



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:03 PM UTC

PDB ID : 3IWP / pdb_00003iwp
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:

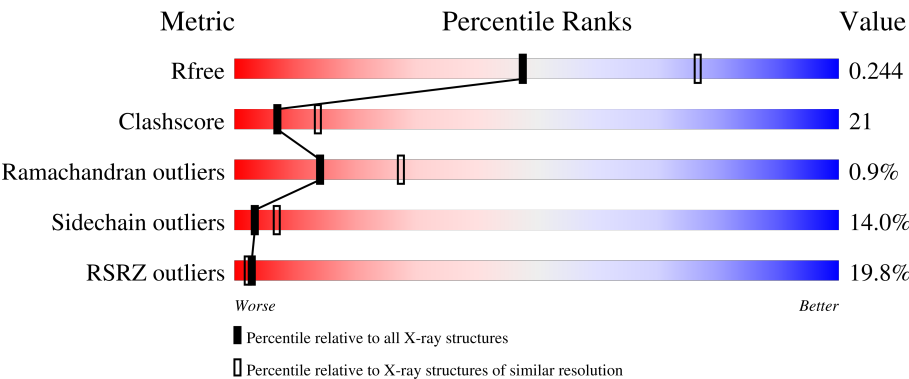
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	287	7% 44% 33% 9% • 13%
1	B	287	2% 54% 24% 7% 15%
1	C	287	3% 54% 25% 6% 14%
1	D	287	4% 45% 31% 10% 15%
1	E	287	19% 52% 26% 6% 16%

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Mol	Chain	Length	Quality of chain
1	F	287	
1	G	287	
1	H	287	
1	I	287	
1	J	287	
1	K	287	
1	L	287	

2 Entry composition

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 145 145	0	0

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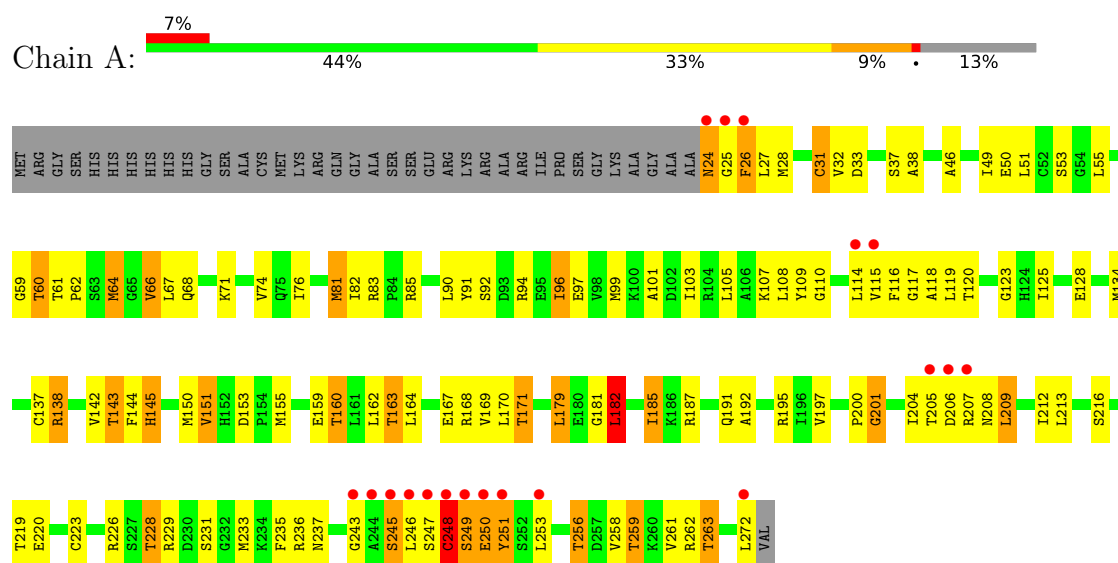
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	134	Total 134	O 134	0	0
2	C	137	Total 137	O 137	0	0
2	D	157	Total 157	O 157	0	0
2	E	58	Total 58	O 58	0	0
2	F	47	Total 47	O 47	0	0
2	G	25	Total 25	O 25	0	0
2	H	33	Total 33	O 33	0	0
2	I	56	Total 56	O 56	0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

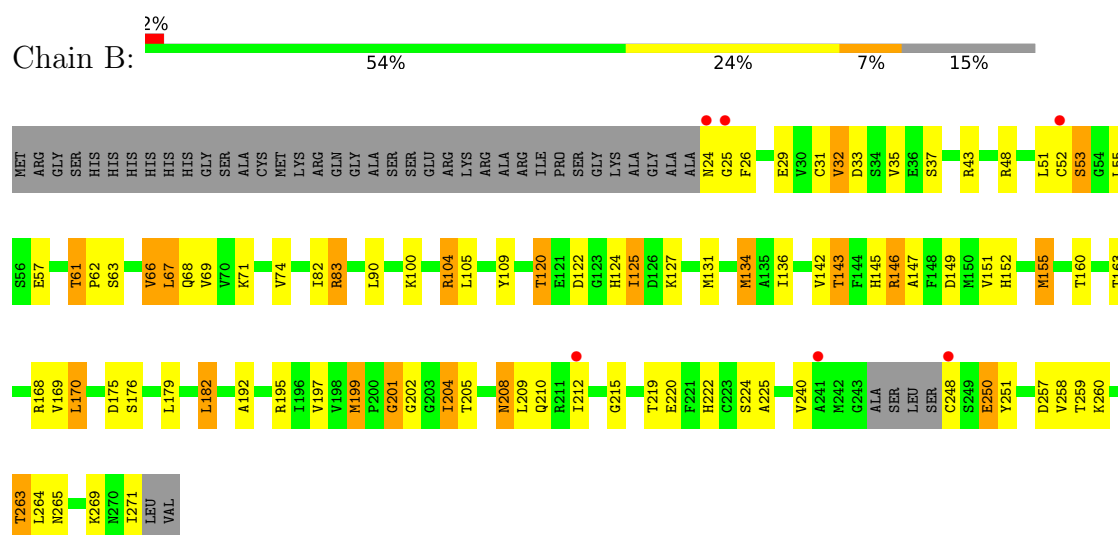
3 Residue-property plots [i](#)

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

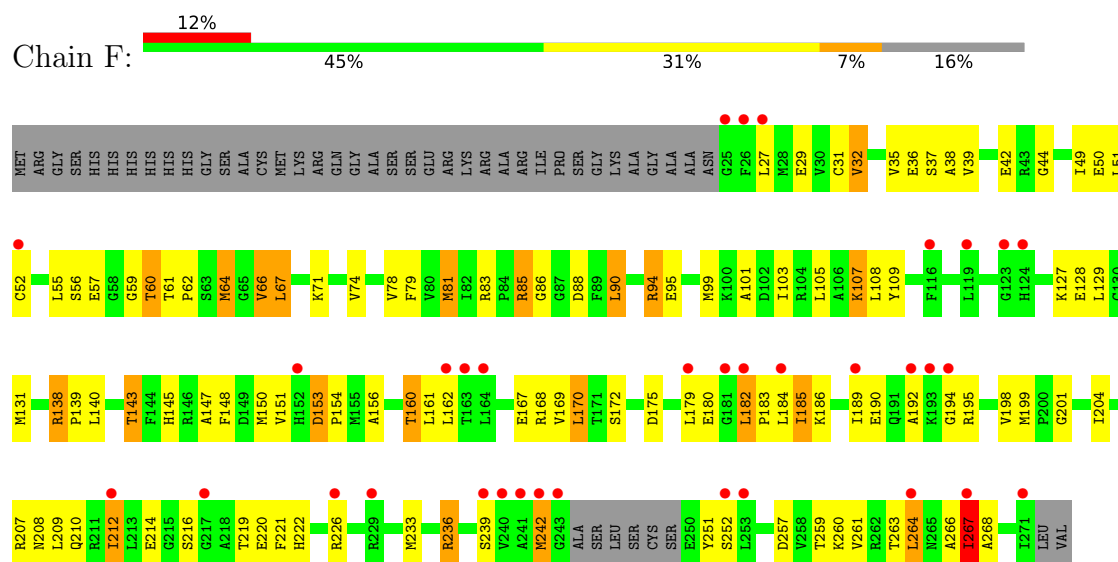


- Molecule 1: Copper homeostasis protein cutC homolog

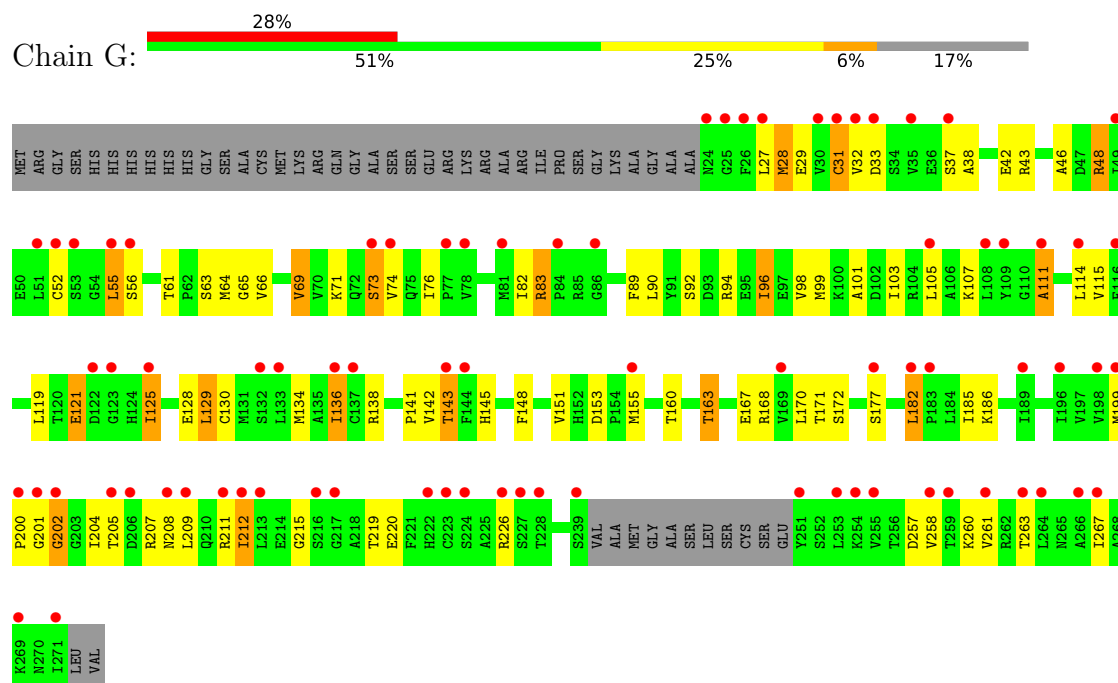


- Molecule 1: Copper homeostasis protein cutC homolog

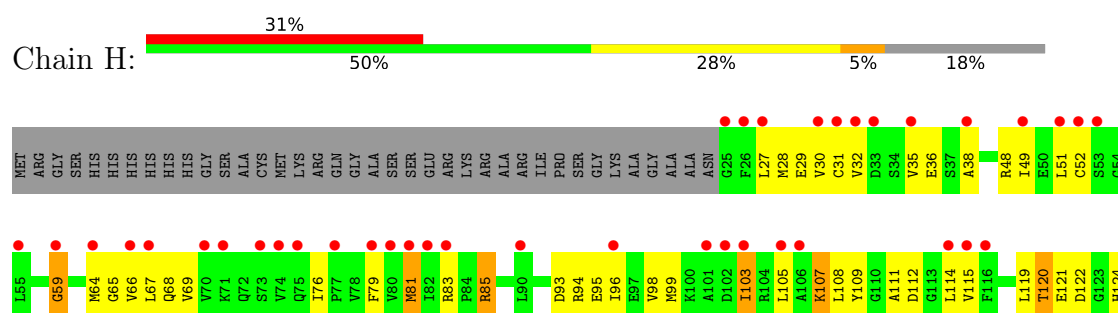


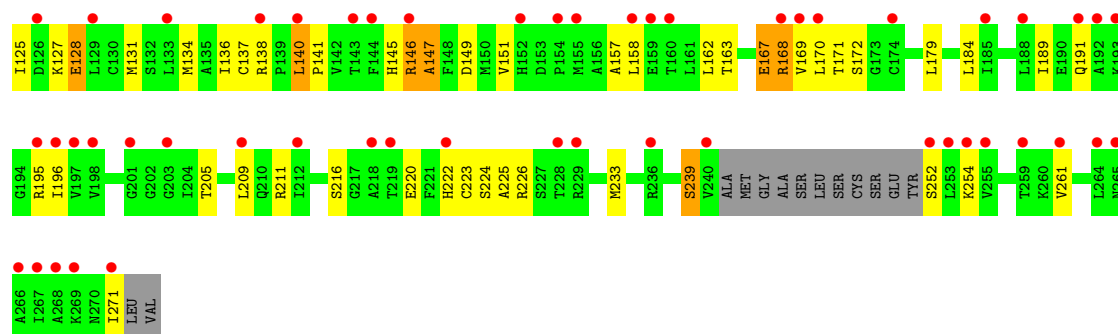


• Molecule 1: Copper homeostasis protein cutC homolog

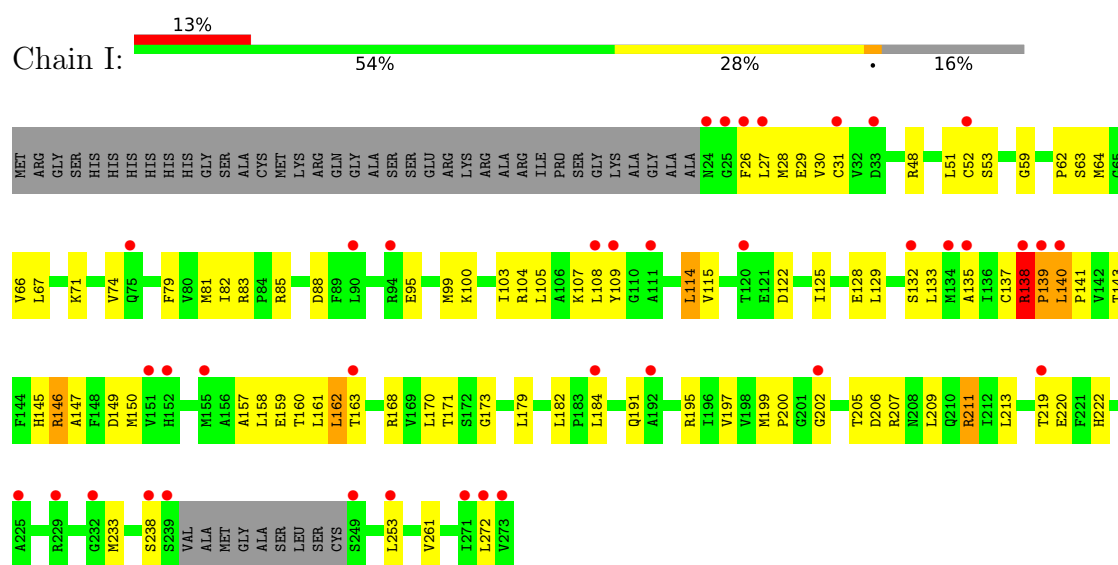


• Molecule 1: Copper homeostasis protein cutC homolog

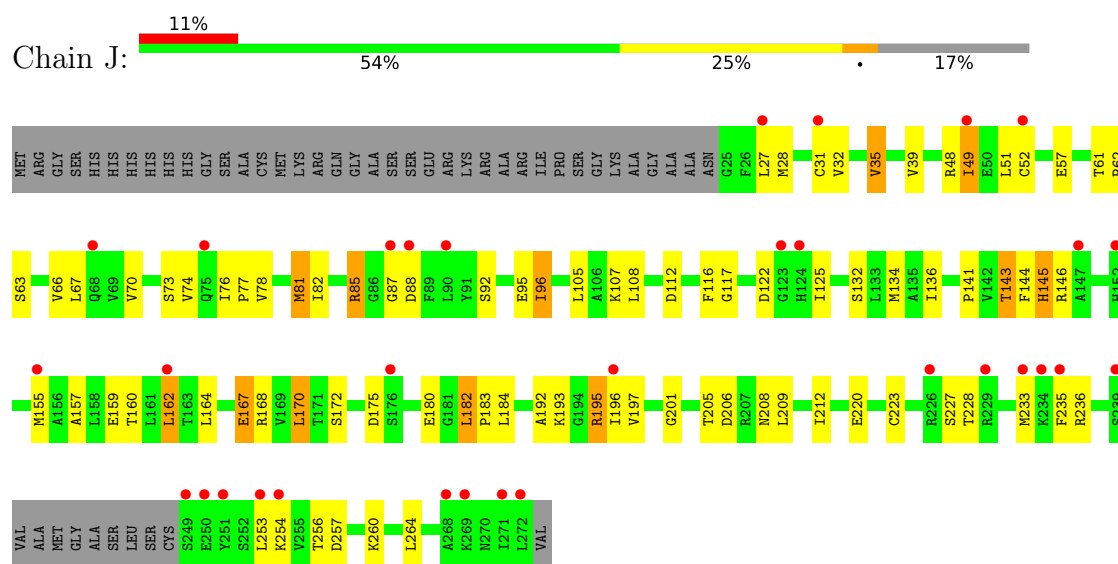




• Molecule 1: Copper homeostasis protein cutC homolog

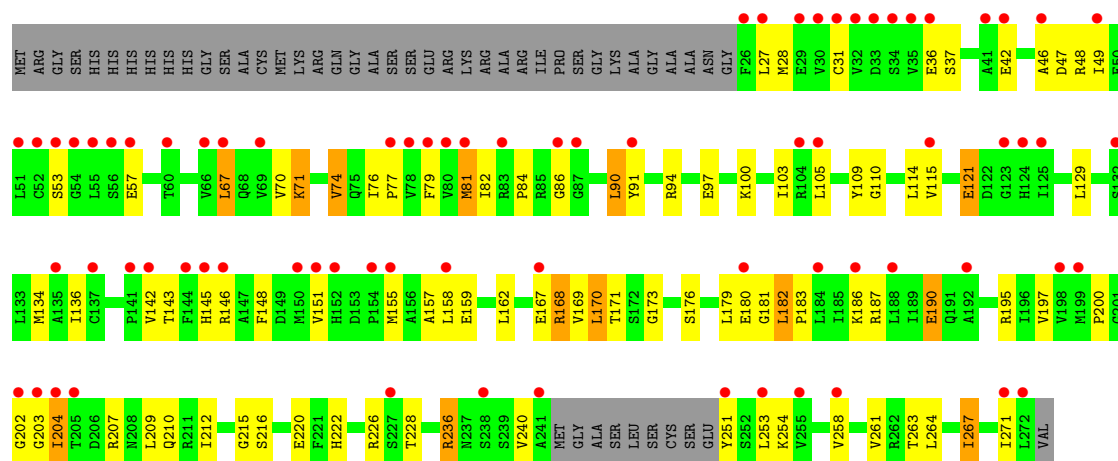


• Molecule 1: Copper homeostasis protein cutC homolog

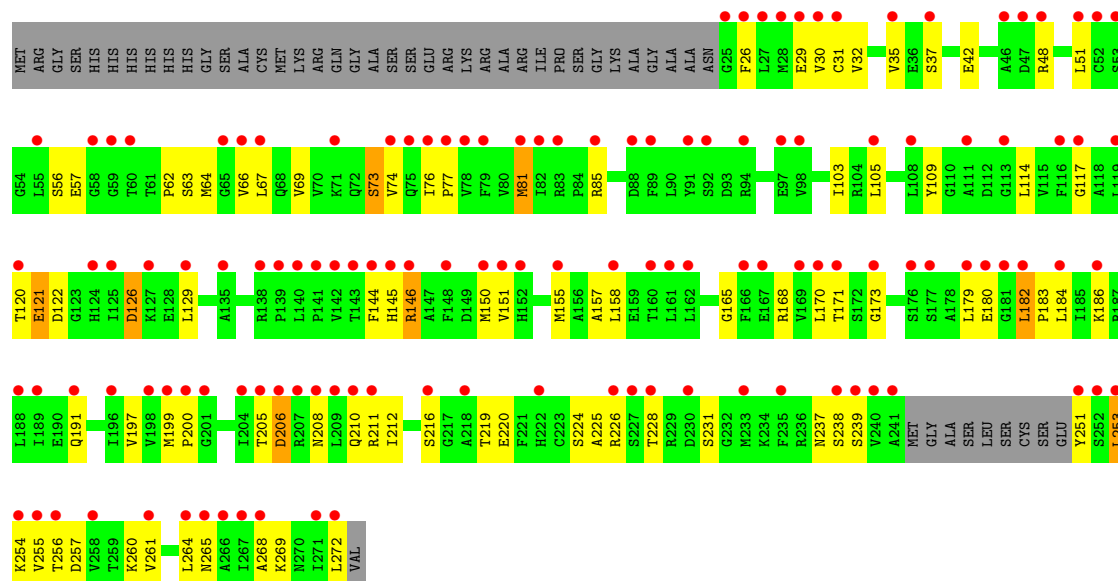
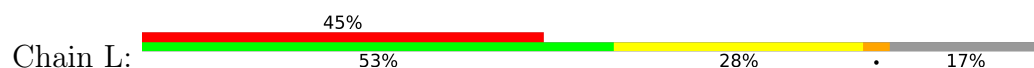


• Molecule 1: Copper homeostasis protein cutC homolog





• Molecule 1: Copper homeostasis protein cutC homolog



4 Data and refinement statistics

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 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.50) 98.5 (50.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.96%)	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)	0.33 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.81	0/1893	1.09	8/2549 (0.3%)
1	B	0.81	1/1859 (0.1%)	1.01	3/2501 (0.1%)
1	C	0.84	1/1878 (0.1%)	1.11	9/2527 (0.4%)
1	D	0.86	0/1865	1.12	9/2509 (0.4%)
1	E	0.58	0/1847	0.90	0/2486
1	F	0.60	0/1839	0.93	3/2474 (0.1%)
1	G	0.50	0/1814	0.86	0/2441
1	H	0.48	0/1800	0.86	2/2422 (0.1%)
1	I	0.54	0/1844	0.94	4/2482 (0.2%)
1	J	0.56	0/1829	0.90	0/2461
1	K	0.47	0/1822	0.88	1/2453 (0.0%)
1	L	0.48	0/1826	0.85	0/2458
All	All	0.65	2/22116 (0.0%)	0.96	39/29763 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	ILE	CA-CB	6.32	1.60	1.53
1	C	125	ILE	CA-CB	5.55	1.59	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	LEU	CA-C-N	-9.07	109.31	119.28
1	C	182	LEU	C-N-CA	-9.07	109.31	119.28
1	I	138	ARG	CA-C-N	8.26	130.16	119.84
1	I	138	ARG	C-N-CA	8.26	130.16	119.84
1	A	182	LEU	CA-C-N	-7.33	111.22	119.28
1	A	182	LEU	C-N-CA	-7.33	111.22	119.28
1	B	182	LEU	CA-C-N	-7.31	111.24	119.28
1	B	182	LEU	C-N-CA	-7.31	111.24	119.28
1	D	182	LEU	CA-C-N	-7.29	110.96	119.05
1	D	182	LEU	C-N-CA	-7.29	110.96	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	VAL	N-CA-C	-6.93	104.01	110.53
1	A	153	ASP	CA-C-N	6.66	126.61	119.28
1	A	153	ASP	C-N-CA	6.66	126.61	119.28
1	A	171	THR	N-CA-C	6.61	119.36	108.99
1	D	82	ILE	CB-CA-C	6.44	118.24	111.09
1	C	66	VAL	CB-CA-C	-6.08	103.83	112.22
1	A	245	SER	N-CA-C	6.04	120.29	107.67
1	A	66	VAL	CB-CA-C	-6.02	103.91	112.22
1	H	147	ALA	N-CA-C	-6.01	105.91	113.18
1	C	208	ASN	N-CA-C	5.85	120.43	113.12
1	C	66	VAL	N-CA-CB	5.81	119.29	110.58
1	C	258	VAL	CB-CA-C	-5.78	104.48	111.88
1	D	199	MET	CB-CA-C	-5.76	104.47	110.17
1	A	243	GLY	N-CA-C	5.66	119.36	111.10
1	B	199	MET	CB-CA-C	-5.64	104.59	110.17
1	C	199	MET	CB-CA-C	-5.60	103.71	110.15
1	D	66	VAL	CB-CA-C	-5.57	104.73	112.02
1	D	53	SER	N-CA-C	-5.54	102.27	110.46
1	F	66	VAL	CB-CA-C	-5.53	104.59	112.22
1	C	53	SER	N-CA-C	-5.38	102.20	109.95
1	H	239	SER	N-CA-C	5.36	117.33	109.24
1	C	145	HIS	N-CA-C	5.16	116.64	109.31
1	D	153	ASP	CA-C-N	5.10	124.27	118.97
1	D	153	ASP	C-N-CA	5.10	124.27	118.97
1	I	140	LEU	CA-C-N	5.09	125.00	119.76
1	I	140	LEU	C-N-CA	5.09	125.00	119.76
1	F	153	ASP	CA-C-N	5.08	124.53	119.24
1	F	153	ASP	C-N-CA	5.08	124.53	119.24
1	K	168	ARG	N-CA-C	5.06	116.88	109.24

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	1870	0	1905	132	0
1	B	1837	0	1867	79	0
1	C	1856	0	1888	75	0
1	D	1843	0	1877	115	0
1	E	1825	0	1855	77	0
1	F	1817	0	1851	80	0
1	G	1792	0	1825	79	0
1	H	1779	0	1819	70	0
1	I	1822	0	1856	67	0
1	J	1807	0	1841	63	0
1	K	1800	0	1841	77	0
1	L	1804	0	1844	56	0
2	A	145	0	0	15	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	9	0
2	F	47	0	0	4	0
2	G	25	0	0	5	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	922	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 21.

All (922) 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
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:28:MET:HE1	1:A:261:VAL:HG13	1.41	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:K:28:MET:HE1	1:K:261:VAL:HG13	1.42	1.00
1:C:143:THR:HG21	2:C:274:HOH:O	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:81:MET:HE1	1:A:145:HIS:CD2	2.04	0.92
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:C:251:TYR:OH	1:D:150:MET:HE2	1.72	0.88
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:I:28:MET:HE1	1:I:261:VAL:HG13	1.55	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:I:107:LYS:HZ2	1:I:138:ARG:HB2	1.43	0.84
1:A:115:VAL:HG13	1:A:143:THR:O	1.78	0.84
1:K:171:THR:HG22	1:K:173:GLY:H	1.39	0.84
1:B:63:SER:OG	1:B:66:VAL:HG23	1.78	0.83
1:D:81:MET:HE1	1:D:145:HIS:HD2	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:195:ARG:HD2	2:E:281:HOH:O	1.81	0.81
1:A:81:MET:HE1	1:A:145:HIS:HD2	1.42	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:F:128:GLU:HA	1:F:131:MET:HE2	1.65	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:168:ARG:HG2	1:A:197:VAL:HB	1.65	0.78
1:C:28:MET:HE1	1:C:261:VAL:HG13	1.65	0.78
1:B:248:CYS:N	1:C:248:CYS:HG	1.81	0.78
1:K:263:THR:O	1:K:267:ILE:HG22	1.84	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
1:L:29:GLU:HG2	1:L:199:MET:HE1	1.67	0.77
1:B:29:GLU:OE2	1:B:222:HIS:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:TYR:CG	1:D:99:MET:HE1	2.19	0.77
1:D:81:MET:HE1	1:D:145:HIS:CD2	2.21	0.76
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:E:240:VAL:HB	1:F:150:MET:HE1	1.68	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:HH11	1:B:104:ARG:CG	2.03	0.69
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:28:MET:HE2	1:A:46:ALA:HA	1.74	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: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:F:81:MET:HE1	1:F:145:HIS:ND1	2.08	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:D:91:TYR:CD2	1:D:99:MET:HE1	2.29	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:E:60:THR:O	1:E:61:THR:C	2.37	0.67
1:F:27:LEU:HB2	1:F:220:GLU:HG2	1.75	0.67
1:H:28:MET:HE1	1:H:261:VAL:HG13	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:27:LEU:HB3	1:H:220:GLU:CG	2.27	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:I:28:MET:CE	1:I:261:VAL:HG13	2.26	0.64
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:A:91:TYR:CD2	1:A:99:MET:HE1	2.32	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: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:I:64:MET:HE3	2:I:481:HOH:O	1.96	0.63
1:A:28:MET:CE	1:A:261:VAL:HG13	2.25	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:B:125:ILE:HD12	1:B:160:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:81:MET:HE3	1:I:83:ARG:HB2	1.82	0.62
1:J:28:MET:CE	1:J:223:CYS:SG	2.88	0.62
1:J:134:MET:HE2	1:J:164:LEU:O	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:206:ASP:CG	2:C:782:HOH:O	2.44	0.59
1:D:81:MET:HE2	1:D:82:ILE:H	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:B:182:LEU:HD23	1:B:182:LEU:C	2.28	0.59
1:D:61:THR:HG22	1:D:83:ARG:O	2.02	0.59
1:F:242:MET:HE3	1:F:242:MET:HA	1.84	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:D:269:LYS:C	2:D:407:HOH:O	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:MET:HE3	1:B:251:TYR:OH	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:E:64:MET:HA	1:E:64:MET:HE2	1.85	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
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:D:226:ARG:NE	2:D:573:HOH:O	2.37	0.57
1:K:28:MET:CE	1:K:261:VAL:HG13	2.28	0.57
1:B:208:ASN:C	1:B:208:ASN:HD22	2.12	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:G:64:MET:HE3	1:G:105:LEU:HB3	1.86	0.57
1:A:208:ASN:C	1:A:208:ASN:OD1	2.48	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:F:266:ALA:C	1:F:268:ALA:H	2.13	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:H:103:ILE:HD12	1:H:137:CYS:SG	2.45	0.56
1:J:107:LYS:NZ	1:J:136:ILE:O	2.37	0.56
1:D:82:ILE:HD11	1:D:114:LEU:HD22	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:I:138:ARG:C	1:I:140:LEU:H	2.12	0.56
1:A:96:ILE:HA	1:A:99:MET:HE3	1.88	0.55
1:A:116:PHE:O	1:A:145:HIS:CE1	2.59	0.55
1:E:88:ASP:HB2	1:F:233:MET:HE2	1.88	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:A:115:VAL:HG13	1:A:143:THR:C	2.31	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:A:68:GLN:OE1	1:B:105:LEU:HD21	2.07	0.55
1:C:28:MET:CE	1:C:261:VAL:HG13	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:125:ILE:C	1:B:125:ILE:HD13	2.32	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:K:37:SER:HG	1:L:85:ARG:HH22	1.55	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: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:E:134:MET:HE1	1:E:138:ARG:NE	2.24	0.53
1:F:143:THR:HB	1:F:168:ARG:CB	2.39	0.53
1:I:85:ARG:HH21	1:I:88:ASP:CG	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:MET:HE2	1:J:223:CYS:SG	2.49	0.52
1:J:183:PRO:HG2	1:L:211:ARG:NH1	2.24	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:I:59:GLY:O	1:I:83:ARG:HD3	2.10	0.52
1:L:145:HIS:CG	1:L:146:ARG:H	2.28	0.52
1:C:28:MET:HE2	1:C:46:ALA:HA	1.91	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: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:H:167:GLU:C	1:H:168:ARG:HG2	2.35	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:E:233:MET:HE3	1:F:90:LEU:HB2	1.92	0.51
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:C:243:GLY:HA2	1:D:57:GLU:C	2.35	0.51
1:E:134:MET:HE3	1:E:142:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:175:ASP:OD2	1:J:180:GLU:CB	2.50	0.51
1:I:107:LYS:HG2	1:I:140:LEU:HD12	1.93	0.51
1:K:151:VAL:HG11	1:K:157:ALA:HB2	1.91	0.51
1:B:134:MET:HE3	1:B:142:VAL:HG21	1.93	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:D:81:MET:HE2	1:D:115:VAL:O	2.10	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: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
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:J:81:MET:HE1	1:J:145:HIS:CD2	2.47	0.50
1:E:146:ARG:NH2	1:E:172:SER:HB3	2.26	0.50
1:G:29:GLU:HB3	1:G:199:MET:HE1	1.93	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:199:MET:HE2	1:B:222:HIS:HB2	1.92	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:D:96:ILE:HA	1:D:99:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61:THR:HA	1:J:81:MET: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: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:29:GLU:HB3	1:B:199:MET:HE1	1.93	0.49
1:B:209:LEU:HD22	1:B:264:LEU:CD2	2.43	0.49
1:C:146:ARG:C	1:C:148:PHE:N	2.70	0.49
1:E:168:ARG:HG2	1:E:197:VAL:HB	1.94	0.49
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:A:114:LEU:C	1:A:115:VAL:CG2	2.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:182:LEU:O	1:C:183:PRO:C	2.51	0.48
1:G:208:ASN:HD21	1:G:211:ARG:HH21	1.59	0.48
1:K:81:MET:HE2	1:K:115:VAL:HG12	1.94	0.48
1:A:116:PHE:O	1:A:145:HIS:CG	2.65	0.48
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:J:28:MET:HE3	1:J:223:CYS:SG	2.54	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:A:114:LEU:C	1:A:115:VAL:HG23	2.39	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:E:71:LYS:NZ	1:E:112:ASP:OD2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:LYS:HD2	1:G:111:ALA:H	1.79	0.48
1:J:85:ARG:HH11	1:J:95:GLU:CD	2.21	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: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:I:168:ARG:HD3	1:I:199:MET:HE2	1.96	0.47
1:C:101:ALA:O	1:C:105:LEU:HD22	2.14	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: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
1:B:29:GLU:CD	1:B:199:MET:HE1	2.40	0.47
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:J:235:PHE:C	1:J:236:ARG:HG2	2.40	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:A:233:MET:HE1	1:B:120:THR:O	2.15	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:C:89:PHE:CZ	1:D:242:MET:HE3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:201:GLY:O	1:B:202:GLY:C	2.58	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
1:E:60:THR:O	1:E:61:THR:O	2.34	0.46
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:A:91:TYR:CG	1:A:99:MET:HE1	2.51	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:H:149:ASP:CG	1:H:172:SER:H	2.24	0.46
1:K:28:MET:HE2	1:K:46:ALA:HA	1.98	0.46
1:F:182:LEU:HB3	1:F:183:PRO:HD3	1.98	0.46
1:B:29:GLU:CB	1:B:199:MET:HE1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:85:ARG:NH2	1:I:88:ASP:CG	2.74	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:F:55:LEU:C	1:F:57:GLU:H	2.25	0.45
1:D:55:LEU:HD13	1:D:226:ARG:CZ	2.47	0.45
1:G:28:MET:HE1	1:G:261:VAL:HG13	1.99	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: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
1:J:197:VAL:HG11	1:J:220:GLU:OE1	2.16	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:A:247:SER:O	1:A:248:CYS:C	2.58	0.44
1:B:24:ASN:CG	1:B:25:GLY:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:105:LEU:O	1:H:109:TYR:CD1	2.71	0.44
1:L:56:SER:HB3	1:L:254:LYS:HZ2	1.82	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:C:210:GLN:HE21	1:C:214:GLU:CD	2.26	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:110:GLY:O	1:C:111:ALA:C	2.60	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:D:88:ASP:OD2	1:D:88:ASP:C	2.60	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:A:205:THR:OG1	1:A:206:ASP:N	2.45	0.44
1:B:182:LEU:C	1:B:182:LEU:CD2	2.91	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:E:134:MET:HE3	1:E:142:VAL:CG2	2.47	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:D:146:ARG:C	1:D:148:PHE:N	2.74	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:K:236:ARG:HE	1:L:150:MET:HE3	1.82	0.43
1:C:55:LEU:CD2	1:C:55:LEU:N	2.68	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:128:GLU:HA	1:H:131:MET:HE2	1.99	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: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:C:158:LEU:HD23	1:C:191:GLN:CD	2.44	0.43
1:I:145:HIS:CD2	1:I:145:HIS:C	2.95	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: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: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:L:237:ASN:C	1:L:239:SER:H	2.26	0.43
1:A:235:PHE:CE1	1:B:152:HIS:ND1	2.86	0.43
1:D:64:MET:HA	1:D:64:MET:HE2	2.00	0.43
1:E:146:ARG:HH11	1:E:146:ARG:HB3	1.84	0.43
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:C:237:ASN:HB3	1:D:150:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:146:ARG:O	1:D:147:ALA:C	2.62	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: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:I:138:ARG:C	1:I:140:LEU:N	2.76	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:A:249:SER:OG	1:A:250:GLU:N	2.50	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:L:120:THR:O	1:L:121:GLU:C	2.63	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:G:128:GLU:CD	2:G:756:HOH:O	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:81:MET:HE2	1:J:82:ILE:N	2.35	0.41
1:A:60:THR:CG2	1:A:61:THR:N	2.83	0.41
1:C:44:GLY:C	1:C:261:VAL:HG12	2.45	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:32:VAL:HG21	1:E:37:SER:C	2.45	0.41
1:E:39:VAL:HG11	1:F:94:ARG:HH11	1.86	0.41
1:E:71:LYS:NZ	2:E:278:HOH:O	2.53	0.41
1:E:182:LEU:C	1:E:182:LEU:HD23	2.45	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:J:85:ARG:NH1	1:J:95:GLU:CD	2.79	0.41
1:K:210:GLN:HG3	1:K:271:ILE:HD11	2.03	0.41
1:D:134:MET:HE2	1:D:164:LEU:O	2.20	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: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:E:134:MET:HE1	1:E:138:ARG:HE	1.85	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:F:42:GLU:C	1:F:44:GLY:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:ARG:HG3	1:E:256:THR:HG22	2.03	0.41
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:F:266:ALA:C	1:F:268:ALA:N	2.79	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:A:81:MET:C	1:A:82:ILE:HD12	2.46	0.41
1:A:134:MET:HE1	1:A:138:ARG:NH2	2.36	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:182:LEU:HD21	1:D:215:GLY:C	2.46	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:F:129:LEU:HD23	1:F:129:LEU:C	2.46	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:A:246:LEU:C	1:A:248:CYS:H	2.26	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:B:146:ARG:O	1:B:147:ALA:C	2.64	0.41
1:I:205:THR:CG2	1:I:206:ASP:H	2.33	0.41
1:L:64:MET:HA	1:L:64:MET:HE2	2.02	0.41
1:A:251:TYR:C	2:A:319:HOH:O	2.64	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:126:ASP:OD2	1:D:126:ASP:C	2.63	0.40
1:E:162:LEU:HB3	1:E:196:ILE:HD13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:MET:CE	1:H:261:VAL:HG13	2.47	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:G:172:SER:HB2	1:G:177:SER:C	2.46	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
1:L:228:THR:HG23	1:L:253:LEU:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/287 (86%)	231 (94%)	13 (5%)	3 (1%)	10	20
1	B	240/287 (84%)	228 (95%)	10 (4%)	2 (1%)	16	31
1	C	243/287 (85%)	237 (98%)	5 (2%)	1 (0%)	30	49
1	D	241/287 (84%)	235 (98%)	6 (2%)	0	100	100
1	E	238/287 (83%)	217 (91%)	18 (8%)	3 (1%)	9	18
1	F	237/287 (83%)	214 (90%)	20 (8%)	3 (1%)	9	18
1	G	233/287 (81%)	208 (89%)	21 (9%)	4 (2%)	7	13
1	H	232/287 (81%)	211 (91%)	20 (9%)	1 (0%)	30	49
1	I	237/287 (83%)	225 (95%)	10 (4%)	2 (1%)	16	31
1	J	235/287 (82%)	216 (92%)	18 (8%)	1 (0%)	30	49
1	K	234/287 (82%)	213 (91%)	17 (7%)	4 (2%)	7	13
1	L	235/287 (82%)	210 (89%)	22 (9%)	3 (1%)	9	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2852/3444 (83%)	2645 (93%)	180 (6%)	27 (1%)	14 27

All (27) Ramachandran outliers are listed below:

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

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%)	166 (81%)	40 (19%)	1	2
1	B	202/233 (87%)	171 (85%)	31 (15%)	3	5
1	C	204/233 (88%)	176 (86%)	28 (14%)	3	7
1	D	203/233 (87%)	164 (81%)	39 (19%)	1	2
1	E	201/233 (86%)	172 (86%)	29 (14%)	3	6
1	F	199/233 (85%)	166 (83%)	33 (17%)	2	4
1	G	197/233 (84%)	176 (89%)	21 (11%)	6	13
1	H	196/233 (84%)	170 (87%)	26 (13%)	4	8
1	I	201/233 (86%)	178 (89%)	23 (11%)	5	12
1	J	199/233 (85%)	172 (86%)	27 (14%)	3	8
1	K	198/233 (85%)	177 (89%)	21 (11%)	6	14
1	L	198/233 (85%)	179 (90%)	19 (10%)	8	17
All	All	2404/2796 (86%)	2067 (86%)	337 (14%)	3	7

All (337) 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	108	LEU
1	A	120	THR
1	A	125	ILE
1	A	138	ARG
1	A	143	THR
1	A	145	HIS
1	A	151	VAL
1	A	159	GLU
1	A	160	THR
1	A	162	LEU

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Mol	Chain	Res	Type
1	A	163	THR
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	187	ARG
1	A	209	LEU
1	A	228	THR
1	A	248	CYS
1	A	249	SER
1	A	250	GLU
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	32	VAL
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	66	VAL
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	146	ARG
1	B	151	VAL
1	B	155	MET
1	B	163	THR
1	B	169	VAL

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Mol	Chain	Res	Type
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	C	31	CYS
1	C	32	VAL
1	C	52	CYS
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
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	151	VAL
1	C	162	LEU
1	C	169	VAL
1	C	170	LEU
1	C	209	LEU
1	C	228	THR
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	51	LEU
1	D	52	CYS
1	D	60	THR
1	D	61	THR

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Mol	Chain	Res	Type
1	D	64	MET
1	D	66	VAL
1	D	67	LEU
1	D	74	VAL
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	152	HIS
1	D	160	THR
1	D	162	LEU
1	D	163	THR
1	D	167	GLU
1	D	169	VAL
1	D	170	LEU
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	240	VAL
1	D	248	CYS
1	D	254	LYS
1	D	263	THR
1	E	31	CYS
1	E	39	VAL
1	E	49	ILE
1	E	61	THR
1	E	66	VAL
1	E	67	LEU
1	E	71	LYS
1	E	74	VAL
1	E	90	LEU
1	E	104	ARG

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Mol	Chain	Res	Type
1	E	105	LEU
1	E	108	LEU
1	E	119	LEU
1	E	120	THR
1	E	125	ILE
1	E	127	LYS
1	E	134	MET
1	E	142	VAL
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	240	VAL
1	E	259	THR
1	F	32	VAL
1	F	52	CYS
1	F	60	THR
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
1	F	94	ARG
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

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Mol	Chain	Res	Type
1	F	190	GLU
1	F	207	ARG
1	F	212	ILE
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	28	MET
1	G	31	CYS
1	G	33	ASP
1	G	48	ARG
1	G	52	CYS
1	G	55	LEU
1	G	69	VAL
1	G	73	SER
1	G	74	VAL
1	G	83	ARG
1	G	96	ILE
1	G	115	VAL
1	G	125	ILE
1	G	129	LEU
1	G	136	ILE
1	G	143	THR
1	G	163	THR
1	G	171	THR
1	G	182	LEU
1	G	212	ILE
1	G	219	THR
1	H	31	CYS
1	H	52	CYS
1	H	64	MET
1	H	67	LEU
1	H	81	MET
1	H	85	ARG
1	H	103	ILE
1	H	107	LYS
1	H	108	LEU
1	H	115	VAL
1	H	120	THR

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Mol	Chain	Res	Type
1	H	128	GLU
1	H	140	LEU
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	H	271	ILE
1	I	30	VAL
1	I	31	CYS
1	I	51	LEU
1	I	52	CYS
1	I	67	LEU
1	I	71	LYS
1	I	74	VAL
1	I	82	ILE
1	I	114	LEU
1	I	146	ARG
1	I	150	MET
1	I	158	LEU
1	I	162	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	219	THR
1	I	233	MET
1	I	238	SER
1	I	253	LEU
1	J	31	CYS
1	J	35	VAL
1	J	49	ILE
1	J	52	CYS

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Mol	Chain	Res	Type
1	J	57	GLU
1	J	67	LEU
1	J	73	SER
1	J	74	VAL
1	J	81	MET
1	J	85	ARG
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	159	GLU
1	J	160	THR
1	J	162	LEU
1	J	167	GLU
1	J	170	LEU
1	J	182	LEU
1	J	184	LEU
1	J	209	LEU
1	J	227	SER
1	J	254	LYS
1	K	31	CYS
1	K	36	GLU
1	K	53	SER
1	K	67	LEU
1	K	71	LYS
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	169	VAL
1	K	170	LEU
1	K	179	LEU
1	K	182	LEU
1	K	190	GLU
1	K	204	ILE
1	K	207	ARG
1	K	236	ARG

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Mol	Chain	Res	Type
1	K	258	VAL
1	K	267	ILE
1	L	31	CYS
1	L	35	VAL
1	L	57	GLU
1	L	67	LEU
1	L	73	SER
1	L	81	MET
1	L	126	ASP
1	L	158	LEU
1	L	170	LEU
1	L	179	LEU
1	L	180	GLU
1	L	182	LEU
1	L	184	LEU
1	L	206	ASP
1	L	219	THR
1	L	231	SER
1	L	253	LEU
1	L	255	VAL
1	L	265	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	124	HIS
1	B	208	ASN
1	B	210	GLN
1	B	222	HIS
1	B	265	ASN
1	C	68	GLN
1	C	210	GLN
1	C	270	ASN
1	D	72	GLN
1	D	75	GLN
1	D	124	HIS
1	D	152	HIS
1	D	237	ASN
1	E	68	GLN
1	F	68	GLN
1	F	124	HIS

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Mol	Chain	Res	Type
1	G	68	GLN
1	H	68	GLN
1	H	124	HIS
1	H	222	HIS
1	I	145	HIS
1	I	191	GLN
1	I	222	HIS
1	I	237	ASN
1	J	68	GLN
1	J	208	ASN
1	K	124	HIS
1	K	152	HIS
1	L	124	HIS
1	L	152	HIS
1	L	191	GLN
1	L	270	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	249/287 (86%)	0.17	19 (7%)	20 17	9, 25, 57, 151	0
1	B	244/287 (85%)	-0.14	6 (2%)	58 54	9, 24, 48, 100	0
1	C	247/287 (86%)	-0.17	8 (3%)	50 46	12, 22, 50, 91	0
1	D	245/287 (85%)	-0.14	11 (4%)	38 33	9, 23, 48, 89	0
1	E	242/287 (84%)	1.33	54 (22%)	2 2	36, 60, 94, 119	0
1	F	241/287 (83%)	0.92	34 (14%)	6 5	26, 55, 89, 113	0
1	G	237/287 (82%)	1.76	79 (33%)	1 1	52, 77, 99, 134	0
1	H	236/287 (82%)	1.84	90 (38%)	1 0	52, 79, 103, 120	0
1	I	241/287 (83%)	1.17	38 (15%)	5 4	37, 57, 91, 136	0
1	J	239/287 (83%)	1.07	32 (13%)	7 5	35, 57, 92, 113	0
1	K	238/287 (82%)	1.76	75 (31%)	1 1	54, 80, 108, 125	0
1	L	239/287 (83%)	2.16	129 (53%)	0 0	61, 87, 121, 143	0
All	All	2898/3444 (84%)	0.97	575 (19%)	3 2	9, 58, 100, 151	0

All (575) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	9.3
1	K	145	HIS	6.6
1	G	52	CYS	5.9
1	H	52	CYS	5.9
1	J	196	ILE	5.7
1	L	26	PHE	5.5
1	G	136	ILE	5.3
1	K	53	SER	5.2
1	J	52	CYS	5.0
1	H	83	ARG	5.0
1	K	272	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	272	LEU	4.9
1	A	272	LEU	4.8
1	F	52	CYS	4.8
1	L	205	THR	4.8
1	L	85	ARG	4.8
1	L	129	LEU	4.8
1	I	273	VAL	4.7
1	A	251	TYR	4.7
1	A	249	SER	4.7
1	L	60	THR	4.7
1	L	272	LEU	4.6
1	G	125	ILE	4.6
1	L	208	ASN	4.6
1	L	271	ILE	4.6
1	L	53	SER	4.5
1	L	27	LEU	4.5
1	K	26	PHE	4.5
1	A	24	ASN	4.5
1	A	244	ALA	4.5
1	L	253	LEU	4.4
1	K	251	TYR	4.4
1	L	52	CYS	4.4
1	L	81	MET	4.3
1	G	271	ILE	4.3
1	F	271	ILE	4.2
1	J	88	ASP	4.2
1	H	271	ILE	4.2
1	A	115	VAL	4.2
1	J	235	PHE	4.2
1	H	240	VAL	4.1
1	K	79	PHE	4.1
1	G	267	ILE	4.1
1	H	169	VAL	4.0
1	H	198	VAL	4.0
1	K	52	CYS	4.0
1	K	205	THR	4.0
1	H	266	ALA	3.9
1	F	240	VAL	3.9
1	L	82	ILE	3.9
1	H	252	SER	3.9
1	G	208	ASN	3.8
1	I	272	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	L	91	TYR	3.8
1	K	150	MET	3.8
1	E	235	PHE	3.8
1	I	26	PHE	3.8
1	H	129	LEU	3.8
1	K	27	LEU	3.8
1	E	119	LEU	3.7
1	H	253	LEU	3.7
1	D	272	LEU	3.7
1	H	27	LEU	3.7
1	L	55	LEU	3.7
1	I	138	ARG	3.7
1	K	66	VAL	3.6
1	K	33	ASP	3.6
1	H	158	LEU	3.6
1	K	49	ILE	3.6
1	G	55	LEU	3.6
1	J	75	GLN	3.6
1	K	35	VAL	3.6
1	H	116	PHE	3.6
1	G	205	THR	3.5
1	L	75	GLN	3.5
1	L	145	HIS	3.5
1	L	222	HIS	3.5
1	E	258	VAL	3.5
1	K	83	ARG	3.5
1	G	261	VAL	3.5
1	L	150	MET	3.5
1	C	244	ALA	3.5
1	E	256	THR	3.5
1	G	209	LEU	3.5
1	I	139	PRO	3.5
1	L	258	VAL	3.4
1	K	241	ALA	3.4
1	L	238	SER	3.4
1	L	28	MET	3.4
1	K	271	ILE	3.4
1	L	135	ALA	3.4
1	F	116	PHE	3.4
1	E	188	LEU	3.4
1	H	170	LEU	3.3
1	I	135	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	137	CYS	3.3
1	H	133	LEU	3.3
1	H	74	VAL	3.3
1	L	256	THR	3.3
1	H	196	ILE	3.3
1	G	109	TYR	3.3
1	F	162	LEU	3.3
1	K	155	MET	3.3
1	C	206	ASP	3.2
1	B	24	ASN	3.2
1	I	184	LEU	3.2
1	F	163	THR	3.2
1	H	64	MET	3.2
1	I	163	THR	3.2
1	E	53	SER	3.2
1	L	67	LEU	3.2
1	A	250	GLU	3.2
1	L	267	ILE	3.2
1	F	192	ALA	3.2
1	K	86	GLY	3.2
1	L	255	VAL	3.2
1	L	254	LYS	3.2
1	E	125	ILE	3.2
1	H	82	ILE	3.2
1	L	108	LEU	3.1
1	H	32	VAL	3.1
1	A	247	SER	3.1
1	L	97	GLU	3.1
1	A	253	LEU	3.1
1	K	203	GLY	3.1
1	L	125	ILE	3.1
1	L	189	ILE	3.1
1	A	248	CYS	3.1
1	B	248	CYS	3.1
1	H	154	PRO	3.1
1	L	158	LEU	3.1
1	B	25	GLY	3.1
1	H	236	ARG	3.1
1	G	49	ILE	3.1
1	F	242	MET	3.1
1	H	155	MET	3.1
1	G	226	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	232	GLY	3.1
1	H	197	VAL	3.1
1	H	255	VAL	3.1
1	F	152	HIS	3.0
1	L	141	PRO	3.0
1	H	26	PHE	3.0
1	H	53	SER	3.0
1	L	143	THR	3.0
1	F	182	LEU	3.0
1	K	137	CYS	3.0
1	A	243	GLY	3.0
1	L	58	GLY	3.0
1	G	258	VAL	3.0
1	K	204	ILE	3.0
1	A	205	THR	3.0
1	L	139	PRO	3.0
1	J	162	LEU	3.0
1	L	25	GLY	3.0
1	E	271	ILE	3.0
1	G	212	ILE	3.0
1	H	38	ALA	3.0
1	H	114	LEU	3.0
1	I	239	SER	3.0
1	L	31	CYS	3.0
1	E	136	ILE	2.9
1	E	240	VAL	2.9
1	C	241	ALA	2.9
1	J	268	ALA	2.9
1	G	144	PHE	2.9
1	G	251	TYR	2.9
1	G	26	PHE	2.9
1	E	25	GLY	2.9
1	I	25	GLY	2.9
1	K	123	GLY	2.9
1	L	206	ASP	2.9
1	K	34	SER	2.9
1	G	189	ILE	2.9
1	H	49	ILE	2.9
1	G	51	LEU	2.9
1	H	90	LEU	2.9
1	I	155	MET	2.9
1	L	155	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	251	TYR	2.9
1	F	243	GLY	2.9
1	C	245	SER	2.8
1	G	73	SER	2.8
1	G	132	SER	2.8
1	J	176	SER	2.8
1	L	48	ARG	2.8
1	F	241	ALA	2.8
1	H	218	ALA	2.8
1	L	266	ALA	2.8
1	G	133	LEU	2.8
1	L	162	LEU	2.8
1	L	209	LEU	2.8
1	E	204	ILE	2.8
1	J	239	SER	2.8
1	G	32	VAL	2.8
1	H	30	VAL	2.8
1	L	51	LEU	2.8
1	L	170	LEU	2.8
1	E	229	ARG	2.8
1	L	169	VAL	2.8
1	E	209	LEU	2.8
1	I	140	LEU	2.8
1	K	105	LEU	2.8
1	K	29	GLU	2.8
1	A	207	ARG	2.8
1	G	201	GLY	2.8
1	H	152	HIS	2.8
1	J	87	GLY	2.8
1	K	152	HIS	2.8
1	A	245	SER	2.8
1	I	192	ALA	2.8
1	H	229	ARG	2.8
1	L	94	ARG	2.8
1	F	123	GLY	2.7
1	G	53	SER	2.7
1	K	258	VAL	2.7
1	L	240	VAL	2.7
1	H	219	THR	2.7
1	H	81	MET	2.7
1	I	134	MET	2.7
1	G	269	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	52	CYS	2.7
1	E	201	GLY	2.7
1	F	181	GLY	2.7
1	L	204	ILE	2.7
1	K	77	PRO	2.7
1	L	77	PRO	2.7
1	L	119	LEU	2.7
1	F	193	LYS	2.7
1	E	248	CYS	2.7
1	I	271	ILE	2.7
1	F	239	SER	2.7
1	G	56	SER	2.7
1	I	132	SER	2.7
1	L	30	VAL	2.7
1	L	261	VAL	2.7
1	J	253	LEU	2.7
1	E	152	HIS	2.7
1	H	25	GLY	2.7
1	I	24	ASN	2.7
1	E	195	ARG	2.7
1	F	27	LEU	2.7
1	G	155	MET	2.7
1	G	199	MET	2.7
1	H	55	LEU	2.7
1	H	115	VAL	2.7
1	I	151	VAL	2.7
1	G	259	THR	2.7
1	I	202	GLY	2.6
1	L	116	PHE	2.6
1	G	239	SER	2.6
1	G	263	THR	2.6
1	A	25	GLY	2.6
1	H	71	LYS	2.6
1	F	212	ILE	2.6
1	H	261	VAL	2.6
1	G	143	THR	2.6
1	L	111	ALA	2.6
1	L	228	THR	2.6
1	G	202	GLY	2.6
1	H	59	GLY	2.6
1	L	181	GLY	2.6
1	G	211	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	212	ILE	2.6
1	L	146	ARG	2.6
1	L	199	MET	2.6
1	B	52	CYS	2.6
1	H	31	CYS	2.6
1	K	253	LEU	2.6
1	L	184	LEU	2.6
1	L	188	LEU	2.6
1	K	78	VAL	2.6
1	K	198	VAL	2.6
1	L	198	VAL	2.6
1	L	177	SER	2.6
1	I	219	THR	2.6
1	I	109	TYR	2.6
1	D	25	GLY	2.6
1	E	183	PRO	2.6
1	F	217	GLY	2.6
1	G	25	GLY	2.6
1	L	88	ASP	2.6
1	L	211	ARG	2.6
1	K	142	VAL	2.6
1	G	31	CYS	2.6
1	J	31	CYS	2.6
1	H	101	ALA	2.6
1	L	216	SER	2.6
1	H	269	LYS	2.6
1	H	144	PHE	2.5
1	K	42	GLU	2.5
1	L	144	PHE	2.5
1	K	184	LEU	2.5
1	H	265	ASN	2.5
1	L	151	VAL	2.5
1	F	124	HIS	2.5
1	K	192	ALA	2.5
1	K	227	SER	2.5
1	L	59	GLY	2.5
1	J	250	GLU	2.5
1	L	167	GLU	2.5
1	E	182	LEU	2.5
1	K	67	LEU	2.5
1	G	30	VAL	2.5
1	K	151	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	142	VAL	2.5
1	E	241	ALA	2.5
1	G	266	ALA	2.5
1	D	247	SER	2.5
1	K	31	CYS	2.5
1	E	154	PRO	2.5
1	K	36	GLU	2.5
1	F	26	PHE	2.5
1	G	27	LEU	2.5
1	L	161	LEU	2.5
1	H	75	GLN	2.5
1	L	210	GLN	2.5
1	I	152	HIS	2.5
1	E	111	ALA	2.5
1	H	168	ARG	2.5
1	I	225	ALA	2.5
1	H	228	THR	2.5
1	I	120	THR	2.5
1	E	117	GLY	2.5
1	G	33	ASP	2.5
1	K	125	ILE	2.5
1	G	182	LEU	2.5
1	H	79	PHE	2.5
1	J	124	HIS	2.5
1	I	94	ARG	2.5
1	L	226	ARG	2.5
1	G	227	SER	2.5
1	L	171	THR	2.5
1	E	200	PRO	2.4
1	L	173	GLY	2.4
1	H	267	ILE	2.4
1	E	253	LEU	2.4
1	F	184	LEU	2.4
1	G	105	LEU	2.4
1	I	253	LEU	2.4
1	E	124	HIS	2.4
1	H	138	ARG	2.4
1	H	146	ARG	2.4
1	G	198	VAL	2.4
1	G	255	VAL	2.4
1	E	131	MET	2.4
1	K	41	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	160	THR	2.4
1	L	37	SER	2.4
1	L	252	SER	2.4
1	K	54	GLY	2.4
1	F	267	ILE	2.4
1	A	114	LEU	2.4
1	I	27	LEU	2.4
1	I	108	LEU	2.4
1	K	146	ARG	2.4
1	J	249	SER	2.4
1	L	227	SER	2.4
1	K	202	GLY	2.4
1	J	271	ILE	2.4
1	C	272	LEU	2.4
1	F	164	LEU	2.4
1	I	75	GLN	2.4
1	H	222	HIS	2.4
1	L	241	ALA	2.4
1	L	268	ALA	2.4
1	G	228	THR	2.4
1	K	60	THR	2.4
1	C	243	GLY	2.4
1	B	212	ILE	2.4
1	G	108	LEU	2.4
1	H	102	ASP	2.4
1	K	51	LEU	2.4
1	K	91	TYR	2.4
1	L	79	PHE	2.4
1	L	89	PHE	2.4
1	H	66	VAL	2.4
1	L	65	GLY	2.3
1	J	27	LEU	2.3
1	L	230	ASP	2.3
1	E	134	MET	2.3
1	K	199	MET	2.3
1	K	144	PHE	2.3
1	H	193	LYS	2.3
1	E	128	GLU	2.3
1	K	135	ALA	2.3
1	K	132	SER	2.3
1	L	113	GLY	2.3
1	G	253	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	140	LEU	2.3
1	I	90	LEU	2.3
1	J	152	HIS	2.3
1	A	26	PHE	2.3
1	C	248	CYS	2.3
1	E	52	CYS	2.3
1	L	66	VAL	2.3
1	L	78	VAL	2.3
1	E	77	PRO	2.3
1	D	243	GLY	2.3
1	F	25	GLY	2.3
1	H	203	GLY	2.3
1	L	92	SER	2.3
1	H	264	LEU	2.3
1	K	188	LEU	2.3
1	G	81	MET	2.3
1	I	33	ASP	2.3
1	K	81	MET	2.3
1	I	31	CYS	2.3
1	K	32	VAL	2.3
1	K	167	GLU	2.3
1	L	98	VAL	2.3
1	B	241	ALA	2.3
1	E	268	ALA	2.3
1	G	111	ALA	2.3
1	K	154	PRO	2.3
1	I	229	ARG	2.3
1	D	152	HIS	2.3
1	G	86	GLY	2.3
1	G	37	SER	2.3
1	G	222	HIS	2.3
1	E	103	ILE	2.3
1	H	67	LEU	2.3
1	H	188	LEU	2.3
1	L	264	LEU	2.3
1	E	150	MET	2.3
1	G	122	ASP	2.3
1	J	254	LYS	2.3
1	E	43	ARG	2.3
1	F	226	ARG	2.3
1	L	83	ARG	2.3
1	L	207	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	87	GLY	2.2
1	E	96	ILE	2.2
1	E	189	ILE	2.2
1	E	199	MET	2.2
1	F	119	LEU	2.2
1	H	105	LEU	2.2
1	A	206	ASP	2.2
1	H	159	GLU	2.2
1	G	200	PRO	2.2
1	L	191	GLN	2.2
1	G	217	GLY	2.2
1	G	254	LYS	2.2
1	D	96	ILE	2.2
1	D	238	SER	2.2
1	I	249	SER	2.2
1	J	49	ILE	2.2
1	K	238	SER	2.2
1	L	196	ILE	2.2
1	G	116	PHE	2.2
1	E	197	VAL	2.2
1	K	115	VAL	2.2
1	K	141	PRO	2.2
1	I	111	ALA	2.2
1	E	234	LYS	2.2
1	H	254	LYS	2.2
1	G	213	LEU	2.2
1	H	51	LEU	2.2
1	E	196	ILE	2.2
1	G	224	SER	2.2
1	L	29	GLU	2.2
1	G	84	PRO	2.2
1	K	255	VAL	2.2
1	L	74	VAL	2.2
1	L	218	ALA	2.2
1	L	265	ASN	2.2
1	H	191	GLN	2.2
1	G	223	CYS	2.2
1	H	209	LEU	2.2
1	K	158	LEU	2.2
1	H	103	ILE	2.2
1	E	227	SER	2.2
1	L	176	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	33	ASP	2.2
1	F	229	ARG	2.2
1	J	226	ARG	2.2
1	J	229	ARG	2.2
1	G	77	PRO	2.2
1	E	78	VAL	2.1
1	G	35	VAL	2.1
1	G	169	VAL	2.1
1	H	70	VAL	2.1
1	H	80	VAL	2.1
1	E	192	ALA	2.1
1	L	233	MET	2.1
1	G	123	GLY	2.1
1	D	271	ILE	2.1
1	E	138	ARG	2.1
1	G	216	SER	2.1
1	E	26	PHE	2.1
1	L	148	PHE	2.1
1	G	74	VAL	2.1
1	K	80	VAL	2.1
1	K	124	HIS	2.1
1	L	152	HIS	2.1
1	H	268	ALA	2.1
1	F	179	LEU	2.1
1	J	123	GLY	2.1
1	L	160	THR	2.1
1	G	196	ILE	2.1
1	L	76	ILE	2.1
1	H	195	ARG	2.1
1	K	57	GLU	2.1
1	K	180	GLU	2.1
1	L	138	ARG	2.1
1	G	177	SER	2.1
1	K	186	LYS	2.1
1	H	77	PRO	2.1
1	J	68	GLN	2.1
1	K	30	VAL	2.1
1	H	106	ALA	2.1
1	H	192	ALA	2.1
1	F	194	GLY	2.1
1	G	114	LEU	2.1
1	K	55	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	105	LEU	2.1
1	H	143	THR	2.1
1	H	259	THR	2.1
1	L	120	THR	2.1
1	L	201	GLY	2.1
1	H	96	ILE	2.1
1	L	180	GLU	2.1
1	J	251	TYR	2.1
1	D	33	ASP	2.1
1	J	269	LYS	2.1
1	L	186	LYS	2.1
1	H	174	CYS	2.1
1	G	183	PRO	2.1
1	J	233	MET	2.1
1	L	124	HIS	2.1
1	H	35	VAL	2.1
1	L	35	VAL	2.1
1	L	235	PHE	2.1
1	F	253	LEU	2.1
1	G	264	LEU	2.1
1	E	194	GLY	2.1
1	H	185	ILE	2.1
1	H	126	ASP	2.1
1	F	252	SER	2.1
1	H	73	SER	2.1
1	K	56	SER	2.1
1	L	239	SER	2.1
1	D	248	CYS	2.1
1	L	200	PRO	2.1
1	E	35	VAL	2.0
1	K	69	VAL	2.0
1	L	166	PHE	2.0
1	D	241	ALA	2.0
1	K	104	ARG	2.0
1	E	24	ASN	2.0
1	F	264	LEU	2.0
1	L	140	LEU	2.0
1	L	182	LEU	2.0
1	H	201	GLY	2.0
1	L	117	GLY	2.0
1	E	143	THR	2.0
1	E	205	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	71	LYS	2.0
1	E	257	ASP	2.0
1	J	155	MET	2.0
1	E	187	ARG	2.0
1	G	78	VAL	2.0
1	J	90	LEU	2.0
1	J	147	ALA	2.0
1	K	46	ALA	2.0
1	L	46	ALA	2.0
1	L	179	LEU	2.0
1	C	270	ASN	2.0
1	G	24	ASN	2.0
1	J	234	LYS	2.0
1	L	127	LYS	2.0
1	F	189	ILE	2.0
1	G	206	ASP	2.0
1	L	47	ASP	2.0
1	I	238	SER	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.