG3	1:F:221:PHE:HA	2.00	0.41
1:J:76:ILE:HB	1:J:77:PRO:HD2	2.02	0.41
1:D:236:ARG:HG2	1:D:251:TYR:CE2	2.55	0.41
1:E:39:VAL:HG11	1:F:94:ARG:HH11	1.86	0.41
1:G:94:ARG:HD2	1:H:36:GLU:HG3	2.02	0.41
1:G:160:THR:O	1:G:163:THR:HG22	2.20	0.41
1:K:210:GLN:HG3	1:K:271:ILE:HD11	2.03	0.41
1:D:81:MET:HE1	1:D:145:HIS:HD2	1.84	0.41
1:E:39:VAL:HG11	1:F:94:ARG:NH1	2.34	0.41
1:E:41:ALA:HB3	1:E:49:ILE:HD11	2.02	0.41
1:F:81:MET:CE	1:F:145:HIS:ND1	2.84	0.41
1:F:153:ASP:HA	1:F:154:PRO:HD2	1.80	0.41
1:G:94:ARG:HD3	1:H:35:VAL:HG12	2.03	0.41
1:H:65:GLY:O	1:H:69:VAL:HG23	2.20	0.41
1:H:223:CYS:SG	1:H:224:SER:N	2.93	0.41
1:I:140:LEU:HA	1:I:141:PRO:HD2	1.73	0.41
1:K:71:LYS:CG	1:K:110:GLY:O	2.69	0.41
1:B:201:GLY:O	1:B:202:GLY:C	2.58	0.41
1:I:137:CYS:O	1:I:138:ARG:O	2.38	0.41
1:K:67:LEU:O	1:K:71:LYS:HB2	2.21	0.41
1:A:33:ASP:OD2	1:A:55:LEU:HD12	2.21	0.41
1:B:170:LEU:HD21	1:B:222:HIS:CB	2.51	0.41
1:H:149:ASP:CG	1:H:172:SER:H	2.24	0.41
1:I:29:GLU:HA	1:I:48:ARG:O	2.21	0.41
1:I:205:THR:CG2	1:I:206:ASP:N	2.83	0.41
1:A:182:LEU:HD21	1:A:216:SER:HB3	2.03	0.41
1:A:250:GLU:HB2	2:A:363:HOH:O	2.12	0.41
1:A:253:LEU:HD23	1:A:253:LEU:N	2.35	0.41
1:C:125:ILE:HD11	1:C:164:LEU:CD1	2.51	0.41
1:C:151:VAL:HG11	1:C:157:ALA:HB2	2.02	0.41
1:D:91:TYR:CG	1:D:99:MET:CE	3.04	0.41
1:E:226:ARG:HG3	1:E:256:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:VAL:HG13	1:L:37:SER:OG	2.21	0.41
1:A:32:VAL:HG11	1:A:38:ALA:N	2.35	0.41
1:F:261:VAL:HA	1:F:264:LEU:HD22	2.02	0.41
1:H:79:PHE:CZ	1:H:141:PRO:HG2	2.55	0.41
1:L:29:GLU:HB2	1:L:48:ARG:O	2.21	0.41
1:L:261:VAL:HA	1:L:264:LEU:HD12	2.03	0.41
1:D:64:MET:CG	1:D:109:TYR:CD1	3.04	0.41
1:D:167:GLU:H	1:D:167:GLU:HG2	1.63	0.41
1:D:193:LYS:HB2	1:D:195:ARG:NH1	2.36	0.41
1:E:40:ASN:ND2	2:E:640:HOH:O	2.40	0.41
1:E:83:ARG:HH12	1:F:242:MET:HG2	1.86	0.41
1:F:50:GLU:HA	1:F:79:PHE:O	2.21	0.41
1:G:32:VAL:HG11	1:G:38:ALA:HB2	2.02	0.41
1:G:257:ASP:CB	1:G:260:LYS:HD3	2.50	0.41
1:H:119:LEU:HD23	1:H:125:ILE:HA	2.03	0.41
1:H:149:ASP:OD1	1:H:171:THR:HG23	2.21	0.41
1:J:172:SER:HB3	1:J:201:GLY:O	2.20	0.41
1:K:76:ILE:HB	1:K:77:PRO:HD2	2.03	0.41
1:B:67:LEU:O	1:B:71:LYS:HB2	2.20	0.41
1:B:104:ARG:HG3	1:B:104:ARG:NH1	2.14	0.41
1:I:205:THR:CG2	1:I:206:ASP:H	2.33	0.41
1:A:28:MET:HE2	1:A:46:ALA:HA	2.02	0.40
1:D:88:ASP:OD2	1:D:88:ASP:C	2.60	0.40
1:J:205:THR:HG22	1:J:206:ASP:N	2.35	0.40
1:J:228:THR:HA	1:J:253:LEU:O	2.20	0.40
1:K:57:GLU:HG3	1:K:86:GLY:HA3	2.03	0.40
1:L:168:ARG:HG2	1:L:197:VAL:HB	2.04	0.40
1:B:224:SER:HA	2:B:308:HOH:O	2.20	0.40
1:D:60:THR:CG2	1:D:61:THR:N	2.83	0.40
1:E:162:LEU:HB3	1:E:196:ILE:HD13	2.01	0.40
1:F:55:LEU:C	1:F:57:GLU:H	2.25	0.40
1:I:168:ARG:NH1	2:I:284:HOH:O	2.48	0.40
1:A:204:ILE:HG12	1:A:212:ILE:HD13	2.02	0.40
1:F:170:LEU:HD21	1:F:222:HIS:HB3	2.04	0.40
1:H:145:HIS:CD2	1:H:147:ALA:H	2.38	0.40
1:B:35:VAL:HG21	1:B:69:VAL:HG12	2.04	0.40
1:B:259:THR:O	1:B:263:THR:CG2	2.70	0.40
1:F:189:ILE:HG12	1:F:198:VAL:HB	2.03	0.40
1:G:96:ILE:HG21	1:G:129:LEU:HD11	2.03	0.40
1:J:81:MET:CE	1:J:145:HIS:CD2	3.04	0.40
1:K:182:LEU:N	1:K:183:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:228:THR:HG23	1:L:253:LEU:H	1.87	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	247/287 (86%)	231 (94%)	13 (5%)	3 (1%)	13	24
1	B	240/287 (84%)	228 (95%)	10 (4%)	2 (1%)	19	35
1	C	243/287 (85%)	237 (98%)	5 (2%)	1 (0%)	34	54
1	D	241/287 (84%)	235 (98%)	6 (2%)	0	100	100
1	E	238/287 (83%)	217 (91%)	18 (8%)	3 (1%)	12	21
1	F	237/287 (83%)	214 (90%)	20 (8%)	3 (1%)	12	21
1	G	233/287 (81%)	208 (89%)	21 (9%)	4 (2%)	9	16
1	H	232/287 (81%)	211 (91%)	20 (9%)	1 (0%)	34	54
1	I	237/287 (83%)	225 (95%)	10 (4%)	2 (1%)	19	35
1	J	235/287 (82%)	216 (92%)	18 (8%)	1 (0%)	34	54
1	K	234/287 (82%)	213 (91%)	17 (7%)	4 (2%)	9	16
1	L	235/287 (82%)	210 (89%)	22 (9%)	3 (1%)	12	21
All	All	2852/3444 (83%)	2645 (93%)	180 (6%)	27 (1%)	17	31

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	CYS
1	F	267	ILE
1	I	138	ARG

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Mol	Chain	Res	Type
1	I	139	PRO
1	L	121	GLU
1	A	26	PHE
1	B	53	SER
1	C	243	GLY
1	G	121	GLU
1	H	59	GLY
1	K	176	SER
1	K	203	GLY
1	L	238	SER
1	B	201	GLY
1	E	215	GLY
1	F	56	SER
1	G	202	GLY
1	K	146	ARG
1	K	202	GLY
1	E	54	GLY
1	E	61	THR
1	F	194	GLY
1	G	111	ALA
1	J	195	ARG
1	L	146	ARG
1	A	201	GLY
1	G	201	GLY

5.3.2 Protein sidechains (i)

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	206/233 (88%)	172 (84%)	34 (16%)	2 4
1	B	202/233 (87%)	176 (87%)	26 (13%)	4 8
1	C	204/233 (88%)	179 (88%)	25 (12%)	4 9
1	D	203/233 (87%)	165 (81%)	38 (19%)	1 2
1	E	201/233 (86%)	179 (89%)	22 (11%)	6 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	199/233 (85%)	169 (85%)	30 (15%)	3 5
1	G	197/233 (84%)	182 (92%)	15 (8%)	13 25
1	H	196/233 (84%)	171 (87%)	25 (13%)	4 8
1	I	201/233 (86%)	185 (92%)	16 (8%)	12 23
1	J	199/233 (85%)	175 (88%)	24 (12%)	5 9
1	K	198/233 (85%)	180 (91%)	18 (9%)	9 18
1	L	198/233 (85%)	180 (91%)	18 (9%)	9 18
All	All	2404/2796 (86%)	2113 (88%)	291 (12%)	5 9

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	31	CYS
1	A	51	LEU
1	A	60	THR
1	A	64	MET
1	A	66	VAL
1	A	67	LEU
1	A	74	VAL
1	A	81	MET
1	A	85	ARG
1	A	90	LEU
1	A	96	ILE
1	A	120	THR
1	A	125	ILE
1	A	143	THR
1	A	145	HIS
1	A	151	VAL
1	A	159	GLU
1	A	160	THR
1	A	162	LEU
1	A	167	GLU
1	A	169	VAL
1	A	170	LEU
1	A	179	LEU
1	A	182	LEU
1	A	185	ILE
1	A	209	LEU
1	A	228	THR

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Mol	Chain	Res	Type
1	A	249	SER
1	A	251	TYR
1	A	256	THR
1	A	259	THR
1	A	263	THR
1	A	272	LEU
1	B	31	CYS
1	B	33	ASP
1	B	43	ARG
1	B	52	CYS
1	B	55	LEU
1	B	57	GLU
1	B	61	THR
1	B	67	LEU
1	B	74	VAL
1	B	83	ARG
1	B	90	LEU
1	B	104	ARG
1	B	120	THR
1	B	125	ILE
1	B	134	MET
1	B	143	THR
1	B	145	HIS
1	B	163	THR
1	B	170	LEU
1	B	176	SER
1	B	204	ILE
1	B	208	ASN
1	B	250	GLU
1	B	258	VAL
1	B	263	THR
1	B	265	ASN
1	C	31	CYS
1	C	32	VAL
1	C	55	LEU
1	C	61	THR
1	C	66	VAL
1	C	67	LEU
1	C	74	VAL
1	C	83	ARG
1	C	90	LEU
1	C	105	LEU

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Mol	Chain	Res	Type
1	C	108	LEU
1	C	125	ILE
1	C	127	LYS
1	C	129	LEU
1	C	143	THR
1	C	145	HIS
1	C	162	LEU
1	C	170	LEU
1	C	186	LYS
1	C	209	LEU
1	C	248	CYS
1	C	253	LEU
1	C	259	THR
1	C	263	THR
1	C	271	ILE
1	D	27	LEU
1	D	31	CYS
1	D	32	VAL
1	D	43	ARG
1	D	51	LEU
1	D	52	CYS
1	D	60	THR
1	D	61	THR
1	D	64	MET
1	D	66	VAL
1	D	67	LEU
1	D	81	MET
1	D	85	ARG
1	D	90	LEU
1	D	96	ILE
1	D	105	LEU
1	D	108	LEU
1	D	122	ASP
1	D	125	ILE
1	D	128	GLU
1	D	129	LEU
1	D	145	HIS
1	D	160	THR
1	D	162	LEU
1	D	163	THR
1	D	167	GLU
1	D	170	LEU

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Mol	Chain	Res	Type
1	D	175	ASP
1	D	179	LEU
1	D	185	ILE
1	D	190	GLU
1	D	193	LYS
1	D	209	LEU
1	D	228	THR
1	D	237	ASN
1	D	240	VAL
1	D	248	CYS
1	D	263	THR
1	E	31	CYS
1	E	39	VAL
1	E	49	ILE
1	E	61	THR
1	E	71	LYS
1	E	90	LEU
1	E	104	ARG
1	E	105	LEU
1	E	119	LEU
1	E	125	ILE
1	E	127	LYS
1	E	134	MET
1	E	143	THR
1	E	145	HIS
1	E	146	ARG
1	E	151	VAL
1	E	170	LEU
1	E	175	ASP
1	E	186	LYS
1	E	188	LEU
1	E	209	LEU
1	E	259	THR
1	F	32	VAL
1	F	52	CYS
1	F	64	MET
1	F	66	VAL
1	F	67	LEU
1	F	74	VAL
1	F	81	MET
1	F	85	ARG
1	F	90	LEU

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Mol	Chain	Res	Type
1	F	107	LYS
1	F	108	LEU
1	F	138	ARG
1	F	140	LEU
1	F	143	THR
1	F	160	THR
1	F	162	LEU
1	F	170	LEU
1	F	179	LEU
1	F	182	LEU
1	F	184	LEU
1	F	185	ILE
1	F	190	GLU
1	F	207	ARG
1	F	219	THR
1	F	226	ARG
1	F	236	ARG
1	F	242	MET
1	F	252	SER
1	F	264	LEU
1	F	267	ILE
1	G	24	ASN
1	G	31	CYS
1	G	33	ASP
1	G	48	ARG
1	G	52	CYS
1	G	55	LEU
1	G	73	SER
1	G	83	ARG
1	G	125	ILE
1	G	129	LEU
1	G	143	THR
1	G	163	THR
1	G	171	THR
1	G	212	ILE
1	G	219	THR
1	H	31	CYS
1	H	33	ASP
1	H	52	CYS
1	H	64	MET
1	H	67	LEU
1	H	81	MET

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Mol	Chain	Res	Type
1	H	85	ARG
1	H	103	ILE
1	H	107	LYS
1	H	120	THR
1	H	128	GLU
1	H	140	LEU
1	H	145	HIS
1	H	146	ARG
1	H	158	LEU
1	H	163	THR
1	H	167	GLU
1	H	168	ARG
1	H	170	LEU
1	H	184	LEU
1	H	191	GLN
1	H	205	THR
1	H	209	LEU
1	H	233	MET
1	H	239	SER
1	I	30	VAL
1	I	31	CYS
1	I	51	LEU
1	I	67	LEU
1	I	71	LYS
1	I	150	MET
1	I	158	LEU
1	I	170	LEU
1	I	179	LEU
1	I	182	LEU
1	I	184	LEU
1	I	209	LEU
1	I	211	ARG
1	I	233	MET
1	I	238	SER
1	I	253	LEU
1	J	31	CYS
1	J	35	VAL
1	J	52	CYS
1	J	57	GLU
1	J	67	LEU
1	J	73	SER
1	J	74	VAL

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Mol	Chain	Res	Type
1	J	81	MET
1	J	85	ARG
1	J	88	ASP
1	J	96	ILE
1	J	105	LEU
1	J	108	LEU
1	J	122	ASP
1	J	143	THR
1	J	145	HIS
1	J	155	MET
1	J	160	THR
1	J	167	GLU
1	J	170	LEU
1	J	182	LEU
1	J	209	LEU
1	J	227	SER
1	J	254	LYS
1	K	31	CYS
1	K	53	SER
1	K	67	LEU
1	K	74	VAL
1	K	81	MET
1	K	90	LEU
1	K	121	GLU
1	K	129	LEU
1	K	158	LEU
1	K	170	LEU
1	K	179	LEU
1	K	182	LEU
1	K	190	GLU
1	K	193	LYS
1	K	204	ILE
1	K	207	ARG
1	K	236	ARG
1	K	267	ILE
1	L	31	CYS
1	L	33	ASP
1	L	57	GLU
1	L	67	LEU
1	L	73	SER
1	L	81	MET
1	L	126	ASP

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Mol	Chain	Res	Type
1	L	158	LEU
1	L	170	LEU
1	L	175	ASP
1	L	179	LEU
1	L	180	GLU
1	L	184	LEU
1	L	206	ASP
1	L	219	THR
1	L	231	SER
1	L	253	LEU
1	L	265	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	124	HIS
1	A	145	HIS
1	A	191	GLN
1	B	24	ASN
1	B	72	GLN
1	B	208	ASN
1	B	210	GLN
1	B	222	HIS
1	B	265	ASN
1	C	75	GLN
1	C	210	GLN
1	D	72	GLN
1	D	124	HIS
1	D	152	HIS
1	D	237	ASN
1	E	24	ASN
1	E	68	GLN
1	G	68	GLN
1	H	68	GLN
1	H	222	HIS
1	I	145	HIS
1	I	191	GLN
1	I	222	HIS
1	J	68	GLN
1	J	208	ASN
1	K	124	HIS

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Mol	Chain	Res	Type
1	L	191	GLN
1	L	270	ASN

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 monosaccharides 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, 95^{th} 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	249/287 (86%)	0.09	10 (4%) 38 41	9, 25, 57, 151	0
1	B	244/287 (85%)	-0.23	2 (0%) 86 87	9, 24, 48, 100	0
1	C	247/287 (86%)	-0.22	3 (1%) 79 80	12, 22, 50, 91	0
1	D	245/287 (85%)	-0.13	3 (1%) 79 80	9, 23, 48, 89	0
1	E	242/287 (84%)	0.58	18 (7%) 14 15	36, 60, 94, 119	0
1	F	241/287 (83%)	0.32	12 (4%) 28 30	26, 55, 89, 113	0
1	G	237/287 (82%)	0.91	30 (12%) 3 3	52, 77, 99, 134	0
1	H	236/287 (82%)	0.86	28 (11%) 4 4	52, 79, 103, 120	0
1	I	241/287 (83%)	0.54	14 (5%) 23 24	37, 57, 91, 136	0
1	J	239/287 (83%)	0.42	21 (8%) 10 10	35, 57, 92, 113	0
1	K	238/287 (82%)	0.96	29 (12%) 4 3	54, 80, 108, 125	0
1	L	239/287 (83%)	1.23	51 (21%) 0 0	61, 87, 121, 143	0
All	All	2898/3444 (84%)	0.44	221 (7%) 13 14	9, 58, 100, 151	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	273	VAL	11.7
1	A	245	SER	9.8
1	A	246	LEU	7.5
1	K	145	HIS	7.2
1	L	271	ILE	7.0
1	K	272	LEU	6.4
1	G	269	LYS	6.1
1	G	271	ILE	6.0
1	I	24	ASN	5.9
1	K	27	LEU	5.7
1	L	52	CYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	I	272	LEU	5.4
1	K	86	GLY	5.3
1	J	272	LEU	5.2
1	L	26	PHE	5.2
1	L	266	ALA	5.0
1	G	258	VAL	5.0
1	H	90	LEU	5.0
1	L	25	GLY	4.8
1	L	27	LEU	4.6
1	J	196	ILE	4.6
1	G	24	ASN	4.5
1	L	254	LYS	4.4
1	I	25	GLY	4.4
1	A	24	ASN	4.4
1	L	60	THR	4.3
1	H	152	HIS	4.3
1	H	52	CYS	4.3
1	A	244	ALA	4.2
1	K	83	ARG	4.2
1	H	155	MET	4.2
1	L	162	LEU	4.1
1	K	26	PHE	4.1
1	F	52	CYS	4.0
1	E	152	HIS	4.0
1	G	52	CYS	4.0
1	K	122	ASP	3.9
1	I	271	ILE	3.9
1	J	235	PHE	3.8
1	I	138	ARG	3.8
1	K	152	HIS	3.8
1	E	187	ARG	3.8
1	L	272	LEU	3.7
1	K	271	ILE	3.7
1	H	240	VAL	3.7
1	G	26	PHE	3.6
1	L	268	ALA	3.6
1	L	85	ARG	3.6
1	K	234	LYS	3.6
1	L	129	LEU	3.6
1	K	79	PHE	3.5
1	L	234	LYS	3.5
1	L	269	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	247	SER	3.5
1	K	155	MET	3.5
1	K	163	THR	3.4
1	H	234	LYS	3.4
1	E	248	CYS	3.4
1	J	152	HIS	3.3
1	A	115	VAL	3.3
1	L	208	ASN	3.2
1	K	123	GLY	3.2
1	C	245	SER	3.2
1	H	195	ARG	3.2
1	G	262	ARG	3.2
1	J	234	LYS	3.2
1	B	24	ASN	3.2
1	H	129	LEU	3.2
1	G	73	SER	3.1
1	L	230	ASP	3.1
1	H	74	VAL	3.1
1	H	83	ARG	3.1
1	L	163	THR	3.1
1	F	271	ILE	3.1
1	E	264	LEU	3.1
1	J	229	ARG	3.0
1	L	139	PRO	3.0
1	G	136	ILE	3.0
1	G	39	VAL	3.0
1	J	88	ASP	3.0
1	A	249	SER	3.0
1	K	53	SER	3.0
1	H	229	ARG	3.0
1	E	24	ASN	2.9
1	K	253	LEU	2.9
1	J	228	THR	2.9
1	G	70	VAL	2.9
1	G	25	GLY	2.9
1	L	121	GLU	2.9
1	J	193	LYS	2.9
1	A	251	TYR	2.9
1	L	270	ASN	2.8
1	H	266	ALA	2.8
1	F	193	LYS	2.8
1	F	192	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	257	ASP	2.8
1	L	122	ASP	2.8
1	K	52	CYS	2.8
1	L	238	SER	2.8
1	A	248	CYS	2.7
1	L	253	LEU	2.7
1	J	262	ARG	2.7
1	J	269	LYS	2.7
1	H	269	LYS	2.7
1	L	150	MET	2.7
1	A	247	SER	2.7
1	L	169	VAL	2.7
1	G	43	ARG	2.7
1	L	75	GLN	2.7
1	G	261	VAL	2.6
1	G	265	ASN	2.6
1	G	74	VAL	2.6
1	L	123	GLY	2.6
1	K	66	VAL	2.6
1	G	121	GLU	2.6
1	L	67	LEU	2.6
1	H	121	GLU	2.6
1	K	232	GLY	2.6
1	L	152	HIS	2.6
1	H	126	ASP	2.6
1	L	229	ARG	2.6
1	E	258	VAL	2.6
1	H	170	LEU	2.5
1	G	267	ILE	2.5
1	H	232	GLY	2.5
1	L	252	SER	2.5
1	L	207	ARG	2.5
1	I	108	LEU	2.5
1	K	35	VAL	2.5
1	E	229	ARG	2.5
1	L	216	SER	2.5
1	G	207	ARG	2.5
1	G	251	TYR	2.5
1	E	128	GLU	2.5
1	L	125	ILE	2.5
1	K	150	MET	2.5
1	E	235	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	192	ALA	2.5
1	H	235	PHE	2.4
1	J	232	GLY	2.4
1	E	188	LEU	2.4
1	K	49	ILE	2.4
1	G	155	MET	2.4
1	I	94	ARG	2.4
1	F	124	HIS	2.4
1	L	120	THR	2.4
1	H	255	VAL	2.4
1	A	25	GLY	2.4
1	F	243	GLY	2.4
1	H	27	LEU	2.4
1	J	43	ARG	2.4
1	L	187	ARG	2.4
1	F	156	ALA	2.4
1	G	120	THR	2.4
1	J	52	CYS	2.4
1	H	133	LEU	2.4
1	F	152	HIS	2.4
1	H	271	ILE	2.4
1	H	75	GLN	2.4
1	E	234	LYS	2.3
1	L	258	VAL	2.3
1	I	229	ARG	2.3
1	E	90	LEU	2.3
1	E	43	ARG	2.3
1	G	125	ILE	2.3
1	E	200	PRO	2.3
1	K	235	PHE	2.3
1	I	239	SER	2.3
1	J	259	THR	2.3
1	C	248	CYS	2.3
1	E	262	ARG	2.3
1	G	266	ALA	2.3
1	J	239	SER	2.3
1	L	235	PHE	2.3
1	L	259	THR	2.3
1	L	55	LEU	2.3
1	L	119	LEU	2.3
1	G	75	GLN	2.2
1	I	230	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	137	CYS	2.2
1	H	122	ASP	2.2
1	L	92	SER	2.2
1	L	131	MET	2.2
1	K	228	THR	2.2
1	B	243	GLY	2.2
1	E	122	ASP	2.2
1	G	235	PHE	2.2
1	G	259	THR	2.2
1	L	28	MET	2.2
1	G	90	LEU	2.2
1	L	251	TYR	2.2
1	J	258	VAL	2.2
1	J	268	ALA	2.2
1	I	139	PRO	2.2
1	D	248	CYS	2.2
1	I	75	GLN	2.1
1	F	183	PRO	2.1
1	J	253	LEU	2.1
1	K	78	VAL	2.1
1	E	121	GLU	2.1
1	L	164	LEU	2.1
1	H	169	VAL	2.1
1	K	186	LYS	2.1
1	L	82	ILE	2.1
1	J	236	ARG	2.1
1	L	236	ARG	2.1
1	G	72	GLN	2.1
1	L	148	PHE	2.1
1	L	81	MET	2.1
1	F	207	ARG	2.1
1	G	233	MET	2.0
1	F	267	ILE	2.0
1	C	272	LEU	2.0
1	D	272	LEU	2.0
1	K	268	ALA	2.0
1	H	66	VAL	2.0
1	H	262	ARG	2.0
1	F	120	THR	2.0
1	J	75	GLN	2.0
1	K	265	ASN	2.0
1	H	253	LEU	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 monosaccharides 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.