



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:12 PM UTC

PDB ID : 6OKB / pdb_00006okb
EMDB ID : EMD-20099
Title : Prohead 2 of the phage T5
Authors : Huet, A.; Duda, R.L.; Boulanger, P.; Conway, J.F.
Deposited on : 2019-04-12
Resolution : 6.70 Å(reported)
Based on initial model : 2FT1

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

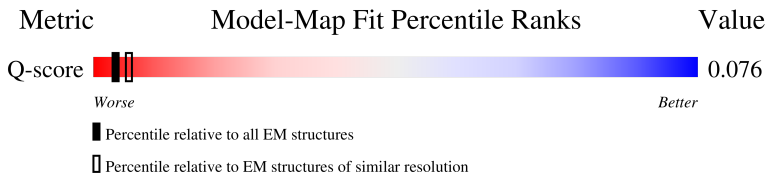
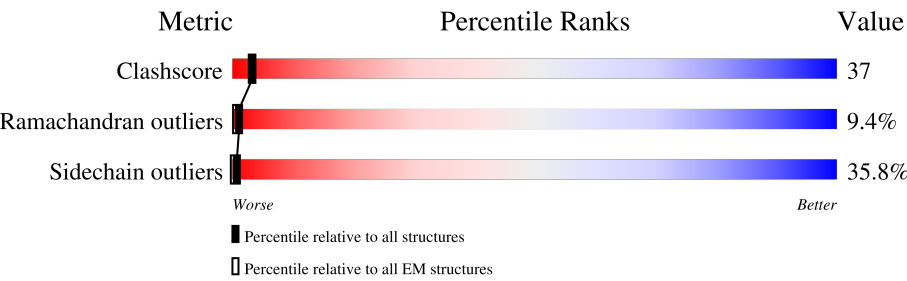
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	523 (6.20 - 7.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	49% 25% 42% 27% • •
1	B	299	52% 19% 48% 25% 5% •
1	C	299	51% 28% 43% 24% • •
1	D	299	48% 24% 44% 25% • •

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Mol	Chain	Length	Quality of chain
1	E	299	49% 23% 41% 30%
1	F	299	53% 23% 41% 27% 5%
1	G	299	50% 21% 46% 24% 6%
1	H	299	51% 18% 43% 32%
1	I	299	52% 20% 49% 25%
1	J	299	55% 20% 49% 24%
1	K	299	54% 20% 47% 25%
1	L	299	54% 26% 42% 25%
1	M	299	77% 36% 42% 17%

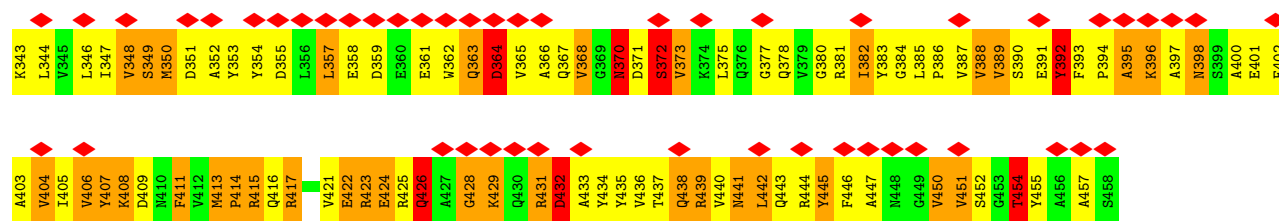
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29211 atoms, of which 0 are hydrogens and 0 are deuteriums.

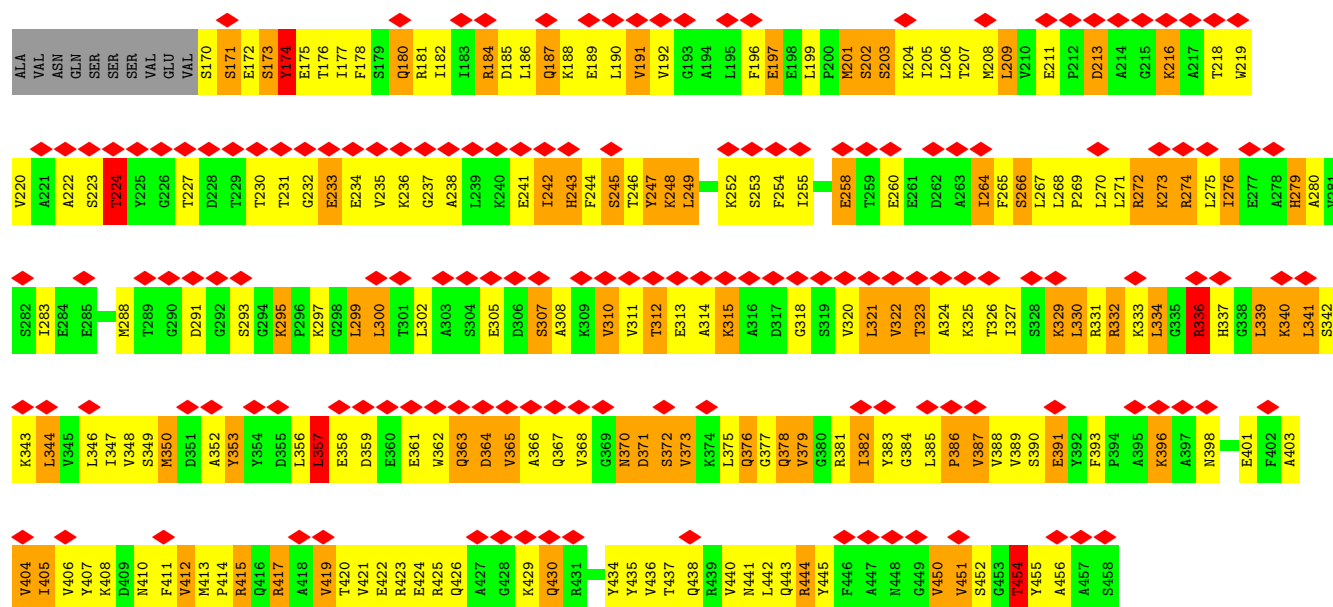
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

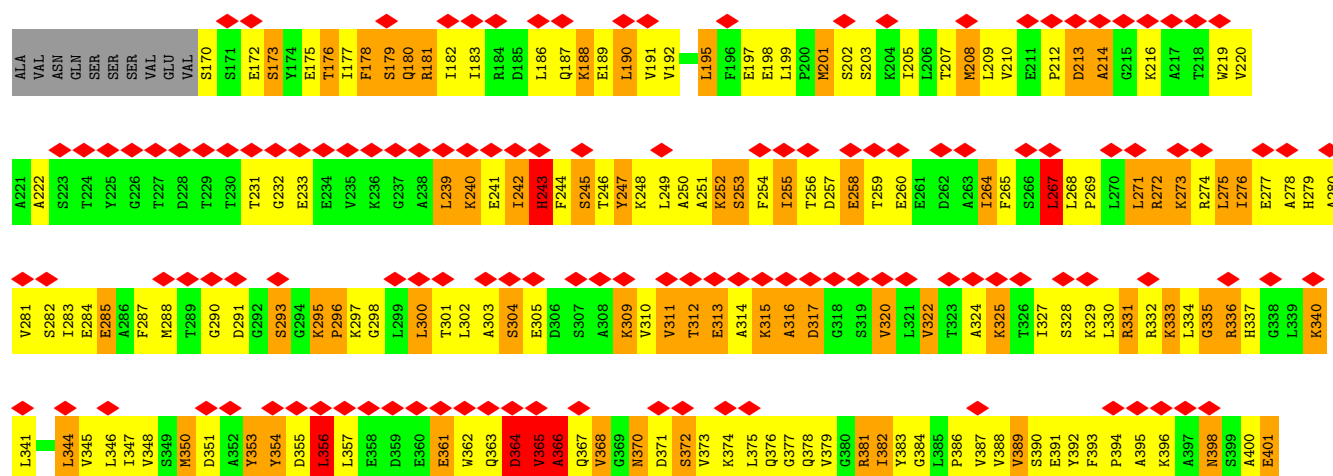
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	B	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	C	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	D	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	E	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	F	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	G	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	H	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	I	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	J	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	K	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	L	289	Total 2247	C 1425	N 379	O 438	S 5	0	0
1	M	289	Total 2247	C 1425	N 379	O 438	S 5	0	0

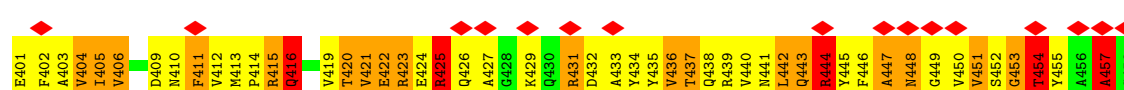
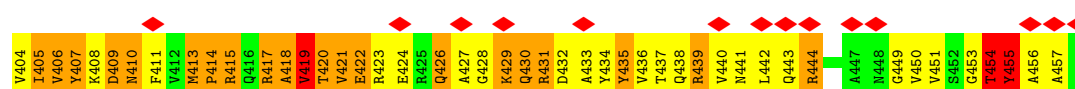


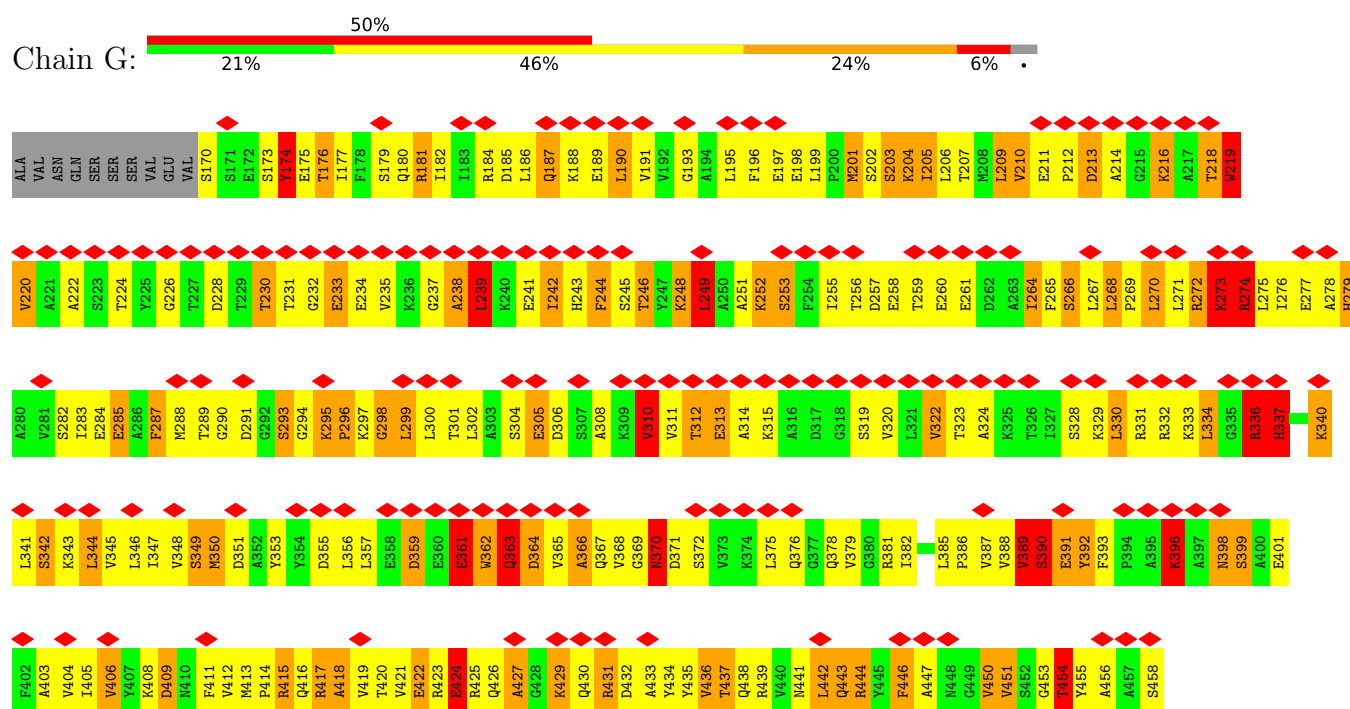
• Molecule 1: Major capsid protein



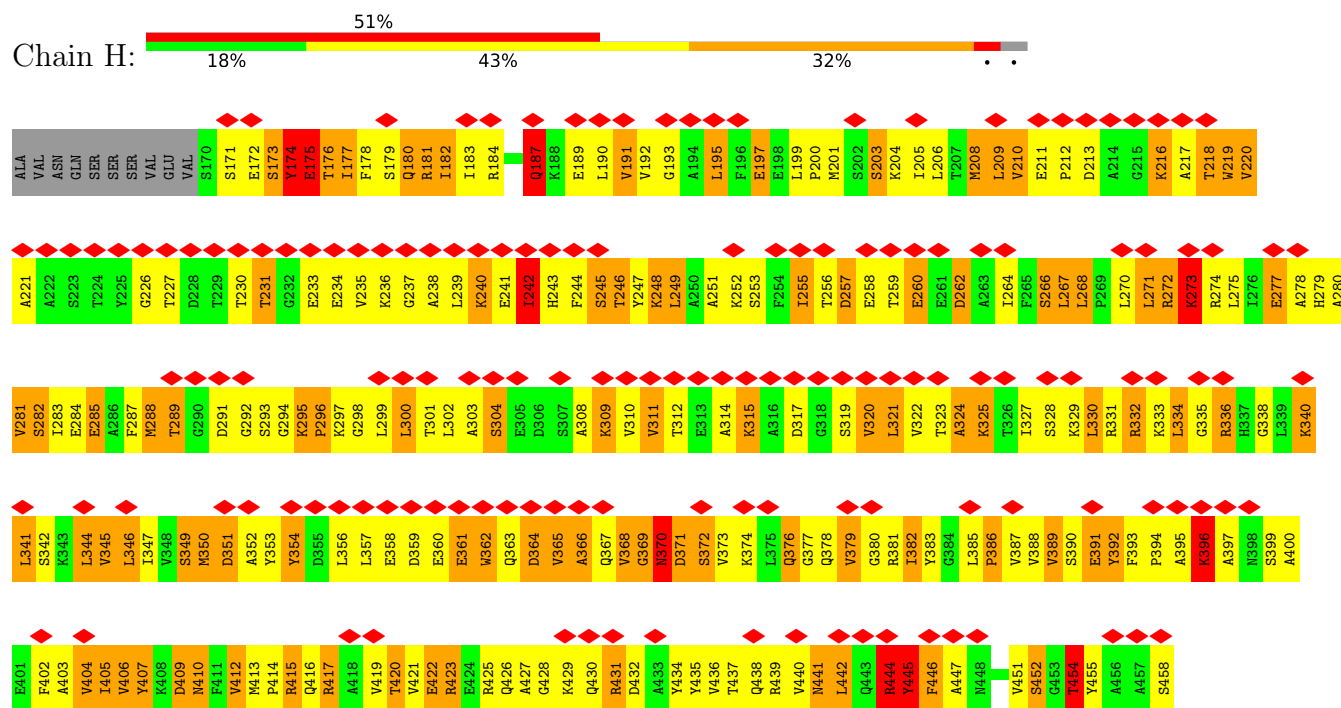
• Molecule 1: Major capsid protein



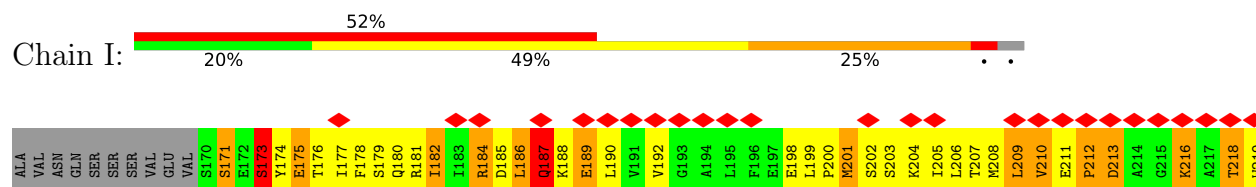


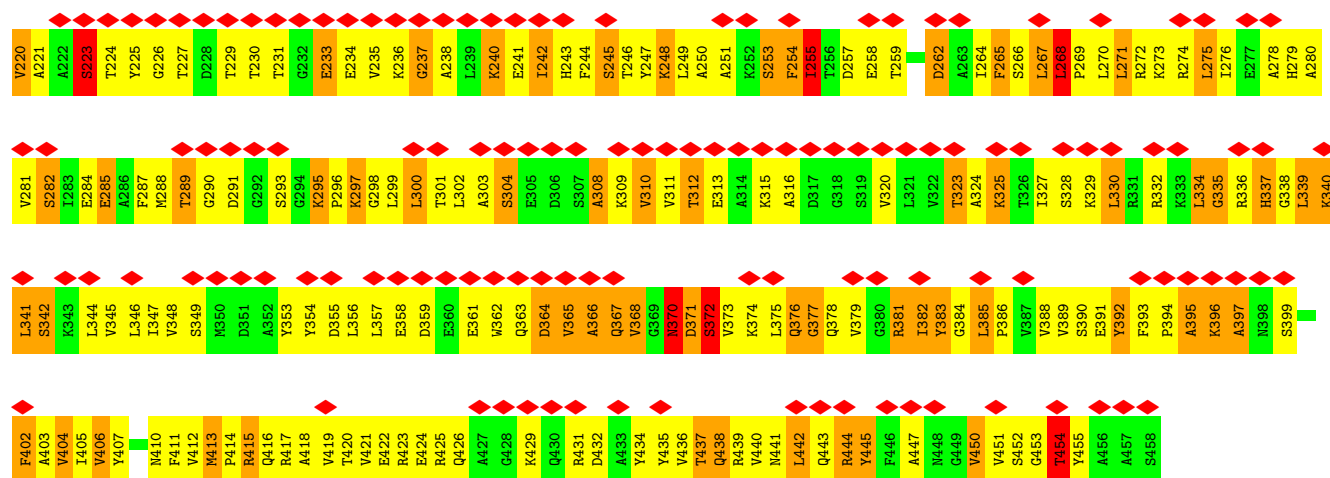


- Molecule 1: Major capsid protein

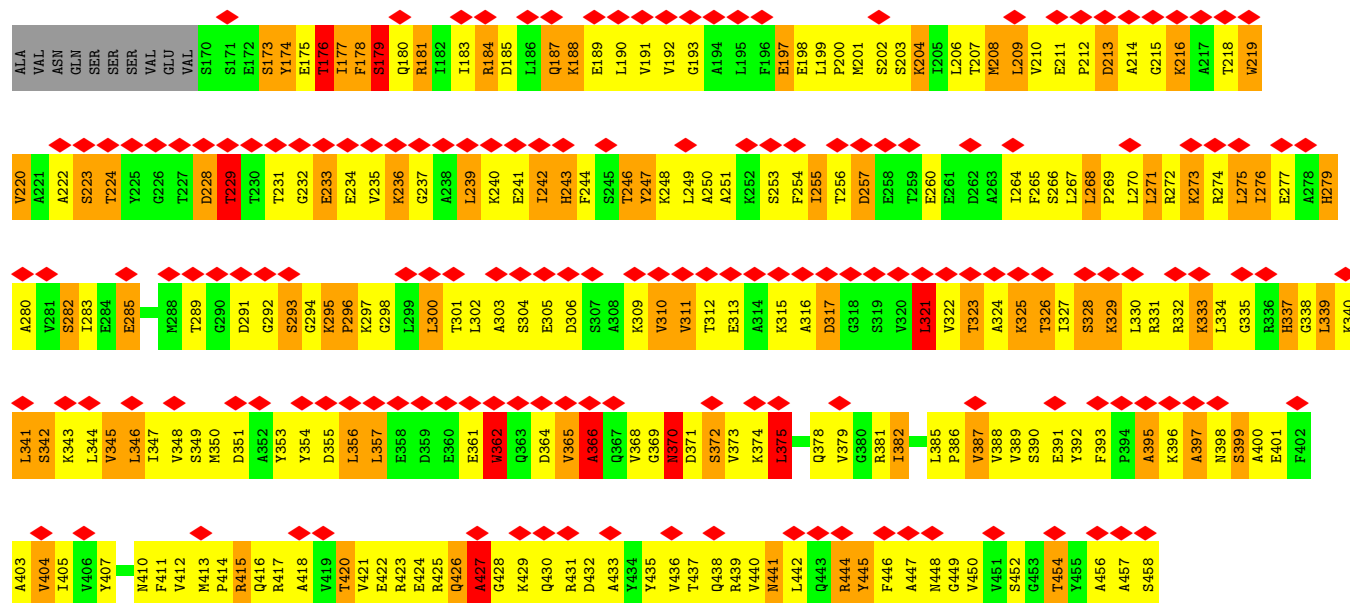
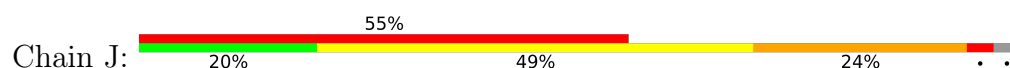


- Molecule 1: Major capsid protein

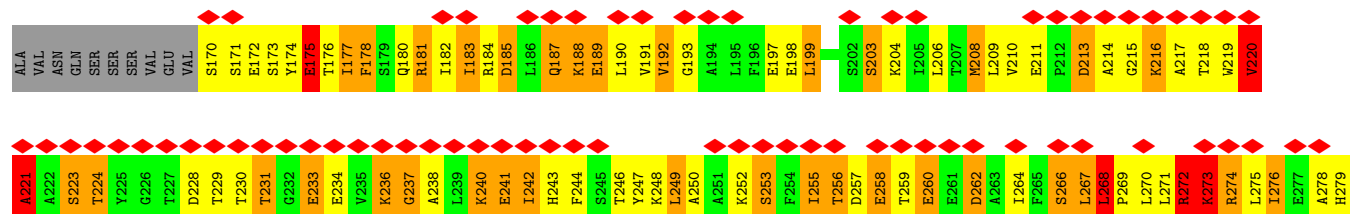
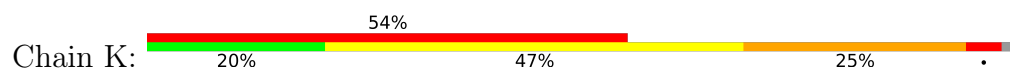


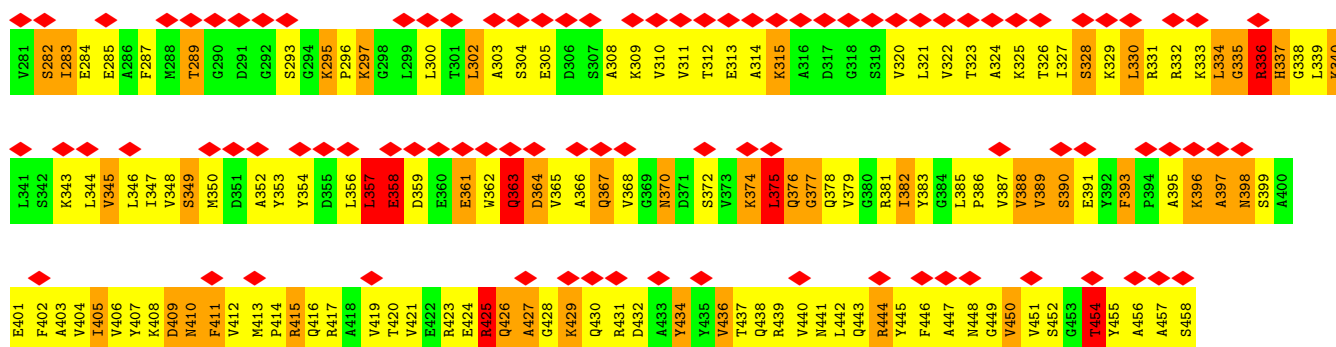


• Molecule 1: Major capsid protein

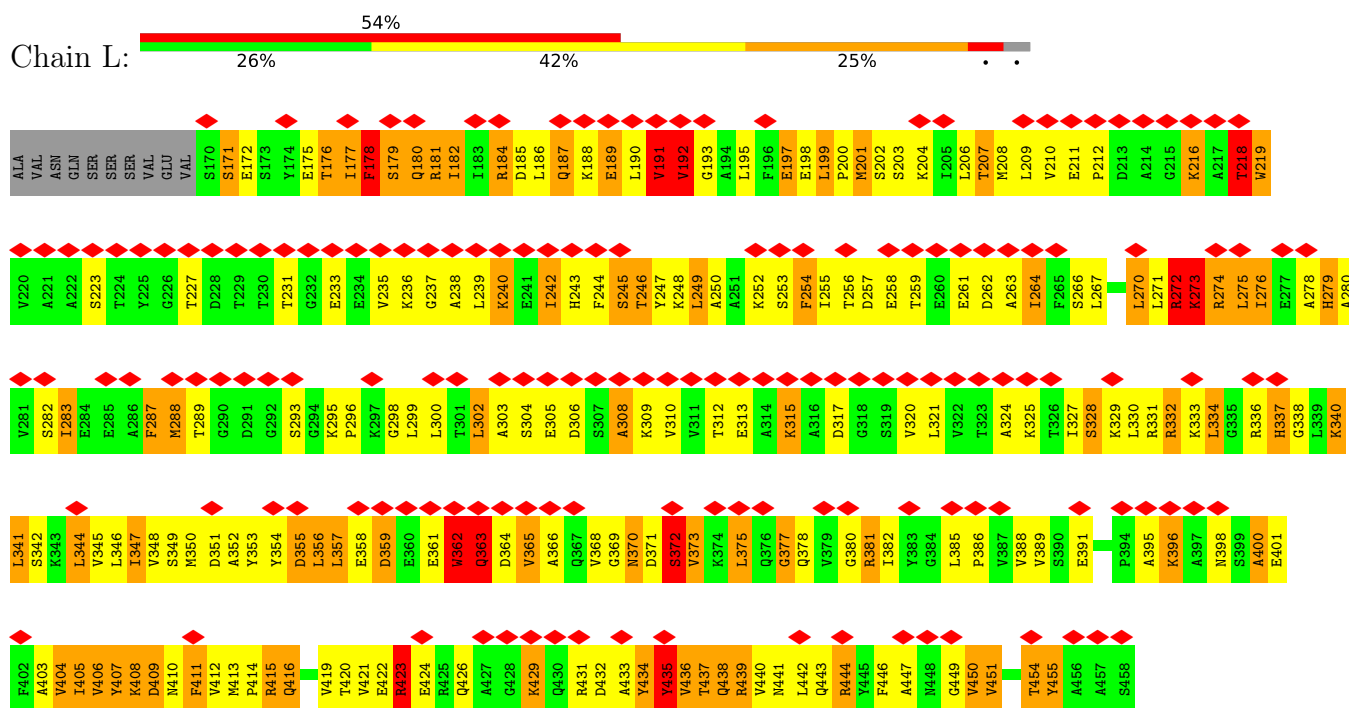


• Molecule 1: Major capsid protein

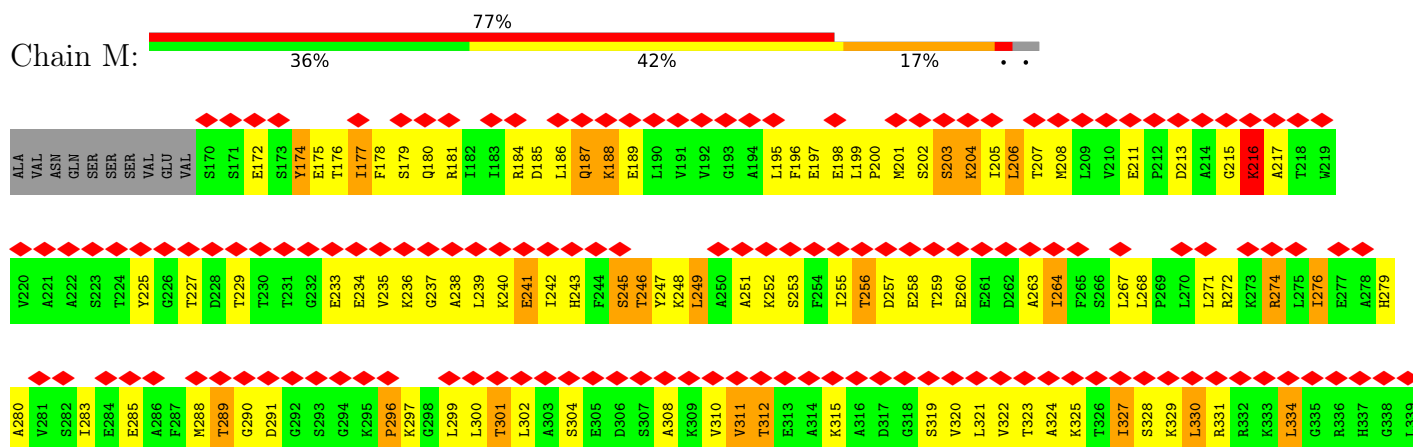




• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	32.443	Depositor
Minimum map value	-15.158	Depositor
Average map value	0.119	Depositor
Map value standard deviation	4.035	Depositor
Recommended contour level	14	Depositor
Map size (Å)	845.05493, 845.05493, 845.05493	wwPDB
Map dimensions	801, 801, 801	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

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	0.70	1/2282 (0.0%)	1.21	22/3082 (0.7%)
1	B	0.76	1/2282 (0.0%)	1.20	20/3082 (0.6%)
1	C	0.68	0/2282	1.21	18/3082 (0.6%)
1	D	0.75	0/2282	1.23	21/3082 (0.7%)
1	E	0.75	1/2282 (0.0%)	1.21	19/3082 (0.6%)
1	F	0.69	1/2282 (0.0%)	1.20	21/3082 (0.7%)
1	G	0.78	1/2282 (0.0%)	1.29	33/3082 (1.1%)
1	H	0.82	1/2282 (0.0%)	1.23	23/3082 (0.7%)
1	I	0.72	1/2282 (0.0%)	1.11	17/3082 (0.6%)
1	J	0.70	1/2282 (0.0%)	1.20	22/3082 (0.7%)
1	K	0.72	1/2282 (0.0%)	1.24	23/3082 (0.7%)
1	L	0.77	2/2282 (0.1%)	1.21	21/3082 (0.7%)
1	M	0.52	0/2282	1.06	16/3082 (0.5%)
All	All	0.72	11/29666 (0.0%)	1.20	276/40066 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	15
1	C	0	14
1	D	0	11
1	E	0	15
1	F	0	11
1	G	0	13
1	H	0	11
1	I	0	14
1	J	0	8
1	K	0	14
1	L	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	9
All	All	0	160

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	210	VAL	C-N	-13.50	1.11	1.33
1	H	267	LEU	CA-CB	-12.57	1.32	1.53
1	L	189	GLU	CA-C	-11.32	1.40	1.53
1	I	267	LEU	CA-CB	-10.35	1.35	1.53
1	L	423	ARG	CA-CB	-9.12	1.38	1.53
1	F	189	GLU	CA-C	-7.88	1.42	1.52
1	K	413	MET	C-N	-7.39	1.26	1.33
1	B	267	LEU	CA-CB	-7.26	1.41	1.53
1	J	243	HIS	CA-CB	-7.04	1.42	1.53
1	A	393	PHE	C-N	-5.34	1.26	1.33
1	E	257	ASP	CA-CB	-5.31	1.46	1.52

All (276) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	401	GLU	N-CA-C	-10.87	96.63	111.96
1	G	366	ALA	N-CA-C	-10.72	102.40	114.62
1	K	221	ALA	N-CA-C	-10.47	101.27	114.56
1	F	188	LYS	CA-C-N	10.43	141.47	121.54
1	F	188	LYS	C-N-CA	10.43	141.47	121.54
1	L	188	LYS	CA-C-N	9.63	136.31	122.05
1	L	188	LYS	C-N-CA	9.63	136.31	122.05
1	E	421	VAL	CA-C-N	-8.69	110.58	122.30
1	E	421	VAL	C-N-CA	-8.69	110.58	122.30
1	B	392	TYR	N-CA-C	-8.59	100.73	113.61
1	J	216	LYS	CA-C-N	8.55	137.09	121.70
1	J	216	LYS	C-N-CA	8.55	137.09	121.70
1	A	192	VAL	N-CA-C	-8.37	105.09	112.12
1	K	220	VAL	N-CA-C	-8.30	103.79	111.67
1	L	400	ALA	CA-C-N	-8.01	109.92	122.49
1	L	400	ALA	C-N-CA	-8.01	109.92	122.49
1	J	426	GLN	CA-C-N	7.93	135.97	121.70
1	J	426	GLN	C-N-CA	7.93	135.97	121.70
1	K	364	ASP	N-CA-C	-7.89	102.69	113.18
1	H	426	GLN	CA-C-N	7.74	135.63	121.70
1	H	426	GLN	C-N-CA	7.74	135.63	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	216	LYS	CA-C-N	7.71	135.57	121.70
1	F	216	LYS	C-N-CA	7.71	135.57	121.70
1	A	426	GLN	CA-C-N	7.59	135.36	121.70
1	A	426	GLN	C-N-CA	7.59	135.36	121.70
1	D	426	GLN	CA-C-N	7.56	135.30	121.70
1	D	426	GLN	C-N-CA	7.56	135.30	121.70
1	G	216	LYS	CA-C-N	7.53	135.25	121.70
1	G	216	LYS	C-N-CA	7.53	135.25	121.70
1	L	216	LYS	CA-C-N	7.43	135.07	121.70
1	L	216	LYS	C-N-CA	7.43	135.07	121.70
1	G	426	GLN	CA-C-N	7.42	135.06	121.70
1	G	426	GLN	C-N-CA	7.42	135.06	121.70
1	J	228	ASP	CA-C-N	7.36	134.95	121.70
1	J	228	ASP	C-N-CA	7.36	134.95	121.70
1	E	216	LYS	CA-C-N	7.34	134.91	121.70
1	E	216	LYS	C-N-CA	7.34	134.91	121.70
1	A	174	TYR	CA-C-N	7.30	135.48	121.54
1	A	174	TYR	C-N-CA	7.30	135.48	121.54
1	K	216	LYS	CA-C-N	7.28	134.81	121.70
1	K	216	LYS	C-N-CA	7.28	134.81	121.70
1	A	216	LYS	CA-C-N	7.27	134.78	121.70
1	A	216	LYS	C-N-CA	7.27	134.78	121.70
1	G	195	LEU	N-CA-C	-7.25	104.17	113.16
1	C	426	GLN	CA-C-N	7.24	134.73	121.70
1	C	426	GLN	C-N-CA	7.24	134.73	121.70
1	E	426	GLN	CA-C-N	7.20	134.67	121.70
1	E	426	GLN	C-N-CA	7.20	134.67	121.70
1	J	454	THR	CA-C-N	7.18	134.63	121.70
1	J	454	THR	C-N-CA	7.18	134.63	121.70
1	J	229	THR	CA-C-N	7.14	134.56	121.70
1	J	229	THR	C-N-CA	7.14	134.56	121.70
1	H	216	LYS	CA-C-N	7.05	134.40	121.70
1	H	216	LYS	C-N-CA	7.05	134.40	121.70
1	M	426	GLN	CA-C-N	7.03	134.36	121.70
1	M	426	GLN	C-N-CA	7.03	134.36	121.70
1	F	454	THR	CA-C-N	7.03	134.35	121.70
1	F	454	THR	C-N-CA	7.03	134.35	121.70
1	I	426	GLN	CA-C-N	7.02	134.34	121.70
1	I	426	GLN	C-N-CA	7.02	134.34	121.70
1	G	424	GLU	CA-C-N	-6.99	115.65	123.13
1	G	424	GLU	C-N-CA	-6.99	115.65	123.13
1	G	210	VAL	CA-C-N	6.96	130.37	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	210	VAL	C-N-CA	6.96	130.37	120.49
1	B	361	GLU	CA-C-N	6.94	134.20	121.70
1	B	361	GLU	C-N-CA	6.94	134.20	121.70
1	D	216	LYS	CA-C-N	6.94	134.19	121.70
1	D	216	LYS	C-N-CA	6.94	134.19	121.70
1	I	216	LYS	CA-C-N	6.89	134.11	121.70
1	I	216	LYS	C-N-CA	6.89	134.11	121.70
1	I	361	GLU	CA-C-N	6.89	134.11	121.70
1	I	361	GLU	C-N-CA	6.89	134.11	121.70
1	C	216	LYS	CA-C-N	6.89	134.10	121.70
1	C	216	LYS	C-N-CA	6.89	134.10	121.70
1	B	232	GLY	CA-C-N	6.86	134.64	121.54
1	B	232	GLY	C-N-CA	6.86	134.64	121.54
1	I	392	TYR	N-CA-C	-6.84	103.51	112.41
1	B	216	LYS	CA-C-N	6.82	133.97	121.70
1	B	216	LYS	C-N-CA	6.82	133.97	121.70
1	L	435	TYR	CA-CB-CG	6.81	126.16	113.90
1	D	232	GLY	CA-C-N	6.77	134.47	121.54
1	D	232	GLY	C-N-CA	6.77	134.47	121.54
1	C	361	GLU	CA-C-N	6.77	133.88	121.70
1	C	361	GLU	C-N-CA	6.77	133.88	121.70
1	J	361	GLU	CA-C-N	6.75	133.84	121.70
1	J	361	GLU	C-N-CA	6.75	133.84	121.70
1	K	361	GLU	CA-C-N	6.74	133.82	121.70
1	K	361	GLU	C-N-CA	6.74	133.82	121.70
1	E	420	THR	N-CA-C	-6.72	100.45	110.06
1	H	361	GLU	CA-C-N	6.71	133.77	121.70
1	H	361	GLU	C-N-CA	6.71	133.77	121.70
1	J	232	GLY	CA-C-N	6.69	134.32	121.54
1	J	232	GLY	C-N-CA	6.69	134.32	121.54
1	G	232	GLY	CA-C-N	6.67	134.29	121.54
1	G	232	GLY	C-N-CA	6.67	134.29	121.54
1	F	426	GLN	CA-C-N	6.65	133.67	121.70
1	F	426	GLN	C-N-CA	6.65	133.67	121.70
1	L	426	GLN	CA-C-N	6.61	133.60	121.70
1	L	426	GLN	C-N-CA	6.61	133.60	121.70
1	E	361	GLU	CA-C-N	6.60	133.58	121.70
1	E	361	GLU	C-N-CA	6.60	133.58	121.70
1	K	454	THR	CA-C-N	6.59	133.57	121.70
1	K	454	THR	C-N-CA	6.59	133.57	121.70
1	D	361	GLU	CA-C-N	6.58	133.54	121.70
1	D	361	GLU	C-N-CA	6.58	133.54	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	366	ALA	N-CA-C	-6.54	105.19	113.43
1	A	361	GLU	CA-C-N	6.51	133.42	121.70
1	A	361	GLU	C-N-CA	6.51	133.42	121.70
1	G	392	TYR	CA-C-N	-6.45	111.88	120.65
1	G	392	TYR	C-N-CA	-6.45	111.88	120.65
1	E	240	LYS	CA-C-N	6.45	133.30	121.70
1	E	240	LYS	C-N-CA	6.45	133.30	121.70
1	M	361	GLU	CA-C-N	6.39	133.20	121.70
1	M	361	GLU	C-N-CA	6.39	133.20	121.70
1	G	446	PHE	N-CA-C	6.35	116.84	108.07
1	H	267	LEU	N-CA-C	-6.35	105.11	112.92
1	B	209	LEU	CA-C-N	-6.35	114.18	122.37
1	B	209	LEU	C-N-CA	-6.35	114.18	122.37
1	D	364	ASP	N-CA-C	-6.34	105.54	113.28
1	G	378	GLN	N-CA-C	6.33	116.35	108.19
1	M	216	LYS	CA-C-N	6.30	133.04	121.70
1	M	216	LYS	C-N-CA	6.30	133.04	121.70
1	A	233	GLU	CA-C-N	6.24	132.93	121.70
1	A	233	GLU	C-N-CA	6.24	132.93	121.70
1	G	372	SER	CA-C-N	6.23	132.92	121.70
1	G	372	SER	C-N-CA	6.23	132.92	121.70
1	H	372	SER	CA-C-N	6.22	132.90	121.70
1	H	372	SER	C-N-CA	6.22	132.90	121.70
1	K	372	SER	CA-C-N	6.21	132.88	121.70
1	K	372	SER	C-N-CA	6.21	132.88	121.70
1	A	240	LYS	CA-C-N	6.18	132.83	121.70
1	A	240	LYS	C-N-CA	6.18	132.83	121.70
1	F	361	GLU	CA-C-N	6.18	132.82	121.70
1	F	361	GLU	C-N-CA	6.18	132.82	121.70
1	F	372	SER	CA-C-N	6.18	132.82	121.70
1	F	372	SER	C-N-CA	6.18	132.82	121.70
1	B	426	GLN	CA-C-N	6.18	132.82	121.70
1	B	426	GLN	C-N-CA	6.18	132.82	121.70
1	B	454	THR	CA-C-N	6.16	132.78	121.70
1	B	454	THR	C-N-CA	6.16	132.78	121.70
1	K	426	GLN	CA-C-N	6.14	132.76	121.70
1	K	426	GLN	C-N-CA	6.14	132.76	121.70
1	M	233	GLU	CA-C-N	6.14	132.75	121.70
1	M	233	GLU	C-N-CA	6.14	132.75	121.70
1	H	195	LEU	N-CA-C	-6.11	104.19	112.26
1	C	454	THR	CA-C-N	6.03	132.55	121.70
1	C	454	THR	C-N-CA	6.03	132.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	240	LYS	CA-C-N	6.00	132.51	121.70
1	K	240	LYS	C-N-CA	6.00	132.51	121.70
1	A	454	THR	CA-C-N	5.99	132.48	121.70
1	A	454	THR	C-N-CA	5.99	132.48	121.70
1	E	372	SER	CA-C-N	5.99	132.47	121.70
1	E	372	SER	C-N-CA	5.99	132.47	121.70
1	H	173	SER	CA-C-N	-5.98	115.02	123.03
1	H	173	SER	C-N-CA	-5.98	115.02	123.03
1	C	295	LYS	N-CA-C	-5.96	102.37	110.36
1	L	233	GLU	CA-C-N	5.95	132.42	121.70
1	L	233	GLU	C-N-CA	5.95	132.42	121.70
1	J	233	GLU	CA-C-N	5.94	132.39	121.70
1	J	233	GLU	C-N-CA	5.94	132.39	121.70
1	M	372	SER	CA-C-N	5.92	132.35	121.70
1	M	372	SER	C-N-CA	5.92	132.35	121.70
1	J	240	LYS	CA-C-N	5.90	132.31	121.70
1	J	240	LYS	C-N-CA	5.90	132.31	121.70
1	D	233	GLU	CA-C-N	5.89	132.31	121.70
1	D	233	GLU	C-N-CA	5.89	132.31	121.70
1	K	233	GLU	CA-C-N	5.88	132.29	121.70
1	K	233	GLU	C-N-CA	5.88	132.29	121.70
1	F	295	LYS	N-CA-C	-5.87	103.38	110.13
1	G	233	GLU	CA-C-N	5.86	132.24	121.70
1	G	233	GLU	C-N-CA	5.86	132.24	121.70
1	C	173	SER	CA-C-N	5.83	132.68	121.54
1	C	173	SER	C-N-CA	5.83	132.68	121.54
1	B	233	GLU	CA-C-N	5.83	132.19	121.70
1	B	233	GLU	C-N-CA	5.83	132.19	121.70
1	B	370	ASN	CA-C-N	5.81	132.15	121.70
1	B	370	ASN	C-N-CA	5.81	132.15	121.70
1	J	370	ASN	CA-C-N	5.81	132.16	121.70
1	J	370	ASN	C-N-CA	5.81	132.16	121.70
1	F	226	GLY	CA-C-N	5.79	132.60	121.54
1	F	226	GLY	C-N-CA	5.79	132.60	121.54
1	K	405	ILE	CA-C-N	-5.77	115.16	122.43
1	K	405	ILE	C-N-CA	-5.77	115.16	122.43
1	G	298	GLY	CA-C-N	5.77	129.47	120.82
1	G	298	GLY	C-N-CA	5.77	129.47	120.82
1	J	366	ALA	N-CA-C	-5.66	98.75	110.80
1	D	240	LYS	CA-C-N	5.65	131.87	121.70
1	D	240	LYS	C-N-CA	5.65	131.87	121.70
1	G	361	GLU	CA-C-N	5.61	131.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	361	GLU	C-N-CA	5.61	131.79	121.70
1	L	454	THR	CA-C-N	5.60	131.78	121.70
1	L	454	THR	C-N-CA	5.60	131.78	121.70
1	H	370	ASN	CA-C-N	5.59	131.76	121.70
1	H	370	ASN	C-N-CA	5.59	131.76	121.70
1	C	191	VAL	N-CA-C	5.58	112.18	106.21
1	L	370	ASN	CA-C-N	5.56	131.71	121.70
1	L	370	ASN	C-N-CA	5.56	131.71	121.70
1	L	372	SER	CA-C-N	5.56	131.71	121.70
1	L	372	SER	C-N-CA	5.56	131.71	121.70
1	A	356	LEU	CA-C-N	-5.53	112.12	122.73
1	A	356	LEU	C-N-CA	-5.53	112.12	122.73
1	H	360	GLU	N-CA-C	-5.53	104.79	113.02
1	H	174	TYR	CA-CB-CG	-5.51	103.98	113.90
1	M	454	THR	CA-C-N	5.51	131.62	121.70
1	M	454	THR	C-N-CA	5.51	131.62	121.70
1	A	370	ASN	CA-C-N	5.50	131.60	121.70
1	A	370	ASN	C-N-CA	5.50	131.60	121.70
1	L	435	TYR	N-CA-CB	5.47	118.61	110.29
1	L	240	LYS	CA-C-N	5.47	131.54	121.70
1	L	240	LYS	C-N-CA	5.47	131.54	121.70
1	E	400	ALA	CA-C-N	-5.46	111.90	122.06
1	E	400	ALA	C-N-CA	-5.46	111.90	122.06
1	I	186	LEU	CA-C-N	-5.46	113.89	122.95
1	I	186	LEU	C-N-CA	-5.46	113.89	122.95
1	I	370	ASN	CA-C-N	5.44	131.49	121.70
1	I	370	ASN	C-N-CA	5.44	131.49	121.70
1	H	240	LYS	CA-C-N	5.43	131.47	121.70
1	H	240	LYS	C-N-CA	5.43	131.47	121.70
1	F	233	GLU	CA-C-N	5.43	131.47	121.70
1	F	233	GLU	C-N-CA	5.43	131.47	121.70
1	A	247	TYR	CA-CB-CG	-5.41	104.16	113.90
1	I	372	SER	CA-C-N	5.41	131.44	121.70
1	I	372	SER	C-N-CA	5.41	131.44	121.70
1	A	372	SER	CA-C-N	5.36	131.35	121.70
1	A	372	SER	C-N-CA	5.36	131.35	121.70
1	C	233	GLU	CA-C-N	5.36	131.35	121.70
1	C	233	GLU	C-N-CA	5.36	131.35	121.70
1	F	370	ASN	CA-C-N	5.35	131.34	121.70
1	F	370	ASN	C-N-CA	5.35	131.34	121.70
1	D	365	VAL	CA-C-N	5.35	131.75	121.54
1	D	365	VAL	C-N-CA	5.35	131.75	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	398	ASN	N-CA-C	5.34	118.14	107.62
1	K	224	THR	N-CA-C	-5.31	106.07	112.54
1	H	324	ALA	N-CA-C	-5.29	106.51	113.17
1	E	260	GLU	N-CA-C	-5.26	106.09	112.88
1	M	411	PHE	CA-C-N	-5.24	115.05	122.34
1	M	411	PHE	C-N-CA	-5.24	115.05	122.34
1	H	233	GLU	CA-C-N	5.24	131.13	121.70
1	H	233	GLU	C-N-CA	5.24	131.13	121.70
1	K	175	GLU	CA-C-N	-5.22	114.87	122.86
1	K	175	GLU	C-N-CA	-5.22	114.87	122.86
1	B	174	TYR	CA-CB-CG	-5.21	104.53	113.90
1	F	240	LYS	CA-C-N	5.19	131.05	121.70
1	F	240	LYS	C-N-CA	5.19	131.05	121.70
1	C	227	THR	CA-C-N	5.19	131.46	121.54
1	C	227	THR	C-N-CA	5.19	131.46	121.54
1	G	238	ALA	CA-C-N	5.17	131.42	121.54
1	G	238	ALA	C-N-CA	5.17	131.42	121.54
1	B	187	GLN	CA-C-N	-5.16	113.57	120.54
1	B	187	GLN	C-N-CA	-5.16	113.57	120.54
1	D	243	HIS	CA-C-N	-5.13	115.49	122.93
1	D	243	HIS	C-N-CA	-5.13	115.49	122.93
1	D	454	THR	CA-C-N	5.11	130.90	121.70
1	D	454	THR	C-N-CA	5.11	130.90	121.70
1	K	376	GLN	CA-CB-CG	5.11	124.31	114.10
1	C	372	SER	CA-C-N	5.10	130.88	121.70
1	C	372	SER	C-N-CA	5.10	130.88	121.70
1	I	233	GLU	CA-C-N	5.10	130.88	121.70
1	I	233	GLU	C-N-CA	5.10	130.88	121.70
1	L	377	GLY	N-CA-C	5.09	125.25	113.18
1	H	392	TYR	N-CA-C	-5.09	104.02	111.30
1	G	273	LYS	CA-C-N	5.08	131.25	121.54
1	G	273	LYS	C-N-CA	5.08	131.25	121.54
1	D	374	LYS	CB-CA-C	-5.05	110.74	116.54
1	I	240	LYS	CA-C-N	5.04	130.78	121.70
1	I	240	LYS	C-N-CA	5.04	130.78	121.70
1	J	427	ALA	N-CA-C	5.04	125.11	111.00
1	G	370	ASN	CA-C-N	5.04	130.76	121.70
1	G	370	ASN	C-N-CA	5.04	130.76	121.70
1	H	366	ALA	N-CA-C	-5.03	106.29	114.09
1	G	454	THR	CA-C-N	5.01	130.72	121.70
1	G	454	THR	C-N-CA	5.01	130.72	121.70
1	E	370	ASN	CA-C-N	5.01	130.72	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	370	ASN	C-N-CA	5.01	130.72	121.70
1	M	263	ALA	CA-C-N	-5.01	118.06	122.97
1	M	263	ALA	C-N-CA	-5.01	118.06	122.97

There are no chirality outliers.

All (160) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	GLN	Peptide
1	A	188	LYS	Peptide
1	A	197	GLU	Peptide
1	A	210	VAL	Peptide
1	A	220	VAL	Peptide
1	A	221	ALA	Peptide
1	A	325	LYS	Peptide
1	A	370	ASN	Peptide
1	A	392	TYR	Peptide
1	A	432	ASP	Peptide
1	B	178	PHE	Peptide
1	B	187	GLN	Peptide
1	B	205	ILE	Peptide
1	B	209	LEU	Peptide
1	B	210	VAL	Peptide
1	B	218	THR	Peptide
1	B	223	SER	Peptide
1	B	288	MET	Peptide
1	B	294	GLY	Peptide
1	B	337	HIS	Peptide
1	B	372	SER	Peptide
1	B	392	TYR	Peptide
1	B	407	TYR	Peptide
1	B	417	ARG	Peptide
1	B	426	GLN	Peptide
1	C	178	PHE	Peptide
1	C	187	GLN	Peptide
1	C	189	GLU	Peptide
1	C	209	LEU	Peptide
1	C	224	THR	Peptide
1	C	254	PHE	Peptide
1	C	265	PHE	Peptide
1	C	266	SER	Peptide
1	C	321	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	C	337	HIS	Peptide
1	C	356	LEU	Peptide
1	C	357	LEU	Peptide
1	C	386	PRO	Peptide
1	C	454	THR	Peptide
1	D	214	ALA	Peptide
1	D	244	PHE	Peptide
1	D	267	LEU	Peptide
1	D	335	GLY	Peptide
1	D	356	LEU	Peptide
1	D	364	ASP	Peptide
1	D	366	ALA	Peptide
1	D	370	ASN	Peptide
1	D	393	PHE	Peptide
1	D	400	ALA	Peptide
1	D	454	THR	Peptide
1	E	187	GLN	Peptide
1	E	189	GLU	Peptide
1	E	220	VAL	Peptide
1	E	250	ALA	Peptide
1	E	260	GLU	Peptide
1	E	265	PHE	Peptide
1	E	294	GLY	Peptide
1	E	321	LEU	Peptide
1	E	325	LYS	Peptide
1	E	356	LEU	Peptide
1	E	379	VAL	Peptide
1	E	389	VAL	Peptide
1	E	398	ASN	Peptide
1	E	428	GLY	Peptide
1	E	454	THR	Peptide
1	F	187	GLN	Peptide
1	F	219	TRP	Peptide
1	F	255	ILE	Peptide
1	F	294	GLY	Peptide
1	F	325	LYS	Peptide
1	F	332	ARG	Peptide
1	F	363	GLN	Peptide
1	F	366	ALA	Peptide
1	F	390	SER	Peptide
1	F	391	GLU	Peptide
1	F	457	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	G	187	GLN	Peptide
1	G	219	TRP	Peptide
1	G	246	THR	Peptide
1	G	249	LEU	Peptide
1	G	336	ARG	Peptide
1	G	361	GLU	Peptide
1	G	369	GLY	Peptide
1	G	370	ASN	Peptide
1	G	390	SER	Peptide
1	G	392	TYR	Peptide
1	G	399	SER	Peptide
1	G	418	ALA	Peptide
1	G	454	THR	Peptide
1	H	187	GLN	Peptide
1	H	209	LEU	Peptide
1	H	220	VAL	Peptide
1	H	294	GLY	Peptide
1	H	315	LYS	Peptide
1	H	356	LEU	Peptide
1	H	364	ASP	Peptide
1	H	405	ILE	Peptide
1	H	410	ASN	Peptide
1	H	423	ARG	Peptide
1	H	454	THR	Peptide
1	I	187	GLN	Peptide
1	I	189	GLU	Peptide
1	I	209	LEU	Peptide
1	I	220	VAL	Peptide
1	I	223	SER	Peptide
1	I	265	PHE	Peptide
1	I	308	ALA	Peptide
1	I	310	VAL	Peptide
1	I	335	GLY	Peptide
1	I	337	HIS	Peptide
1	I	356	LEU	Peptide
1	I	370	ASN	Peptide
1	I	377	GLY	Peptide
1	I	454	THR	Peptide
1	J	178	PHE	Peptide
1	J	209	LEU	Peptide
1	J	294	GLY	Peptide
1	J	321	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	J	325	LYS	Peptide
1	J	356	LEU	Peptide
1	J	362	TRP	Peptide
1	J	375	LEU	Peptide
1	K	187	GLN	Peptide
1	K	220	VAL	Peptide
1	K	221	ALA	Peptide
1	K	260	GLU	Peptide
1	K	266	SER	Peptide
1	K	268	LEU	Peptide
1	K	272	ARG	Peptide
1	K	336	ARG	Peptide
1	K	357	LEU	Peptide
1	K	358	GLU	Peptide
1	K	363	GLN	Peptide
1	K	366	ALA	Peptide
1	K	389	VAL	Peptide
1	K	399	SER	Peptide
1	L	178	PHE	Peptide
1	L	187	GLN	Peptide
1	L	218	THR	Peptide
1	L	219	TRP	Peptide
1	L	254	PHE	Peptide
1	L	308	ALA	Peptide
1	L	315	LYS	Peptide
1	L	325	LYS	Peptide
1	L	356	LEU	Peptide
1	L	361	GLU	Peptide
1	L	362	TRP	Peptide
1	L	363	GLN	Peptide
1	L	366	ALA	Peptide
1	L	400	ALA	Peptide
1	L	409	ASP	Peptide
1	M	187	GLN	Peptide
1	M	216	LYS	Peptide
1	M	356	LEU	Peptide
1	M	373	VAL	Peptide
1	M	410	ASN	Peptide
1	M	418	ALA	Peptide
1	M	421	VAL	Peptide
1	M	436	VAL	Peptide
1	M	454	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2247	0	2275	187	0
1	B	2247	0	2275	177	0
1	C	2247	0	2275	164	0
1	D	2247	0	2275	182	0
1	E	2247	0	2275	163	0
1	F	2247	0	2275	171	0
1	G	2247	0	2274	186	0
1	H	2247	0	2275	214	0
1	I	2247	0	2275	179	0
1	J	2247	0	2274	172	0
1	K	2247	0	2275	187	0
1	L	2247	0	2275	148	0
1	M	2247	0	2275	119	0
All	All	29211	0	29573	2181	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 37.

All (2181) 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:A:352:ALA:O	1:A:356:LEU:HB2	1.54	1.07
1:K:327:ILE:O	1:K:331:ARG:HB2	1.60	1.01
1:L:351:ASP:O	1:L:355:ASP:HB2	1.64	0.95
1:B:350:MET:O	1:B:354:TYR:HB2	1.73	0.89
1:E:377:GLY:H	1:E:378:GLN:HG2	1.42	0.82
1:E:275:LEU:O	1:E:279:HIS:HB3	1.81	0.81
1:F:351:ASP:O	1:F:355:ASP:HB2	1.80	0.80
1:K:275:LEU:O	1:K:279:HIS:HB3	1.81	0.80
1:L:416:GLN:H	1:L:440:VAL:HA	1.44	0.80
1:D:411:PHE:H	1:D:444:ARG:HA	1.46	0.79
1:K:405:ILE:HG13	1:K:410:ASN:HD22	1.47	0.77
1:M:308:ALA:HB1	1:M:452:SER:H	1.49	0.76
1:F:405:ILE:HG12	1:F:410:ASN:HD22	1.49	0.76
1:B:176:THR:HG1	1:B:272:ARG:HH21	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:391:GLU:HG2	1:H:393:PHE:H	1.50	0.76
1:F:416:GLN:H	1:F:440:VAL:HA	1.50	0.76
1:H:369:GLY:HA2	1:H:380:GLY:H	1.51	0.76
1:E:246:THR:OG1	1:E:247:TYR:N	2.18	0.75
1:H:341:LEU:H	1:H:344:LEU:HD22	1.51	0.75
1:B:176:THR:OG1	1:B:272:ARG:NH2	2.18	0.75
1:G:344:LEU:HA	1:G:406:VAL:HA	1.67	0.74
1:E:357:LEU:HA	1:E:367:GLN:HE22	1.50	0.74
1:B:283:ILE:O	1:B:287:PHE:HB2	1.88	0.74
1:A:176:THR:O	1:A:423:ARG:NH1	2.21	0.74
1:M:346:LEU:HB2	1:M:385:LEU:HB3	1.69	0.74
1:C:364:ASP:HB2	1:C:383:TYR:HA	1.69	0.74
1:C:267:LEU:H	1:C:269:PRO:HD2	1.53	0.74
1:F:274:ARG:O	1:F:278:ALA:HB2	1.88	0.73
1:D:176:THR:HG1	1:D:180:GLN:HE22	1.33	0.73
1:G:362:TRP:HD1	1:G:367:GLN:H	1.34	0.73
1:B:176:THR:O	1:B:180:GLN:NE2	2.21	0.73
1:F:199:LEU:HB3	1:F:414:PRO:HA	1.70	0.73
1:J:184:ARG:O	1:J:188:LYS:HB2	1.88	0.72
1:B:290:GLY:H	1:B:298:GLY:HA3	1.54	0.72
1:B:174:TYR:HA	1:B:177:ILE:HD11	1.69	0.72
1:B:246:THR:OG1	1:B:247:TYR:N	2.21	0.72
1:B:421:VAL:HG13	1:B:436:VAL:HG22	1.72	0.72
1:F:327:ILE:O	1:F:331:ARG:HB2	1.90	0.71
1:G:308:ALA:HB1	1:G:451:VAL:HA	1.72	0.71
1:H:281:VAL:O	1:H:285:GLU:HB2	1.90	0.71
1:B:308:ALA:HB1	1:B:451:VAL:HA	1.72	0.71
1:C:314:ALA:HB1	1:C:320:VAL:HB	1.72	0.71
1:G:310:VAL:HG21	1:G:330:LEU:HD11	1.72	0.71
1:K:177:ILE:HG12	1:K:423:ARG:HD2	1.72	0.71
1:F:180:GLN:HE21	1:F:421:VAL:HG11	1.55	0.71
1:G:252:LYS:NZ	1:G:434:TYR:O	2.23	0.71
1:H:268:LEU:HA	1:H:271:LEU:HB2	1.72	0.71
1:E:402:PHE:HB2	1:E:453:GLY:H	1.56	0.71
1:H:249:LEU:HB2	1:H:438:GLN:HB3	1.73	0.70
1:K:309:LYS:HB3	1:K:454:THR:HG23	1.72	0.70
1:J:246:THR:OG1	1:J:247:TYR:N	2.23	0.70
1:C:248:LYS:NZ	1:D:220:VAL:O	2.23	0.70
1:M:267:LEU:O	1:M:271:LEU:HB2	1.91	0.70
1:E:249:LEU:HB2	1:E:438:GLN:HB3	1.71	0.70
1:J:257:ASP:OD2	1:J:257:ASP:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:HIS:O	1:B:443:GLN:NE2	2.24	0.70
1:D:417:ARG:HH11	1:D:419:VAL:HA	1.56	0.70
1:F:429:LYS:HB2	1:F:431:ARG:HD3	1.72	0.70
1:G:357:LEU:HA	1:G:367:GLN:HE22	1.57	0.70
1:L:249:LEU:HB2	1:L:438:GLN:HB3	1.72	0.70
1:B:267:LEU:HG	1:B:270:LEU:HD11	1.73	0.70
1:D:332:ARG:HH22	1:D:340:LYS:HD2	1.57	0.70
1:G:272:ARG:HH12	1:G:275:LEU:H	1.40	0.70
1:J:351:ASP:HA	1:J:354:TYR:HB3	1.73	0.70
1:I:269:PRO:HA	1:I:272:ARG:HB2	1.72	0.69
1:H:308:ALA:HB1	1:H:451:VAL:HA	1.73	0.69
1:H:366:ALA:HA	1:H:382:ILE:HA	1.73	0.69
1:G:220:VAL:HG11	1:G:226:GLY:HA3	1.73	0.69
1:E:184:ARG:NH1	1:E:185:ASP:OD1	2.25	0.69
1:G:297:LYS:HB3	1:G:302:LEU:HD11	1.73	0.69
1:I:354:TYR:HA	1:I:357:LEU:HB3	1.74	0.69
1:E:410:ASN:ND2	1:E:449:GLY:O	2.25	0.69
1:K:410:ASN:ND2	1:K:449:GLY:O	2.25	0.69
1:I:207:THR:HA	1:I:243:HIS:HA	1.74	0.69
1:M:176:THR:OG1	1:M:180:GLN:NE2	2.26	0.69
1:M:246:THR:HA	1:M:441:ASN:HB2	1.74	0.69
1:D:199:LEU:HB3	1:D:414:PRO:HA	1.74	0.69
1:A:391:GLU:HA	1:A:393:PHE:HB2	1.75	0.69
1:A:411:PHE:H	1:A:444:ARG:HA	1.56	0.68
1:K:362:TRP:HD1	1:K:365:VAL:HA	1.58	0.68
1:C:422:GLU:HB2	1:C:435:TYR:HB2	1.76	0.68
1:M:201:MET:HB2	1:M:416:GLN:HA	1.74	0.68
1:B:342:SER:H	1:B:344:LEU:HD13	1.59	0.68
1:G:181:ARG:NH1	1:G:185:ASP:OD2	2.25	0.68
1:K:267:LEU:O	1:K:271:LEU:N	2.25	0.68
1:F:268:LEU:HA	1:F:271:LEU:HB3	1.74	0.68
1:F:314:ALA:H	1:F:455:TYR:H	1.40	0.68
1:I:362:TRP:HA	1:I:366:ALA:HB3	1.74	0.68
1:M:184:ARG:NH1	1:M:417:ARG:O	2.27	0.68
1:C:271:LEU:HA	1:C:274:ARG:HH12	1.58	0.68
1:F:410:ASN:ND2	1:F:449:GLY:O	2.27	0.68
1:G:405:ILE:HB	1:G:450:VAL:HB	1.76	0.68
1:J:347:ILE:HB	1:J:403:ALA:HB3	1.76	0.68
1:L:176:THR:H	1:L:423:ARG:HH22	1.42	0.68
1:F:257:ASP:OD1	1:F:257:ASP:N	2.27	0.68
1:I:206:LEU:HB3	1:I:244:PHE:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:TYR:HA	1:H:177:ILE:HD11	1.76	0.67
1:L:308:ALA:HB1	1:L:451:VAL:HA	1.75	0.67
1:L:347:ILE:H	1:L:403:ALA:HB3	1.59	0.67
1:L:246:THR:HA	1:L:441:ASN:HB2	1.75	0.67
1:L:340:LYS:HB3	1:L:341:LEU:HD22	1.77	0.67
1:B:402:PHE:HB2	1:B:452:SER:HA	1.77	0.67
1:L:171:SER:OG	1:L:172:GLU:N	2.26	0.67
1:B:331:ARG:HD2	1:B:341:LEU:HD11	1.75	0.67
1:F:332:ARG:HH22	1:F:340:LYS:HA	1.60	0.67
1:G:444:ARG:NH2	1:G:446:PHE:O	2.27	0.67
1:A:332:ARG:HH12	1:A:336:ARG:HE	1.42	0.67
1:A:406:VAL:O	1:A:410:ASN:ND2	2.27	0.67
1:D:208:MET:HG2	1:D:242:ILE:HB	1.76	0.67
1:B:289:THR:HG21	1:B:392:TYR:HB2	1.77	0.67
1:G:341:LEU:H	1:G:344:LEU:HD22	1.59	0.67
1:I:291:ASP:H	1:I:295:LYS:HE2	1.58	0.67
1:M:410:ASN:OD1	1:M:410:ASN:N	2.28	0.67
1:H:246:THR:OG1	1:H:247:TYR:N	2.25	0.67
1:K:176:THR:O	1:K:180:GLN:NE2	2.23	0.67
1:D:220:VAL:HG13	1:D:222:ALA:H	1.59	0.66
1:H:176:THR:OG1	1:H:180:GLN:NE2	2.29	0.66
1:A:343:LYS:NZ	1:A:344:LEU:O	2.28	0.66
1:H:353:TYR:O	1:H:357:LEU:N	2.25	0.66
1:M:348:VAL:HG21	1:M:353:TYR:HB2	1.75	0.66
1:I:243:HIS:O	1:I:443:GLN:NE2	2.28	0.66
1:E:262:ASP:OD1	1:E:262:ASP:N	2.28	0.66
1:J:280:ALA:HA	1:J:283:ILE:HD12	1.76	0.66
1:L:250:ALA:HA	1:L:437:THR:HA	1.78	0.66
1:A:314:ALA:HA	1:A:321:LEU:HB2	1.77	0.66
1:B:187:GLN:NE2	1:B:189:GLU:O	2.29	0.66
1:D:246:THR:OG1	1:D:247:TYR:N	2.27	0.66
1:E:348:VAL:N	1:E:388:VAL:O	2.25	0.66
1:I:366:ALA:HA	1:I:382:ILE:HA	1.78	0.66
1:M:172:GLU:HB3	1:M:423:ARG:HG2	1.78	0.66
1:F:270:LEU:O	1:F:274:ARG:NH2	2.29	0.66
1:I:248:LYS:NZ	1:J:220:VAL:O	2.29	0.66
1:I:255:ILE:H	1:I:432:ASP:HB2	1.61	0.66
1:K:176:THR:OG1	1:K:180:GLN:NE2	2.29	0.66
1:I:353:TYR:O	1:I:357:LEU:N	2.22	0.66
1:A:295:LYS:O	1:A:295:LYS:NZ	2.29	0.66
1:H:172:GLU:OE1	1:H:423:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:334:LEU:O	1:I:338:GLY:N	2.27	0.66
1:K:246:THR:OG1	1:K:247:TYR:N	2.27	0.66
1:L:175:GLU:OE2	1:L:423:ARG:NH1	2.29	0.66
1:L:178:PHE:O	1:L:182:ILE:HB	1.96	0.66
1:C:313:GLU:O	1:C:315:LYS:NZ	2.27	0.66
1:C:376:GLN:HE22	1:C:386:PRO:HB2	1.61	0.66
1:E:185:ASP:OD1	1:E:188:LYS:NZ	2.28	0.66
1:F:173:SER:OG	1:F:174:TYR:N	2.28	0.66
1:J:272:ARG:HG3	1:J:273:LYS:HD3	1.78	0.65
1:J:344:LEU:HA	1:J:407:TYR:H	1.61	0.65
1:L:210:VAL:HG22	1:L:242:ILE:HG13	1.76	0.65
1:G:415:ARG:NH1	1:G:417:ARG:O	2.30	0.65
1:M:203:SER:OG	1:M:204:LYS:N	2.30	0.65
1:B:179:SER:OG	1:B:180:GLN:NE2	2.29	0.65
1:E:171:SER:OG	1:E:172:GLU:N	2.27	0.65
1:F:334:LEU:HD22	1:F:338:GLY:H	1.61	0.65
1:L:350:MET:HA	1:L:353:TYR:HB3	1.78	0.65
1:B:431:ARG:NH2	1:B:431:ARG:O	2.30	0.65
1:E:351:ASP:OD1	1:E:351:ASP:N	2.28	0.65
1:F:225:TYR:HB3	1:F:227:THR:H	1.61	0.65
1:G:267:LEU:O	1:G:271:LEU:N	2.27	0.65
1:H:274:ARG:HA	1:H:277:GLU:HB3	1.78	0.65
1:H:342:SER:H	1:H:344:LEU:HD13	1.62	0.65
1:J:323:THR:HA	1:J:356:LEU:HD11	1.76	0.65
1:B:353:TYR:O	1:B:357:LEU:N	2.24	0.65
1:D:346:LEU:HD13	1:D:404:VAL:HG23	1.77	0.65
1:I:184:ARG:NH1	1:I:185:ASP:OD1	2.29	0.65
1:J:303:ALA:HA	1:J:306:ASP:HB2	1.78	0.65
1:M:341:LEU:H	1:M:344:LEU:HD22	1.61	0.65
1:D:312:THR:OG1	1:D:315:LYS:NZ	2.29	0.65
1:I:176:THR:OG1	1:I:423:ARG:NH2	2.28	0.65
1:J:272:ARG:HA	1:J:275:LEU:HD21	1.79	0.65
1:E:327:ILE:O	1:E:331:ARG:HB3	1.97	0.65
1:C:381:ARG:HH21	1:C:384:GLY:HA2	1.62	0.65
1:C:411:PHE:HB3	1:C:442:LEU:HD11	1.77	0.65
1:K:428:GLY:O	1:K:431:ARG:NH2	2.30	0.65
1:C:370:ASN:HD22	1:C:371:ASP:HA	1.61	0.65
1:F:338:GLY:HA3	1:F:406:VAL:HG11	1.79	0.64
1:K:185:ASP:N	1:K:185:ASP:OD1	2.26	0.64
1:K:187:GLN:NE2	1:K:189:GLU:O	2.30	0.64
1:A:382:ILE:O	1:A:385:LEU:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:HD12	1:B:403:ALA:H	1.62	0.64
1:I:275:LEU:HD12	1:I:276:ILE:HG13	1.78	0.64
1:J:209:LEU:HA	1:J:241:GLU:HB2	1.80	0.64
1:B:367:GLN:NE2	1:B:371:ASP:OD2	2.31	0.64
1:K:323:THR:OG1	1:K:324:ALA:N	2.27	0.64
1:A:181:ARG:NH1	1:A:185:ASP:OD2	2.29	0.64
1:B:246:THR:HB	1:B:441:ASN:HB2	1.79	0.64
1:E:186:LEU:HG	1:E:187:GLN:HE21	1.61	0.64
1:L:276:ILE:HA	1:L:279:HIS:HB3	1.80	0.64
1:A:315:LYS:H	1:A:320:VAL:HG12	1.62	0.64
1:B:212:PRO:O	1:B:238:ALA:N	2.28	0.64
1:G:269:PRO:HA	1:G:272:ARG:HB2	1.80	0.64
1:K:347:ILE:HG23	1:K:388:VAL:HB	1.78	0.64
1:H:425:ARG:NH2	1:H:432:ASP:OD1	2.31	0.64
1:K:272:ARG:HH12	1:K:276:ILE:H	1.46	0.64
1:D:253:SER:OG	1:D:254:PHE:N	2.27	0.64
1:J:201:MET:HB2	1:J:416:GLN:HA	1.78	0.64
1:J:250:ALA:HA	1:J:437:THR:HA	1.79	0.64
1:K:198:GLU:HB3	1:K:415:ARG:HG2	1.80	0.64
1:M:179:SER:OG	1:M:180:GLN:NE2	2.31	0.64
1:C:330:LEU:HA	1:C:333:LYS:HB3	1.79	0.63
1:J:424:GLU:HA	1:J:425:ARG:HH11	1.63	0.63
1:K:275:LEU:O	1:K:279:HIS:CB	2.46	0.63
1:A:180:GLN:HG3	1:A:272:ARG:HH11	1.62	0.63
1:B:341:LEU:H	1:B:344:LEU:HD22	1.63	0.63
1:K:417:ARG:HB3	1:K:439:ARG:H	1.63	0.63
1:A:417:ARG:HH22	1:A:439:ARG:HG3	1.62	0.63
1:D:275:LEU:O	1:D:279:HIS:HB2	1.99	0.63
1:D:412:VAL:N	1:D:443:GLN:O	2.32	0.63
1:H:274:ARG:NH2	1:I:445:TYR:OH	2.31	0.63
1:H:370:ASN:OD1	1:H:370:ASN:N	2.30	0.63
1:J:208:MET:HB2	1:J:210:VAL:HG13	1.80	0.63
1:A:432:ASP:N	1:A:432:ASP:OD1	2.32	0.63
1:C:413:MET:HG3	1:C:441:ASN:H	1.64	0.63
1:D:265:PHE:HB3	1:D:268:LEU:HD11	1.78	0.63
1:F:322:VAL:HB	1:F:356:LEU:HG	1.81	0.63
1:G:368:VAL:HG13	1:G:370:ASN:H	1.62	0.63
1:H:359:ASP:HB2	1:H:361:GLU:H	1.64	0.63
1:J:206:LEU:HB3	1:J:244:PHE:HB2	1.80	0.63
1:C:421:VAL:HG13	1:C:436:VAL:HG22	1.80	0.63
1:D:249:LEU:N	1:D:438:GLN:O	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ARG:HA	1:F:277:GLU:HB2	1.79	0.63
1:H:200:PRO:HA	1:H:415:ARG:HG3	1.80	0.63
1:J:276:ILE:HA	1:J:279:HIS:HB3	1.80	0.63
1:L:332:ARG:O	1:L:336:ARG:N	2.31	0.63
1:B:349:SER:H	1:B:352:ALA:HB3	1.60	0.63
1:H:415:ARG:HA	1:H:440:VAL:HA	1.81	0.63
1:I:249:LEU:N	1:I:438:GLN:O	2.32	0.63
1:A:288:MET:HB3	1:A:289:THR:HG23	1.80	0.62
1:C:372:SER:OG	1:C:381:ARG:NH1	2.32	0.62
1:D:356:LEU:HD21	1:D:363:GLN:HE21	1.64	0.62
1:E:339:LEU:HD12	1:E:342:SER:HB3	1.81	0.62
1:G:202:SER:O	1:G:416:GLN:NE2	2.32	0.62
1:I:198:GLU:HA	1:I:413:MET:HB3	1.81	0.62
1:J:422:GLU:N	1:J:435:TYR:O	2.30	0.62
1:M:411:PHE:H	1:M:444:ARG:HA	1.64	0.62
1:F:251:ALA:N	1:F:436:VAL:O	2.30	0.62
1:G:348:VAL:N	1:G:388:VAL:O	2.31	0.62
1:J:428:GLY:O	1:J:431:ARG:NH2	2.33	0.62
1:L:420:THR:O	1:L:437:THR:OG1	2.17	0.62
1:C:176:THR:OG1	1:C:423:ARG:NH2	2.32	0.62
1:F:184:ARG:NH1	1:F:185:ASP:OD1	2.32	0.62
1:G:204:LYS:HA	1:G:439:ARG:HH12	1.64	0.62
1:G:293:SER:O	1:G:295:LYS:NZ	2.32	0.62
1:H:331:ARG:HH21	1:H:332:ARG:HH22	1.46	0.62
1:H:349:SER:H	1:H:352:ALA:HB3	1.65	0.62
1:I:240:LYS:NZ	1:I:241:GLU:O	2.30	0.62
1:D:325:LYS:H	1:D:325:LYS:HZ3	1.47	0.62
1:G:275:LEU:O	1:G:279:HIS:HB3	2.00	0.62
1:I:421:VAL:HG13	1:I:436:VAL:HG22	1.80	0.62
1:B:272:ARG:O	1:B:273:LYS:NZ	2.29	0.62
1:C:176:THR:OG1	1:C:180:GLN:NE2	2.29	0.62
1:C:272:ARG:O	1:C:274:ARG:NH2	2.32	0.62
1:D:246:THR:HA	1:D:441:ASN:HD22	1.64	0.62
1:D:267:LEU:HD12	1:D:271:LEU:HB2	1.82	0.62
1:E:353:TYR:O	1:E:357:LEU:N	2.19	0.62
1:H:347:ILE:H	1:H:403:ALA:HB3	1.63	0.62
1:A:334:LEU:HD13	1:A:337:HIS:HB2	1.81	0.62
1:B:173:SER:O	1:B:423:ARG:NH2	2.33	0.62
1:C:352:ALA:HB2	1:C:401:GLU:HB2	1.80	0.62
1:C:359:ASP:O	1:C:367:GLN:NE2	2.33	0.62
1:K:421:VAL:HG22	1:K:436:VAL:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ALA:HA	1:C:382:ILE:HA	1.82	0.62
1:F:256:THR:O	1:F:259:THR:OG1	2.18	0.62
1:F:303:ALA:O	1:F:309:LYS:NZ	2.32	0.62
1:G:333:LYS:O	1:G:336:ARG:NH2	2.32	0.62
1:D:205:ILE:HG12	1:D:245:SER:HB3	1.81	0.62
1:F:351:ASP:OD1	1:F:351:ASP:N	2.23	0.62
1:H:267:LEU:HD21	1:I:206:LEU:HD21	1.82	0.62
1:A:431:ARG:O	1:A:431:ARG:NH2	2.33	0.62
1:D:443:GLN:HE21	1:D:444:ARG:H	1.46	0.62
1:F:203:SER:OG	1:F:204:LYS:N	2.33	0.62
1:F:245:SER:O	1:F:441:ASN:ND2	2.33	0.62
1:I:315:LYS:HB2	1:I:320:VAL:HA	1.81	0.62
1:M:246:THR:OG1	1:M:247:TYR:N	2.30	0.62
1:G:381:ARG:HA	1:G:386:PRO:HA	1.82	0.62
1:M:342:SER:H	1:M:344:LEU:HD13	1.65	0.62
1:A:206:LEU:HB3	1:A:244:PHE:HB2	1.81	0.61
1:F:181:ARG:O	1:F:184:ARG:NH1	2.33	0.61
1:D:335:GLY:O	1:D:340:LYS:NZ	2.32	0.61
1:D:376:GLN:HE21	1:D:378:GLN:HE22	1.46	0.61
1:I:248:LYS:HZ1	1:J:220:VAL:HG12	1.65	0.61
1:J:269:PRO:O	1:J:273:LYS:NZ	2.29	0.61
1:L:252:LYS:HG3	1:L:435:TYR:HB3	1.80	0.61
1:A:376:GLN:NE2	1:A:377:GLY:O	2.33	0.61
1:F:350:MET:HA	1:F:353:TYR:HB3	1.80	0.61
1:G:322:VAL:HG11	1:G:355:ASP:HB3	1.81	0.61
1:I:181:ARG:HH22	1:I:418:ALA:HB1	1.65	0.61
1:L:363:GLN:HE22	1:L:382:ILE:HG23	1.65	0.61
1:L:406:VAL:HG22	1:L:409:ASP:H	1.64	0.61
1:M:315:LYS:H	1:M:320:VAL:HG12	1.66	0.61
1:B:422:GLU:N	1:B:435:TYR:O	2.28	0.61
1:E:422:GLU:O	1:E:435:TYR:N	2.32	0.61
1:J:370:ASN:OD1	1:J:370:ASN:N	2.25	0.61
1:K:203:SER:O	1:K:416:GLN:NE2	2.33	0.61
1:M:343:LYS:H	1:M:406:VAL:HA	1.66	0.61
1:M:351:ASP:OD1	1:M:351:ASP:N	2.32	0.61
1:C:211:GLU:HA	1:C:238:ALA:H	1.66	0.61
1:C:414:PRO:HD2	1:C:441:ASN:HB3	1.82	0.61
1:D:272:ARG:O	1:D:273:LYS:NZ	2.31	0.61
1:E:296:PRO:HG3	1:E:442:LEU:H	1.65	0.61
1:E:409:ASP:OD1	1:E:409:ASP:N	2.33	0.61
1:F:175:GLU:OE2	1:F:423:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:184:ARG:NH1	1:H:187:GLN:O	2.32	0.61
1:I:422:GLU:N	1:I:435:TYR:O	2.31	0.61
1:A:308:ALA:HB1	1:A:451:VAL:HA	1.83	0.61
1:B:328:SER:HA	1:B:331:ARG:HB3	1.83	0.61
1:D:324:ALA:O	1:D:328:SER:N	2.32	0.61
1:G:331:ARG:HG2	1:G:332:ARG:HH11	1.64	0.61
1:I:250:ALA:HA	1:I:437:THR:HA	1.82	0.61
1:J:173:SER:O	1:J:423:ARG:NH2	2.33	0.61
1:D:173:SER:O	1:D:423:ARG:NH2	2.29	0.61
1:E:310:VAL:N	1:E:454:THR:OG1	2.33	0.61
1:H:415:ARG:HB2	1:H:440:VAL:HG12	1.83	0.61
1:I:187:GLN:NE2	1:I:189:GLU:O	2.33	0.61
1:J:184:ARG:HH12	1:J:188:LYS:HZ3	1.49	0.61
1:M:353:TYR:O	1:M:357:LEU:N	2.33	0.61
1:A:258:GLU:OE2	1:A:426:GLN:NE2	2.31	0.61
1:A:298:GLY:O	1:A:301:THR:OG1	2.18	0.61
1:K:243:HIS:O	1:K:443:GLN:NE2	2.34	0.61
1:K:361:GLU:O	1:K:367:GLN:NE2	2.29	0.61
1:E:312:THR:O	1:E:315:LYS:NZ	2.34	0.61
1:E:398:ASN:HA	1:E:456:ALA:HA	1.83	0.61
1:H:378:GLN:H	1:H:386:PRO:HB3	1.66	0.61
1:C:258:GLU:OE2	1:C:430:GLN:NE2	2.34	0.60
1:D:176:THR:OG1	1:D:180:GLN:NE2	2.32	0.60
1:G:245:SER:OG	1:G:246:THR:N	2.29	0.60
1:I:211:GLU:HG3	1:I:238:ALA:H	1.66	0.60
1:K:259:THR:HB	1:M:204:LYS:HD3	1.83	0.60
1:L:206:LEU:HB3	1:L:244:PHE:HB2	1.82	0.60
1:B:203:SER:OG	1:B:204:LYS:N	2.35	0.60
1:B:383:TYR:HB2	1:B:385:LEU:HG	1.83	0.60
1:D:314:ALA:HB2	1:D:322:VAL:HG13	1.83	0.60
1:E:291:ASP:OD1	1:E:295:LYS:NZ	2.32	0.60
1:H:208:MET:HG3	1:H:210:VAL:HG13	1.83	0.60
1:H:420:THR:O	1:H:437:THR:OG1	2.19	0.60
1:K:409:ASP:N	1:K:409:ASP:OD1	2.33	0.60
1:B:334:LEU:O	1:B:337:HIS:ND1	2.34	0.60
1:B:365:VAL:HG13	1:B:382:ILE:HA	1.84	0.60
1:C:375:LEU:HD22	1:C:386:PRO:HG3	1.83	0.60
1:H:423:ARG:HB3	1:H:425:ARG:HD3	1.83	0.60
1:M:349:SER:OG	1:M:391:GLU:OE2	2.20	0.60
1:A:273:LYS:O	1:A:277:GLU:N	2.34	0.60
1:B:424:GLU:N	1:B:433:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:405:ILE:HB	1:K:450:VAL:HB	1.83	0.60
1:A:203:SER:OG	1:A:204:LYS:N	2.34	0.60
1:D:344:LEU:HA	1:D:406:VAL:HA	1.82	0.60
1:H:179:SER:OG	1:H:180:GLN:NE2	2.34	0.60
1:L:252:LYS:HA	1:L:435:TYR:HA	1.82	0.60
1:C:370:ASN:ND2	1:C:371:ASP:OD1	2.34	0.60
1:E:343:LYS:H	1:E:406:VAL:HG23	1.65	0.60
1:J:353:TYR:O	1:J:357:LEU:N	2.33	0.60
1:K:173:SER:OG	1:K:175:GLU:OE1	2.18	0.60
1:A:421:VAL:HG22	1:A:436:VAL:HA	1.82	0.60
1:B:195:LEU:N	1:B:407:TYR:OH	2.34	0.60
1:C:269:PRO:O	1:C:273:LYS:NZ	2.31	0.60
1:C:377:GLY:O	1:C:378:GLN:NE2	2.34	0.60
1:D:347:ILE:HB	1:D:403:ALA:HB3	1.83	0.60
1:F:243:HIS:O	1:F:443:GLN:NE2	2.35	0.60
1:F:332:ARG:NH2	1:F:339:LEU:O	2.35	0.60
1:H:201:MET:HE1	1:H:245:SER:HA	1.82	0.60
1:H:362:TRP:HA	1:H:366:ALA:HB3	1.84	0.60
1:C:272:ARG:HB3	1:C:273:LYS:HD3	1.84	0.60
1:B:339:LEU:H	1:B:344:LEU:HD11	1.67	0.60
1:C:218:THR:OG1	1:C:219:TRP:N	2.33	0.60
1:D:280:ALA:HA	1:D:283:ILE:HD12	1.83	0.60
1:D:416:GLN:OE1	1:D:439:ARG:NH2	2.34	0.60
1:H:181:ARG:HD2	1:H:182:ILE:HG12	1.84	0.60
1:H:335:GLY:O	1:H:340:LYS:NZ	2.35	0.60
1:L:267:LEU:HA	1:L:270:LEU:HB3	1.83	0.60
1:M:272:ARG:HB3	1:M:276:ILE:HD11	1.83	0.60
1:M:346:LEU:HD12	1:M:403:ALA:H	1.67	0.60
1:A:332:ARG:O	1:A:336:ARG:NH2	2.35	0.59
1:B:310:VAL:O	1:B:454:THR:N	2.28	0.59
1:D:269:PRO:HB2	1:D:273:LYS:HD3	1.84	0.59
1:E:382:ILE:HB	1:E:385:LEU:HB2	1.83	0.59
1:H:199:LEU:N	1:H:413:MET:O	2.30	0.59
1:J:253:SER:OG	1:J:254:PHE:N	2.33	0.59
1:A:324:ALA:O	1:A:328:SER:N	2.35	0.59
1:B:199:LEU:N	1:B:413:MET:O	2.31	0.59
1:D:250:ALA:O	1:E:220:VAL:N	2.34	0.59
1:E:291:ASP:H	1:E:295:LYS:HE2	1.65	0.59
1:F:423:ARG:HA	1:F:434:TYR:HA	1.84	0.59
1:G:314:ALA:O	1:G:455:TYR:N	2.35	0.59
1:H:288:MET:SD	1:H:392:TYR:N	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:414:PRO:O	1:K:441:ASN:N	2.31	0.59
1:L:288:MET:O	1:L:300:LEU:N	2.29	0.59
1:M:325:LYS:NZ	1:M:383:TYR:OH	2.35	0.59
1:B:408:LYS:O	1:B:408:LYS:NZ	2.33	0.59
1:E:316:ALA:HA	1:E:457:ALA:HA	1.84	0.59
1:H:248:LYS:NZ	1:I:221:ALA:O	2.31	0.59
1:I:335:GLY:O	1:I:340:LYS:NZ	2.32	0.59
1:M:271:LEU:O	1:M:274:ARG:NH1	2.36	0.59
1:E:199:LEU:HB3	1:E:414:PRO:HA	1.84	0.59
1:H:171:SER:O	1:H:425:ARG:NH1	2.35	0.59
1:I:274:ARG:NH1	1:J:445:TYR:OH	2.36	0.59
1:L:191:VAL:HB	1:L:378:GLN:HG2	1.82	0.59
1:C:172:GLU:OE2	1:C:423:ARG:NH2	2.36	0.59
1:I:177:ILE:HD11	1:I:423:ARG:HD2	1.84	0.59
1:I:184:ARG:HH12	1:I:188:LYS:HZ3	1.49	0.59
1:L:177:ILE:HA	1:L:180:GLN:HG2	1.83	0.59
1:L:333:LYS:O	1:L:337:HIS:ND1	2.34	0.59
1:C:249:LEU:HB2	1:C:438:GLN:HB3	1.85	0.59
1:G:274:ARG:NH1	1:H:445:TYR:OH	2.36	0.59
1:H:301:THR:OG1	1:H:302:LEU:N	2.34	0.59
1:H:349:SER:O	1:H:353:TYR:N	2.31	0.59
1:J:267:LEU:O	1:J:271:LEU:N	2.25	0.59
1:K:213:ASP:N	1:K:213:ASP:OD1	2.36	0.59
1:A:249:LEU:HD21	1:A:296:PRO:HD3	1.85	0.59
1:A:420:THR:O	1:A:420:THR:OG1	2.20	0.59
1:C:341:LEU:H	1:C:344:LEU:HD22	1.68	0.59
1:E:339:LEU:O	1:E:340:LYS:NZ	2.35	0.59
1:F:187:GLN:HA	1:F:189:GLU:HB2	1.84	0.59
1:G:362:TRP:HB2	1:G:367:GLN:HG2	1.85	0.59
1:I:299:LEU:HA	1:I:302:LEU:HB2	1.84	0.59
1:K:180:GLN:HG2	1:K:423:ARG:HH12	1.67	0.59
1:H:176:THR:O	1:H:180:GLN:NE2	2.28	0.59
1:J:246:THR:HB	1:J:441:ASN:HB2	1.84	0.59
1:K:223:SER:OG	1:K:224:THR:N	2.33	0.59
1:G:216:LYS:NZ	1:G:237:GLY:O	2.33	0.59
1:K:444:ARG:NH1	1:K:447:ALA:O	2.29	0.59
1:B:267:LEU:HA	1:B:270:LEU:HD21	1.85	0.58
1:B:273:LYS:O	1:B:277:GLU:N	2.34	0.58
1:E:344:LEU:H	1:E:406:VAL:HA	1.68	0.58
1:H:365:VAL:HG13	1:H:383:TYR:HD1	1.66	0.58
1:K:271:LEU:O	1:K:274:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:343:LYS:H	1:K:408:LYS:HZ2	1.50	0.58
1:L:243:HIS:O	1:L:443:GLN:NE2	2.36	0.58
1:F:333:LYS:O	1:F:337:HIS:ND1	2.36	0.58
1:H:270:LEU:O	1:H:274:ARG:NH2	2.36	0.58
1:J:207:THR:HA	1:J:243:HIS:HA	1.84	0.58
1:M:421:VAL:HG13	1:M:435:TYR:H	1.67	0.58
1:D:176:THR:O	1:D:179:SER:OG	2.20	0.58
1:E:240:LYS:NZ	1:E:241:GLU:O	2.32	0.58
1:E:441:ASN:HD21	1:E:443:GLN:HB2	1.68	0.58
1:I:370:ASN:OD1	1:I:370:ASN:N	2.36	0.58
1:I:415:ARG:NH2	1:I:416:GLN:O	2.36	0.58
1:J:335:GLY:O	1:J:340:LYS:NZ	2.27	0.58
1:L:349:SER:O	1:L:353:TYR:N	2.36	0.58
1:A:368:VAL:HG23	1:A:380:GLY:H	1.68	0.58
1:C:348:VAL:N	1:C:388:VAL:O	2.34	0.58
1:D:258:GLU:OE2	1:D:426:GLN:NE2	2.36	0.58
1:G:353:TYR:O	1:G:357:LEU:N	2.25	0.58
1:J:293:SER:O	1:J:295:LYS:NZ	2.37	0.58
1:J:420:THR:N	1:J:437:THR:O	2.33	0.58
1:K:249:LEU:HD13	1:K:283:ILE:HD11	1.84	0.58
1:K:258:GLU:HG3	1:K:259:THR:HG23	1.84	0.58
1:L:413:MET:HA	1:L:442:LEU:HA	1.84	0.58
1:A:349:SER:O	1:A:353:TYR:N	2.34	0.58
1:A:444:ARG:HH21	1:A:445:TYR:H	1.51	0.58
1:D:293:SER:O	1:D:295:LYS:NZ	2.37	0.58
1:J:414:PRO:O	1:J:441:ASN:N	2.35	0.58
1:M:176:THR:O	1:M:179:SER:OG	2.20	0.58
1:C:170:SER:N	1:C:175:GLU:OE1	2.36	0.58
1:D:278:ALA:O	1:D:282:SER:OG	2.21	0.58
1:F:344:LEU:HA	1:F:406:VAL:HA	1.85	0.58
1:F:369:GLY:N	1:F:371:ASP:OD2	2.32	0.58
1:F:382:ILE:O	1:F:385:LEU:N	2.37	0.58
1:G:272:ARG:HH11	1:G:276:ILE:HG12	1.69	0.58
1:I:272:ARG:HH22	1:I:421:VAL:HG11	1.68	0.58
1:L:181:ARG:NH2	1:L:185:ASP:OD2	2.36	0.58
1:M:207:THR:HA	1:M:243:HIS:HA	1.84	0.58
1:C:207:THR:HA	1:C:243:HIS:HA	1.85	0.58
1:D:410:ASN:HD21	1:D:446:PHE:HB2	1.68	0.58
1:E:341:LEU:H	1:E:344:LEU:HD22	1.69	0.58
1:E:370:ASN:O	1:E:374:LYS:N	2.37	0.58
1:H:262:ASP:N	1:H:262:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:349:SER:HA	1:K:390:SER:H	1.69	0.58
1:L:298:GLY:O	1:L:302:LEU:N	2.36	0.58
1:C:176:THR:O	1:C:180:GLN:NE2	2.36	0.58
1:E:333:LYS:HA	1:E:336:ARG:HH21	1.69	0.58
1:F:179:SER:OG	1:F:180:GLN:OE1	2.21	0.58
1:G:312:THR:OG1	1:G:314:ALA:O	2.21	0.58
1:I:323:THR:HG1	1:I:363:GLN:NE2	2.01	0.58
1:A:245:SER:O	1:A:441:ASN:ND2	2.37	0.58
1:E:199:LEU:N	1:E:413:MET:O	2.32	0.58
1:E:346:LEU:HD13	1:E:385:LEU:HD23	1.86	0.58
1:H:199:LEU:HB3	1:H:414:PRO:HA	1.86	0.58
1:I:341:LEU:H	1:I:344:LEU:HD22	1.68	0.58
1:I:346:LEU:HD11	1:I:402:PHE:HB3	1.86	0.58
1:J:267:LEU:HD12	1:J:270:LEU:HB3	1.86	0.58
1:J:365:VAL:HG22	1:J:382:ILE:HG13	1.84	0.58
1:M:184:ARG:O	1:M:188:LYS:NZ	2.34	0.58
1:M:331:ARG:HA	1:M:404:VAL:HG11	1.86	0.58
1:F:201:MET:HG3	1:F:416:GLN:HA	1.86	0.58
1:H:324:ALA:O	1:H:328:SER:N	2.36	0.58
1:J:247:TYR:OH	1:J:292:GLY:O	2.22	0.58
1:J:331:ARG:HE	1:J:332:ARG:HD3	1.68	0.58
1:B:251:ALA:O	1:B:436:VAL:N	2.30	0.57
1:E:170:SER:OG	1:E:171:SER:N	2.34	0.57
1:H:414:PRO:HD2	1:H:442:LEU:HA	1.86	0.57
1:C:346:LEU:HB2	1:C:385:LEU:HD23	1.86	0.57
1:H:416:GLN:HB3	1:H:417:ARG:HG3	1.86	0.57
1:A:349:SER:H	1:A:352:ALA:HB3	1.68	0.57
1:B:186:LEU:O	1:B:187:GLN:NE2	2.29	0.57
1:B:249:LEU:N	1:B:438:GLN:O	2.38	0.57
1:E:342:SER:O	1:E:408:LYS:NZ	2.37	0.57
1:H:260:GLU:HG2	1:H:264:ILE:HD12	1.85	0.57
1:H:344:LEU:HA	1:H:406:VAL:HA	1.86	0.57
1:K:258:GLU:HB3	1:K:430:GLN:HB3	1.84	0.57
1:E:257:ASP:HB2	1:E:431:ARG:HA	1.86	0.57
1:C:417:ARG:NH1	1:C:437:THR:O	2.37	0.57
1:G:429:LYS:HE2	1:G:431:ARG:HH11	1.69	0.57
1:H:213:ASP:HB3	1:H:216:LYS:HD3	1.85	0.57
1:I:257:ASP:OD2	1:I:425:ARG:NH1	2.38	0.57
1:A:246:THR:OG1	1:A:247:TYR:N	2.38	0.57
1:C:186:LEU:O	1:C:187:GLN:NE2	2.37	0.57
1:C:346:LEU:HB3	1:C:387:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ARG:HH11	1:D:440:VAL:HG12	1.68	0.57
1:G:313:GLU:O	1:G:315:LYS:NZ	2.38	0.57
1:G:362:TRP:HD1	1:G:366:ALA:H	1.51	0.57
1:I:213:ASP:OD1	1:I:213:ASP:N	2.36	0.57
1:J:324:ALA:O	1:J:328:SER:N	2.34	0.57
1:L:175:GLU:HG2	1:L:176:THR:HG22	1.86	0.57
1:L:271:LEU:O	1:L:273:LYS:NZ	2.37	0.57
1:L:414:PRO:HG2	1:L:441:ASN:HB3	1.86	0.57
1:M:211:GLU:OE1	1:M:216:LYS:NZ	2.33	0.57
1:A:381:ARG:HA	1:A:386:PRO:HA	1.86	0.57
1:D:187:GLN:HA	1:D:190:LEU:HD22	1.86	0.57
1:F:180:GLN:HA	1:F:183:ILE:HD12	1.86	0.57
1:F:419:VAL:HG23	1:F:438:GLN:HB2	1.86	0.57
1:G:422:GLU:HG2	1:G:435:TYR:HB2	1.85	0.57
1:H:415:ARG:NH2	1:H:417:ARG:O	2.37	0.57
1:D:333:LYS:HE2	1:D:336:ARG:HH12	1.70	0.57
1:G:264:ILE:HD12	1:G:267:LEU:HD22	1.87	0.57
1:H:176:THR:OG1	1:H:272:ARG:NH2	2.34	0.57
1:H:329:LYS:HA	1:H:332:ARG:HG2	1.87	0.57
1:M:370:ASN:OD1	1:M:370:ASN:N	2.32	0.57
1:A:300:LEU:O	1:A:304:SER:OG	2.21	0.57
1:C:318:GLY:H	1:C:320:VAL:HG13	1.68	0.57
1:C:347:ILE:HA	1:C:388:VAL:HB	1.86	0.57
1:C:411:PHE:H	1:C:444:ARG:HA	1.69	0.57
1:F:181:ARG:HB2	1:F:184:ARG:HH11	1.70	0.57
1:F:356:LEU:O	1:F:362:TRP:NE1	2.38	0.57
1:G:346:LEU:HD23	1:G:387:VAL:HG22	1.87	0.57
1:I:268:LEU:O	1:I:272:ARG:N	2.37	0.57
1:K:181:ARG:NH1	1:K:185:ASP:OD1	2.37	0.57
1:K:271:LEU:HD11	1:L:210:VAL:HG21	1.86	0.57
1:K:338:GLY:O	1:K:340:LYS:NZ	2.37	0.57
1:L:405:ILE:HD11	1:L:410:ASN:HB2	1.85	0.57
1:E:193:GLY:O	1:E:407:TYR:OH	2.21	0.57
1:F:271:LEU:HA	1:F:274:ARG:HH12	1.70	0.57
1:L:353:TYR:O	1:L:357:LEU:N	2.38	0.57
1:D:404:VAL:O	1:D:451:VAL:N	2.31	0.56
1:F:267:LEU:HA	1:F:270:LEU:HD23	1.86	0.56
1:G:324:ALA:O	1:G:328:SER:N	2.39	0.56
1:I:416:GLN:HG2	1:I:417:ARG:HG3	1.87	0.56
1:J:203:SER:OG	1:J:204:LYS:N	2.38	0.56
1:J:420:THR:HG1	1:J:437:THR:HG1	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:414:PRO:HG2	1:K:441:ASN:HB3	1.86	0.56
1:L:348:VAL:N	1:L:388:VAL:O	2.28	0.56
1:E:298:GLY:O	1:E:302:LEU:N	2.34	0.56
1:L:257:ASP:OD1	1:L:434:TYR:OH	2.23	0.56
1:A:288:MET:O	1:A:299:LEU:N	2.37	0.56
1:D:271:LEU:O	1:D:274:ARG:NH1	2.39	0.56
1:E:203:SER:OG	1:E:204:LYS:N	2.36	0.56
1:E:306:ASP:N	1:E:306:ASP:OD1	2.38	0.56
1:H:241:GLU:O	1:H:243:HIS:ND1	2.38	0.56
1:H:320:VAL:HB	1:H:322:VAL:HG23	1.88	0.56
1:K:176:THR:HG1	1:K:180:GLN:NE2	2.02	0.56
1:K:425:ARG:NH2	1:K:432:ASP:OD2	2.38	0.56
1:L:421:VAL:HG13	1:L:436:VAL:HG13	1.87	0.56
1:D:313:GLU:O	1:D:315:LYS:NZ	2.36	0.56
1:H:300:LEU:O	1:H:304:SER:OG	2.22	0.56
1:H:371:ASP:OD1	1:H:381:ARG:NE	2.38	0.56
1:I:264:ILE:HG22	1:I:266:SER:H	1.69	0.56
1:M:249:LEU:HB3	1:M:279:HIS:HE1	1.71	0.56
1:A:247:TYR:HB2	1:A:296:PRO:HG3	1.88	0.56
1:B:370:ASN:N	1:B:370:ASN:OD1	2.38	0.56
1:C:404:VAL:N	1:C:451:VAL:O	2.37	0.56
1:C:421:VAL:HG22	1:C:436:VAL:HG13	1.87	0.56
1:H:251:ALA:O	1:H:436:VAL:N	2.37	0.56
1:L:207:THR:HA	1:L:243:HIS:HA	1.87	0.56
1:A:415:ARG:NH1	1:A:417:ARG:O	2.39	0.56
1:F:176:THR:H	1:F:423:ARG:HH22	1.52	0.56
1:F:272:ARG:HE	1:F:276:ILE:HD11	1.70	0.56
1:G:181:ARG:O	1:G:184:ARG:NH1	2.39	0.56
1:G:414:PRO:O	1:G:441:ASN:N	2.39	0.56
1:H:264:ILE:O	1:H:266:SER:OG	2.22	0.56
1:H:298:GLY:O	1:H:301:THR:OG1	2.21	0.56
1:I:313:GLU:O	1:I:315:LYS:NZ	2.38	0.56
1:K:348:VAL:HG23	1:K:389:VAL:HG12	1.87	0.56
1:B:352:ALA:HB2	1:B:401:GLU:HB2	1.86	0.56
1:C:249:LEU:HD22	1:C:283:ILE:HG12	1.87	0.56
1:D:256:THR:HG23	1:D:258:GLU:HG3	1.88	0.56
1:F:176:THR:O	1:F:423:ARG:NH2	2.39	0.56
1:F:208:MET:N	1:F:241:GLU:OE1	2.38	0.56
1:J:300:LEU:O	1:J:304:SER:N	2.35	0.56
1:K:199:LEU:HB3	1:K:414:PRO:HA	1.87	0.56
1:K:326:THR:HA	1:K:329:LYS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ALA:O	1:B:396:LYS:NZ	2.35	0.56
1:D:241:GLU:HG2	1:D:243:HIS:H	1.71	0.56
1:E:266:SER:HA	1:E:269:PRO:HD2	1.86	0.56
1:I:342:SER:H	1:I:344:LEU:HD13	1.71	0.56
1:I:424:GLU:O	1:I:425:ARG:NH2	2.39	0.56
1:M:238:ALA:HB1	1:M:447:ALA:H	1.71	0.56
1:C:223:SER:OG	1:C:224:THR:N	2.39	0.56
1:E:368:VAL:HG22	1:E:371:ASP:HA	1.87	0.56
1:F:349:SER:O	1:F:353:TYR:N	2.38	0.56
1:G:429:LYS:HB2	1:G:431:ARG:HE	1.70	0.56
1:H:257:ASP:OD1	1:H:257:ASP:N	2.38	0.56
1:H:425:ARG:NH2	1:H:434:TYR:OH	2.39	0.56
1:L:444:ARG:NH2	1:L:447:ALA:O	2.39	0.56
1:B:382:ILE:HB	1:B:385:LEU:HD12	1.88	0.56
1:F:176:THR:OG1	1:F:180:GLN:OE1	2.24	0.56
1:G:206:LEU:N	1:G:244:PHE:O	2.39	0.56
1:G:323:THR:O	1:G:363:GLN:NE2	2.38	0.56
1:I:262:ASP:N	1:I:262:ASP:OD1	2.37	0.56
1:K:176:THR:O	1:K:176:THR:OG1	2.22	0.56
1:M:206:LEU:HD21	1:M:208:MET:HE3	1.88	0.56
1:A:246:THR:HA	1:A:441:ASN:HB2	1.87	0.55
1:B:185:ASP:OD1	1:B:188:LYS:NZ	2.31	0.55
1:B:317:ASP:OD1	1:B:317:ASP:N	2.35	0.55
1:C:342:SER:H	1:C:344:LEU:HD13	1.71	0.55
1:E:249:LEU:HA	1:F:219:TRP:HZ3	1.71	0.55
1:F:278:ALA:O	1:F:282:SER:OG	2.23	0.55
1:F:404:VAL:N	1:F:451:VAL:O	2.38	0.55
1:G:350:MET:HA	1:G:353:TYR:HB3	1.88	0.55
1:I:349:SER:O	1:I:353:TYR:N	2.38	0.55
1:L:345:VAL:HG12	1:L:386:PRO:HD2	1.89	0.55
1:E:324:ALA:O	1:E:328:SER:N	2.40	0.55
1:E:423:ARG:HA	1:E:434:TYR:HA	1.87	0.55
1:F:413:MET:HA	1:F:442:LEU:HA	1.87	0.55
1:E:346:LEU:HB2	1:E:385:LEU:HB3	1.87	0.55
1:G:212:PRO:O	1:G:216:LYS:NZ	2.34	0.55
1:K:347:ILE:O	1:K:403:ALA:N	2.39	0.55
1:D:327:ILE:HA	1:D:330:LEU:HD22	1.88	0.55
1:F:295:LYS:NZ	1:F:296:PRO:O	2.39	0.55
1:L:198:GLU:HA	1:L:413:MET:HB3	1.87	0.55
1:L:406:VAL:O	1:L:410:ASN:ND2	2.39	0.55
1:C:322:VAL:HG22	1:C:325:LYS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ASP:OD1	1:C:359:ASP:N	2.37	0.55
1:D:310:VAL:N	1:D:454:THR:OG1	2.40	0.55
1:F:381:ARG:HA	1:F:386:PRO:HA	1.89	0.55
1:G:203:SER:O	1:G:416:GLN:NE2	2.39	0.55
1:J:346:LEU:HD13	1:J:404:VAL:HG22	1.87	0.55
1:K:233:GLU:OE1	1:K:236:LYS:NZ	2.40	0.55
1:B:432:ASP:OD1	1:B:432:ASP:N	2.40	0.55
1:C:308:ALA:HB1	1:C:451:VAL:HA	1.88	0.55
1:E:257:ASP:OD1	1:E:434:TYR:OH	2.24	0.55
1:I:299:LEU:O	1:I:303:ALA:N	2.38	0.55
1:L:378:GLN:HB3	1:L:386:PRO:HB2	1.88	0.55
1:D:275:LEU:O	1:D:279:HIS:CB	2.55	0.55
1:D:350:MET:O	1:D:354:TYR:N	2.34	0.55
1:J:338:GLY:O	1:J:340:LYS:NZ	2.35	0.55
1:L:203:SER:O	1:L:416:GLN:NE2	2.39	0.55
1:A:423:ARG:HA	1:A:434:TYR:HD1	1.71	0.55
1:B:241:GLU:HG2	1:B:243:HIS:CG	2.42	0.55
1:E:308:ALA:HB1	1:E:451:VAL:HA	1.87	0.55
1:G:290:GLY:H	1:G:298:GLY:HA3	1.70	0.55
1:I:324:ALA:O	1:I:328:SER:N	2.40	0.55
1:I:334:LEU:O	1:I:337:HIS:N	2.39	0.55
1:I:345:VAL:N	1:I:405:ILE:O	2.40	0.55
1:L:344:LEU:HD12	1:L:406:VAL:HB	1.89	0.55
1:L:349:SER:OG	1:L:352:ALA:N	2.37	0.55
1:B:180:GLN:O	1:B:184:ARG:HB3	2.07	0.55
1:D:421:VAL:HG22	1:D:436:VAL:HA	1.89	0.55
1:F:356:LEU:HD22	1:F:362:TRP:HB2	1.88	0.55
1:F:404:VAL:O	1:F:451:VAL:N	2.38	0.55
1:G:201:MET:N	1:G:415:ARG:O	2.37	0.55
1:L:334:LEU:HD23	1:L:337:HIS:HB2	1.89	0.55
1:M:416:GLN:HG3	1:M:417:ARG:HG3	1.89	0.55
1:A:310:VAL:O	1:A:454:THR:N	2.37	0.55
1:C:375:LEU:HD13	1:C:386:PRO:HB3	1.88	0.55
1:E:405:ILE:HB	1:E:450:VAL:HB	1.88	0.55
1:F:369:GLY:HA2	1:F:380:GLY:HA2	1.89	0.55
1:H:197:GLU:HG2	1:H:412:VAL:HA	1.88	0.55
1:H:428:GLY:O	1:H:431:ARG:NE	2.40	0.55
1:I:272:ARG:HA	1:I:275:LEU:HD21	1.87	0.55
1:I:394:PRO:O	1:I:399:SER:OG	2.24	0.55
1:J:346:LEU:HD12	1:J:403:ALA:H	1.72	0.55
1:L:245:SER:OG	1:L:246:THR:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LYS:HZ3	1:B:274:ARG:H	1.55	0.54
1:C:171:SER:O	1:C:425:ARG:NH2	2.39	0.54
1:C:206:LEU:O	1:C:244:PHE:N	2.39	0.54
1:D:303:ALA:HB1	1:D:452:SER:HB3	1.88	0.54
1:F:176:THR:O	1:F:180:GLN:NE2	2.39	0.54
1:H:212:PRO:HD2	1:H:239:LEU:HD12	1.88	0.54
1:H:278:ALA:O	1:H:282:SER:OG	2.25	0.54
1:H:444:ARG:NH1	1:H:447:ALA:O	2.41	0.54
1:L:334:LEU:O	1:L:338:GLY:N	2.41	0.54
1:A:255:ILE:H	1:A:434:TYR:HE2	1.55	0.54
1:B:187:GLN:HB3	1:B:190:LEU:HB2	1.89	0.54
1:B:405:ILE:HB	1:B:450:VAL:HA	1.87	0.54
1:E:275:LEU:O	1:E:279:HIS:CB	2.55	0.54
1:E:275:LEU:HD12	1:E:276:ILE:HG12	1.89	0.54
1:F:272:ARG:HH11	1:F:276:ILE:HG12	1.73	0.54
1:I:365:VAL:HG13	1:I:383:TYR:HD1	1.72	0.54
1:L:405:ILE:HG13	1:L:450:VAL:HB	1.89	0.54
1:M:422:GLU:H	1:M:435:TYR:HB2	1.71	0.54
1:A:257:ASP:OD1	1:A:434:TYR:OH	2.18	0.54
1:D:178:PHE:HA	1:D:181:ARG:HE	1.72	0.54
1:G:199:LEU:N	1:G:413:MET:O	2.40	0.54
1:H:351:ASP:OD1	1:H:351:ASP:N	2.30	0.54
1:I:323:THR:OG1	1:I:324:ALA:N	2.38	0.54
1:M:383:TYR:HB2	1:M:385:LEU:HD13	1.88	0.54
1:C:203:SER:OG	1:C:204:LYS:N	2.40	0.54
1:E:268:LEU:HA	1:E:271:LEU:HB3	1.89	0.54
1:F:233:GLU:H	1:F:234:GLU:HA	1.72	0.54
1:B:193:GLY:O	1:B:407:TYR:OH	2.18	0.54
1:B:362:TRP:HD1	1:B:365:VAL:HA	1.72	0.54
1:C:323:THR:OG1	1:C:324:ALA:N	2.31	0.54
1:H:251:ALA:HB3	1:H:436:VAL:HB	1.90	0.54
1:J:421:VAL:HA	1:J:436:VAL:HA	1.89	0.54
1:L:405:ILE:HG12	1:L:410:ASN:HD22	1.72	0.54
1:C:415:ARG:HA	1:C:440:VAL:HA	1.90	0.54
1:D:291:ASP:N	1:D:296:PRO:O	2.35	0.54
1:H:183:ILE:O	1:H:187:GLN:N	2.38	0.54
1:J:415:ARG:O	1:J:415:ARG:NH2	2.41	0.54
1:K:302:LEU:HD13	1:K:411:PHE:HZ	1.73	0.54
1:L:267:LEU:O	1:L:271:LEU:N	2.38	0.54
1:C:343:LYS:H	1:C:406:VAL:HG23	1.72	0.54
1:D:333:LYS:HA	1:D:336:ARG:HH22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:ASP:OD1	1:G:409:ASP:N	2.39	0.54
1:H:208:MET:HG3	1:H:210:VAL:H	1.73	0.54
1:J:381:ARG:HA	1:J:386:PRO:HA	1.89	0.54
1:K:267:LEU:HD23	1:K:268:LEU:HD23	1.89	0.54
1:L:201:MET:SD	1:L:202:SER:N	2.73	0.54
1:A:354:TYR:HE1	1:B:329:LYS:HA	1.72	0.54
1:B:421:VAL:HA	1:B:436:VAL:HA	1.90	0.54
1:C:288:MET:N	1:C:288:MET:SD	2.80	0.54
1:I:410:ASN:HB3	1:I:445:TYR:H	1.73	0.54
1:K:314:ALA:HB3	1:K:455:TYR:HA	1.90	0.54
1:E:365:VAL:HG13	1:E:383:TYR:H	1.73	0.54
1:F:187:GLN:NE2	1:F:189:GLU:O	2.34	0.54
1:F:411:PHE:HE1	1:F:444:ARG:HH11	1.56	0.54
1:H:350:MET:O	1:I:332:ARG:NH2	2.41	0.54
1:I:285:GLU:O	1:I:289:THR:OG1	2.24	0.54
1:K:349:SER:H	1:K:352:ALA:HB3	1.73	0.54
1:K:411:PHE:HA	1:K:444:ARG:HA	1.90	0.54
1:L:369:GLY:O	1:L:380:GLY:N	2.38	0.54
1:B:299:LEU:HA	1:B:302:LEU:HB2	1.90	0.54
1:E:349:SER:O	1:E:353:TYR:N	2.41	0.54
1:F:415:ARG:NH1	1:F:416:GLN:O	2.41	0.54
1:H:203:SER:OG	1:H:204:LYS:N	2.41	0.54
1:H:257:ASP:OD2	1:H:434:TYR:OH	2.26	0.54
1:H:346:LEU:HB3	1:H:387:VAL:HG22	1.90	0.54
1:I:438:GLN:HE21	1:I:440:VAL:HG13	1.72	0.54
1:J:349:SER:HB3	1:J:401:GLU:HB2	1.89	0.54
1:G:302:LEU:O	1:G:306:ASP:N	2.38	0.53
1:H:400:ALA:HB1	1:H:452:SER:HB2	1.90	0.53
1:M:198:GLU:HB3	1:M:415:ARG:HG2	1.89	0.53
1:A:248:LYS:HA	1:A:439:ARG:HA	1.90	0.53
1:D:362:TRP:CG	1:D:367:GLN:HB3	2.44	0.53
1:J:208:MET:O	1:J:242:ILE:N	2.39	0.53
1:L:201:MET:HE3	1:L:206:LEU:HD22	1.89	0.53
1:M:405:ILE:HD12	1:M:450:VAL:HB	1.89	0.53
1:B:377:GLY:HA2	1:B:386:PRO:HA	1.91	0.53
1:E:223:SER:OG	1:E:224:THR:N	2.38	0.53
1:E:362:TRP:HD1	1:E:365:VAL:HA	1.72	0.53
1:G:268:LEU:HA	1:G:271:LEU:HB2	1.91	0.53
1:G:401:GLU:HG2	1:G:453:GLY:HA2	1.90	0.53
1:H:347:ILE:HG12	1:H:388:VAL:HB	1.88	0.53
1:H:367:GLN:HG2	1:H:368:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:353:TYR:OH	1:J:374:LYS:NZ	2.37	0.53
1:B:272:ARG:O	1:B:274:ARG:N	2.41	0.53
1:B:378:GLN:HG3	1:B:388:VAL:HG13	1.90	0.53
1:E:176:THR:OG1	1:E:177:ILE:N	2.41	0.53
1:K:312:THR:OG1	1:K:313:GLU:N	2.41	0.53
1:A:272:ARG:HA	1:A:275:LEU:HD12	1.90	0.53
1:A:376:GLN:OE1	1:A:378:GLN:NE2	2.40	0.53
1:B:415:ARG:NH1	1:B:417:ARG:O	2.42	0.53
1:C:349:SER:O	1:C:353:TYR:N	2.39	0.53
1:F:313:GLU:O	1:F:315:LYS:NZ	2.41	0.53
1:G:342:SER:H	1:G:344:LEU:HD13	1.74	0.53
1:J:327:ILE:O	1:J:331:ARG:CB	2.57	0.53
1:K:358:GLU:N	1:K:367:GLN:OE1	2.37	0.53
1:L:352:ALA:HB2	1:L:401:GLU:HB2	1.90	0.53
1:M:247:TYR:HB2	1:M:296:PRO:HG3	1.90	0.53
1:A:378:GLN:HB2	1:A:386:PRO:HB2	1.89	0.53
1:A:416:GLN:OE1	1:A:439:ARG:NH2	2.41	0.53
1:D:213:ASP:OD1	1:D:213:ASP:N	2.34	0.53
1:D:366:ALA:HA	1:D:382:ILE:HG12	1.89	0.53
1:D:429:LYS:HZ3	1:D:431:ARG:HH22	1.57	0.53
1:E:421:VAL:HG22	1:E:436:VAL:HA	1.90	0.53
1:F:444:ARG:NH2	1:F:447:ALA:O	2.42	0.53
1:G:218:THR:HG1	1:G:219:TRP:CD1	2.27	0.53
1:G:265:PHE:H	1:G:268:LEU:HD21	1.74	0.53
1:H:325:LYS:N	1:H:325:LYS:HZ2	2.06	0.53
1:I:348:VAL:N	1:I:388:VAL:O	2.37	0.53
1:L:240:LYS:HB3	1:L:242:ILE:HD13	1.91	0.53
1:L:327:ILE:HG22	1:L:331:ARG:HH21	1.73	0.53
1:M:246:THR:OG1	1:M:439:ARG:NH1	2.41	0.53
1:C:349:SER:H	1:C:352:ALA:HB3	1.73	0.53
1:D:297:LYS:NZ	1:D:305:GLU:OE2	2.37	0.53
1:G:266:SER:OG	1:G:267:LEU:N	2.42	0.53
1:G:390:SER:O	1:G:390:SER:OG	2.24	0.53
1:H:328:SER:HB3	1:H:332:ARG:HH21	1.72	0.53
1:I:223:SER:OG	1:I:224:THR:N	2.41	0.53
1:K:174:TYR:HA	1:K:177:ILE:HG13	1.90	0.53
1:K:192:VAL:HA	1:K:388:VAL:HG11	1.90	0.53
1:K:259:THR:O	1:M:204:LYS:NZ	2.40	0.53
1:L:208:MET:HG2	1:L:242:ILE:HB	1.91	0.53
1:M:327:ILE:HA	1:M:330:LEU:HB2	1.89	0.53
1:A:176:THR:O	1:A:176:THR:OG1	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ALA:O	1:B:328:SER:N	2.41	0.53
1:E:361:GLU:HB3	1:E:363:GLN:HG2	1.90	0.53
1:L:365:VAL:HG21	1:L:381:ARG:HH12	1.73	0.53
1:L:412:VAL:HG23	1:L:414:PRO:HD3	1.91	0.53
1:M:328:SER:OG	1:M:383:TYR:OH	2.24	0.53
1:B:381:ARG:HH21	1:B:384:GLY:H	1.56	0.53
1:D:170:SER:O	1:D:170:SER:OG	2.21	0.53
1:E:184:ARG:HH22	1:E:188:LYS:HZ2	1.57	0.53
1:G:362:TRP:CD1	1:G:366:ALA:H	2.27	0.53
1:I:344:LEU:HA	1:I:406:VAL:HA	1.90	0.53
1:K:323:THR:HG1	1:K:324:ALA:H	1.56	0.53
1:K:345:VAL:HG12	1:K:386:PRO:HD2	1.90	0.53
1:L:197:GLU:HB3	1:L:412:VAL:HA	1.89	0.53
1:L:246:THR:OG1	1:L:247:TYR:N	2.42	0.53
1:E:248:LYS:HG3	1:E:417:ARG:HH12	1.74	0.53
1:G:203:SER:OG	1:G:204:LYS:N	2.40	0.53
1:G:431:ARG:O	1:G:431:ARG:NH2	2.42	0.53
1:J:220:VAL:HG13	1:J:222:ALA:H	1.73	0.53
1:J:298:GLY:O	1:J:301:THR:OG1	2.21	0.53
1:K:255:ILE:HG23	1:K:434:TYR:HE2	1.74	0.53
1:C:343:LYS:HD2	1:C:407:TYR:HB3	1.90	0.52
1:D:265:PHE:HA	1:D:268:LEU:HD21	1.90	0.52
1:F:246:THR:OG1	1:F:439:ARG:NE	2.41	0.52
1:F:249:LEU:N	1:F:438:GLN:O	2.35	0.52
1:H:353:TYR:HB3	1:I:332:ARG:HH22	1.73	0.52
1:J:302:LEU:O	1:J:306:ASP:N	2.42	0.52
1:K:253:SER:N	1:K:434:TYR:O	2.32	0.52
1:K:304:SER:OG	1:K:309:LYS:NZ	2.40	0.52
1:L:272:ARG:O	1:L:274:ARG:N	2.42	0.52
1:L:349:SER:H	1:L:352:ALA:HB3	1.72	0.52
1:L:423:ARG:HA	1:L:434:TYR:HA	1.91	0.52
1:A:427:ALA:HB3	1:A:432:ASP:HA	1.91	0.52
1:D:353:TYR:OH	1:D:366:ALA:O	2.24	0.52
1:D:414:PRO:O	1:D:441:ASN:N	2.42	0.52
1:F:239:LEU:HB2	1:J:224:THR:HG22	1.90	0.52
1:F:422:GLU:N	1:F:435:TYR:O	2.40	0.52
1:G:177:ILE:HG12	1:G:421:VAL:HB	1.90	0.52
1:H:421:VAL:HG22	1:H:436:VAL:HG13	1.90	0.52
1:I:171:SER:O	1:I:425:ARG:NH1	2.42	0.52
1:B:202:SER:O	1:B:416:GLN:NE2	2.41	0.52
1:B:267:LEU:HB3	1:B:271:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ALA:HB2	1:C:382:ILE:HG23	1.90	0.52
1:D:207:THR:HA	1:D:243:HIS:HA	1.91	0.52
1:D:290:GLY:H	1:D:298:GLY:HA3	1.74	0.52
1:E:362:TRP:NE1	1:E:367:GLN:O	2.42	0.52
1:F:199:LEU:N	1:F:413:MET:O	2.42	0.52
1:G:444:ARG:HD2	1:G:446:PHE:H	1.74	0.52
1:H:291:ASP:OD2	1:H:293:SER:OG	2.22	0.52
1:I:201:MET:N	1:I:415:ARG:O	2.43	0.52
1:K:233:GLU:H	1:K:234:GLU:HA	1.74	0.52
1:M:249:LEU:HD13	1:M:283:ILE:HG12	1.92	0.52
1:C:421:VAL:HA	1:C:436:VAL:HA	1.92	0.52
1:E:424:GLU:N	1:E:433:ALA:O	2.42	0.52
1:F:364:ASP:OD2	1:F:383:TYR:N	2.42	0.52
1:G:174:TYR:HA	1:G:177:ILE:HD12	1.91	0.52
1:G:206:LEU:O	1:G:244:PHE:N	2.27	0.52
1:H:359:ASP:N	1:H:359:ASP:OD1	2.41	0.52
1:I:415:ARG:HA	1:I:440:VAL:HA	1.90	0.52
1:L:299:LEU:HA	1:L:302:LEU:HB2	1.91	0.52
1:D:329:LYS:O	1:D:333:LYS:HB2	2.10	0.52
1:D:405:ILE:HB	1:D:450:VAL:HA	1.92	0.52
1:E:424:GLU:O	1:E:433:ALA:N	2.42	0.52
1:G:391:GLU:OE2	1:H:336:ARG:NH2	2.43	0.52
1:H:315:LYS:NZ	1:H:319:SER:O	2.36	0.52
1:H:444:ARG:HH21	1:H:446:PHE:H	1.58	0.52
1:I:284:GLU:HA	1:I:287:PHE:HB2	1.91	0.52
1:L:415:ARG:NH2	1:L:416:GLN:O	2.41	0.52
1:H:297:LYS:HG3	1:H:302:LEU:HD21	1.92	0.52
1:J:415:ARG:NH2	1:J:416:GLN:O	2.43	0.52
1:K:330:LEU:HA	1:K:333:LYS:HD3	1.91	0.52
1:M:200:PRO:HA	1:M:415:ARG:HH21	1.75	0.52
1:A:270:LEU:O	1:A:273:LYS:NZ	2.28	0.52
1:A:288:MET:HA	1:A:299:LEU:HG	1.92	0.52
1:B:331:ARG:HG2	1:B:332:ARG:HE	1.74	0.52
1:G:257:ASP:OD2	1:G:432:ASP:N	2.38	0.52
1:J:337:HIS:NE2	1:J:448:ASN:O	2.37	0.52
1:L:249:LEU:HD11	1:L:440:VAL:HG22	1.92	0.52
1:L:382:ILE:HB	1:L:385:LEU:HB2	1.90	0.52
1:L:404:VAL:N	1:L:451:VAL:O	2.43	0.52
1:M:200:PRO:HA	1:M:415:ARG:HD3	1.90	0.52
1:A:210:VAL:HG22	1:F:255:ILE:HG12	1.92	0.52
1:B:389:VAL:O	1:B:391:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:TRP:CD1	1:F:363:GLN:HG2	2.45	0.52
1:G:293:SER:N	1:G:295:LYS:O	2.42	0.52
1:J:324:ALA:O	1:J:328:SER:OG	2.26	0.52
1:K:300:LEU:HA	1:K:303:ALA:HB3	1.91	0.52
1:M:415:ARG:NH2	1:M:416:GLN:O	2.43	0.52
1:C:420:THR:OG1	1:C:422:GLU:OE2	2.27	0.52
1:G:260:GLU:OE2	1:G:434:TYR:OH	2.27	0.52
1:I:203:SER:OG	1:I:205:ILE:O	2.23	0.52
1:I:265:PHE:HB3	1:I:268:LEU:HD21	1.92	0.52
1:I:415:ARG:HB3	1:I:440:VAL:HG12	1.92	0.52
1:J:272:ARG:HB2	1:J:275:LEU:HD11	1.92	0.52
1:L:324:ALA:O	1:L:328:SER:OG	2.26	0.52
1:C:246:THR:OG1	1:C:247:TYR:N	2.38	0.52
1:D:189:GLU:OE1	1:D:189:GLU:N	2.42	0.52
1:E:410:ASN:OD1	1:E:410:ASN:N	2.41	0.52
1:E:421:VAL:HA	1:E:437:THR:HG23	1.91	0.52
1:G:180:GLN:HE22	1:G:272:ARG:HG3	1.75	0.52
1:G:412:VAL:HG23	1:G:414:PRO:HD3	1.92	0.52
1:I:370:ASN:HB2	1:I:373:VAL:HG22	1.93	0.52
1:I:405:ILE:HB	1:I:450:VAL:HB	1.91	0.52
1:J:176:THR:O	1:J:176:THR:OG1	2.24	0.52
1:B:175:GLU:OE1	1:B:423:ARG:NH2	2.43	0.51
1:D:176:THR:OG1	1:D:423:ARG:NH1	2.42	0.51
1:D:176:THR:HG23	1:D:423:ARG:HH22	1.75	0.51
1:D:279:HIS:O	1:D:282:SER:OG	2.24	0.51
1:E:256:THR:HG23	1:F:209:LEU:HB2	1.92	0.51
1:H:349:SER:HB2	1:H:391:GLU:HG3	1.91	0.51
1:H:414:PRO:O	1:H:441:ASN:N	2.43	0.51
1:K:250:ALA:HB2	1:K:437:THR:HA	1.92	0.51
1:M:285:GLU:O	1:M:289:THR:OG1	2.26	0.51
1:A:192:VAL:HA	1:A:388:VAL:HG21	1.92	0.51
1:C:315:LYS:HE2	1:C:321:LEU:HD12	1.92	0.51
1:C:362:TRP:NE1	1:C:367:GLN:O	2.43	0.51
1:E:172:GLU:OE1	1:E:434:TYR:OH	2.28	0.51
1:G:173:SER:OG	1:G:175:GLU:OE1	2.27	0.51
1:J:180:GLN:HB3	1:J:183:ILE:HD12	1.92	0.51
1:J:184:ARG:NE	1:J:185:ASP:OD1	2.33	0.51
1:J:332:ARG:HA	1:J:332:ARG:HH11	1.75	0.51
1:J:350:MET:HB2	1:J:391:GLU:HB2	1.92	0.51
1:K:271:LEU:HD21	1:L:210:VAL:HG11	1.91	0.51
1:K:272:ARG:HE	1:K:273:LYS:N	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:ILE:HB	1:K:403:ALA:HB3	1.92	0.51
1:B:251:ALA:N	1:B:436:VAL:O	2.32	0.51
1:B:415:ARG:HA	1:B:440:VAL:HA	1.93	0.51
1:C:291:ASP:OD1	1:C:291:ASP:N	2.38	0.51
1:D:181:ARG:HB2	1:D:181:ARG:HH21	1.75	0.51
1:E:184:ARG:HH12	1:E:188:LYS:HZ2	1.57	0.51
1:E:381:ARG:HG3	1:E:384:GLY:H	1.75	0.51
1:H:414:PRO:HG2	1:H:441:ASN:HB3	1.92	0.51
1:I:324:ALA:HA	1:I:327:ILE:HD12	1.92	0.51
1:J:178:PHE:HE1	1:J:418:ALA:HB3	1.75	0.51
1:J:198:GLU:HA	1:J:413:MET:HB3	1.92	0.51
1:B:278:ALA:O	1:B:282:SER:OG	2.24	0.51
1:B:421:VAL:HG22	1:B:436:VAL:HG13	1.92	0.51
1:C:174:TYR:HA	1:C:423:ARG:HD3	1.93	0.51
1:D:316:ALA:H	1:D:320:VAL:HG13	1.75	0.51
1:D:404:VAL:HB	1:D:451:VAL:HB	1.92	0.51
1:G:270:LEU:HD13	1:H:199:LEU:HD13	1.92	0.51
1:G:314:ALA:HB3	1:G:455:TYR:HB2	1.92	0.51
1:H:272:ARG:O	1:H:275:LEU:N	2.34	0.51
1:K:216:LYS:NZ	1:K:237:GLY:O	2.42	0.51
1:L:287:PHE:HE1	1:L:296:PRO:HG2	1.74	0.51
1:M:351:ASP:HA	1:M:354:TYR:HB3	1.92	0.51
1:D:255:ILE:HG22	1:E:210:VAL:HG11	1.91	0.51
1:E:181:ARG:O	1:E:185:ASP:N	2.44	0.51
1:F:274:ARG:O	1:F:278:ALA:CB	2.58	0.51
1:H:176:THR:HG1	1:H:272:ARG:HH21	1.54	0.51
1:H:206:LEU:O	1:H:244:PHE:N	2.36	0.51
1:H:362:TRP:HD1	1:H:366:ALA:H	1.59	0.51
1:J:415:ARG:NH1	1:J:417:ARG:O	2.43	0.51
1:M:197:GLU:HB2	1:M:412:VAL:HG11	1.93	0.51
1:B:411:PHE:H	1:B:445:TYR:HB2	1.74	0.51
1:F:353:TYR:O	1:F:357:LEU:N	2.44	0.51
1:F:362:TRP:HE1	1:F:366:ALA:HB3	1.76	0.51
1:G:278:ALA:O	1:G:282:SER:OG	2.26	0.51
1:H:176:THR:O	1:H:180:GLN:N	2.39	0.51
1:H:349:SER:HA	1:H:391:GLU:HB2	1.92	0.51
1:I:206:LEU:O	1:I:244:PHE:N	2.44	0.51
1:I:325:LYS:HD3	1:I:363:GLN:HE22	1.74	0.51
1:M:290:GLY:O	1:M:301:THR:OG1	2.26	0.51
1:C:396:LYS:O	1:C:398:ASN:N	2.43	0.51
1:H:256:THR:HG22	1:H:258:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:GLU:O	1:H:289:THR:N	2.43	0.51
1:A:347:ILE:HB	1:A:403:ALA:HB3	1.91	0.51
1:C:275:LEU:O	1:C:279:HIS:HB3	2.10	0.51
1:C:347:ILE:H	1:C:403:ALA:HB3	1.76	0.51
1:D:186:LEU:HA	1:D:189:GLU:HB2	1.93	0.51
1:F:452:SER:O	1:F:454:THR:OG1	2.26	0.51
1:K:444:ARG:HB2	1:K:444:ARG:HH21	1.76	0.51
1:M:330:LEU:O	1:M:334:LEU:HB2	2.11	0.51
1:C:324:ALA:HA	1:C:327:ILE:HD12	1.93	0.51
1:F:250:ALA:HA	1:F:437:THR:HA	1.92	0.51
1:G:256:THR:HB	1:H:210:VAL:HG12	1.91	0.51
1:H:272:ARG:HE	1:H:275:LEU:HD12	1.75	0.51
1:H:327:ILE:HA	1:H:330:LEU:HB2	1.93	0.51
1:H:346:LEU:HD11	1:H:402:PHE:HB3	1.91	0.51
1:I:251:ALA:O	1:I:253:SER:OG	2.29	0.51
1:K:382:ILE:O	1:K:385:LEU:N	2.38	0.51
1:C:331:ARG:HH21	1:C:332:ARG:HE	1.58	0.51
1:J:316:ALA:HB1	1:J:397:ALA:HB1	1.93	0.51
1:M:398:ASN:HB2	1:M:457:ALA:HB2	1.91	0.51
1:C:350:MET:HA	1:C:353:TYR:HB2	1.93	0.50
1:C:420:THR:O	1:C:437:THR:N	2.42	0.50
1:D:284:GLU:HA	1:D:287:PHE:HB2	1.92	0.50
1:H:422:GLU:HB2	1:H:435:TYR:HB2	1.92	0.50
1:A:181:ARG:HB2	1:A:184:ARG:HH11	1.77	0.50
1:A:219:TRP:HZ3	1:F:249:LEU:HD22	1.76	0.50
1:A:417:ARG:NE	1:A:418:ALA:O	2.45	0.50
1:D:251:ALA:N	1:D:436:VAL:O	2.32	0.50
1:F:181:ARG:HH21	1:F:182:ILE:HG13	1.76	0.50
1:G:219:TRP:CZ2	1:L:249:LEU:HA	2.46	0.50
1:J:251:ALA:HB3	1:J:436:VAL:HB	1.92	0.50
1:K:415:ARG:HA	1:K:440:VAL:HA	1.92	0.50
1:L:357:LEU:HA	1:L:362:TRP:CE2	2.45	0.50
1:B:416:GLN:N	1:B:439:ARG:O	2.43	0.50
1:B:417:ARG:NH1	1:B:439:ARG:HG3	2.26	0.50
1:C:184:ARG:HG3	1:C:419:VAL:HG11	1.93	0.50
1:C:331:ARG:O	1:C:332:ARG:NH1	2.44	0.50
1:H:299:LEU:O	1:H:303:ALA:N	2.40	0.50
1:H:310:VAL:O	1:H:454:THR:N	2.38	0.50
1:H:317:ASP:HA	1:H:320:VAL:HG13	1.93	0.50
1:I:206:LEU:N	1:I:244:PHE:O	2.35	0.50
1:J:371:ASP:OD2	1:J:381:ARG:NH1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:365:VAL:HG11	1:K:381:ARG:CZ	2.42	0.50
1:L:346:LEU:HB2	1:L:385:LEU:HD23	1.93	0.50
1:L:359:ASP:OD1	1:L:359:ASP:N	2.43	0.50
1:A:362:TRP:NE1	1:A:367:GLN:O	2.44	0.50
1:D:201:MET:HE2	1:D:202:SER:H	1.77	0.50
1:D:249:LEU:HB2	1:D:438:GLN:HB3	1.92	0.50
1:D:256:THR:HG22	1:D:259:THR:H	1.75	0.50
1:D:277:GLU:O	1:D:280:ALA:N	2.43	0.50
1:D:426:GLN:NE2	1:D:427:ALA:O	2.45	0.50
1:H:272:ARG:O	1:H:274:ARG:N	2.45	0.50
1:F:364:ASP:HB2	1:F:365:VAL:HG12	1.93	0.50
1:G:342:SER:OG	1:L:391:GLU:OE2	2.28	0.50
1:I:300:LEU:O	1:I:304:SER:OG	2.26	0.50
1:K:420:THR:O	1:K:437:THR:OG1	2.23	0.50
1:L:278:ALA:O	1:L:282:SER:OG	2.23	0.50
1:A:238:ALA:HB1	1:A:240:LYS:HG2	1.94	0.50
1:B:211:GLU:HG3	1:B:239:LEU:HD13	1.93	0.50
1:B:249:LEU:HA	1:C:219:TRP:HE1	1.76	0.50
1:B:351:ASP:HA	1:B:354:TYR:HB3	1.93	0.50
1:K:334:LEU:HA	1:K:336:ARG:HB3	1.93	0.50
1:M:372:SER:HB3	1:M:374:LYS:HD2	1.92	0.50
1:A:351:ASP:HA	1:A:354:TYR:HB3	1.93	0.50
1:F:363:GLN:NE2	1:F:364:ASP:OD2	2.38	0.50
1:H:255:ILE:HG22	1:I:210:VAL:HG11	1.92	0.50
1:I:362:TRP:CG	1:I:367:GLN:HB3	2.47	0.50
1:J:369:GLY:O	1:J:381:ARG:N	2.45	0.50
1:L:410:ASN:ND2	1:L:449:GLY:O	2.44	0.50
1:L:435:TYR:H	1:L:435:TYR:HD2	1.60	0.50
1:A:347:ILE:HG12	1:A:388:VAL:HB	1.93	0.50
1:A:362:TRP:HD1	1:A:366:ALA:H	1.58	0.50
1:D:257:ASP:OD2	1:D:434:TYR:OH	2.25	0.50
1:E:278:ALA:O	1:E:282:SER:OG	2.29	0.50
1:G:179:SER:HA	1:G:182:ILE:HB	1.93	0.50
1:G:295:LYS:HD3	1:H:219:TRP:HE1	1.77	0.50
1:H:353:TYR:HD2	1:I:332:ARG:HH12	1.60	0.50
1:A:267:LEU:O	1:A:271:LEU:N	2.44	0.50
1:I:272:ARG:HH21	1:I:423:ARG:HH12	1.58	0.50
1:J:190:LEU:HD21	1:K:339:LEU:HD11	1.93	0.50
1:B:330:LEU:HA	1:B:333:LYS:HD3	1.94	0.49
1:C:405:ILE:HA	1:C:450:VAL:HA	1.94	0.49
1:E:304:SER:OG	1:E:309:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:THR:HG21	1:G:439:ARG:HE	1.76	0.49
1:G:382:ILE:O	1:G:385:LEU:N	2.44	0.49
1:H:279:HIS:NE2	1:H:438:GLN:OE1	2.37	0.49
1:H:285:GLU:O	1:H:289:THR:OG1	2.22	0.49
1:I:269:PRO:HB2	1:I:273:LYS:HD2	1.94	0.49
1:I:359:ASP:OD1	1:I:359:ASP:N	2.28	0.49
1:I:421:VAL:HG22	1:I:436:VAL:HG13	1.92	0.49
1:K:356:LEU:O	1:K:367:GLN:NE2	2.44	0.49
1:K:417:ARG:HB2	1:K:439:ARG:HB2	1.94	0.49
1:L:199:LEU:O	1:L:415:ARG:N	2.44	0.49
1:M:172:GLU:OE1	1:M:423:ARG:NH2	2.45	0.49
1:M:252:LYS:HA	1:M:436:VAL:H	1.76	0.49
1:A:197:GLU:HG3	1:A:412:VAL:HG12	1.94	0.49
1:D:413:MET:HG2	1:D:415:ARG:HB3	1.94	0.49
1:E:397:ALA:HA	1:E:455:TYR:CZ	2.47	0.49
1:H:314:ALA:HB1	1:H:320:VAL:HG12	1.93	0.49
1:H:365:VAL:HG13	1:H:383:TYR:HA	1.93	0.49
1:I:184:ARG:HH22	1:I:188:LYS:HG3	1.76	0.49
1:K:378:GLN:N	1:K:386:PRO:HB3	2.27	0.49
1:C:208:MET:N	1:C:242:ILE:O	2.37	0.49
1:E:272:ARG:O	1:E:274:ARG:N	2.37	0.49
1:F:381:ARG:HH21	1:F:384:GLY:HA2	1.77	0.49
1:J:389:VAL:O	1:J:391:GLU:N	2.43	0.49
1:A:272:ARG:O	1:A:274:ARG:N	2.45	0.49
1:A:285:GLU:O	1:A:289:THR:OG1	2.26	0.49
1:A:291:ASP:H	1:A:295:LYS:NZ	2.09	0.49
1:B:396:LYS:O	1:B:398:ASN:N	2.44	0.49
1:C:362:TRP:N	1:C:366:ALA:HB3	2.28	0.49
1:H:323:THR:HB	1:H:325:LYS:HG2	1.93	0.49
1:I:310:VAL:O	1:I:454:THR:OG1	2.28	0.49
1:J:282:SER:HA	1:J:285:GLU:HB2	1.95	0.49
1:B:348:VAL:N	1:B:388:VAL:O	2.44	0.49
1:I:323:THR:OG1	1:I:363:GLN:NE2	2.45	0.49
1:M:308:ALA:HA	1:M:451:VAL:HA	1.94	0.49
1:A:341:LEU:H	1:A:344:LEU:HD22	1.78	0.49
1:B:198:GLU:HB3	1:B:415:ARG:HG2	1.95	0.49
1:C:365:VAL:O	1:C:383:TYR:N	2.30	0.49
1:F:253:SER:O	1:F:434:TYR:N	2.38	0.49
1:G:264:ILE:HG21	1:G:267:LEU:HD13	1.93	0.49
1:G:368:VAL:N	1:G:371:ASP:OD2	2.39	0.49
1:L:330:LEU:HA	1:L:333:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:O	1:B:304:SER:OG	2.23	0.49
1:C:267:LEU:O	1:C:271:LEU:N	2.45	0.49
1:D:410:ASN:ND2	1:D:446:PHE:HB2	2.28	0.49
1:F:267:LEU:O	1:F:271:LEU:N	2.45	0.49
1:G:181:ARG:HA	1:G:184:ARG:HB3	1.95	0.49
1:G:433:ALA:HB1	1:G:435:TYR:HE2	1.76	0.49
1:H:279:HIS:O	1:H:282:SER:OG	2.26	0.49
1:I:199:LEU:HD12	1:I:200:PRO:HD2	1.94	0.49
1:I:259:THR:HG21	1:J:209:LEU:H	1.77	0.49
1:I:372:SER:HB2	1:I:374:LYS:HD2	1.95	0.49
1:J:331:ARG:HH21	1:J:332:ARG:HD3	1.78	0.49
1:K:173:SER:O	1:K:176:THR:N	2.45	0.49
1:K:203:SER:OG	1:K:204:LYS:N	2.43	0.49
1:K:314:ALA:H	1:K:455:TYR:H	1.61	0.49
1:M:346:LEU:HB3	1:M:387:VAL:HA	1.94	0.49
1:A:177:ILE:HG13	1:A:423:ARG:HH11	1.78	0.49
1:A:213:ASP:OD1	1:A:213:ASP:N	2.44	0.49
1:A:349:SER:OG	1:A:351:ASP:N	2.46	0.49
1:D:195:LEU:O	1:D:407:TYR:OH	2.26	0.49
1:D:415:ARG:HE	1:D:440:VAL:HG12	1.77	0.49
1:F:382:ILE:N	1:F:385:LEU:O	2.46	0.49
1:H:345:VAL:HA	1:H:385:LEU:HG	1.94	0.49
1:I:272:ARG:HD2	1:I:423:ARG:HH12	1.78	0.49
1:I:290:GLY:H	1:I:298:GLY:HA3	1.78	0.49
1:I:362:TRP:CD2	1:I:367:GLN:HB3	2.47	0.49
1:I:371:ASP:OD1	1:I:381:ARG:NE	2.46	0.49
1:K:279:HIS:O	1:K:283:ILE:HB	2.13	0.49
1:L:331:ARG:HG2	1:L:332:ARG:HH11	1.77	0.49
1:M:260:GLU:HB3	1:M:264:ILE:HG13	1.94	0.49
1:B:423:ARG:O	1:B:425:ARG:NH2	2.43	0.49
1:D:208:MET:HB2	1:D:210:VAL:HG22	1.95	0.49
1:D:241:GLU:OE2	1:D:243:HIS:ND1	2.45	0.49
1:E:362:TRP:CD1	1:E:366:ALA:H	2.31	0.49
1:J:285:GLU:HG3	1:J:392:TYR:HE1	1.78	0.49
1:K:300:LEU:HD21	1:K:393:PHE:HE1	1.78	0.49
1:A:186:LEU:O	1:A:187:GLN:NE2	2.46	0.49
1:B:417:ARG:HB2	1:B:439:ARG:N	2.28	0.49
1:F:246:THR:C	1:F:439:ARG:HH11	2.21	0.49
1:F:293:SER:H	1:F:295:LYS:NZ	2.11	0.49
1:F:357:LEU:HA	1:F:362:TRP:CZ2	2.48	0.49
1:I:389:VAL:O	1:I:391:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:272:ARG:HH11	1:J:276:ILE:HD13	1.78	0.49
1:J:396:LYS:O	1:J:398:ASN:N	2.46	0.49
1:K:300:LEU:HD22	1:K:309:LYS:HE2	1.94	0.49
1:M:272:ARG:O	1:M:274:ARG:NH2	2.46	0.49
1:M:409:ASP:HB3	1:M:446:PHE:CE2	2.48	0.49
1:D:290:GLY:HA2	1:D:295:LYS:HE2	1.94	0.48
1:D:331:ARG:HH11	1:D:341:LEU:HD11	1.78	0.48
1:E:274:ARG:NH1	1:F:211:GLU:O	2.46	0.48
1:E:312:THR:O	1:E:312:THR:OG1	2.27	0.48
1:F:288:MET:O	1:F:299:LEU:N	2.46	0.48
1:H:208:MET:HG2	1:H:242:ILE:HG13	1.95	0.48
1:H:212:PRO:HD2	1:H:239:LEU:HA	1.94	0.48
1:H:364:ASP:OD2	1:H:383:TYR:OH	2.26	0.48
1:K:170:SER:O	1:K:173:SER:OG	2.31	0.48
1:K:389:VAL:HG23	1:K:390:SER:HB3	1.95	0.48
1:A:211:GLU:HA	1:A:238:ALA:C	2.38	0.48
1:A:398:ASN:HB2	1:A:457:ALA:H	1.78	0.48
1:C:312:THR:HB	1:C:456:ALA:HB3	1.96	0.48
1:D:314:ALA:HB3	1:D:455:TYR:HA	1.94	0.48
1:E:419:VAL:HG23	1:E:421:VAL:HG23	1.94	0.48
1:F:272:ARG:O	1:F:274:ARG:NH2	2.45	0.48
1:F:352:ALA:HB2	1:F:401:GLU:HB2	1.95	0.48
1:I:180:GLN:O	1:I:184:ARG:HB2	2.12	0.48
1:K:260:GLU:OE2	1:K:264:ILE:N	2.45	0.48
1:K:331:ARG:HG2	1:K:340:LYS:HD2	1.94	0.48
1:A:362:TRP:CG	1:A:367:GLN:HG2	2.48	0.48
1:A:390:SER:HG	1:B:340:LYS:HZ1	1.54	0.48
1:B:206:LEU:O	1:B:244:PHE:N	2.39	0.48
1:B:362:TRP:CD1	1:B:365:VAL:HA	2.48	0.48
1:D:248:LYS:HA	1:D:439:ARG:HG2	1.95	0.48
1:D:353:TYR:O	1:E:332:ARG:NH2	2.46	0.48
1:D:364:ASP:OD2	1:D:383:TYR:OH	2.22	0.48
1:G:181:ARG:HE	1:G:184:ARG:HH11	1.60	0.48
1:G:347:ILE:HB	1:G:403:ALA:HB3	1.95	0.48
1:H:292:GLY:N	1:H:296:PRO:O	2.33	0.48
1:I:270:LEU:HD13	1:J:200:PRO:HG2	1.95	0.48
1:J:313:GLU:HG3	1:J:326:THR:HA	1.95	0.48
1:L:375:LEU:HD12	1:L:377:GLY:H	1.78	0.48
1:A:300:LEU:O	1:A:304:SER:N	2.47	0.48
1:A:396:LYS:O	1:A:398:ASN:N	2.46	0.48
1:A:419:VAL:HG23	1:A:437:THR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASP:HA	1:B:301:THR:HG21	1.96	0.48
1:D:179:SER:HA	1:D:182:ILE:HG13	1.96	0.48
1:E:405:ILE:HG13	1:E:410:ASN:HD22	1.78	0.48
1:G:176:THR:O	1:G:176:THR:OG1	2.29	0.48
1:G:350:MET:SD	1:H:336:ARG:NH2	2.86	0.48
1:I:346:LEU:HD13	1:I:404:VAL:HG13	1.95	0.48
1:K:410:ASN:OD1	1:K:410:ASN:N	2.46	0.48
1:C:208:MET:HB2	1:C:242:ILE:HB	1.95	0.48
1:D:317:ASP:OD1	1:D:317:ASP:N	2.44	0.48
1:G:199:LEU:HG	1:G:201:MET:HG2	1.95	0.48
1:G:246:THR:HA	1:G:441:ASN:HB2	1.94	0.48
1:J:422:GLU:O	1:J:435:TYR:N	2.43	0.48
1:K:398:ASN:CG	1:K:457:ALA:H	2.21	0.48
1:L:253:SER:O	1:L:253:SER:OG	2.28	0.48
1:M:241:GLU:O	1:M:243:HIS:ND1	2.42	0.48
1:B:415:ARG:NH2	1:B:416:GLN:O	2.47	0.48
1:G:201:MET:HB2	1:G:416:GLN:HA	1.95	0.48
1:J:265:PHE:HA	1:J:268:LEU:HD21	1.95	0.48
1:K:253:SER:HB2	1:K:434:TYR:HD2	1.78	0.48
1:M:353:TYR:HA	1:M:356:LEU:HB2	1.95	0.48
1:A:326:THR:OG1	1:A:327:ILE:N	2.47	0.48
1:B:250:ALA:HA	1:B:437:THR:HA	1.95	0.48
1:B:362:TRP:CD1	1:B:366:ALA:H	2.32	0.48
1:D:365:VAL:HG21	1:D:383:TYR:H	1.78	0.48
1:F:298:GLY:O	1:F:301:THR:OG1	2.31	0.48
1:G:170:SER:OG	1:G:175:GLU:OE1	2.28	0.48
1:H:370:ASN:HB2	1:H:373:VAL:HG22	1.96	0.48
1:J:270:LEU:HD22	1:K:199:LEU:HD13	1.95	0.48
1:L:179:SER:OG	1:L:180:GLN:N	2.44	0.48
1:L:201:MET:SD	1:L:203:SER:N	2.80	0.48
1:M:378:GLN:H	1:M:386:PRO:HB3	1.78	0.48
1:D:331:ARG:HD3	1:D:341:LEU:HD21	1.94	0.48
1:G:187:GLN:OE1	1:G:190:LEU:N	2.47	0.48
1:I:251:ALA:HB3	1:I:436:VAL:HB	1.95	0.48
1:K:378:GLN:H	1:K:386:PRO:HB3	1.78	0.48
1:L:248:LYS:HA	1:L:439:ARG:HG2	1.96	0.48
1:F:311:VAL:HA	1:F:312:THR:HA	1.60	0.48
1:F:341:LEU:HD13	1:F:344:LEU:HD22	1.95	0.48
1:F:424:GLU:N	1:F:433:ALA:O	2.47	0.48
1:I:377:GLY:HA2	1:I:386:PRO:HA	1.96	0.48
1:K:398:ASN:HA	1:K:456:ALA:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:O	1:A:282:SER:OG	2.29	0.48
1:B:207:THR:HA	1:B:243:HIS:HA	1.96	0.48
1:C:175:GLU:HG2	1:C:423:ARG:HH11	1.78	0.48
1:C:248:LYS:HD2	1:C:249:LEU:C	2.39	0.48
1:C:389:VAL:O	1:C:391:GLU:N	2.45	0.48
1:D:188:LYS:HB3	1:D:188:LYS:HE2	1.63	0.48
1:D:278:ALA:HB1	1:E:217:ALA:HB2	1.94	0.48
1:E:349:SER:H	1:E:352:ALA:HB3	1.79	0.48
1:F:261:GLU:O	1:F:263:ALA:N	2.47	0.48
1:G:359:ASP:HB2	1:G:361:GLU:H	1.79	0.48
1:I:412:VAL:HG23	1:I:414:PRO:HD3	1.96	0.48
1:J:312:THR:OG1	1:J:313:GLU:N	2.46	0.48
1:J:327:ILE:O	1:J:331:ARG:HB3	2.13	0.48
1:K:397:ALA:HB3	1:K:457:ALA:HB2	1.95	0.48
1:L:192:VAL:HG22	1:L:288:MET:HE2	1.95	0.48
1:M:419:VAL:HB	1:M:438:GLN:HA	1.95	0.48
1:A:249:LEU:HB2	1:A:438:GLN:HB2	1.96	0.47
1:A:389:VAL:O	1:A:391:GLU:N	2.47	0.47
1:C:372:SER:H	1:C:373:VAL:HA	1.78	0.47
1:D:203:SER:O	1:D:416:GLN:NE2	2.47	0.47
1:D:405:ILE:HB	1:D:450:VAL:HG23	1.96	0.47
1:F:289:THR:HG22	1:F:300:LEU:HD12	1.96	0.47
1:H:256:THR:OG1	1:H:430:GLN:O	2.32	0.47
1:K:297:LYS:HB3	1:K:442:LEU:HD23	1.96	0.47
1:L:206:LEU:O	1:L:244:PHE:N	2.47	0.47
1:A:272:ARG:NH1	1:A:423:ARG:HH12	2.12	0.47
1:A:353:TYR:O	1:A:357:LEU:N	2.35	0.47
1:C:307:SER:O	1:C:307:SER:OG	2.26	0.47
1:C:424:GLU:HB3	1:C:435:TYR:HE2	1.78	0.47
1:E:333:LYS:O	1:E:336:ARG:NE	2.47	0.47
1:F:413:MET:HG3	1:F:442:LEU:HB2	1.97	0.47
1:G:243:HIS:O	1:G:443:GLN:NE2	2.47	0.47
1:G:424:GLU:N	1:G:433:ALA:O	2.47	0.47
1:K:278:ALA:O	1:K:282:SER:OG	2.32	0.47
1:L:181:ARG:HD3	1:L:182:ILE:HG13	1.96	0.47
1:L:370:ASN:HB3	1:L:373:VAL:HG22	1.96	0.47
1:L:396:LYS:HE2	1:L:396:LYS:HB3	1.61	0.47
1:M:249:LEU:HB2	1:M:438:GLN:HB3	1.95	0.47
1:C:280:ALA:HA	1:C:283:ILE:HD12	1.96	0.47
1:E:359:ASP:N	1:E:359:ASP:OD1	2.47	0.47
1:F:172:GLU:OE1	1:F:423:ARG:NE	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:VAL:HB	1:F:451:VAL:HG23	1.97	0.47
1:G:301:THR:OG1	1:G:302:LEU:N	2.45	0.47
1:G:415:ARG:HB2	1:G:438:GLN:HE22	1.79	0.47
1:J:276:ILE:H	1:J:276:ILE:HG12	1.37	0.47
1:L:288:MET:O	1:L:299:LEU:N	2.47	0.47
1:B:257:ASP:OD1	1:B:434:TYR:OH	2.32	0.47
1:C:422:GLU:N	1:C:435:TYR:O	2.40	0.47
1:F:239:LEU:HD13	1:F:239:LEU:HA	1.78	0.47
1:F:326:THR:OG1	1:F:327:ILE:N	2.46	0.47
1:G:284:GLU:HA	1:G:287:PHE:HB2	1.96	0.47
1:G:297:LYS:NZ	1:G:305:GLU:OE2	2.39	0.47
1:K:170:SER:OG	1:K:171:SER:O	2.31	0.47
1:A:288:MET:HE1	1:A:300:LEU:HG	1.96	0.47
1:A:317:ASP:OD1	1:A:317:ASP:N	2.47	0.47
1:C:196:PHE:HB3	1:C:197:GLU:H	1.56	0.47
1:C:220:VAL:HG22	1:C:222:ALA:H	1.79	0.47
1:D:333:LYS:O	1:D:336:ARG:NH1	2.47	0.47
1:E:180:GLN:OE1	1:E:272:ARG:NE	2.47	0.47
1:E:199:LEU:HD23	1:E:414:PRO:HB3	1.95	0.47
1:E:244:PHE:HE1	1:E:443:GLN:HB3	1.79	0.47
1:F:230:THR:O	1:F:230:THR:OG1	2.33	0.47
1:I:250:ALA:HB3	1:J:220:VAL:HB	1.97	0.47
1:K:228:ASP:OD1	1:K:228:ASP:N	2.38	0.47
1:M:343:LYS:HG3	1:M:408:LYS:HD2	1.96	0.47
1:M:345:VAL:HG12	1:M:386:PRO:HD2	1.96	0.47
1:A:180:GLN:CD	1:A:272:ARG:HE	2.23	0.47
1:A:339:LEU:HD22	1:A:340:LYS:H	1.79	0.47
1:C:205:ILE:HG12	1:C:245:SER:HA	1.95	0.47
1:D:272:ARG:HB3	1:D:276:ILE:HD11	1.96	0.47
1:G:336:ARG:HB2	1:G:337:HIS:CE1	2.49	0.47
1:H:267:LEU:HD12	1:H:267:LEU:HA	1.78	0.47
1:H:395:ALA:HB3	1:H:396:LYS:HE3	1.97	0.47
1:J:187:GLN:HE22	1:J:190:LEU:HD13	1.78	0.47
1:A:323:THR:O	1:A:326:THR:OG1	2.33	0.47
1:A:362:TRP:HA	1:A:366:ALA:H	1.80	0.47
1:B:273:LYS:HE2	1:B:273:LYS:HB2	1.74	0.47
1:B:423:ARG:HA	1:B:434:TYR:HD1	1.79	0.47
1:C:252:LYS:HZ1	1:C:434:TYR:H	1.63	0.47
1:D:333:LYS:HA	1:D:336:ARG:NH2	2.29	0.47
1:E:211:GLU:HB3	1:E:238:ALA:H	1.80	0.47
1:F:240:LYS:NZ	1:F:241:GLU:O	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:GLU:OE2	1:G:437:THR:OG1	2.27	0.47
1:H:208:MET:HE2	1:H:208:MET:HB3	1.75	0.47
1:H:315:LYS:HE3	1:H:321:LEU:HD12	1.96	0.47
1:I:180:GLN:HG3	1:I:272:ARG:CZ	2.45	0.47
1:I:298:GLY:O	1:I:301:THR:OG1	2.24	0.47
1:J:273:LYS:H	1:J:276:ILE:HD11	1.78	0.47
1:J:317:ASP:OD1	1:J:317:ASP:N	2.44	0.47
1:J:339:LEU:H	1:J:339:LEU:HG	1.41	0.47
1:K:330:LEU:HA	1:K:333:LYS:HB2	1.96	0.47
1:M:410:ASN:HD22	1:M:444:ARG:NH2	2.12	0.47
1:A:427:ALA:HB1	1:A:431:ARG:HH22	1.80	0.47
1:B:260:GLU:HG2	1:B:264:ILE:HD12	1.96	0.47
1:C:311:VAL:HA	1:C:312:THR:HA	1.69	0.47
1:F:208:MET:HB2	1:F:242:ILE:HB	1.96	0.47
1:J:228:ASP:H	1:J:229:THR:HG23	1.78	0.47
1:A:267:LEU:HG	1:A:271:LEU:HG	1.96	0.47
1:F:253:SER:N	1:F:434:TYR:O	2.48	0.47
1:G:176:THR:OG1	1:G:423:ARG:NH1	2.48	0.47
1:G:201:MET:HE3	1:G:201:MET:HB3	1.68	0.47
1:H:399:SER:HB2	1:H:455:TYR:HE2	1.80	0.47
1:J:212:PRO:O	1:J:214:ALA:N	2.48	0.47
1:J:249:LEU:HB3	1:K:219:TRP:CZ2	2.50	0.47
1:L:330:LEU:HA	1:L:333:LYS:HB2	1.97	0.47
1:L:372:SER:H	1:L:373:VAL:HA	1.80	0.47
1:C:186:LEU:HG	1:C:187:GLN:HG2	1.96	0.47
1:C:359:ASP:OD1	1:C:367:GLN:NE2	2.44	0.47
1:C:403:ALA:HA	1:C:452:SER:HA	1.97	0.47
1:D:172:GLU:OE1	1:D:423:ARG:NE	2.48	0.47
1:E:401:GLU:H	1:E:401:GLU:HG2	1.56	0.47
1:F:334:LEU:HD21	1:F:406:VAL:HG12	1.96	0.47
1:H:328:SER:O	1:H:332:ARG:NE	2.48	0.47
1:K:171:SER:OG	1:K:175:GLU:OE2	2.29	0.47
1:K:249:LEU:N	1:K:438:GLN:O	2.48	0.47
1:K:264:ILE:O	1:K:266:SER:N	2.48	0.47
1:L:272:ARG:CZ	1:L:275:LEU:HD12	2.45	0.47
1:C:339:LEU:HD13	1:C:340:LYS:H	1.79	0.46
1:G:207:THR:HA	1:G:243:HIS:HA	1.96	0.46
1:H:211:GLU:HG3	1:H:238:ALA:O	2.15	0.46
1:H:444:ARG:HD3	1:H:446:PHE:H	1.80	0.46
1:I:216:LYS:HD3	1:I:218:THR:HG23	1.97	0.46
1:I:278:ALA:O	1:I:282:SER:OG	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:300:LEU:O	1:J:304:SER:OG	2.26	0.46
1:J:414:PRO:HD2	1:J:441:ASN:C	2.40	0.46
1:A:292:GLY:N	1:A:296:PRO:O	2.48	0.46
1:B:199:LEU:HD12	1:B:200:PRO:HD2	1.98	0.46
1:C:172:GLU:H	1:C:423:ARG:NH1	2.13	0.46
1:F:240:LYS:HG2	1:F:243:HIS:CE1	2.50	0.46
1:F:367:GLN:HG2	1:F:368:VAL:HA	1.97	0.46
1:I:224:THR:OG1	1:I:225:TYR:N	2.48	0.46
1:K:336:ARG:O	1:K:337:HIS:ND1	2.48	0.46
1:B:212:PRO:HD2	1:B:240:LYS:H	1.81	0.46
1:C:249:LEU:O	1:C:438:GLN:N	2.36	0.46
1:D:300:LEU:O	1:D:304:SER:OG	2.33	0.46
1:D:362:TRP:CD1	1:D:367:GLN:H	2.33	0.46
1:D:370:ASN:ND2	1:D:372:SER:OG	2.49	0.46
1:D:414:PRO:HG2	1:D:441:ASN:HB3	1.97	0.46
1:E:264:ILE:HB	1:E:267:LEU:HD22	1.97	0.46
1:G:249:LEU:HD11	1:G:296:PRO:HD3	1.98	0.46
1:G:401:GLU:H	1:G:453:GLY:HA2	1.80	0.46
1:I:212:PRO:HB2	1:I:213:ASP:H	1.52	0.46
1:I:267:LEU:HB3	1:I:271:LEU:HD12	1.97	0.46
1:J:417:ARG:CZ	1:J:439:ARG:HG3	2.44	0.46
1:K:208:MET:HB2	1:K:242:ILE:HD12	1.97	0.46
1:K:370:ASN:OD1	1:K:370:ASN:N	2.46	0.46
1:L:264:ILE:O	1:L:266:SER:N	2.47	0.46
1:L:328:SER:O	1:L:332:ARG:NH1	2.48	0.46
1:M:215:GLY:O	1:M:234:GLU:N	2.48	0.46
1:A:257:ASP:HA	1:A:260:GLU:HB2	1.98	0.46
1:A:279:HIS:CE1	1:A:283:ILE:HD11	2.51	0.46
1:B:183:ILE:HG21	1:B:273:LYS:HA	1.96	0.46
1:E:300:LEU:HD11	1:E:399:SER:HB3	1.98	0.46
1:G:331:ARG:HH11	1:G:341:LEU:HD11	1.80	0.46
1:I:246:THR:OG1	1:I:247:TYR:N	2.49	0.46
1:I:423:ARG:HA	1:I:434:TYR:HD1	1.80	0.46
1:K:268:LEU:O	1:K:272:ARG:HG3	2.15	0.46
1:L:187:GLN:HA	1:L:189:GLU:HB2	1.97	0.46
1:A:177:ILE:O	1:A:180:GLN:N	2.49	0.46
1:D:443:GLN:HE21	1:D:444:ARG:N	2.12	0.46
1:E:236:LYS:HA	1:E:237:GLY:HA2	1.61	0.46
1:E:432:ASP:HB3	1:E:434:TYR:CZ	2.50	0.46
1:E:455:TYR:HD1	1:E:455:TYR:HA	1.54	0.46
1:F:420:THR:O	1:F:437:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:LYS:HA	1:G:439:ARG:HA	1.97	0.46
1:I:272:ARG:HH11	1:I:276:ILE:HD11	1.80	0.46
1:I:411:PHE:H	1:I:444:ARG:HA	1.80	0.46
1:L:369:GLY:N	1:L:371:ASP:OD2	2.48	0.46
1:L:423:ARG:HG2	1:L:434:TYR:HB3	1.96	0.46
1:A:188:LYS:NZ	1:A:413:MET:SD	2.73	0.46
1:A:309:LYS:HB3	1:A:454:THR:HG23	1.97	0.46
1:A:414:PRO:HD2	1:A:441:ASN:C	2.41	0.46
1:B:171:SER:O	1:B:425:ARG:NH1	2.49	0.46
1:B:196:PHE:CZ	1:B:411:PHE:HB2	2.51	0.46
1:B:307:SER:O	1:B:307:SER:OG	2.32	0.46
1:B:429:LYS:HD2	1:B:431:ARG:HH11	1.81	0.46
1:H:267:LEU:HG	1:H:270:LEU:HB3	1.97	0.46
1:H:334:LEU:HD13	1:H:338:GLY:HA3	1.97	0.46
1:I:365:VAL:HG23	1:I:381:ARG:HH12	1.81	0.46
1:K:272:ARG:HH11	1:K:273:LYS:HA	1.79	0.46
1:M:184:ARG:HH12	1:M:415:ARG:HH11	1.64	0.46
1:M:199:LEU:HG	1:M:201:MET:HG2	1.97	0.46
1:A:316:ALA:HB2	1:A:455:TYR:HA	1.98	0.46
1:A:350:MET:O	1:A:354:TYR:HB2	2.16	0.46
1:B:212:PRO:HB2	1:B:238:ALA:HB3	1.98	0.46
1:B:372:SER:OG	1:B:373:VAL:O	2.29	0.46
1:B:381:ARG:NH2	1:B:384:GLY:H	2.13	0.46
1:D:415:ARG:HA	1:D:440:VAL:HA	1.97	0.46
1:G:209:LEU:HB3	1:G:239:LEU:HD11	1.98	0.46
1:H:240:LYS:HE3	1:H:240:LYS:HB3	1.82	0.46
1:H:248:LYS:HE3	1:H:248:LYS:HB3	1.67	0.46
1:J:215:GLY:HA2	1:J:235:VAL:HG22	1.97	0.46
1:J:306:ASP:OD2	1:J:444:ARG:NH1	2.46	0.46
1:J:426:GLN:HA	1:J:427:ALA:C	2.40	0.46
1:M:376:GLN:HG3	1:M:386:PRO:HG2	1.97	0.46
1:B:348:VAL:HG22	1:B:387:VAL:HG12	1.97	0.46
1:C:349:SER:HA	1:C:391:GLU:HG2	1.97	0.46
1:H:177:ILE:HG23	1:H:423:ARG:HH21	1.79	0.46
1:I:211:GLU:HG3	1:I:238:ALA:N	2.29	0.46
1:I:291:ASP:OD1	1:I:291:ASP:N	2.46	0.46
1:I:453:GLY:HA3	1:I:454:THR:HG23	1.98	0.46
1:K:246:THR:O	1:K:439:ARG:NH1	2.49	0.46
1:K:361:GLU:HB3	1:K:363:GLN:HB3	1.98	0.46
1:F:376:GLN:HE22	1:F:386:PRO:HG2	1.81	0.46
1:I:273:LYS:HA	1:I:276:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:381:ARG:HD2	1:I:384:GLY:HA2	1.98	0.46
1:J:297:LYS:HD3	1:J:297:LYS:HA	1.76	0.46
1:J:311:VAL:HA	1:J:312:THR:HA	1.69	0.46
1:J:448:ASN:OD1	1:J:449:GLY:N	2.49	0.46
1:K:219:TRP:HE3	1:K:221:ALA:HA	1.81	0.46
1:L:195:LEU:O	1:L:407:TYR:OH	2.29	0.46
1:L:257:ASP:N	1:L:432:ASP:OD1	2.37	0.46
1:A:267:LEU:HD22	1:B:206:LEU:HD21	1.97	0.46
1:A:405:ILE:HB	1:A:450:VAL:HB	1.96	0.46
1:B:205:ILE:HA	1:B:245:SER:HB3	1.97	0.46
1:G:204:LYS:HB3	1:G:205:ILE:H	1.57	0.46
1:G:346:LEU:HD13	1:G:404:VAL:HG22	1.98	0.46
1:H:311:VAL:HG12	1:H:312:THR:HA	1.98	0.46
1:I:327:ILE:HA	1:I:330:LEU:HB2	1.97	0.46
1:K:377:GLY:O	1:K:378:GLN:NE2	2.49	0.46
1:M:237:GLY:HA3	1:M:238:ALA:HA	1.67	0.46
1:M:245:SER:O	1:M:441:ASN:ND2	2.49	0.46
1:M:280:ALA:HA	1:M:283:ILE:HD12	1.97	0.46
1:M:380:GLY:O	1:M:387:VAL:N	2.47	0.46
1:D:351:ASP:OD1	1:D:351:ASP:N	2.46	0.45
1:E:260:GLU:HG3	1:E:264:ILE:HG13	1.98	0.45
1:G:368:VAL:HG21	1:H:365:VAL:HG12	1.98	0.45
1:H:350:MET:O	1:H:354:TYR:HB2	2.15	0.45
1:K:362:TRP:HA	1:K:365:VAL:HA	1.96	0.45
1:K:396:LYS:O	1:K:398:ASN:N	2.46	0.45
1:M:243:HIS:O	1:M:443:GLN:NE2	2.48	0.45
1:M:252:LYS:HG3	1:M:435:TYR:HA	1.97	0.45
1:A:272:ARG:HB3	1:A:273:LYS:H	1.49	0.45
1:A:284:GLU:HA	1:A:287:PHE:HB2	1.97	0.45
1:D:183:ILE:HB	1:D:276:ILE:HG21	1.99	0.45
1:E:230:THR:HA	1:E:231:THR:HA	1.72	0.45
1:E:314:ALA:HB3	1:E:455:TYR:HA	1.98	0.45
1:G:230:THR:HA	1:G:231:THR:HA	1.61	0.45
1:H:314:ALA:H	1:H:455:TYR:H	1.64	0.45
1:I:201:MET:HE2	1:I:201:MET:HB3	1.81	0.45
1:J:310:VAL:O	1:J:454:THR:N	2.35	0.45
1:J:346:LEU:HB2	1:J:404:VAL:HG13	1.98	0.45
1:K:199:LEU:HD23	1:K:414:PRO:HB3	1.97	0.45
1:L:201:MET:N	1:L:415:ARG:O	2.39	0.45
1:L:345:VAL:HG23	1:L:405:ILE:HG23	1.97	0.45
1:M:334:LEU:HD12	1:M:344:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HA	1:A:231:THR:HA	1.70	0.45
1:C:288:MET:HA	1:C:299:LEU:HB2	1.98	0.45
1:D:278:ALA:HA	1:D:281:VAL:HB	1.98	0.45
1:F:291:ASP:OD1	1:F:291:ASP:N	2.40	0.45
1:G:272:ARG:HD2	1:G:272:ARG:HA	1.70	0.45
1:G:285:GLU:O	1:G:289:THR:OG1	2.26	0.45
1:H:284:GLU:HA	1:H:287:PHE:CD2	2.52	0.45
1:H:325:LYS:NZ	1:H:363:GLN:OE1	2.30	0.45
1:H:406:VAL:HG22	1:H:409:ASP:N	2.31	0.45
1:J:197:GLU:O	1:J:413:MET:N	2.40	0.45
1:J:342:SER:HA	1:J:343:LYS:HD3	1.97	0.45
1:K:249:LEU:O	1:K:438:GLN:N	2.49	0.45
1:K:324:ALA:HB1	1:K:327:ILE:HB	1.97	0.45
1:L:351:ASP:HA	1:L:354:TYR:CE2	2.51	0.45
1:A:212:PRO:HG2	1:A:238:ALA:HB3	1.98	0.45
1:A:276:ILE:H	1:A:276:ILE:HG12	1.49	0.45
1:B:363:GLN:CD	1:B:364:ASP:H	2.23	0.45
1:C:313:GLU:OE1	1:C:326:THR:OG1	2.35	0.45
1:D:253:SER:O	1:D:434:TYR:N	2.42	0.45
1:D:271:LEU:HG	1:D:274:ARG:HH12	1.81	0.45
1:D:279:HIS:CE1	1:D:438:GLN:HG3	2.52	0.45
1:G:181:ARG:HH11	1:G:184:ARG:HH12	1.63	0.45
1:H:249:LEU:O	1:H:438:GLN:N	2.49	0.45
1:H:280:ALA:HA	1:H:283:ILE:HB	1.99	0.45
1:H:295:LYS:HZ3	1:H:295:LYS:HG3	1.71	0.45
1:J:292:GLY:N	1:J:296:PRO:O	2.46	0.45
1:M:340:LYS:HD3	1:M:340:LYS:HA	1.62	0.45
1:M:441:ASN:OD1	1:M:442:LEU:N	2.50	0.45
1:A:401:GLU:OE2	1:A:455:TYR:N	2.50	0.45
1:B:362:TRP:CZ2	1:B:367:GLN:HB2	2.52	0.45
1:C:252:LYS:HZ2	1:C:253:SER:N	2.14	0.45
1:C:367:GLN:HA	1:C:368:VAL:HA	1.66	0.45
1:D:378:GLN:HB2	1:D:386:PRO:HB2	1.97	0.45
1:J:197:GLU:HG2	1:J:412:VAL:HA	1.99	0.45
1:K:272:ARG:NH1	1:K:276:ILE:H	2.14	0.45
1:A:312:THR:OG1	1:A:314:ALA:O	2.35	0.45
1:A:362:TRP:CD1	1:A:365:VAL:HA	2.52	0.45
1:C:176:THR:H	1:C:423:ARG:NH1	2.15	0.45
1:C:332:ARG:HH11	1:C:332:ARG:HA	1.80	0.45
1:E:183:ILE:HG21	1:E:273:LYS:HG2	1.99	0.45
1:E:198:GLU:HA	1:E:413:MET:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LYS:NZ	1:E:336:ARG:HE	2.14	0.45
1:F:288:MET:HE2	1:F:392:TYR:HB3	1.99	0.45
1:G:417:ARG:HB2	1:G:418:ALA:H	1.53	0.45
1:H:249:LEU:HB3	1:I:219:TRP:CH2	2.51	0.45
1:H:264:ILE:HG21	1:H:267:LEU:HB2	1.99	0.45
1:H:421:VAL:HA	1:H:436:VAL:HA	1.99	0.45
1:J:175:GLU:HG2	1:J:176:THR:H	1.80	0.45
1:J:176:THR:HG1	1:J:180:GLN:HE22	1.56	0.45
1:J:275:LEU:HD12	1:J:276:ILE:HG23	1.97	0.45
1:J:415:ARG:HA	1:J:440:VAL:HA	1.99	0.45
1:K:183:ILE:HD13	1:K:273:LYS:HB3	1.99	0.45
1:K:230:THR:HA	1:K:231:THR:HA	1.60	0.45
1:L:244:PHE:HD1	1:L:414:PRO:HG3	1.80	0.45
1:L:256:THR:HG23	1:L:258:GLU:HG3	1.98	0.45
1:A:291:ASP:N	1:A:296:PRO:O	2.50	0.45
1:A:349:SER:N	1:A:352:ALA:HB3	2.32	0.45
1:B:291:ASP:H	1:B:295:LYS:HE2	1.80	0.45
1:C:184:ARG:O	1:C:188:LYS:N	2.40	0.45
1:D:389:VAL:O	1:D:391:GLU:N	2.50	0.45
1:D:423:ARG:HA	1:D:434:TYR:HA	1.98	0.45
1:E:417:ARG:HB2	1:E:418:ALA:H	1.59	0.45
1:F:331:ARG:HE	1:F:332:ARG:NE	2.15	0.45
1:G:241:GLU:OE1	1:G:242:ILE:N	2.50	0.45
1:G:291:ASP:OD1	1:G:295:LYS:NZ	2.48	0.45
1:G:350:MET:N	1:G:391:GLU:OE1	2.50	0.45
1:H:354:TYR:CZ	1:I:332:ARG:HG3	2.52	0.45
1:J:431:ARG:HB2	1:J:432:ASP:H	1.54	0.45
1:K:170:SER:OG	1:K:171:SER:N	2.49	0.45
1:K:300:LEU:O	1:K:304:SER:OG	2.25	0.45
1:L:240:LYS:HE3	1:L:242:ILE:HA	1.97	0.45
1:L:280:ALA:HA	1:L:283:ILE:HB	1.97	0.45
1:L:313:GLU:H	1:L:455:TYR:H	1.63	0.45
1:A:420:THR:N	1:A:437:THR:OG1	2.46	0.45
1:B:333:LYS:HZ3	1:B:333:LYS:HG2	1.62	0.45
1:B:346:LEU:HB2	1:B:404:VAL:HG13	1.99	0.45
1:C:331:ARG:HH21	1:C:332:ARG:NE	2.15	0.45
1:D:313:GLU:HG2	1:D:454:THR:H	1.82	0.45
1:F:173:SER:N	1:F:175:GLU:OE2	2.49	0.45
1:F:295:LYS:HD3	1:F:295:LYS:H	1.82	0.45
1:F:347:ILE:HB	1:F:403:ALA:HB3	1.99	0.45
1:G:331:ARG:O	1:G:332:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:LEU:HB2	1:H:385:LEU:HD23	1.99	0.45
1:I:289:THR:HG23	1:I:393:PHE:HE1	1.82	0.45
1:I:385:LEU:HD12	1:I:385:LEU:HA	1.77	0.45
1:J:236:LYS:HA	1:J:237:GLY:HA3	1.71	0.45
1:J:285:GLU:O	1:J:289:THR:OG1	2.30	0.45
1:K:178:PHE:HA	1:K:181:ARG:HG2	1.99	0.45
1:K:367:GLN:HA	1:K:368:VAL:HA	1.72	0.45
1:A:301:THR:O	1:A:305:GLU:N	2.39	0.45
1:B:196:PHE:HB3	1:B:197:GLU:H	1.55	0.45
1:B:290:GLY:O	1:B:298:GLY:N	2.50	0.45
1:C:420:THR:OG1	1:C:437:THR:OG1	2.31	0.45
1:G:291:ASP:OD1	1:G:291:ASP:N	2.42	0.45
1:H:264:ILE:HD13	1:H:267:LEU:HD22	1.99	0.45
1:J:176:THR:O	1:J:180:GLN:NE2	2.49	0.45
1:J:340:LYS:O	1:J:342:SER:OG	2.35	0.45
1:K:330:LEU:HD12	1:K:333:LYS:HD3	1.98	0.45
1:M:195:LEU:HD12	1:M:195:LEU:HA	1.77	0.45
1:D:212:PRO:O	1:D:214:ALA:N	2.50	0.45
1:D:356:LEU:HD22	1:D:356:LEU:HA	1.84	0.45
1:E:288:MET:C	1:E:299:LEU:H	2.25	0.45
1:G:241:GLU:OE2	1:G:243:HIS:ND1	2.41	0.45
1:I:278:ALA:HA	1:I:281:VAL:HB	1.98	0.45
1:J:274:ARG:HH11	1:K:208:MET:HE1	1.82	0.45
1:K:357:LEU:HA	1:K:367:GLN:HE22	1.81	0.45
1:K:396:LYS:HE3	1:K:396:LYS:HB3	1.70	0.45
1:L:351:ASP:HA	1:L:354:TYR:HE2	1.82	0.45
1:A:208:MET:H	1:A:209:LEU:HD12	1.82	0.44
1:C:216:LYS:H	1:C:216:LYS:HG3	1.46	0.44
1:C:320:VAL:HG11	1:C:455:TYR:HE1	1.81	0.44
1:C:417:ARG:NH1	1:C:419:VAL:HA	2.32	0.44
1:E:353:TYR:CG	1:E:357:LEU:HB2	2.51	0.44
1:F:176:THR:N	1:F:423:ARG:HH22	2.15	0.44
1:H:330:LEU:HD23	1:H:404:VAL:HG21	1.98	0.44
1:K:214:ALA:HB3	1:K:237:GLY:H	1.82	0.44
1:K:247:TYR:HA	1:K:439:ARG:HH11	1.82	0.44
1:K:284:GLU:HA	1:K:287:PHE:HB2	1.99	0.44
1:A:196:PHE:HB3	1:A:197:GLU:H	1.50	0.44
1:A:301:THR:OG1	1:A:302:LEU:N	2.49	0.44
1:B:177:ILE:HG23	1:B:423:ARG:HD2	1.99	0.44
1:C:213:ASP:OD1	1:C:213:ASP:N	2.49	0.44
1:E:201:MET:HE2	1:E:201:MET:HB3	1.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:LYS:HA	1:E:297:LYS:HD2	1.81	0.44
1:E:299:LEU:O	1:E:303:ALA:N	2.42	0.44
1:F:421:VAL:HG13	1:F:436:VAL:HG22	1.99	0.44
1:J:211:GLU:HG3	1:J:239:LEU:N	2.31	0.44
1:J:256:THR:OG1	1:J:430:GLN:O	2.28	0.44
1:K:353:TYR:CE1	1:K:357:LEU:HD13	2.51	0.44
1:A:208:MET:SD	1:F:267:LEU:HB3	2.57	0.44
1:A:272:ARG:HG2	1:A:276:ILE:HD11	1.98	0.44
1:B:343:LYS:HB2	1:B:408:LYS:HG2	1.99	0.44
1:C:237:GLY:HA3	1:C:238:ALA:HA	1.76	0.44
1:D:398:ASN:HA	1:D:456:ALA:HA	1.98	0.44
1:F:181:ARG:HB2	1:F:181:ARG:HE	1.62	0.44
1:G:187:GLN:HE22	1:G:189:GLU:HB3	1.83	0.44
1:G:398:ASN:HA	1:G:456:ALA:HA	2.00	0.44
1:H:446:PHE:HB3	1:H:447:ALA:H	1.59	0.44
1:J:382:ILE:HD13	1:J:387:VAL:HB	1.98	0.44
1:K:262:ASP:OD1	1:K:262:ASP:N	2.50	0.44
1:L:347:ILE:HA	1:L:388:VAL:HB	1.98	0.44
1:M:410:ASN:HD22	1:M:444:ARG:HH22	1.63	0.44
1:A:235:VAL:HB	1:A:236:LYS:H	1.67	0.44
1:A:265:PHE:HA	1:A:268:LEU:HD21	2.00	0.44
1:A:353:TYR:CE2	1:A:357:LEU:HD22	2.53	0.44
1:A:368:VAL:O	1:A:381:ARG:N	2.51	0.44
1:A:410:ASN:HA	1:A:445:TYR:HD2	1.82	0.44
1:D:331:ARG:HD3	1:D:341:LEU:HD11	1.99	0.44
1:G:173:SER:H	1:G:423:ARG:NH2	2.15	0.44
1:G:241:GLU:CD	1:G:243:HIS:HD1	2.25	0.44
1:G:300:LEU:O	1:G:304:SER:HB3	2.18	0.44
1:H:205:ILE:HA	1:H:245:SER:HB3	1.99	0.44
1:I:247:TYR:N	1:I:441:ASN:OD1	2.35	0.44
1:I:395:ALA:N	1:I:396:LYS:HZ3	2.15	0.44
1:K:378:GLN:HG2	1:K:388:VAL:HG22	1.99	0.44
1:C:379:VAL:HG13	1:C:389:VAL:H	1.82	0.44
1:C:398:ASN:HA	1:C:456:ALA:HA	1.99	0.44
1:D:429:LYS:HB2	1:D:431:ARG:HG3	2.00	0.44
1:H:285:GLU:HG3	1:H:392:TYR:CG	2.53	0.44
1:I:254:PHE:CZ	1:J:211:GLU:HB2	2.52	0.44
1:J:181:ARG:HH11	1:J:418:ALA:HB2	1.82	0.44
1:K:237:GLY:HA3	1:K:238:ALA:HA	1.83	0.44
1:K:402:PHE:O	1:K:452:SER:HB3	2.18	0.44
1:K:425:ARG:HB2	1:K:426:GLN:H	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:271:LEU:HD12	1:M:271:LEU:HA	1.83	0.44
1:B:182:ILE:H	1:B:182:ILE:HG13	1.52	0.44
1:B:230:THR:HA	1:B:231:THR:HA	1.66	0.44
1:B:340:LYS:O	1:B:342:SER:OG	2.29	0.44
1:D:178:PHE:O	1:D:181:ARG:NH1	2.51	0.44
1:D:202:SER:OG	1:D:203:SER:N	2.43	0.44
1:D:367:GLN:HA	1:D:368:VAL:HA	1.81	0.44
1:E:309:LYS:H	1:E:309:LYS:HG2	1.43	0.44
1:E:311:VAL:HA	1:E:312:THR:HA	1.73	0.44
1:F:188:LYS:H	1:F:188:LYS:HG3	1.52	0.44
1:G:272:ARG:O	1:G:274:ARG:N	2.49	0.44
1:G:454:THR:HG23	1:G:456:ALA:HB2	1.99	0.44
1:H:171:SER:O	1:H:173:SER:OG	2.34	0.44
1:J:446:PHE:HB3	1:J:447:ALA:H	1.64	0.44
1:K:221:ALA:HB3	1:K:223:SER:HB2	1.99	0.44
1:K:268:LEU:H	1:K:268:LEU:HG	1.25	0.44
1:B:426:GLN:CD	1:B:428:GLY:HA2	2.43	0.44
1:C:364:ASP:OD2	1:C:364:ASP:N	2.48	0.44
1:D:378:GLN:H	1:D:386:PRO:HB2	1.82	0.44
1:G:406:VAL:HG22	1:G:408:LYS:H	1.82	0.44
1:H:251:ALA:N	1:H:436:VAL:O	2.43	0.44
1:I:184:ARG:O	1:I:184:ARG:NH2	2.51	0.44
1:I:297:LYS:HA	1:I:297:LYS:HD2	1.65	0.44
1:I:339:LEU:O	1:I:340:LYS:NZ	2.44	0.44
1:J:348:VAL:HG21	1:J:353:TYR:HB2	2.00	0.44
1:J:411:PHE:H	1:J:444:ARG:HA	1.83	0.44
1:J:444:ARG:HB2	1:J:445:TYR:H	1.55	0.44
1:M:353:TYR:HA	1:M:356:LEU:HD12	1.99	0.44
1:B:269:PRO:O	1:B:272:ARG:N	2.50	0.44
1:B:394:PRO:HB2	1:B:396:LYS:HZ1	1.83	0.44
1:D:353:TYR:HB3	1:E:332:ARG:HH22	1.83	0.44
1:G:181:ARG:HE	1:G:181:ARG:HB2	1.63	0.44
1:H:278:ALA:HA	1:H:281:VAL:HB	1.99	0.44
1:H:280:ALA:HA	1:H:283:ILE:HD12	2.00	0.44
1:I:347:ILE:HG23	1:I:388:VAL:HB	2.00	0.44
1:L:317:ASP:OD1	1:L:455:TYR:OH	2.36	0.44
1:A:201:MET:SD	1:A:416:GLN:NE2	2.90	0.44
1:B:220:VAL:HG21	1:B:226:GLY:HA2	2.00	0.44
1:C:314:ALA:N	1:C:455:TYR:H	2.16	0.44
1:C:326:THR:HA	1:C:329:LYS:HE3	2.00	0.44
1:C:367:GLN:NE2	1:C:368:VAL:HG23	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LEU:HD12	1:D:240:LYS:H	1.82	0.44
1:D:272:ARG:HE	1:D:276:ILE:HD11	1.82	0.44
1:E:300:LEU:O	1:E:304:SER:OG	2.21	0.44
1:E:340:LYS:HD3	1:E:340:LYS:HA	1.69	0.44
1:F:412:VAL:HG23	1:F:414:PRO:HD3	2.00	0.44
1:G:214:ALA:HB3	1:G:237:GLY:H	1.83	0.44
1:G:345:VAL:N	1:G:405:ILE:O	2.30	0.44
1:H:242:ILE:HA	1:H:244:PHE:CZ	2.52	0.44
1:H:376:GLN:O	1:H:378:GLN:N	2.51	0.44
1:I:173:SER:HB2	1:I:174:TYR:H	1.64	0.44
1:J:448:ASN:OD1	1:J:450:VAL:N	2.38	0.44
1:L:237:GLY:HA3	1:L:238:ALA:HA	1.77	0.44
1:A:175:GLU:HG2	1:A:176:THR:HG22	2.00	0.43
1:A:207:THR:HG23	1:A:243:HIS:HB3	2.00	0.43
1:B:173:SER:N	1:B:175:GLU:OE2	2.49	0.43
1:B:176:THR:O	1:B:179:SER:OG	2.31	0.43
1:D:252:LYS:HA	1:D:436:VAL:H	1.83	0.43
1:D:330:LEU:HA	1:D:451:VAL:HG11	1.99	0.43
1:E:350:MET:HA	1:E:353:TYR:HB2	1.99	0.43
1:G:429:LYS:HB2	1:G:431:ARG:NE	2.33	0.43
1:H:172:GLU:O	1:H:425:ARG:NE	2.51	0.43
1:H:288:MET:HG3	1:H:392:TYR:HD2	1.83	0.43
1:H:379:VAL:HG13	1:H:389:VAL:HG23	1.99	0.43
1:I:316:ALA:HB1	1:I:397:ALA:HB1	2.00	0.43
1:J:395:ALA:O	1:J:399:SER:OG	2.30	0.43
1:K:257:ASP:HB2	1:K:431:ARG:HA	2.00	0.43
1:K:302:LEU:HD22	1:K:411:PHE:HE2	1.83	0.43
1:M:253:SER:O	1:M:434:TYR:N	2.37	0.43
1:A:341:LEU:HD13	1:A:341:LEU:HA	1.76	0.43
1:A:362:TRP:CD1	1:A:367:GLN:HG2	2.53	0.43
1:D:309:LYS:H	1:D:309:LYS:HG3	1.51	0.43
1:E:351:ASP:HA	1:E:354:TYR:HB2	2.00	0.43
1:F:216:LYS:HB3	1:F:218:THR:HG22	2.01	0.43
1:I:411:PHE:HB3	1:I:442:LEU:HD11	2.00	0.43
1:J:300:LEU:HA	1:J:303:ALA:HB3	2.00	0.43
1:K:308:ALA:HA	1:K:451:VAL:HA	1.99	0.43
1:L:275:LEU:H	1:L:275:LEU:HG	1.52	0.43
1:A:208:MET:HE3	1:F:274:ARG:NH1	2.34	0.43
1:A:218:THR:O	1:F:251:ALA:HA	2.18	0.43
1:B:381:ARG:HD2	1:B:384:GLY:HA2	2.00	0.43
1:D:170:SER:OG	1:D:175:GLU:OE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:LYS:HA	1:D:436:VAL:N	2.34	0.43
1:E:298:GLY:C	1:E:301:THR:HG1	2.23	0.43
1:G:179:SER:HA	1:G:182:ILE:HD12	1.99	0.43
1:G:213:ASP:N	1:G:213:ASP:OD1	2.51	0.43
1:H:246:THR:HB	1:H:441:ASN:HB2	2.00	0.43
1:I:209:LEU:HA	1:I:241:GLU:HG3	2.00	0.43
1:I:241:GLU:HB2	1:I:242:ILE:HG12	2.00	0.43
1:J:249:LEU:HB2	1:J:438:GLN:HB3	1.99	0.43
1:J:346:LEU:HA	1:J:404:VAL:HA	2.00	0.43
1:J:382:ILE:O	1:J:385:LEU:N	2.52	0.43
1:M:240:LYS:HZ3	1:M:240:LYS:HG2	1.67	0.43
1:A:267:LEU:HD12	1:A:270:LEU:HB3	1.99	0.43
1:B:176:THR:OG1	1:B:423:ARG:NH1	2.51	0.43
1:C:177:ILE:O	1:C:180:GLN:HG2	2.18	0.43
1:D:252:LYS:O	1:E:218:THR:OG1	2.31	0.43
1:D:353:TYR:CE1	1:D:357:LEU:HD13	2.53	0.43
1:E:248:LYS:HE3	1:E:248:LYS:HB2	1.80	0.43
1:H:189:GLU:N	1:H:189:GLU:OE1	2.52	0.43
1:H:272:ARG:HH22	1:H:423:ARG:HH22	1.65	0.43
1:I:285:GLU:HG3	1:I:392:TYR:CG	2.53	0.43
1:I:323:THR:HG1	1:I:363:GLN:CD	2.27	0.43
1:K:236:LYS:HZ3	1:K:236:LYS:HG2	1.67	0.43
1:L:412:VAL:O	1:L:443:GLN:N	2.38	0.43
1:L:441:ASN:OD1	1:L:442:LEU:N	2.52	0.43
1:M:217:ALA:HB2	1:M:234:GLU:HG3	2.01	0.43
1:A:181:ARG:H	1:A:181:ARG:HG3	1.64	0.43
1:B:414:PRO:O	1:B:441:ASN:N	2.52	0.43
1:D:348:VAL:N	1:D:388:VAL:O	2.30	0.43
1:F:346:LEU:HB3	1:F:387:VAL:HG13	2.00	0.43
1:G:270:LEU:O	1:G:273:LYS:NZ	2.51	0.43
1:G:350:MET:HE3	1:H:332:ARG:HD2	2.00	0.43
1:I:202:SER:O	1:I:416:GLN:NE2	2.52	0.43
1:I:236:LYS:HA	1:I:237:GLY:HA2	1.60	0.43
1:J:364:ASP:HB2	1:J:365:VAL:H	1.52	0.43
1:J:374:LYS:HB3	1:J:375:LEU:H	1.50	0.43
1:K:240:LYS:HE3	1:K:242:ILE:HA	2.00	0.43
1:K:401:GLU:H	1:K:401:GLU:HG2	1.70	0.43
1:L:176:THR:O	1:L:423:ARG:NH2	2.51	0.43
1:M:197:GLU:H	1:M:412:VAL:HB	1.84	0.43
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.84	0.43
1:C:201:MET:HE2	1:C:202:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LEU:HD11	1:D:208:MET:HE2	2.01	0.43
1:C:379:VAL:N	1:C:387:VAL:O	2.52	0.43
1:E:195:LEU:HD12	1:E:195:LEU:HA	1.68	0.43
1:E:249:LEU:HA	1:F:219:TRP:CZ3	2.52	0.43
1:E:376:GLN:HB3	1:E:378:GLN:CD	2.43	0.43
1:G:446:PHE:HB3	1:G:447:ALA:H	1.56	0.43
1:H:253:SER:HB2	1:H:434:TYR:HB2	2.00	0.43
1:I:199:LEU:N	1:I:413:MET:O	2.51	0.43
1:I:308:ALA:HB1	1:I:451:VAL:HG13	2.00	0.43
1:K:330:LEU:HG	1:K:451:VAL:HB	2.00	0.43
1:L:254:PHE:HB3	1:L:433:ALA:HA	2.01	0.43
1:M:311:VAL:HA	1:M:312:THR:HA	1.62	0.43
1:M:311:VAL:HG13	1:M:454:THR:HB	1.99	0.43
1:A:171:SER:OG	1:A:261:GLU:OE2	2.32	0.43
1:A:272:ARG:O	1:A:273:LYS:NZ	2.42	0.43
1:A:423:ARG:HA	1:A:434:TYR:CD1	2.52	0.43
1:D:287:PHE:HD1	1:D:287:PHE:HA	1.73	0.43
1:D:302:LEU:HA	1:D:305:GLU:HG2	2.01	0.43
1:E:207:THR:HA	1:E:243:HIS:HA	1.99	0.43
1:F:316:ALA:HA	1:F:457:ALA:HA	2.00	0.43
1:H:231:THR:OG1	1:H:234:GLU:OE1	2.30	0.43
1:J:174:TYR:HA	1:J:177:ILE:HD11	2.01	0.43
1:M:271:LEU:C	1:M:274:ARG:HH12	2.27	0.43
1:A:238:ALA:O	1:A:240:LYS:N	2.52	0.43
1:A:265:PHE:HA	1:A:265:PHE:HD1	1.63	0.43
1:A:291:ASP:OD1	1:A:293:SER:N	2.52	0.43
1:A:293:SER:H	1:A:295:LYS:NZ	2.16	0.43
1:A:389:VAL:HG23	1:B:340:LYS:HE3	2.00	0.43
1:C:271:LEU:HA	1:C:271:LEU:HD23	1.76	0.43
1:E:426:GLN:HE22	1:E:430:GLN:H	1.66	0.43
1:F:324:ALA:C	1:F:325:LYS:HZ2	2.26	0.43
1:H:190:LEU:HA	1:H:190:LEU:HD12	1.77	0.43
1:I:230:THR:HA	1:I:231:THR:HA	1.71	0.43
1:J:255:ILE:HG21	1:J:271:LEU:HD11	1.99	0.43
1:J:362:TRP:CD1	1:J:365:VAL:HA	2.54	0.43
1:K:236:LYS:HD3	1:K:236:LYS:HA	1.76	0.43
1:K:285:GLU:O	1:K:289:THR:OG1	2.23	0.43
1:M:349:SER:OG	1:M:350:MET:N	2.49	0.43
1:A:190:LEU:HD12	1:A:190:LEU:HA	1.86	0.43
1:B:327:ILE:H	1:B:327:ILE:HG13	1.67	0.43
1:B:429:LYS:N	1:B:429:LYS:HZ2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:THR:HA	1:C:231:THR:HA	1.67	0.43
1:C:323:THR:OG1	1:C:363:GLN:OE1	2.36	0.43
1:E:211:GLU:OE2	1:E:216:LYS:NZ	2.39	0.43
1:E:353:TYR:HD1	1:E:353:TYR:HA	1.55	0.43
1:H:367:GLN:HA	1:H:368:VAL:HA	1.57	0.43
1:K:249:LEU:HA	1:L:219:TRP:CD2	2.54	0.43
1:K:311:VAL:HA	1:K:312:THR:HA	1.62	0.43
1:M:252:LYS:HA	1:M:436:VAL:N	2.34	0.43
1:E:272:ARG:HD2	1:E:275:LEU:HD21	2.01	0.43
1:F:255:ILE:HG13	1:F:434:TYR:HE2	1.83	0.43
1:F:394:PRO:HB2	1:F:396:LYS:HZ2	1.84	0.43
1:K:315:LYS:HE2	1:K:321:LEU:HB2	2.00	0.43
1:K:346:LEU:HD23	1:K:387:VAL:HG22	2.01	0.43
1:L:211:GLU:HG3	1:L:238:ALA:H	1.84	0.43
1:A:172:GLU:HB3	1:A:423:ARG:HB2	2.01	0.42
1:A:252:LYS:NZ	1:A:434:TYR:H	2.17	0.42
1:A:346:LEU:HB3	1:A:387:VAL:HG22	2.01	0.42
1:A:401:GLU:H	1:A:401:GLU:HG2	1.39	0.42
1:B:398:ASN:OD1	1:B:457:ALA:N	2.51	0.42
1:C:248:LYS:HD3	1:C:437:THR:HG22	2.01	0.42
1:D:264:ILE:H	1:D:264:ILE:HG12	1.58	0.42
1:D:275:LEU:H	1:D:275:LEU:HG	1.53	0.42
1:E:272:ARG:HE	1:E:272:ARG:HB3	1.55	0.42
1:E:358:GLU:HG3	1:F:325:LYS:HG3	2.01	0.42
1:G:197:GLU:O	1:G:199:LEU:N	2.52	0.42
1:I:205:ILE:HG12	1:I:245:SER:HB3	2.00	0.42
1:I:285:GLU:O	1:I:289:THR:N	2.52	0.42
1:I:425:ARG:CZ	1:I:425:ARG:HA	2.49	0.42
1:K:423:ARG:HA	1:K:434:TYR:HD1	1.84	0.42
1:M:276:ILE:H	1:M:276:ILE:HG12	1.47	0.42
1:M:361:GLU:HB3	1:M:363:GLN:HG2	2.00	0.42
1:A:268:LEU:H	1:A:268:LEU:HG	1.49	0.42
1:B:368:VAL:N	1:B:371:ASP:OD1	2.52	0.42
1:C:249:LEU:HD23	1:D:219:TRP:CE3	2.55	0.42
1:F:453:GLY:HA3	1:F:454:THR:HA	1.65	0.42
1:G:204:LYS:O	1:G:206:LEU:N	2.52	0.42
1:G:342:SER:HA	1:G:343:LYS:HA	1.77	0.42
1:G:367:GLN:HA	1:G:368:VAL:HA	1.60	0.42
1:I:345:VAL:HA	1:I:385:LEU:HG	2.01	0.42
1:J:329:LYS:H	1:J:329:LYS:HG3	1.67	0.42
1:A:252:LYS:N	1:B:218:THR:OG1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:SER:O	1:C:408:LYS:NZ	2.49	0.42
1:E:355:ASP:OD1	1:E:355:ASP:N	2.53	0.42
1:F:212:PRO:O	1:F:214:ALA:N	2.52	0.42
1:G:416:GLN:HB3	1:G:417:ARG:H	1.65	0.42
1:H:410:ASN:HB3	1:H:445:TYR:N	2.35	0.42
1:I:323:THR:HG21	1:I:325:LYS:HE2	2.01	0.42
1:J:454:THR:HB	1:J:456:ALA:N	2.34	0.42
1:K:314:ALA:HB3	1:K:455:TYR:HD1	1.84	0.42
1:K:315:LYS:H	1:K:320:VAL:HG12	1.83	0.42
1:K:349:SER:O	1:K:353:TYR:N	2.53	0.42
1:A:212:PRO:HD2	1:A:238:ALA:O	2.19	0.42
1:A:362:TRP:CD1	1:A:367:GLN:H	2.37	0.42
1:A:378:GLN:H	1:A:386:PRO:HB2	1.84	0.42
1:C:314:ALA:H	1:C:455:TYR:H	1.65	0.42
1:D:181:ARG:H	1:D:181:ARG:HG3	1.32	0.42
1:D:394:PRO:HB2	1:D:396:LYS:HG2	2.00	0.42
1:E:256:THR:O	1:E:259:THR:OG1	2.33	0.42
1:F:181:ARG:NH2	1:F:182:ILE:HG13	2.33	0.42
1:G:246:THR:HG21	1:G:439:ARG:HB3	2.01	0.42
1:H:273:LYS:HE2	1:H:273:LYS:HB2	1.84	0.42
1:I:455:TYR:HD1	1:I:455:TYR:HA	1.55	0.42
1:J:345:VAL:H	1:J:407:TYR:HB2	1.84	0.42
1:J:424:GLU:N	1:J:433:ALA:O	2.53	0.42
1:L:357:LEU:HA	1:L:362:TRP:NE1	2.33	0.42
1:A:272:ARG:C	1:A:273:LYS:HZ3	2.25	0.42
1:A:421:VAL:HA	1:A:435:TYR:O	2.20	0.42
1:B:180:GLN:HE22	1:B:272:ARG:HG3	1.85	0.42
1:B:406:VAL:HG13	1:B:411:PHE:HE2	1.85	0.42
1:C:264:ILE:HD13	1:C:267:LEU:HD22	2.02	0.42
1:D:172:GLU:C	1:D:423:ARG:HD3	2.45	0.42
1:D:347:ILE:HG23	1:D:388:VAL:HB	2.02	0.42
1:D:412:VAL:HG23	1:D:414:PRO:HD3	2.01	0.42
1:E:382:ILE:C	1:E:385:LEU:H	2.27	0.42
1:F:237:GLY:HA3	1:F:238:ALA:HA	1.81	0.42
1:G:425:ARG:O	1:G:433:ALA:N	2.43	0.42
1:H:174:TYR:N	1:H:175:GLU:OE1	2.52	0.42
1:J:249:LEU:O	1:J:438:GLN:N	2.53	0.42
1:J:249:LEU:N	1:J:438:GLN:O	2.33	0.42
1:L:276:ILE:H	1:L:276:ILE:HG12	1.38	0.42
1:A:394:PRO:HB2	1:A:396:LYS:HE2	2.00	0.42
1:A:396:LYS:HZ3	1:A:396:LYS:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:OG	1:B:224:THR:N	2.52	0.42
1:B:314:ALA:HB3	1:B:455:TYR:CD1	2.54	0.42
1:D:410:ASN:HB3	1:D:445:TYR:N	2.33	0.42
1:F:279:HIS:NE2	1:F:283:ILE:HD11	2.35	0.42
1:F:327:ILE:HD11	1:F:402:PHE:CZ	2.54	0.42
1:G:258:GLU:HB2	1:G:430:GLN:HB3	2.00	0.42
1:G:340:LYS:HB2	1:G:340:LYS:HE2	1.87	0.42
1:G:396:LYS:O	1:G:398:ASN:N	2.50	0.42
1:H:195:LEU:HB3	1:H:407:TYR:CE2	2.54	0.42
1:H:417:ARG:HG3	1:H:417:ARG:H	1.51	0.42
1:I:187:GLN:HG3	1:I:280:ALA:HB3	2.01	0.42
1:I:308:ALA:HB1	1:I:451:VAL:HA	2.02	0.42
1:I:336:ARG:HG3	1:I:337:HIS:CG	2.55	0.42
1:I:367:GLN:HA	1:I:368:VAL:HA	1.63	0.42
1:J:177:ILE:N	1:J:179:SER:OG	2.49	0.42
1:J:332:ARG:HA	1:J:332:ARG:HD2	1.82	0.42
1:J:412:VAL:HG23	1:J:414:PRO:HD3	2.01	0.42
1:K:173:SER:H	1:K:176:THR:HG22	1.83	0.42
1:K:246:THR:HG1	1:K:247:TYR:H	1.61	0.42
1:M:308:ALA:HA	1:M:451:VAL:HG22	2.01	0.42
1:M:319:SER:O	1:M:319:SER:OG	2.30	0.42
1:A:414:PRO:HG2	1:A:441:ASN:HB3	2.02	0.42
1:B:274:ARG:HA	1:B:277:GLU:HB2	2.00	0.42
1:B:310:VAL:HG21	1:B:330:LEU:HG	2.01	0.42
1:B:323:THR:OG1	1:B:326:THR:N	2.39	0.42
1:B:353:TYR:CE1	1:B:380:GLY:HA3	2.54	0.42
1:C:300:LEU:HG	1:C:393:PHE:CE1	2.55	0.42
1:C:382:ILE:O	1:C:384:GLY:N	2.52	0.42
1:D:272:ARG:HA	1:D:275:LEU:HG	2.01	0.42
1:E:394:PRO:O	1:E:399:SER:OG	2.29	0.42
1:F:395:ALA:H	1:F:396:LYS:NZ	2.18	0.42
1:H:354:TYR:HD2	1:H:354:TYR:HA	1.64	0.42
1:I:355:ASP:O	1:I:359:ASP:HB3	2.20	0.42
1:J:236:LYS:HA	1:J:236:LYS:HD3	1.79	0.42
1:J:372:SER:HA	1:J:373:VAL:HA	1.55	0.42
1:K:218:THR:O	1:K:218:THR:OG1	2.37	0.42
1:K:293:SER:O	1:K:295:LYS:NZ	2.36	0.42
1:K:444:ARG:HH21	1:K:445:TYR:H	1.68	0.42
1:L:187:GLN:C	1:L:189:GLU:H	2.26	0.42
1:M:174:TYR:HA	1:M:177:ILE:HD11	2.01	0.42
1:M:181:ARG:HD3	1:M:181:ARG:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:334:LEU:HG	1:M:404:VAL:HG12	2.01	0.42
1:A:214:ALA:HA	1:A:446:PHE:CZ	2.55	0.42
1:B:287:PHE:CE1	1:B:442:LEU:HB3	2.54	0.42
1:B:445:TYR:HB3	1:B:446:PHE:H	1.52	0.42
1:C:255:ILE:HB	1:C:434:TYR:OH	2.20	0.42
1:C:310:VAL:N	1:C:454:THR:OG1	2.53	0.42
1:D:357:LEU:HD12	1:D:357:LEU:HA	1.65	0.42
1:E:264:ILE:O	1:E:266:SER:OG	2.30	0.42
1:E:287:PHE:CE1	1:E:442:LEU:HB2	2.55	0.42
1:F:170:SER:OG	1:F:425:ARG:NH2	2.53	0.42
1:F:378:GLN:HB3	1:F:379:VAL:H	1.77	0.42
1:F:444:ARG:HE	1:F:444:ARG:HB3	1.73	0.42
1:G:272:ARG:HH12	1:G:275:LEU:N	2.12	0.42
1:G:272:ARG:HB3	1:G:273:LYS:H	1.68	0.42
1:G:334:LEU:O	1:G:337:HIS:ND1	2.37	0.42
1:H:394:PRO:O	1:H:399:SER:OG	2.28	0.42
1:I:282:SER:HA	1:I:285:GLU:HB2	2.00	0.42
1:I:347:ILE:HA	1:I:388:VAL:H	1.85	0.42
1:J:333:LYS:HZ2	1:J:333:LYS:C	2.28	0.42
1:J:347:ILE:HA	1:J:388:VAL:HB	2.01	0.42
1:K:190:LEU:HD12	1:K:190:LEU:HA	1.79	0.42
1:M:205:ILE:HG12	1:M:245:SER:HB3	2.02	0.42
1:M:256:THR:O	1:M:259:THR:OG1	2.37	0.42
1:A:344:LEU:HA	1:A:344:LEU:HD12	1.83	0.42
1:B:184:ARG:NH1	1:B:185:ASP:OD2	2.52	0.42
1:B:185:ASP:HA	1:B:188:LYS:HB2	2.00	0.42
1:C:414:PRO:HG2	1:C:443:GLN:HB2	2.02	0.42
1:D:285:GLU:HG3	1:D:392:TYR:CD1	2.54	0.42
1:D:291:ASP:N	1:D:291:ASP:OD1	2.52	0.42
1:D:327:ILE:HA	1:D:330:LEU:HB2	2.01	0.42
1:E:291:ASP:OD2	1:E:293:SER:OG	2.35	0.42
1:F:309:LYS:HA	1:F:454:THR:HG21	2.00	0.42
1:F:425:ARG:HA	1:F:425:ARG:HD2	1.84	0.42
1:G:322:VAL:HG21	1:G:355:ASP:HB3	2.02	0.42
1:G:431:ARG:HH21	1:G:431:ARG:HB2	1.85	0.42
1:H:272:ARG:NH2	1:H:423:ARG:HH12	2.17	0.42
1:H:345:VAL:N	1:H:405:ILE:O	2.36	0.42
1:H:409:ASP:HB3	1:H:410:ASN:HD22	1.85	0.42
1:H:444:ARG:HB2	1:H:445:TYR:H	1.63	0.42
1:I:177:ILE:HA	1:I:180:GLN:HG2	2.02	0.42
1:J:291:ASP:OD1	1:J:292:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:342:SER:HA	1:J:343:LYS:HA	1.87	0.42
1:L:332:ARG:O	1:L:336:ARG:NE	2.35	0.42
1:L:404:VAL:HB	1:L:451:VAL:HG23	2.01	0.42
1:M:324:ALA:O	1:M:383:TYR:OH	2.37	0.42
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.83	0.42
1:A:264:ILE:HG22	1:A:267:LEU:H	1.84	0.42
1:C:264:ILE:O	1:C:266:SER:N	2.53	0.42
1:D:311:VAL:HA	1:D:312:THR:HA	1.80	0.42
1:E:267:LEU:HD12	1:F:208:MET:HE3	2.02	0.42
1:E:411:PHE:CZ	1:E:444:ARG:HB3	2.55	0.42
1:F:272:ARG:HB2	1:F:273:LYS:NZ	2.34	0.42
1:G:251:ALA:N	1:G:436:VAL:O	2.32	0.42
1:G:302:LEU:HA	1:G:305:GLU:HG2	2.02	0.42
1:G:347:ILE:HG23	1:G:388:VAL:HB	2.00	0.42
1:G:441:ASN:ND2	1:G:442:LEU:H	2.17	0.42
1:H:180:GLN:NE2	1:H:272:ARG:HD3	2.35	0.42
1:J:351:ASP:O	1:J:355:ASP:N	2.41	0.42
1:M:411:PHE:N	1:M:444:ARG:HA	2.33	0.42
1:A:211:GLU:CD	1:A:239:LEU:HB2	2.45	0.41
1:A:362:TRP:HD1	1:A:366:ALA:N	2.18	0.41
1:B:260:GLU:HA	1:B:264:ILE:HD12	2.02	0.41
1:B:312:THR:OG1	1:B:315:LYS:NZ	2.53	0.41
1:D:439:ARG:HH21	1:D:439:ARG:HD3	1.72	0.41
1:G:272:ARG:NH1	1:G:276:ILE:HG12	2.34	0.41
1:G:277:GLU:H	1:G:277:GLU:HG3	1.59	0.41
1:H:171:SER:OG	1:H:172:GLU:N	2.52	0.41
1:H:324:ALA:N	1:H:363:GLN:OE1	2.38	0.41
1:I:370:ASN:CG	1:I:371:ASP:HA	2.44	0.41
1:A:252:LYS:HZ1	1:A:434:TYR:H	1.67	0.41
1:A:446:PHE:HB3	1:A:447:ALA:H	1.49	0.41
1:B:186:LEU:O	1:B:189:GLU:HB2	2.20	0.41
1:B:330:LEU:HA	1:B:333:LYS:HB3	2.01	0.41
1:B:365:VAL:HG21	1:B:381:ARG:HH12	1.85	0.41
1:B:406:VAL:HG21	1:B:409:ASP:HB2	2.02	0.41
1:D:353:TYR:CE2	1:D:357:LEU:HD22	2.55	0.41
1:E:362:TRP:CD1	1:E:365:VAL:HA	2.52	0.41
1:G:177:ILE:HG13	1:G:423:ARG:NH2	2.34	0.41
1:G:424:GLU:HB2	1:G:433:ALA:HB3	2.02	0.41
1:H:365:VAL:HG22	1:H:383:TYR:H	1.85	0.41
1:I:182:ILE:H	1:I:182:ILE:HG13	1.46	0.41
1:I:267:LEU:HD21	1:J:206:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:199:LEU:N	1:J:413:MET:O	2.52	0.41
1:K:375:LEU:HD12	1:K:376:GLN:H	1.85	0.41
1:C:184:ARG:HA	1:C:184:ARG:HD2	1.81	0.41
1:C:264:ILE:O	1:C:266:SER:OG	2.30	0.41
1:C:288:MET:HE1	1:C:299:LEU:HD12	2.01	0.41
1:D:273:LYS:HE2	1:D:273:LYS:HB2	1.83	0.41
1:D:276:ILE:O	1:D:279:HIS:HB3	2.21	0.41
1:E:228:ASP:OD1	1:E:228:ASP:N	2.51	0.41
1:E:290:GLY:H	1:E:301:THR:HG21	1.85	0.41
1:E:307:SER:O	1:E:307:SER:OG	2.29	0.41
1:G:330:LEU:HD23	1:G:404:VAL:HG21	2.02	0.41
1:G:365:VAL:HG11	1:G:381:ARG:NE	2.35	0.41
1:G:422:GLU:H	1:G:422:GLU:CD	2.28	0.41
1:H:314:ALA:HB3	1:H:455:TYR:HA	2.01	0.41
1:I:311:VAL:HA	1:I:312:THR:HA	1.83	0.41
1:M:297:LYS:HA	1:M:297:LYS:HD2	1.86	0.41
1:M:312:THR:O	1:M:312:THR:OG1	2.38	0.41
1:A:368:VAL:HG13	1:A:370:ASN:H	1.86	0.41
1:A:417:ARG:HB2	1:A:418:ALA:H	1.54	0.41
1:B:391:GLU:HA	1:B:393:PHE:HB2	2.03	0.41
1:C:288:MET:HB3	1:C:393:PHE:HE1	1.85	0.41
1:C:362:TRP:CD1	1:C:367:GLN:H	2.38	0.41
1:D:247:TYR:HD2	1:D:249:LEU:HD21	1.85	0.41
1:E:268:LEU:H	1:E:268:LEU:HG	1.32	0.41
1:F:323:THR:O	1:F:326:THR:OG1	2.27	0.41
1:F:375:LEU:HB2	1:F:376:GLN:H	1.70	0.41
1:G:187:GLN:NE2	1:G:189:GLU:HB3	2.35	0.41
1:G:322:VAL:HG12	1:G:356:LEU:HG	2.01	0.41
1:H:365:VAL:H	1:H:383:TYR:HE1	1.67	0.41
1:I:184:ARG:HH12	1:I:188:LYS:NZ	2.17	0.41
1:J:302:LEU:HD23	1:J:302:LEU:HA	1.93	0.41
1:J:356:LEU:HB3	1:J:366:ALA:HB1	2.03	0.41
1:J:424:GLU:HA	1:J:425:ARG:HE	1.85	0.41
1:K:177:ILE:O	1:K:181:ARG:N	2.54	0.41
1:K:206:LEU:O	1:K:244:PHE:N	2.54	0.41
1:K:271:LEU:HD12	1:K:271:LEU:HA	1.84	0.41
1:A:276:ILE:HA	1:A:279:HIS:HB3	2.02	0.41
1:A:293:SER:H	1:A:295:LYS:HZ1	1.68	0.41
1:A:324:ALA:O	1:A:328:SER:OG	2.32	0.41
1:C:276:ILE:H	1:C:276:ILE:HG12	1.44	0.41
1:D:314:ALA:HB3	1:D:455:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:HIS:O	1:F:283:ILE:HG13	2.21	0.41
1:F:405:ILE:HD11	1:F:410:ASN:HB2	2.02	0.41
1:G:331:ARG:HG2	1:G:332:ARG:HD2	2.02	0.41
1:H:230:THR:HA	1:H:231:THR:HA	1.65	0.41
1:K:188:LYS:NZ	1:K:198:GLU:OE1	2.45	0.41
1:M:235:VAL:HB	1:M:236:LYS:H	1.68	0.41
1:M:353:TYR:CD1	1:M:387:VAL:HG11	2.56	0.41
1:B:179:SER:O	1:B:183:ILE:HG13	2.21	0.41
1:B:183:ILE:H	1:B:183:ILE:HG13	1.66	0.41
1:C:235:VAL:HB	1:C:236:LYS:H	1.68	0.41
1:D:381:ARG:O	1:D:384:GLY:N	2.49	0.41
1:E:382:ILE:H	1:E:385:LEU:N	2.19	0.41
1:F:421:VAL:HG22	1:F:436:VAL:HG13	2.02	0.41
1:G:278:ALA:HB1	1:H:217:ALA:H	1.85	0.41
1:H:201:MET:HE3	1:H:206:LEU:HB2	2.02	0.41
1:H:364:ASP:HB2	1:H:383:TYR:HE1	1.85	0.41
1:I:300:LEU:HD23	1:I:300:LEU:HA	1.87	0.41
1:I:376:GLN:HB3	1:I:378:GLN:HE22	1.85	0.41
1:K:325:LYS:O	1:K:328:SER:OG	2.25	0.41
1:K:382:ILE:HG22	1:K:383:TYR:HD2	1.85	0.41
1:K:444:ARG:HD3	1:K:445:TYR:N	2.36	0.41
1:L:245:SER:C	1:L:441:ASN:HD22	2.29	0.41
1:L:356:LEU:HD13	1:L:363:GLN:HG2	2.03	0.41
1:A:334:LEU:HD22	1:A:337:HIS:CG	2.56	0.41
1:B:309:LYS:H	1:B:309:LYS:HG2	1.53	0.41
1:C:232:GLY:H	1:C:234:GLU:HG2	1.86	0.41
1:D:345:VAL:HG23	1:D:405:ILE:HG23	2.02	0.41
1:E:247:TYR:O	1:E:439:ARG:HA	2.21	0.41
1:E:336:ARG:NH1	1:E:336:ARG:HA	2.35	0.41
1:F:241:GLU:H	1:F:241:GLU:HG3	1.59	0.41
1:H:236:LYS:HA	1:H:237:GLY:HA2	1.70	0.41
1:K:335:GLY:HA2	1:K:340:LYS:HZ2	1.86	0.41
1:L:184:ARG:HE	1:L:184:ARG:HB3	1.28	0.41
1:L:342:SER:O	1:L:408:LYS:NZ	2.40	0.41
1:B:334:LEU:HD22	1:B:337:HIS:CE1	2.56	0.41
1:B:347:ILE:HB	1:B:403:ALA:HB3	2.03	0.41
1:B:403:ALA:O	1:B:405:ILE:HG22	2.21	0.41
1:C:297:LYS:HG3	1:C:302:LEU:HG	2.03	0.41
1:F:337:HIS:CD2	1:F:448:ASN:HD22	2.39	0.41
1:G:288:MET:HA	1:G:299:LEU:H	1.84	0.41
1:G:363:GLN:HB2	1:G:364:ASP:H	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:LYS:O	1:H:277:GLU:N	2.32	0.41
1:H:349:SER:OG	1:H:351:ASP:OD1	2.29	0.41
1:H:353:TYR:CE2	1:H:357:LEU:HB2	2.55	0.41
1:J:247:TYR:O	1:J:439:ARG:HG2	2.20	0.41
1:K:429:LYS:HD2	1:K:431:ARG:CZ	2.51	0.41
1:L:321:LEU:HD23	1:L:321:LEU:HA	1.74	0.41
1:L:410:ASN:HB3	1:L:444:ARG:HH11	1.86	0.41
1:B:253:SER:OG	1:B:254:PHE:N	2.52	0.41
1:B:297:LYS:HD3	1:B:297:LYS:HA	1.74	0.41
1:B:346:LEU:HD13	1:B:404:VAL:HG22	2.03	0.41
1:C:357:LEU:HA	1:C:359:ASP:CG	2.46	0.41
1:D:209:LEU:HD22	1:D:241:GLU:HG3	2.03	0.41
1:D:296:PRO:HB2	1:D:297:LYS:H	1.67	0.41
1:D:372:SER:HA	1:D:373:VAL:HA	1.73	0.41
1:E:176:THR:O	1:E:180:GLN:N	2.54	0.41
1:E:216:LYS:HB2	1:E:218:THR:HG22	2.02	0.41
1:E:248:LYS:HG3	1:E:417:ARG:HH22	1.85	0.41
1:F:264:ILE:HG23	1:F:267:LEU:HD13	2.03	0.41
1:G:253:SER:HB3	1:G:275:LEU:HD13	2.03	0.41
1:G:389:VAL:HB	1:G:390:SER:H	1.58	0.41
1:H:187:GLN:NE2	1:H:189:GLU:O	2.40	0.41
1:H:197:GLU:O	1:H:413:MET:N	2.52	0.41
1:H:314:ALA:N	1:H:455:TYR:H	2.19	0.41
1:H:421:VAL:HG13	1:H:436:VAL:HG22	2.02	0.41
1:I:175:GLU:H	1:I:177:ILE:HD12	1.86	0.41
1:I:233:GLU:H	1:I:234:GLU:HA	1.86	0.41
1:I:288:MET:HA	1:I:299:LEU:HG	2.02	0.41
1:K:255:ILE:HG23	1:K:434:TYR:CE2	2.55	0.41
1:K:315:LYS:NZ	1:K:321:LEU:H	2.19	0.41
1:K:456:ALA:HB1	1:K:458:SER:H	1.86	0.41
1:L:176:THR:HG23	1:L:423:ARG:HH12	1.86	0.41
1:L:200:PRO:HA	1:L:415:ARG:HD3	2.02	0.41
1:L:344:LEU:O	1:L:385:LEU:HG	2.21	0.41
1:M:346:LEU:HD12	1:M:346:LEU:HA	1.67	0.41
1:M:413:MET:HE2	1:M:440:VAL:HG21	2.03	0.41
1:A:210:VAL:HA	1:F:255:ILE:HG23	2.02	0.41
1:A:300:LEU:HD21	1:A:393:PHE:CE1	2.56	0.41
1:B:354:TYR:HD1	1:B:357:LEU:HD23	1.86	0.41
1:C:273:LYS:HZ3	1:C:273:LYS:HB2	1.86	0.41
1:C:334:LEU:O	1:C:336:ARG:N	2.54	0.41
1:D:288:MET:HB3	1:D:392:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:LEU:N	1:E:438:GLN:O	2.38	0.41
1:E:285:GLU:O	1:E:289:THR:OG1	2.31	0.41
1:E:336:ARG:O	1:E:337:HIS:ND1	2.54	0.41
1:E:453:GLY:HA3	1:E:454:THR:HA	1.70	0.41
1:I:357:LEU:HG	1:I:358:GLU:HG3	2.02	0.41
1:J:422:GLU:HB2	1:J:435:TYR:HB2	2.01	0.41
1:L:254:PHE:CE2	1:L:431:ARG:HB2	2.56	0.41
1:L:406:VAL:HG22	1:L:409:ASP:N	2.34	0.41
1:D:331:ARG:HD2	1:D:332:ARG:HH11	1.86	0.40
1:D:340:LYS:HB2	1:D:340:LYS:HE2	1.91	0.40
1:E:285:GLU:O	1:E:289:THR:N	2.54	0.40
1:F:196:PHE:HB3	1:F:197:GLU:H	1.65	0.40
1:F:248:LYS:HE3	1:F:248:LYS:HB3	1.82	0.40
1:F:259:THR:OG1	1:F:260:GLU:N	2.54	0.40
1:F:406:VAL:HG22	1:F:409:ASP:H	1.87	0.40
1:H:204:LYS:HB3	1:H:205:ILE:H	1.55	0.40
1:I:325:LYS:NZ	1:I:363:GLN:OE1	2.45	0.40
1:J:398:ASN:OD1	1:J:457:ALA:N	2.55	0.40
1:J:417:ARG:HG2	1:J:439:ARG:HB2	2.02	0.40
1:K:241:GLU:O	1:K:243:HIS:N	2.52	0.40
1:M:177:ILE:H	1:M:177:ILE:HG12	1.53	0.40
1:A:282:SER:HA	1:A:285:GLU:HB2	2.03	0.40
1:A:415:ARG:HA	1:A:440:VAL:HG12	2.03	0.40
1:B:326:THR:O	1:B:330:LEU:HD22	2.21	0.40
1:C:268:LEU:O	1:C:272:ARG:N	2.54	0.40
1:C:313:GLU:N	1:C:454:THR:O	2.46	0.40
1:E:341:LEU:HA	1:E:344:LEU:HB2	2.03	0.40
1:E:415:ARG:HB2	1:E:440:VAL:HG12	2.03	0.40
1:G:219:TRP:CE2	1:L:249:LEU:HA	2.56	0.40
1:G:293:SER:O	1:G:295:LYS:N	2.55	0.40
1:H:201:MET:N	1:H:415:ARG:O	2.34	0.40
1:H:246:THR:HG23	1:H:439:ARG:NH1	2.36	0.40
1:I:248:LYS:HD3	1:I:437:THR:HB	2.03	0.40
1:I:345:VAL:HG12	1:I:386:PRO:HD2	2.04	0.40
1:A:290:GLY:HA2	1:A:295:LYS:HE2	2.04	0.40
1:A:333:LYS:C	1:A:336:ARG:HH22	2.29	0.40
1:B:199:LEU:O	1:B:415:ARG:N	2.53	0.40
1:B:346:LEU:HA	1:B:403:ALA:O	2.21	0.40
1:C:267:LEU:HD12	1:C:270:LEU:HB3	2.02	0.40
1:D:344:LEU:HG	1:D:406:VAL:HB	2.02	0.40
1:D:361:GLU:HB3	1:D:363:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ARG:HA	1:E:440:VAL:HA	2.02	0.40
1:F:415:ARG:HE	1:F:415:ARG:HB2	1.59	0.40
1:G:419:VAL:HA	1:G:437:THR:O	2.21	0.40
1:G:427:ALA:HB3	1:G:432:ASP:HA	2.03	0.40
1:H:327:ILE:H	1:H:327:ILE:HG13	1.71	0.40
1:J:184:ARG:NH2	1:J:188:LYS:HG3	2.37	0.40
1:L:242:ILE:H	1:L:242:ILE:HG12	1.67	0.40
1:L:303:ALA:HA	1:L:306:ASP:HB2	2.04	0.40
1:A:233:GLU:HB3	1:A:234:GLU:C	2.47	0.40
1:A:378:GLN:HG2	1:A:388:VAL:HG23	2.02	0.40
1:B:233:GLU:CD	1:B:236:LYS:HZ2	2.29	0.40
1:C:182:ILE:HA	1:C:185:ASP:CG	2.46	0.40
1:F:313:GLU:CD	1:F:329:LYS:HZ1	2.29	0.40
1:F:325:LYS:HD3	1:F:325:LYS:HA	1.81	0.40
1:G:204:LYS:HE2	1:G:204:LYS:HB2	1.93	0.40
1:J:341:LEU:HA	1:J:341:LEU:HD13	1.62	0.40
1:K:172:GLU:HA	1:K:423:ARG:HE	1.85	0.40
1:M:198:GLU:HA	1:M:413:MET:O	2.22	0.40
1:M:289:THR:HG22	1:M:300:LEU:HB2	2.04	0.40
1:A:264:ILE:HG21	1:A:267:LEU:HB2	2.04	0.40
1:A:331:ARG:HD2	1:A:340:LYS:HG3	2.02	0.40
1:B:396:LYS:HZ3	1:B:396:LYS:HG2	1.78	0.40
1:C:272:ARG:O	1:C:274:ARG:N	2.54	0.40
1:C:412:VAL:N	1:C:443:GLN:O	2.43	0.40
1:D:254:PHE:HA	1:D:433:ALA:HA	2.04	0.40
1:E:173:SER:OG	1:E:175:GLU:OE1	2.25	0.40
1:F:288:MET:HB3	1:F:289:THR:H	1.56	0.40
1:G:349:SER:OG	1:G:391:GLU:OE1	2.30	0.40
1:H:295:LYS:HG2	1:I:219:TRP:CE2	2.56	0.40
1:J:173:SER:HB2	1:J:174:TYR:H	1.67	0.40
1:J:223:SER:HB3	1:J:224:THR:H	1.60	0.40
1:K:211:GLU:C	1:K:238:ALA:H	2.30	0.40
1:K:359:ASP:H	1:K:367:GLN:NE2	2.19	0.40
1:K:427:ALA:HB3	1:K:432:ASP:HA	2.03	0.40
1:M:268:LEU:O	1:M:272:ARG:N	2.54	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 PDB entries followed by that with respect to all EM entries.

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	287/299 (96%)	188 (66%)	71 (25%)	28 (10%)	0	7
1	B	287/299 (96%)	190 (66%)	68 (24%)	29 (10%)	0	7
1	C	38/299 (13%)	24 (63%)	11 (29%)	3 (8%)	1	9
1	D	182/299 (61%)	117 (64%)	45 (25%)	20 (11%)	0	5
1	E	287/299 (96%)	191 (67%)	71 (25%)	25 (9%)	0	9
1	F	287/299 (96%)	190 (66%)	63 (22%)	34 (12%)	0	4
1	G	287/299 (96%)	193 (67%)	65 (23%)	29 (10%)	0	7
1	H	287/299 (96%)	185 (64%)	71 (25%)	31 (11%)	0	6
1	I	287/299 (96%)	180 (63%)	83 (29%)	24 (8%)	0	9
1	J	287/299 (96%)	188 (66%)	77 (27%)	22 (8%)	1	10
1	K	287/299 (96%)	200 (70%)	58 (20%)	29 (10%)	0	7
1	L	287/299 (96%)	190 (66%)	72 (25%)	25 (9%)	0	9
1	M	287/299 (96%)	190 (66%)	80 (28%)	17 (6%)	1	13
All	All	3377/3887 (87%)	2226 (66%)	835 (25%)	316 (9%)	1	8

All (316) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	A	446	PHE
1	B	233	GLU
1	B	273	LYS
1	B	390	SER
1	C	174	TYR
1	D	336	ARG
1	D	365	VAL
1	D	366	ALA
1	D	390	SER

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Mol	Chain	Res	Type
1	D	436	VAL
1	E	266	SER
1	E	364	ASP
1	F	189	GLU
1	F	227	THR
1	F	288	MET
1	F	423	ARG
1	F	457	ALA
1	G	233	GLU
1	G	239	LEU
1	G	274	ARG
1	G	337	HIS
1	G	396	LYS
1	H	221	ALA
1	H	242	ILE
1	H	266	SER
1	H	273	LYS
1	H	296	PRO
1	H	336	ARG
1	H	377	GLY
1	H	396	LYS
1	I	268	LEU
1	I	390	SER
1	J	204	LYS
1	J	213	ASP
1	J	233	GLU
1	J	326	THR
1	J	400	ALA
1	J	427	ALA
1	K	189	GLU
1	K	267	LEU
1	K	446	PHE
1	L	272	ARG
1	L	273	LYS
1	L	364	ASP
1	L	395	ALA
1	L	455	TYR
1	M	389	VAL
1	M	425	ARG
1	A	175	GLU
1	A	217	ALA
1	A	273	LYS

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Mol	Chain	Res	Type
1	A	316	ALA
1	A	317	ASP
1	A	418	ALA
1	B	198	GLU
1	B	219	TRP
1	B	319	SER
1	B	423	ARG
1	C	336	ARG
1	D	354	TYR
1	D	377	GLY
1	D	427	ALA
1	D	428	GLY
1	D	445	TYR
1	E	203	SER
1	E	258	GLU
1	E	296	PRO
1	E	309	LYS
1	E	377	GLY
1	E	378	GLN
1	E	390	SER
1	E	418	ALA
1	E	427	ALA
1	E	455	TYR
1	F	272	ARG
1	F	377	GLY
1	F	396	LYS
1	F	425	ARG
1	F	447	ALA
1	G	266	SER
1	G	362	TRP
1	G	363	GLN
1	G	411	PHE
1	H	203	SER
1	H	219	TRP
1	H	227	THR
1	H	309	LYS
1	H	374	LYS
1	H	390	SER
1	H	397	ALA
1	H	444	ARG
1	I	173	SER
1	I	212	PRO

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Mol	Chain	Res	Type
1	I	237	GLY
1	I	255	ILE
1	I	309	LYS
1	I	339	LEU
1	J	176	THR
1	J	366	ALA
1	J	372	SER
1	K	203	SER
1	K	223	SER
1	K	256	THR
1	K	273	LYS
1	K	344	LEU
1	K	390	SER
1	K	391	GLU
1	K	411	PHE
1	L	245	SER
1	M	203	SER
1	M	345	VAL
1	M	349	SER
1	M	416	GLN
1	A	212	PRO
1	A	214	ALA
1	A	272	ARG
1	A	296	PRO
1	A	299	LEU
1	A	344	LEU
1	A	399	SER
1	B	189	GLU
1	B	196	PHE
1	B	227	THR
1	B	272	ARG
1	B	400	ALA
1	D	372	SER
1	D	395	ALA
1	E	224	THR
1	E	227	THR
1	E	326	THR
1	F	191	VAL
1	F	213	ASP
1	F	262	ASP
1	F	263	ALA
1	F	391	GLU

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Mol	Chain	Res	Type
1	F	397	ALA
1	G	174	TYR
1	G	193	GLY
1	G	198	GLU
1	G	204	LYS
1	G	205	ILE
1	G	238	ALA
1	G	294	GLY
1	G	296	PRO
1	G	319	SER
1	G	344	LEU
1	G	399	SER
1	H	175	GLU
1	H	218	THR
1	H	362	TRP
1	H	369	GLY
1	H	427	ALA
1	I	223	SER
1	I	226	GLY
1	I	227	THR
1	I	296	PRO
1	I	376	GLN
1	I	397	ALA
1	I	447	ALA
1	J	177	ILE
1	J	179	SER
1	J	202	SER
1	J	266	SER
1	J	321	LEU
1	J	397	ALA
1	J	399	SER
1	K	296	PRO
1	K	336	ARG
1	K	375	LEU
1	K	395	ALA
1	L	212	PRO
1	L	227	THR
1	L	263	ALA
1	L	309	LYS
1	L	337	HIS
1	L	344	LEU
1	L	389	VAL

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Mol	Chain	Res	Type
1	L	407	TYR
1	L	411	PHE
1	L	429	LYS
1	M	227	THR
1	M	229	THR
1	M	251	ALA
1	M	322	VAL
1	A	256	THR
1	A	322	VAL
1	A	326	THR
1	A	337	HIS
1	A	397	ALA
1	A	427	ALA
1	A	449	GLY
1	B	229	THR
1	B	268	LEU
1	B	395	ALA
1	B	432	ASP
1	B	447	ALA
1	D	296	PRO
1	D	344	LEU
1	D	389	VAL
1	D	449	GLY
1	E	188	LYS
1	E	192	VAL
1	E	252	LYS
1	E	344	LEU
1	E	429	LYS
1	F	259	THR
1	F	266	SER
1	F	296	PRO
1	F	337	HIS
1	F	362	TRP
1	F	411	PHE
1	F	416	GLN
1	F	444	ARG
1	G	219	TRP
1	G	222	ALA
1	G	389	VAL
1	G	427	ALA
1	H	386	PRO
1	H	391	GLU

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Mol	Chain	Res	Type
1	H	445	TYR
1	I	229	THR
1	I	366	ALA
1	I	395	ALA
1	I	403	ALA
1	J	219	TRP
1	J	296	PRO
1	J	390	SER
1	K	229	THR
1	K	269	PRO
1	K	374	LYS
1	K	425	ARG
1	K	427	ALA
1	L	179	SER
1	L	218	THR
1	L	423	ARG
1	M	213	ASP
1	M	427	ALA
1	A	211	GLU
1	A	237	GLY
1	A	395	ALA
1	B	248	LYS
1	B	318	GLY
1	B	364	ASP
1	B	397	ALA
1	B	414	PRO
1	D	316	ALA
1	D	410	ASN
1	D	455	TYR
1	E	372	SER
1	F	232	GLY
1	F	344	LEU
1	F	427	ALA
1	F	445	TYR
1	G	235	VAL
1	G	273	LYS
1	G	336	ARG
1	H	272	ARG
1	H	344	LEU
1	H	446	PHE
1	I	171	SER
1	I	175	GLU

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Mol	Chain	Res	Type
1	I	279	HIS
1	I	364	ASP
1	I	372	SER
1	J	193	GLY
1	J	395	ALA
1	K	217	ALA
1	K	272	ARG
1	K	274	ARG
1	K	397	ALA
1	L	191	VAL
1	L	362	TRP
1	M	196	PHE
1	M	257	ASP
1	M	296	PRO
1	M	401	GLU
1	A	398	ASN
1	C	344	LEU
1	D	430	GLN
1	F	270	LEU
1	F	273	LYS
1	F	453	GLY
1	G	203	SER
1	J	239	LEU
1	K	193	GLY
1	L	270	LEU
1	A	235	VAL
1	B	193	GLY
1	B	373	VAL
1	E	212	PRO
1	E	414	PRO
1	K	377	GLY
1	L	235	VAL
1	B	428	GLY
1	H	191	VAL
1	K	237	GLY
1	L	193	GLY
1	A	412	VAL
1	B	368	VAL
1	E	193	GLY
1	F	264	ILE
1	G	310	VAL
1	H	226	GLY

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Mol	Chain	Res	Type
1	K	215	GLY
1	B	237	GLY
1	B	264	ILE
1	E	419	VAL
1	F	237	GLY
1	F	389	VAL
1	H	193	GLY
1	H	389	VAL
1	K	335	GLY
1	L	192	VAL
1	M	255	ILE
1	B	348	VAL

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 PDB entries followed by that with respect to all EM entries.

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	196/250 (78%)	120 (61%)	76 (39%)	0	1
1	B	241/250 (96%)	154 (64%)	87 (36%)	0	1
1	C	241/250 (96%)	157 (65%)	84 (35%)	0	1
1	D	241/250 (96%)	160 (66%)	81 (34%)	0	2
1	E	241/250 (96%)	149 (62%)	92 (38%)	0	1
1	F	241/250 (96%)	147 (61%)	94 (39%)	0	1
1	G	241/250 (96%)	154 (64%)	87 (36%)	0	1
1	H	241/250 (96%)	153 (64%)	88 (36%)	0	1
1	I	241/250 (96%)	163 (68%)	78 (32%)	0	2
1	J	241/250 (96%)	153 (64%)	88 (36%)	0	1
1	K	241/250 (96%)	155 (64%)	86 (36%)	0	1
1	L	241/250 (96%)	148 (61%)	93 (39%)	0	1
1	M	241/250 (96%)	170 (70%)	71 (30%)	0	2
All	All	3088/3250 (95%)	1983 (64%)	1105 (36%)	1	1

All (1105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	ARG
1	A	182	ILE
1	A	229	THR
1	A	235	VAL
1	A	239	LEU
1	A	242	ILE
1	A	245	SER
1	A	246	THR
1	A	252	LYS
1	A	257	ASP
1	A	259	THR
1	A	261	GLU
1	A	265	PHE
1	A	267	LEU
1	A	268	LEU
1	A	269	PRO
1	A	273	LYS
1	A	276	ILE
1	A	281	VAL
1	A	282	SER
1	A	284	GLU
1	A	285	GLU
1	A	288	MET
1	A	293	SER
1	A	295	LYS
1	A	297	LYS
1	A	299	LEU
1	A	304	SER
1	A	311	VAL
1	A	312	THR
1	A	315	LYS
1	A	320	VAL
1	A	321	LEU
1	A	322	VAL
1	A	325	LYS
1	A	334	LEU
1	A	336	ARG
1	A	339	LEU
1	A	340	LYS
1	A	341	LEU
1	A	350	MET
1	A	362	TRP

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Mol	Chain	Res	Type
1	A	364	ASP
1	A	365	VAL
1	A	367	GLN
1	A	368	VAL
1	A	372	SER
1	A	375	LEU
1	A	379	VAL
1	A	381	ARG
1	A	382	ILE
1	A	388	VAL
1	A	389	VAL
1	A	391	GLU
1	A	396	LYS
1	A	401	GLU
1	A	405	ILE
1	A	406	VAL
1	A	410	ASN
1	A	415	ARG
1	A	417	ARG
1	A	421	VAL
1	A	422	GLU
1	A	423	ARG
1	A	426	GLN
1	A	429	LYS
1	A	431	ARG
1	A	432	ASP
1	A	435	TYR
1	A	439	ARG
1	A	442	LEU
1	A	444	ARG
1	A	450	VAL
1	A	454	THR
1	A	455	TYR
1	A	458	SER
1	B	170	SER
1	B	175	GLU
1	B	177	ILE
1	B	181	ARG
1	B	183	ILE
1	B	184	ARG
1	B	190	LEU
1	B	192	VAL

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Mol	Chain	Res	Type
1	B	195	LEU
1	B	201	MET
1	B	205	ILE
1	B	208	MET
1	B	216	LYS
1	B	218	THR
1	B	224	THR
1	B	225	TYR
1	B	234	GLU
1	B	239	LEU
1	B	240	LYS
1	B	242	ILE
1	B	244	PHE
1	B	246	THR
1	B	248	LYS
1	B	252	LYS
1	B	255	ILE
1	B	259	THR
1	B	260	GLU
1	B	270	LEU
1	B	272	ARG
1	B	273	LYS
1	B	274	ARG
1	B	276	ILE
1	B	277	GLU
1	B	279	HIS
1	B	282	SER
1	B	287	PHE
1	B	289	THR
1	B	293	SER
1	B	297	LYS
1	B	309	LYS
1	B	310	VAL
1	B	313	GLU
1	B	315	LYS
1	B	317	ASP
1	B	320	VAL
1	B	321	LEU
1	B	326	THR
1	B	330	LEU
1	B	333	LYS
1	B	334	LEU

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Mol	Chain	Res	Type
1	B	342	SER
1	B	349	SER
1	B	350	MET
1	B	355	ASP
1	B	357	LEU
1	B	358	GLU
1	B	359	ASP
1	B	363	GLN
1	B	364	ASP
1	B	370	ASN
1	B	372	SER
1	B	375	LEU
1	B	382	ILE
1	B	388	VAL
1	B	389	VAL
1	B	396	LYS
1	B	398	ASN
1	B	404	VAL
1	B	406	VAL
1	B	408	LYS
1	B	411	PHE
1	B	413	MET
1	B	415	ARG
1	B	422	GLU
1	B	424	GLU
1	B	429	LYS
1	B	431	ARG
1	B	432	ASP
1	B	438	GLN
1	B	439	ARG
1	B	441	ASN
1	B	442	LEU
1	B	444	ARG
1	B	445	TYR
1	B	450	VAL
1	B	451	VAL
1	B	454	THR
1	C	171	SER
1	C	173	SER
1	C	174	TYR
1	C	180	GLN
1	C	181	ARG

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Mol	Chain	Res	Type
1	C	184	ARG
1	C	190	LEU
1	C	191	VAL
1	C	192	VAL
1	C	197	GLU
1	C	199	LEU
1	C	201	MET
1	C	202	SER
1	C	203	SER
1	C	209	LEU
1	C	213	ASP
1	C	224	THR
1	C	233	GLU
1	C	241	GLU
1	C	242	ILE
1	C	243	HIS
1	C	245	SER
1	C	247	TYR
1	C	248	LYS
1	C	249	LEU
1	C	258	GLU
1	C	260	GLU
1	C	264	ILE
1	C	272	ARG
1	C	273	LYS
1	C	274	ARG
1	C	276	ILE
1	C	279	HIS
1	C	293	SER
1	C	295	LYS
1	C	299	LEU
1	C	300	LEU
1	C	305	GLU
1	C	307	SER
1	C	310	VAL
1	C	312	THR
1	C	315	LYS
1	C	322	VAL
1	C	323	THR
1	C	329	LYS
1	C	330	LEU
1	C	332	ARG

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Mol	Chain	Res	Type
1	C	334	LEU
1	C	336	ARG
1	C	339	LEU
1	C	340	LYS
1	C	341	LEU
1	C	350	MET
1	C	353	TYR
1	C	357	LEU
1	C	358	GLU
1	C	363	GLN
1	C	364	ASP
1	C	365	VAL
1	C	370	ASN
1	C	371	ASP
1	C	373	VAL
1	C	376	GLN
1	C	378	GLN
1	C	379	VAL
1	C	382	ILE
1	C	387	VAL
1	C	390	SER
1	C	391	GLU
1	C	396	LYS
1	C	404	VAL
1	C	405	ILE
1	C	410	ASN
1	C	412	VAL
1	C	415	ARG
1	C	417	ARG
1	C	419	VAL
1	C	429	LYS
1	C	430	GLN
1	C	444	ARG
1	C	445	TYR
1	C	450	VAL
1	C	451	VAL
1	C	454	THR
1	D	173	SER
1	D	176	THR
1	D	177	ILE
1	D	178	PHE
1	D	179	SER

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Mol	Chain	Res	Type
1	D	180	GLN
1	D	181	ARG
1	D	188	LYS
1	D	190	LEU
1	D	191	VAL
1	D	192	VAL
1	D	195	LEU
1	D	197	GLU
1	D	198	GLU
1	D	201	MET
1	D	208	MET
1	D	213	ASP
1	D	231	THR
1	D	239	LEU
1	D	242	ILE
1	D	243	HIS
1	D	245	SER
1	D	247	TYR
1	D	252	LYS
1	D	253	SER
1	D	255	ILE
1	D	258	GLU
1	D	260	GLU
1	D	264	ILE
1	D	267	LEU
1	D	271	LEU
1	D	272	ARG
1	D	273	LYS
1	D	275	LEU
1	D	276	ILE
1	D	285	GLU
1	D	293	SER
1	D	295	LYS
1	D	300	LEU
1	D	301	THR
1	D	304	SER
1	D	309	LYS
1	D	311	VAL
1	D	312	THR
1	D	313	GLU
1	D	315	LYS
1	D	317	ASP

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Mol	Chain	Res	Type
1	D	320	VAL
1	D	322	VAL
1	D	325	LYS
1	D	331	ARG
1	D	333	LYS
1	D	334	LEU
1	D	337	HIS
1	D	340	LYS
1	D	350	MET
1	D	353	TYR
1	D	355	ASP
1	D	356	LEU
1	D	368	VAL
1	D	371	ASP
1	D	375	LEU
1	D	379	VAL
1	D	381	ARG
1	D	382	ILE
1	D	387	VAL
1	D	398	ASN
1	D	401	GLU
1	D	406	VAL
1	D	408	LYS
1	D	412	VAL
1	D	415	ARG
1	D	419	VAL
1	D	425	ARG
1	D	438	GLN
1	D	442	LEU
1	D	443	GLN
1	D	450	VAL
1	D	452	SER
1	D	454	THR
1	D	458	SER
1	E	170	SER
1	E	181	ARG
1	E	184	ARG
1	E	188	LYS
1	E	190	LEU
1	E	207	THR
1	E	208	MET
1	E	210	VAL

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Mol	Chain	Res	Type
1	E	211	GLU
1	E	216	LYS
1	E	219	TRP
1	E	220	VAL
1	E	239	LEU
1	E	242	ILE
1	E	245	SER
1	E	246	THR
1	E	256	THR
1	E	259	THR
1	E	261	GLU
1	E	262	ASP
1	E	268	LEU
1	E	270	LEU
1	E	271	LEU
1	E	273	LYS
1	E	275	LEU
1	E	282	SER
1	E	287	PHE
1	E	289	THR
1	E	291	ASP
1	E	293	SER
1	E	295	LYS
1	E	299	LEU
1	E	301	THR
1	E	302	LEU
1	E	306	ASP
1	E	307	SER
1	E	309	LYS
1	E	311	VAL
1	E	312	THR
1	E	313	GLU
1	E	315	LYS
1	E	320	VAL
1	E	321	LEU
1	E	322	VAL
1	E	325	LYS
1	E	331	ARG
1	E	333	LYS
1	E	334	LEU
1	E	340	LYS
1	E	341	LEU

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Mol	Chain	Res	Type
1	E	343	LYS
1	E	348	VAL
1	E	349	SER
1	E	350	MET
1	E	351	ASP
1	E	353	TYR
1	E	355	ASP
1	E	358	GLU
1	E	363	GLN
1	E	364	ASP
1	E	365	VAL
1	E	367	GLN
1	E	368	VAL
1	E	376	GLN
1	E	379	VAL
1	E	382	ILE
1	E	383	TYR
1	E	390	SER
1	E	396	LYS
1	E	398	ASN
1	E	399	SER
1	E	401	GLU
1	E	404	VAL
1	E	405	ILE
1	E	406	VAL
1	E	407	TYR
1	E	409	ASP
1	E	410	ASN
1	E	413	MET
1	E	415	ARG
1	E	417	ARG
1	E	419	VAL
1	E	420	THR
1	E	422	GLU
1	E	429	LYS
1	E	430	GLN
1	E	431	ARG
1	E	435	TYR
1	E	439	ARG
1	E	444	ARG
1	E	454	THR
1	E	455	TYR

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Mol	Chain	Res	Type
1	F	172	GLU
1	F	176	THR
1	F	178	PHE
1	F	181	ARG
1	F	182	ILE
1	F	184	ARG
1	F	185	ASP
1	F	186	LEU
1	F	187	GLN
1	F	188	LYS
1	F	191	VAL
1	F	192	VAL
1	F	197	GLU
1	F	199	LEU
1	F	201	MET
1	F	203	SER
1	F	207	THR
1	F	208	MET
1	F	210	VAL
1	F	213	ASP
1	F	218	THR
1	F	220	VAL
1	F	224	THR
1	F	230	THR
1	F	235	VAL
1	F	239	LEU
1	F	246	THR
1	F	255	ILE
1	F	257	ASP
1	F	260	GLU
1	F	261	GLU
1	F	264	ILE
1	F	265	PHE
1	F	270	LEU
1	F	271	LEU
1	F	273	LYS
1	F	274	ARG
1	F	276	ILE
1	F	282	SER
1	F	288	MET
1	F	289	THR
1	F	295	LYS

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Mol	Chain	Res	Type
1	F	306	ASP
1	F	309	LYS
1	F	310	VAL
1	F	312	THR
1	F	315	LYS
1	F	321	LEU
1	F	323	THR
1	F	329	LYS
1	F	333	LYS
1	F	340	LYS
1	F	341	LEU
1	F	345	VAL
1	F	350	MET
1	F	351	ASP
1	F	353	TYR
1	F	356	LEU
1	F	357	LEU
1	F	359	ASP
1	F	363	GLN
1	F	364	ASP
1	F	365	VAL
1	F	368	VAL
1	F	371	ASP
1	F	375	LEU
1	F	379	VAL
1	F	382	ILE
1	F	387	VAL
1	F	392	TYR
1	F	393	PHE
1	F	396	LYS
1	F	399	SER
1	F	404	VAL
1	F	405	ILE
1	F	406	VAL
1	F	415	ARG
1	F	416	GLN
1	F	420	THR
1	F	421	VAL
1	F	422	GLU
1	F	425	ARG
1	F	431	ARG
1	F	432	ASP

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Mol	Chain	Res	Type
1	F	436	VAL
1	F	437	THR
1	F	442	LEU
1	F	443	GLN
1	F	444	ARG
1	F	446	PHE
1	F	448	ASN
1	F	450	VAL
1	F	451	VAL
1	F	454	THR
1	G	174	TYR
1	G	176	THR
1	G	181	ARG
1	G	186	LEU
1	G	188	LYS
1	G	190	LEU
1	G	191	VAL
1	G	196	PHE
1	G	201	MET
1	G	209	LEU
1	G	210	VAL
1	G	211	GLU
1	G	213	ASP
1	G	218	THR
1	G	220	VAL
1	G	224	THR
1	G	228	ASP
1	G	230	THR
1	G	234	GLU
1	G	239	LEU
1	G	242	ILE
1	G	244	PHE
1	G	248	LYS
1	G	249	LEU
1	G	252	LYS
1	G	253	SER
1	G	255	ILE
1	G	259	THR
1	G	261	GLU
1	G	264	ILE
1	G	268	LEU
1	G	270	LEU

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Mol	Chain	Res	Type
1	G	272	ARG
1	G	273	LYS
1	G	274	ARG
1	G	279	HIS
1	G	283	ILE
1	G	285	GLU
1	G	287	PHE
1	G	293	SER
1	G	295	LYS
1	G	299	LEU
1	G	305	GLU
1	G	310	VAL
1	G	311	VAL
1	G	312	THR
1	G	313	GLU
1	G	320	VAL
1	G	322	VAL
1	G	329	LYS
1	G	330	LEU
1	G	334	LEU
1	G	337	HIS
1	G	340	LYS
1	G	342	SER
1	G	349	SER
1	G	350	MET
1	G	351	ASP
1	G	359	ASP
1	G	363	GLN
1	G	364	ASP
1	G	370	ASN
1	G	375	LEU
1	G	376	GLN
1	G	379	VAL
1	G	389	VAL
1	G	390	SER
1	G	391	GLU
1	G	393	PHE
1	G	396	LYS
1	G	406	VAL
1	G	409	ASP
1	G	415	ARG
1	G	417	ARG

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Mol	Chain	Res	Type
1	G	420	THR
1	G	422	GLU
1	G	424	GLU
1	G	429	LYS
1	G	431	ARG
1	G	436	VAL
1	G	437	THR
1	G	442	LEU
1	G	443	GLN
1	G	444	ARG
1	G	450	VAL
1	G	451	VAL
1	G	458	SER
1	H	174	TYR
1	H	175	GLU
1	H	176	THR
1	H	177	ILE
1	H	178	PHE
1	H	180	GLN
1	H	181	ARG
1	H	182	ILE
1	H	187	GLN
1	H	191	VAL
1	H	192	VAL
1	H	197	GLU
1	H	208	MET
1	H	209	LEU
1	H	210	VAL
1	H	218	THR
1	H	220	VAL
1	H	231	THR
1	H	235	VAL
1	H	242	ILE
1	H	245	SER
1	H	246	THR
1	H	248	LYS
1	H	249	LEU
1	H	252	LYS
1	H	255	ILE
1	H	257	ASP
1	H	259	THR
1	H	260	GLU

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Mol	Chain	Res	Type
1	H	262	ASP
1	H	268	LEU
1	H	271	LEU
1	H	273	LYS
1	H	277	GLU
1	H	281	VAL
1	H	282	SER
1	H	285	GLU
1	H	288	MET
1	H	289	THR
1	H	295	LYS
1	H	300	LEU
1	H	304	SER
1	H	309	LYS
1	H	311	VAL
1	H	320	VAL
1	H	321	LEU
1	H	325	LYS
1	H	330	LEU
1	H	332	ARG
1	H	333	LYS
1	H	334	LEU
1	H	340	LYS
1	H	341	LEU
1	H	345	VAL
1	H	346	LEU
1	H	349	SER
1	H	350	MET
1	H	351	ASP
1	H	354	TYR
1	H	358	GLU
1	H	365	VAL
1	H	368	VAL
1	H	370	ASN
1	H	371	ASP
1	H	372	SER
1	H	376	GLN
1	H	379	VAL
1	H	382	ILE
1	H	396	LYS
1	H	404	VAL
1	H	406	VAL

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Mol	Chain	Res	Type
1	H	407	TYR
1	H	409	ASP
1	H	412	VAL
1	H	415	ARG
1	H	417	ARG
1	H	419	VAL
1	H	420	THR
1	H	422	GLU
1	H	429	LYS
1	H	431	ARG
1	H	441	ASN
1	H	442	LEU
1	H	444	ARG
1	H	445	TYR
1	H	452	SER
1	H	454	THR
1	H	458	SER
1	I	173	SER
1	I	178	PHE
1	I	179	SER
1	I	182	ILE
1	I	184	ARG
1	I	186	LEU
1	I	187	GLN
1	I	190	LEU
1	I	192	VAL
1	I	201	MET
1	I	204	LYS
1	I	208	MET
1	I	210	VAL
1	I	213	ASP
1	I	218	THR
1	I	220	VAL
1	I	235	VAL
1	I	242	ILE
1	I	245	SER
1	I	248	LYS
1	I	253	SER
1	I	254	PHE
1	I	255	ILE
1	I	258	GLU
1	I	262	ASP

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Mol	Chain	Res	Type
1	I	268	LEU
1	I	271	LEU
1	I	275	LEU
1	I	282	SER
1	I	285	GLU
1	I	289	THR
1	I	293	SER
1	I	295	LYS
1	I	297	LYS
1	I	300	LEU
1	I	304	SER
1	I	312	THR
1	I	323	THR
1	I	325	LYS
1	I	329	LYS
1	I	330	LEU
1	I	334	LEU
1	I	340	LYS
1	I	341	LEU
1	I	342	SER
1	I	364	ASP
1	I	365	VAL
1	I	367	GLN
1	I	368	VAL
1	I	370	ASN
1	I	371	ASP
1	I	372	SER
1	I	375	LEU
1	I	379	VAL
1	I	381	ARG
1	I	382	ILE
1	I	383	TYR
1	I	385	LEU
1	I	396	LYS
1	I	402	PHE
1	I	404	VAL
1	I	406	VAL
1	I	407	TYR
1	I	413	MET
1	I	415	ARG
1	I	419	VAL
1	I	420	THR

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Mol	Chain	Res	Type
1	I	429	LYS
1	I	431	ARG
1	I	437	THR
1	I	438	GLN
1	I	439	ARG
1	I	442	LEU
1	I	444	ARG
1	I	445	TYR
1	I	450	VAL
1	I	452	SER
1	I	454	THR
1	J	173	SER
1	J	174	TYR
1	J	176	THR
1	J	179	SER
1	J	181	ARG
1	J	184	ARG
1	J	187	GLN
1	J	188	LYS
1	J	189	GLU
1	J	191	VAL
1	J	192	VAL
1	J	197	GLU
1	J	208	MET
1	J	213	ASP
1	J	216	LYS
1	J	218	THR
1	J	219	TRP
1	J	220	VAL
1	J	223	SER
1	J	224	THR
1	J	229	THR
1	J	231	THR
1	J	234	GLU
1	J	236	LYS
1	J	242	ILE
1	J	246	THR
1	J	247	TYR
1	J	248	LYS
1	J	255	ILE
1	J	257	ASP
1	J	260	GLU

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Mol	Chain	Res	Type
1	J	264	ILE
1	J	268	LEU
1	J	271	LEU
1	J	273	LYS
1	J	275	LEU
1	J	276	ILE
1	J	277	GLU
1	J	279	HIS
1	J	282	SER
1	J	285	GLU
1	J	293	SER
1	J	295	LYS
1	J	300	LEU
1	J	305	GLU
1	J	309	LYS
1	J	310	VAL
1	J	311	VAL
1	J	315	LYS
1	J	317	ASP
1	J	321	LEU
1	J	322	VAL
1	J	323	THR
1	J	325	LYS
1	J	328	SER
1	J	329	LYS
1	J	330	LEU
1	J	333	LYS
1	J	334	LEU
1	J	337	HIS
1	J	339	LEU
1	J	341	LEU
1	J	342	SER
1	J	345	VAL
1	J	346	LEU
1	J	357	LEU
1	J	362	TRP
1	J	365	VAL
1	J	368	VAL
1	J	370	ASN
1	J	375	LEU
1	J	378	GLN
1	J	379	VAL

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Mol	Chain	Res	Type
1	J	382	ILE
1	J	387	VAL
1	J	393	PHE
1	J	404	VAL
1	J	405	ILE
1	J	410	ASN
1	J	415	ARG
1	J	420	THR
1	J	429	LYS
1	J	441	ASN
1	J	442	LEU
1	J	444	ARG
1	J	445	TYR
1	J	452	SER
1	J	458	SER
1	K	175	GLU
1	K	177	ILE
1	K	178	PHE
1	K	181	ARG
1	K	182	ILE
1	K	183	ILE
1	K	184	ARG
1	K	185	ASP
1	K	188	LYS
1	K	191	VAL
1	K	192	VAL
1	K	197	GLU
1	K	199	LEU
1	K	208	MET
1	K	209	LEU
1	K	210	VAL
1	K	213	ASP
1	K	220	VAL
1	K	231	THR
1	K	236	LYS
1	K	241	GLU
1	K	242	ILE
1	K	248	LYS
1	K	249	LEU
1	K	252	LYS
1	K	253	SER
1	K	255	ILE

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Mol	Chain	Res	Type
1	K	256	THR
1	K	258	GLU
1	K	262	ASP
1	K	268	LEU
1	K	270	LEU
1	K	272	ARG
1	K	273	LYS
1	K	276	ILE
1	K	282	SER
1	K	283	ILE
1	K	289	THR
1	K	295	LYS
1	K	297	LYS
1	K	302	LEU
1	K	305	GLU
1	K	310	VAL
1	K	315	LYS
1	K	322	VAL
1	K	328	SER
1	K	330	LEU
1	K	332	ARG
1	K	334	LEU
1	K	337	HIS
1	K	340	LYS
1	K	345	VAL
1	K	349	SER
1	K	350	MET
1	K	354	TYR
1	K	357	LEU
1	K	358	GLU
1	K	363	GLN
1	K	364	ASP
1	K	367	GLN
1	K	370	ASN
1	K	374	LYS
1	K	375	LEU
1	K	379	VAL
1	K	382	ILE
1	K	388	VAL
1	K	393	PHE
1	K	396	LYS
1	K	398	ASN

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Mol	Chain	Res	Type
1	K	404	VAL
1	K	406	VAL
1	K	407	TYR
1	K	409	ASP
1	K	410	ASN
1	K	412	VAL
1	K	415	ARG
1	K	419	VAL
1	K	424	GLU
1	K	425	ARG
1	K	429	LYS
1	K	434	TYR
1	K	436	VAL
1	K	444	ARG
1	K	448	ASN
1	K	450	VAL
1	K	454	THR
1	L	171	SER
1	L	176	THR
1	L	177	ILE
1	L	178	PHE
1	L	180	GLN
1	L	181	ARG
1	L	182	ILE
1	L	184	ARG
1	L	186	LEU
1	L	190	LEU
1	L	191	VAL
1	L	192	VAL
1	L	197	GLU
1	L	199	LEU
1	L	201	MET
1	L	204	LYS
1	L	207	THR
1	L	209	LEU
1	L	216	LYS
1	L	218	THR
1	L	223	SER
1	L	231	THR
1	L	236	LYS
1	L	239	LEU
1	L	242	ILE

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Mol	Chain	Res	Type
1	L	246	THR
1	L	249	LEU
1	L	255	ILE
1	L	259	THR
1	L	261	GLU
1	L	262	ASP
1	L	264	ILE
1	L	272	ARG
1	L	273	LYS
1	L	274	ARG
1	L	275	LEU
1	L	276	ILE
1	L	279	HIS
1	L	283	ILE
1	L	287	PHE
1	L	288	MET
1	L	289	THR
1	L	293	SER
1	L	295	LYS
1	L	302	LEU
1	L	304	SER
1	L	305	GLU
1	L	310	VAL
1	L	312	THR
1	L	315	LYS
1	L	320	VAL
1	L	328	SER
1	L	329	LYS
1	L	332	ARG
1	L	334	LEU
1	L	340	LYS
1	L	341	LEU
1	L	347	ILE
1	L	355	ASP
1	L	357	LEU
1	L	358	GLU
1	L	359	ASP
1	L	363	GLN
1	L	365	VAL
1	L	368	VAL
1	L	372	SER
1	L	373	VAL

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Mol	Chain	Res	Type
1	L	375	LEU
1	L	381	ARG
1	L	396	LYS
1	L	398	ASN
1	L	404	VAL
1	L	405	ILE
1	L	406	VAL
1	L	408	LYS
1	L	411	PHE
1	L	415	ARG
1	L	416	GLN
1	L	419	VAL
1	L	422	GLU
1	L	424	GLU
1	L	429	LYS
1	L	434	TYR
1	L	435	TYR
1	L	436	VAL
1	L	437	THR
1	L	438	GLN
1	L	439	ARG
1	L	444	ARG
1	L	446	PHE
1	L	450	VAL
1	L	451	VAL
1	L	454	THR
1	M	174	TYR
1	M	175	GLU
1	M	177	ILE
1	M	178	PHE
1	M	185	ASP
1	M	186	LEU
1	M	187	GLN
1	M	188	LYS
1	M	189	GLU
1	M	202	SER
1	M	204	LYS
1	M	206	LEU
1	M	225	TYR
1	M	239	LEU
1	M	241	GLU
1	M	242	ILE

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Mol	Chain	Res	Type
1	M	245	SER
1	M	246	THR
1	M	248	LYS
1	M	249	LEU
1	M	256	THR
1	M	258	GLU
1	M	264	ILE
1	M	274	ARG
1	M	276	ILE
1	M	288	MET
1	M	289	THR
1	M	291	ASP
1	M	299	LEU
1	M	301	THR
1	M	302	LEU
1	M	304	SER
1	M	310	VAL
1	M	311	VAL
1	M	312	THR
1	M	321	LEU
1	M	323	THR
1	M	327	ILE
1	M	329	LYS
1	M	330	LEU
1	M	334	LEU
1	M	340	LYS
1	M	341	LEU
1	M	350	MET
1	M	351	ASP
1	M	354	TYR
1	M	357	LEU
1	M	363	GLN
1	M	364	ASP
1	M	367	GLN
1	M	370	ASN
1	M	375	LEU
1	M	376	GLN
1	M	379	VAL
1	M	389	VAL
1	M	391	GLU
1	M	398	ASN
1	M	402	PHE

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Mol	Chain	Res	Type
1	M	405	ILE
1	M	406	VAL
1	M	407	TYR
1	M	409	ASP
1	M	410	ASN
1	M	411	PHE
1	M	415	ARG
1	M	419	VAL
1	M	436	VAL
1	M	437	THR
1	M	439	ARG
1	M	446	PHE
1	M	450	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	279	HIS
1	A	367	GLN
1	B	279	HIS
1	B	410	ASN
1	B	416	GLN
1	B	438	GLN
1	C	180	GLN
1	C	367	GLN
1	C	370	ASN
1	C	448	ASN
1	D	180	GLN
1	D	363	GLN
1	D	370	ASN
1	D	376	GLN
1	D	426	GLN
1	E	187	GLN
1	E	279	HIS
1	E	363	GLN
1	E	378	GLN
1	E	410	ASN
1	E	430	GLN
1	F	363	GLN
1	F	376	GLN
1	F	378	GLN

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Mol	Chain	Res	Type
1	F	410	ASN
1	F	430	GLN
1	F	448	ASN
1	G	367	GLN
1	G	438	GLN
1	H	180	GLN
1	H	376	GLN
1	I	337	HIS
1	I	376	GLN
1	I	438	GLN
1	J	279	HIS
1	K	180	GLN
1	K	376	GLN
1	K	378	GLN
1	K	410	ASN
1	K	443	GLN
1	L	363	GLN
1	L	378	GLN
1	L	410	ASN
1	M	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	210:VAL	C	211:GLU	N	1.11
1	J	294:GLY	C	295:LYS	N	1.08

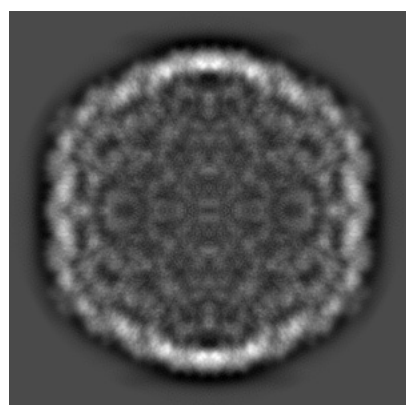
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20099. These allow visual inspection of the internal detail of the map and identification of artifacts.

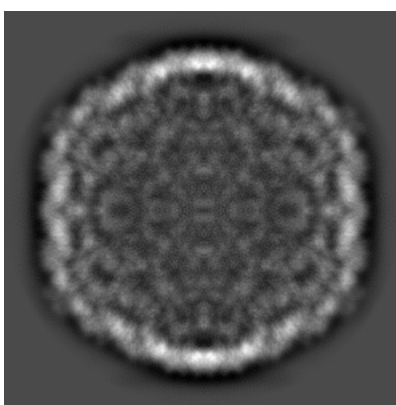
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

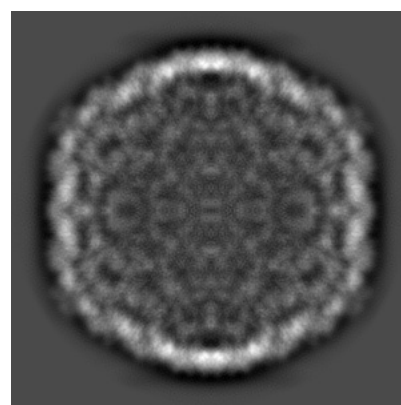
6.1.1 Primary map



X



Y

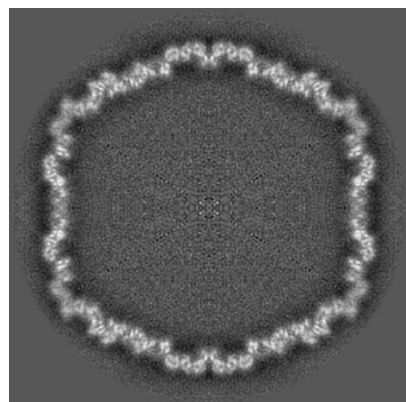


Z

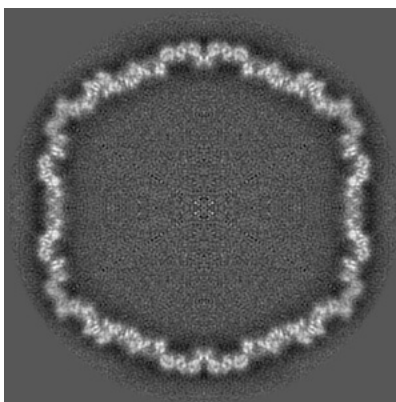
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

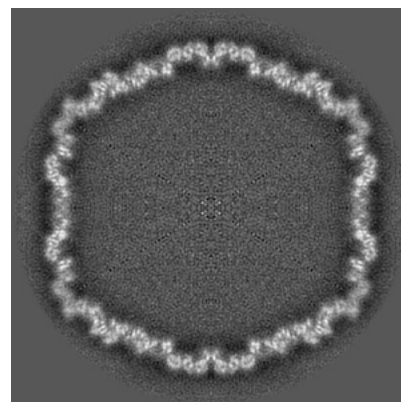
6.2.1 Primary map



X Index: 400



Y Index: 400

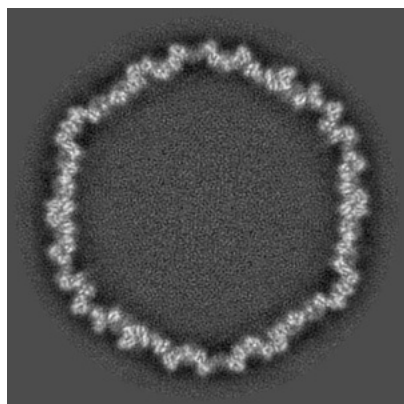


Z Index: 400

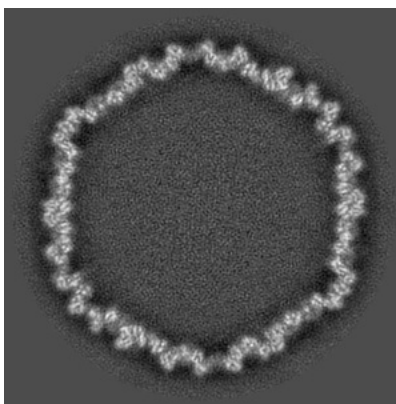
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

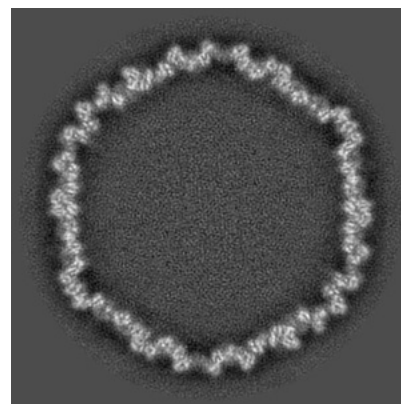
6.3.1 Primary map



X Index: 318



Y Index: 318

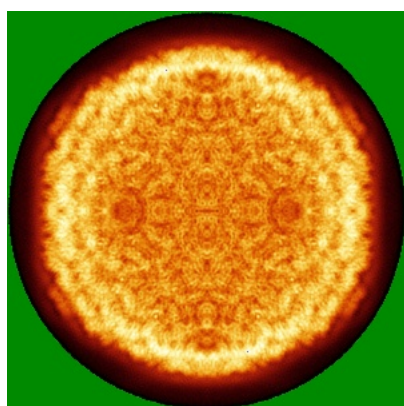


Z Index: 482

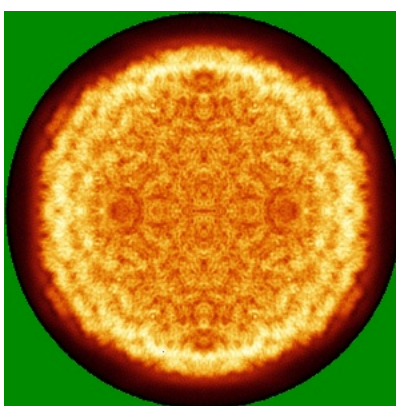
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

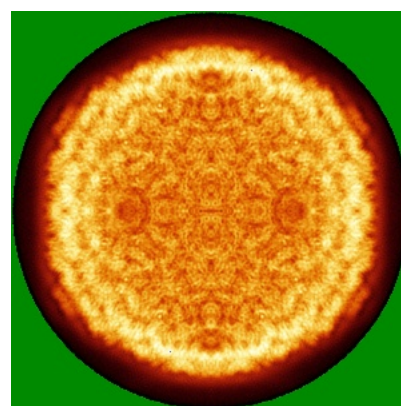
6.4.1 Primary map



X



Y

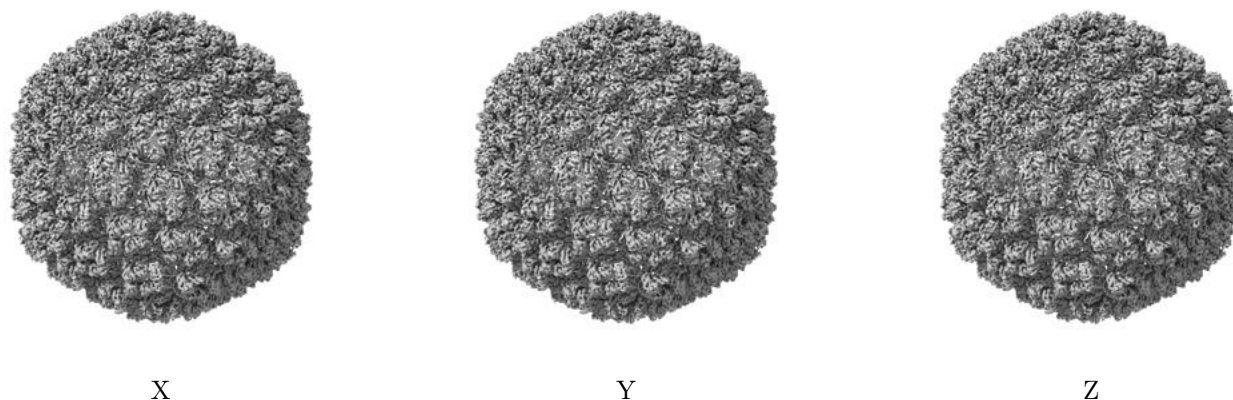


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 14.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

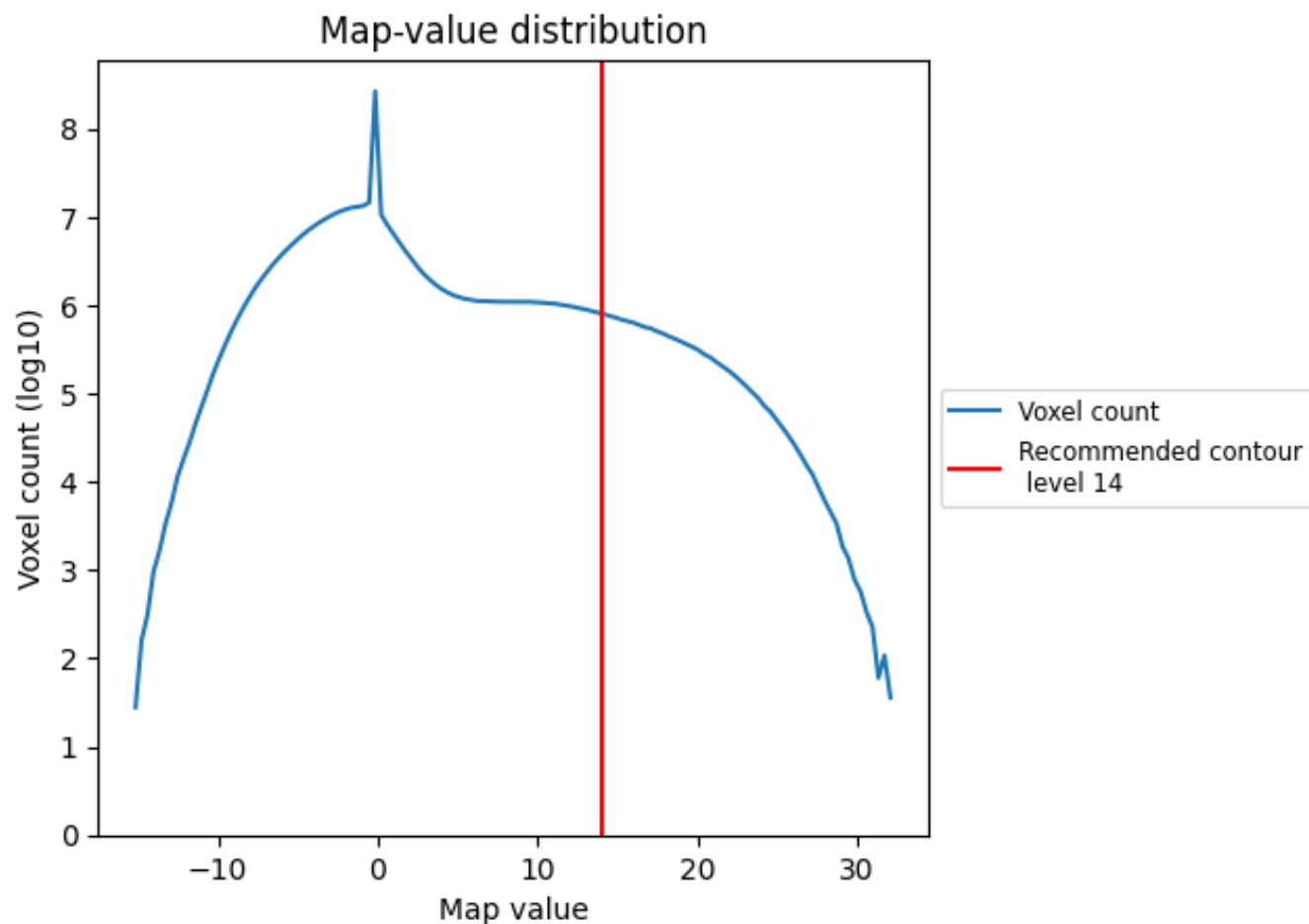
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

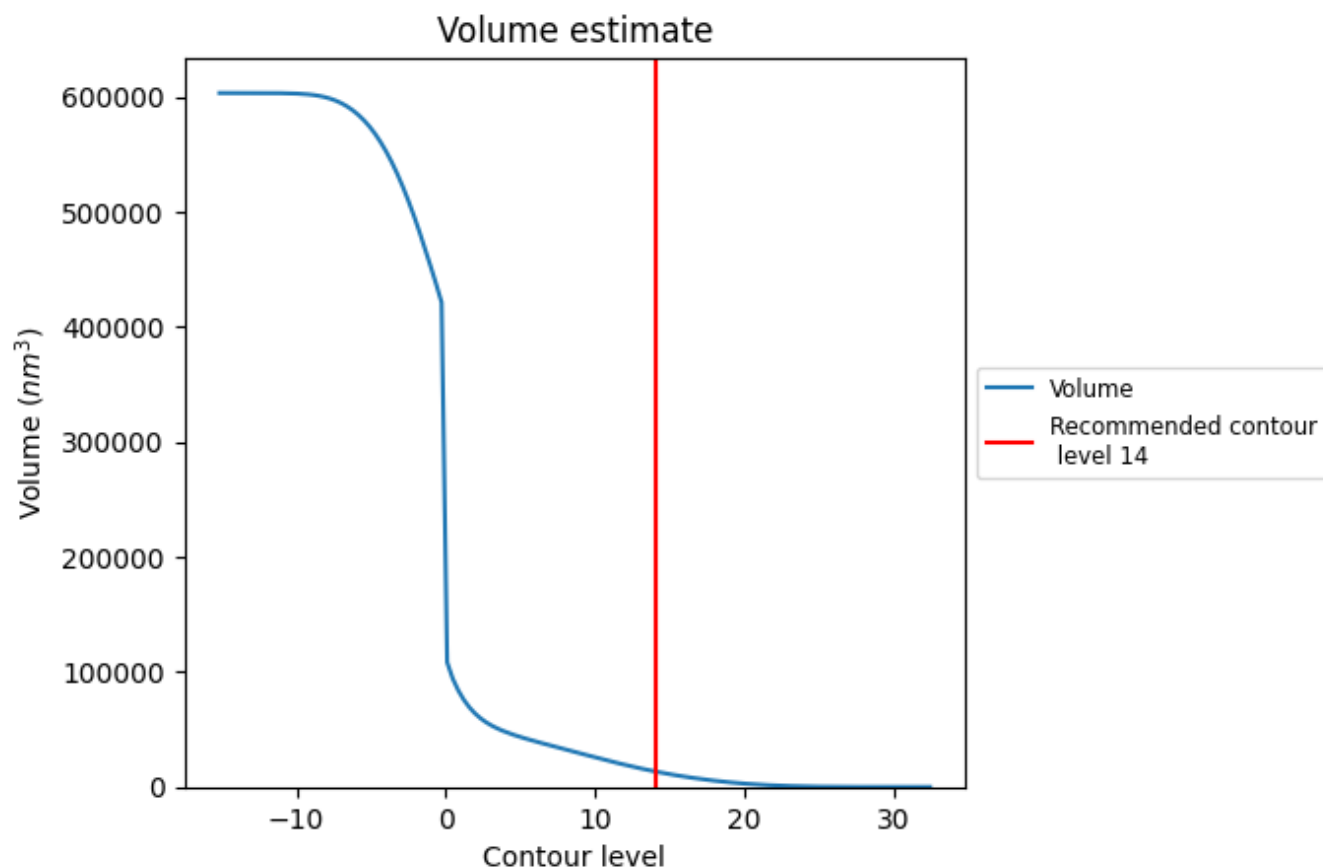
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

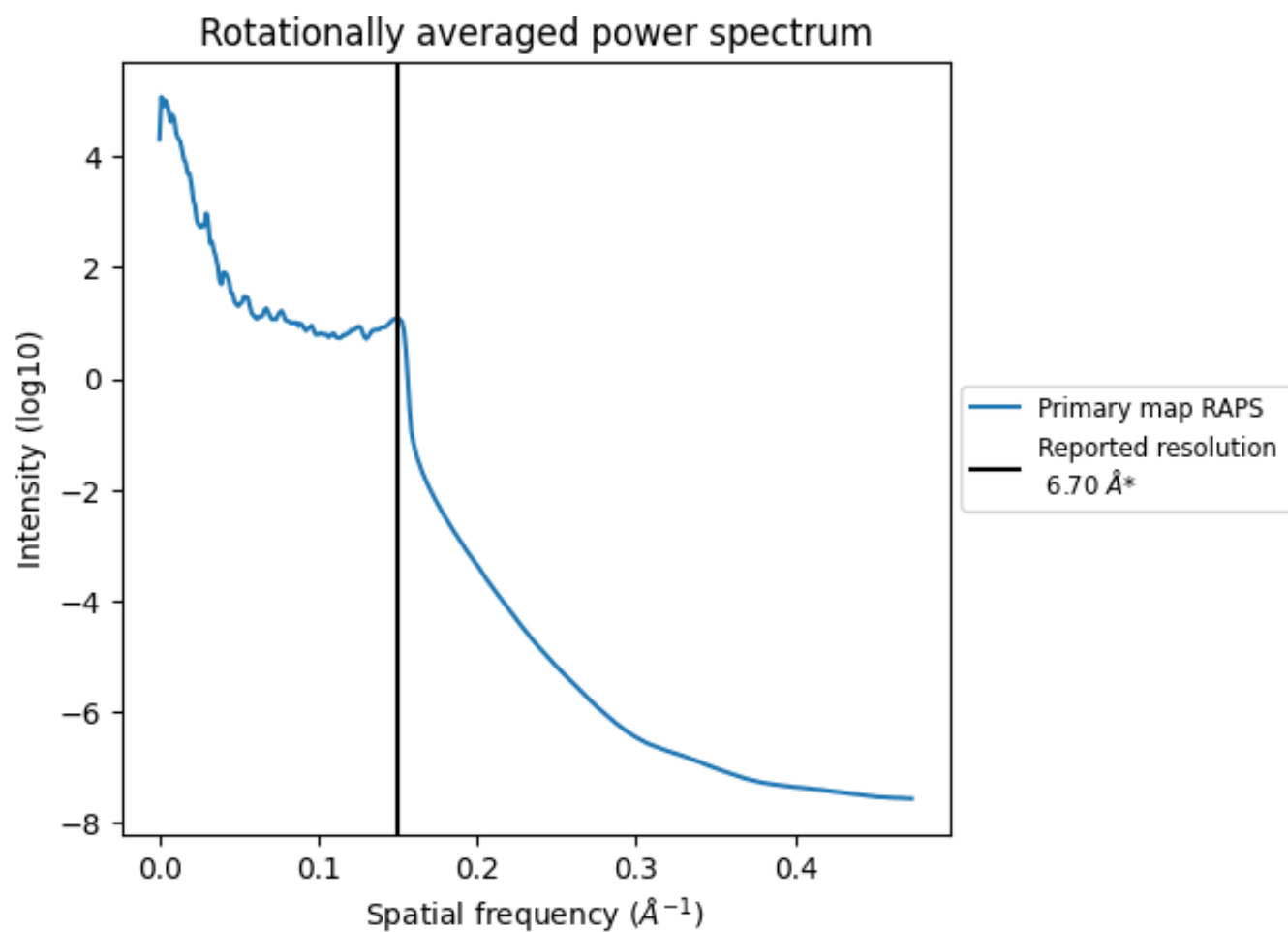
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135533 nm³; this corresponds to an approximate mass of 12243 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

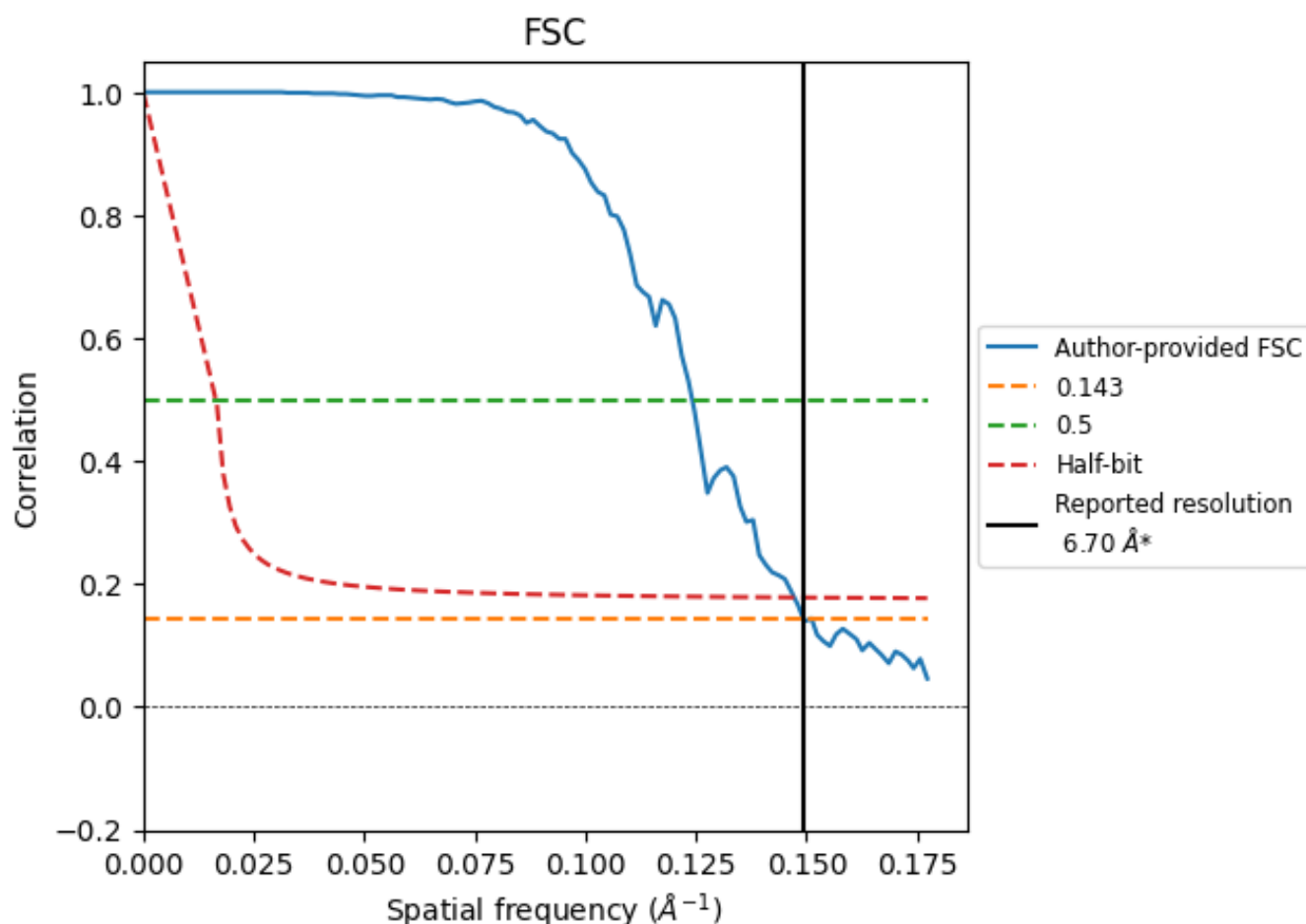


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	6.70	8.06	6.79
Unmasked-calculated*	-	-	-

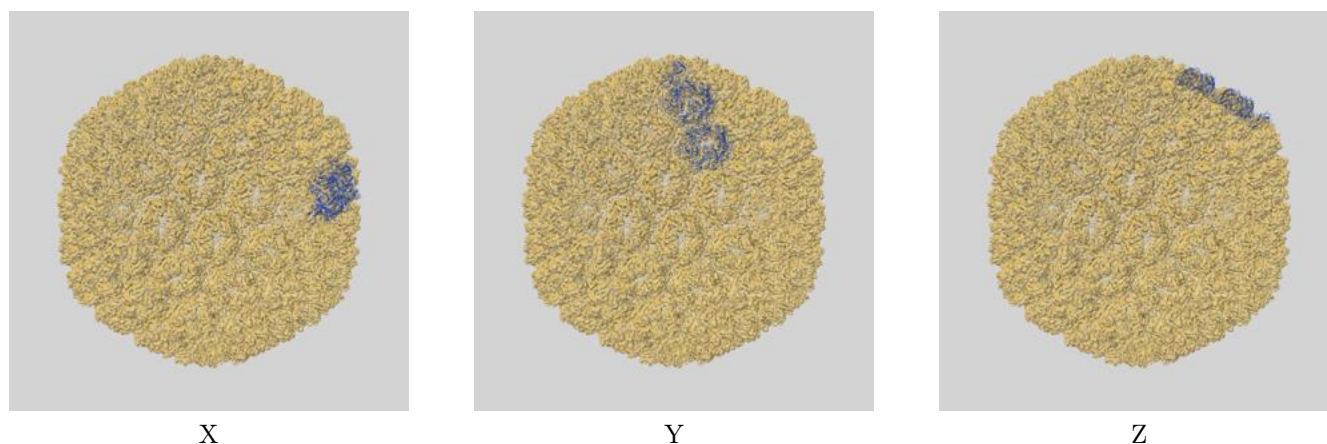
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

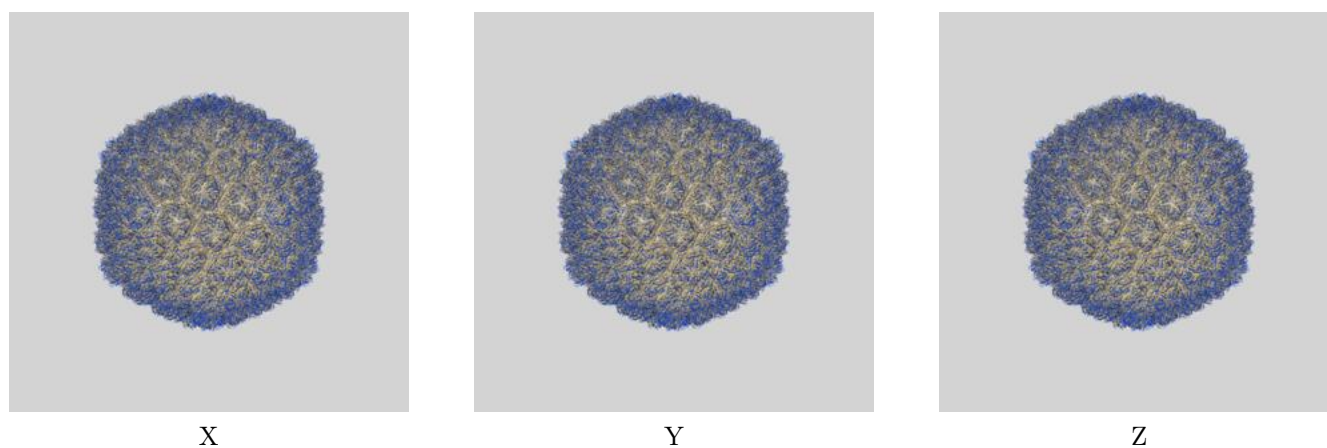
This section contains information regarding the fit between EMDB map EMD-20099 and PDB model 6OKB. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

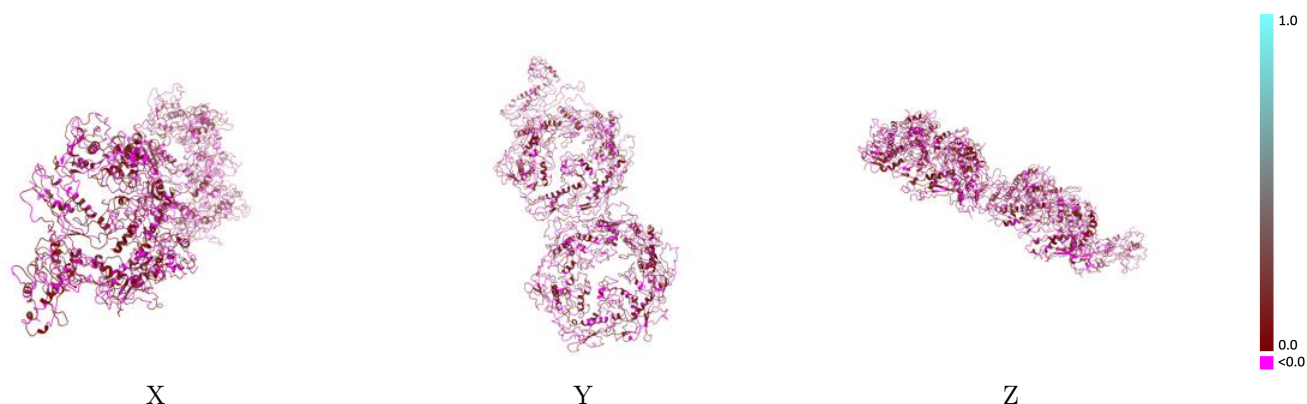


9.1.2 Map-model assembly overlay [i](#)



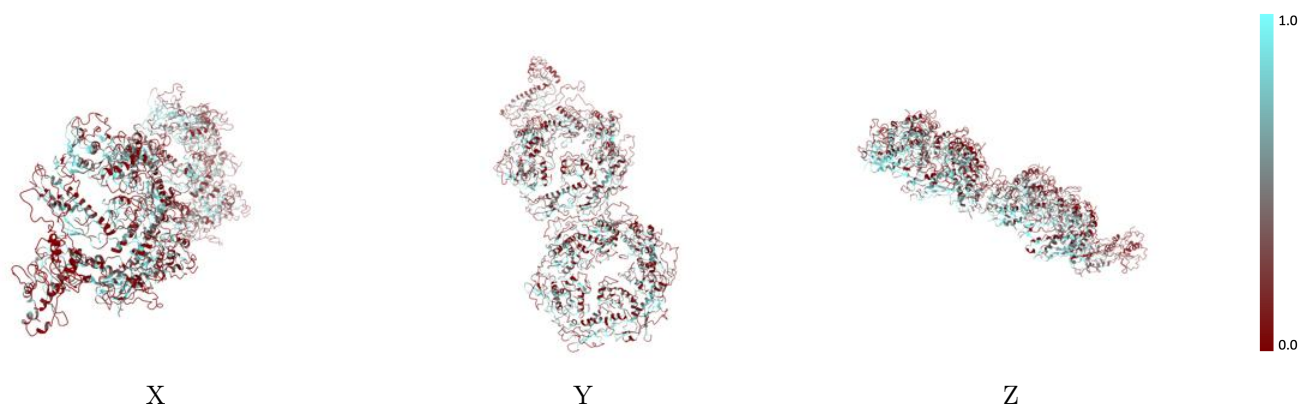
The images above show the 3D surface view of the map at the recommended contour level 14.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



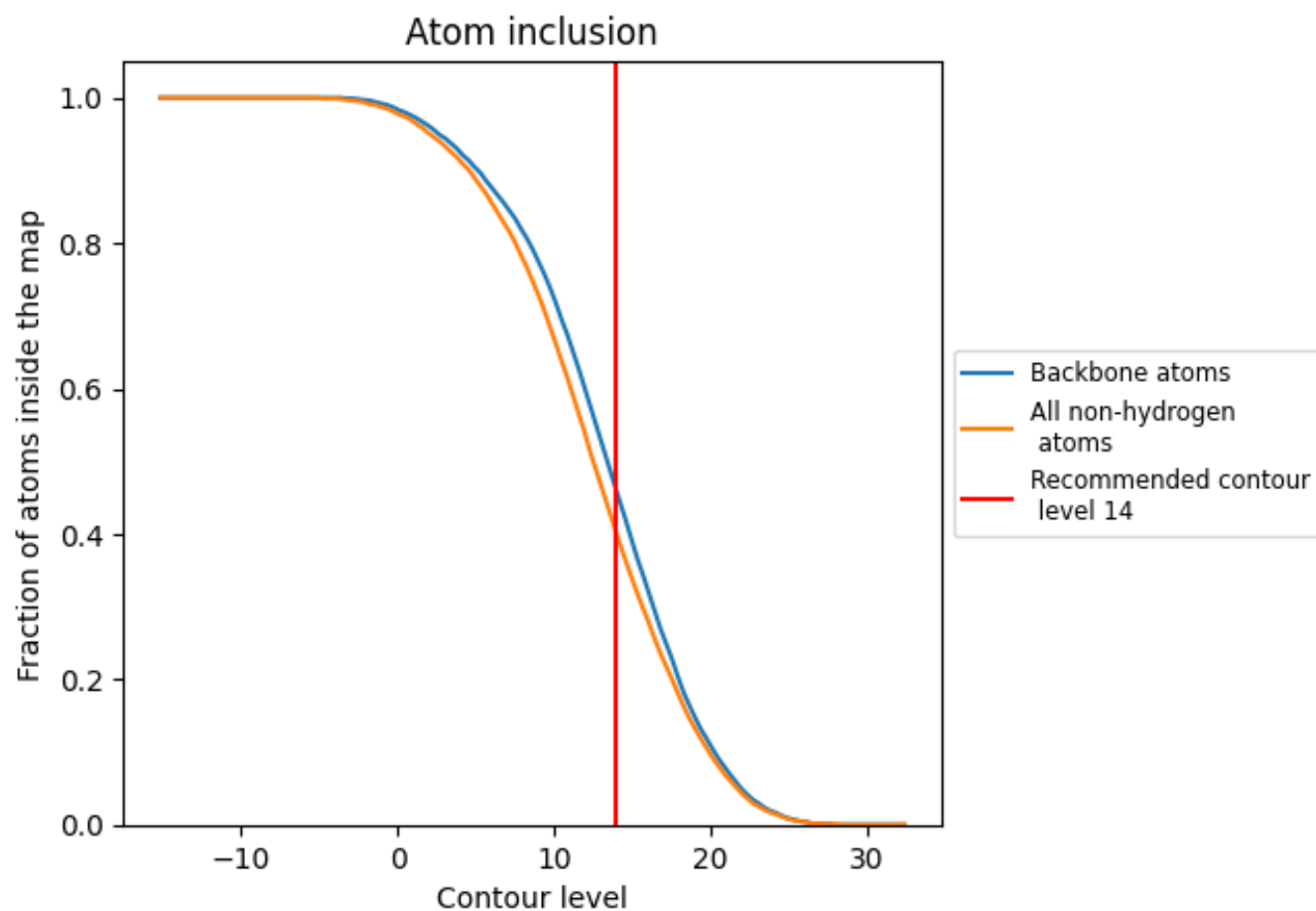
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4000	0.0760
A	0.4330	0.0880
B	0.4220	0.0790
C	0.4180	0.0670
D	0.4510	0.0790
E	0.4350	0.0710
F	0.4110	0.0720
G	0.4090	0.0660
H	0.4080	0.0760
I	0.4130	0.0740
J	0.4050	0.0660
K	0.4020	0.0800
L	0.3980	0.0830
M	0.1970	0.0830

