



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:01 AM UTC

PDB ID : 7AST / pdb_00007ast
EMDB ID : EMD-11904
Title : Apo Human RNA Polymerase III
Authors : Ramsay, E.P.; Abascal-Palacios, G.; Daiss, J.L.; King, H.; Gouge, J.; Pils, M.;
Beuron, F.; Morris, E.; Gunkel, P.; Engel, C.; Vannini, A.
Deposited on : 2020-10-28
Resolution : 4.00 Å(reported)

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

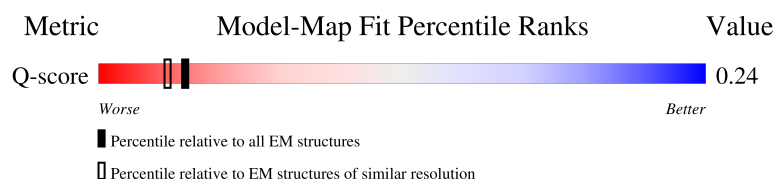
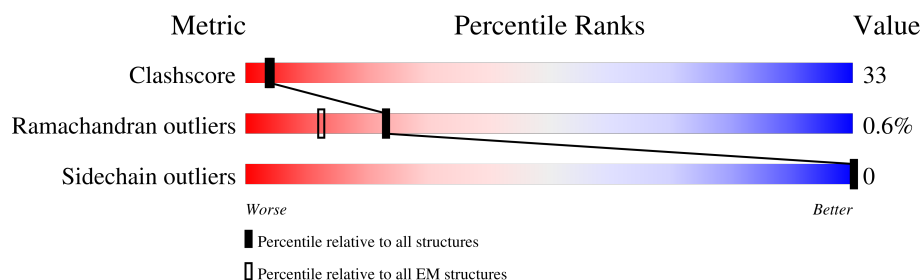
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



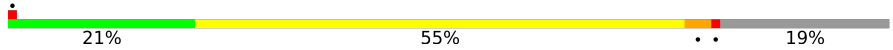
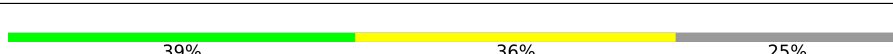
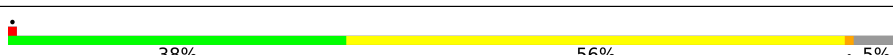
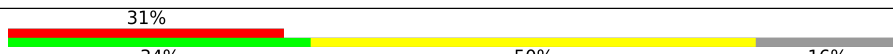
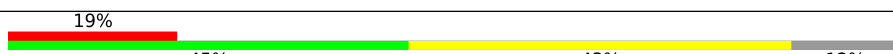
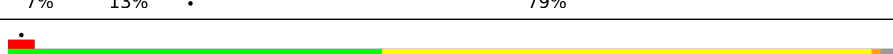
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	N	1390	
2	A	108	
3	B	67	
4	C	58	

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Mol	Chain	Length	Quality of chain
5	D	150	
6	E	127	
7	F	210	
8	G	133	
9	H	346	
10	I	148	
11	J	204	
12	K	708	
13	L	398	
14	M	1133	
15	Z	316	
16	X	534	
17	Y	36	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 34518 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 DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	1238	Total	C	N	O	S	0	0
			9385	5928	1643	1746	68		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	37	Total	C	N	O	S	0	0
			288	179	55	49	5		

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	121	Total	C	N	O	S	0	0
			972	627	160	179	6		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	81	Total	C	N	O	S	0	0
			649	414	111	119	5		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	100	Total	C	N	O	S	0	0
			794	493	142	152	7		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	329	Total	C	N	O	S	0	0
			2635	1663	472	489	11		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	125	Total	C	N	O	S	0	0
			1008	631	175	199	3		

- Molecule 11 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	179	Total	C	N	O	S	0	0
			1442	938	226	271	7		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	137	Total	C	N	O	S	0	0
			1119	718	192	204	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	82	Total	C	N	O	S	0	0
			620	397	104	115	4		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	1114	Total	C	N	O	S	0	0
			8811	5581	1540	1621	69		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	63	Total	C	N	O	S	0	0
			518	337	78	99	4		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	440	Total	C	N	O	S	0	0
			3487	2193	607	665	22		

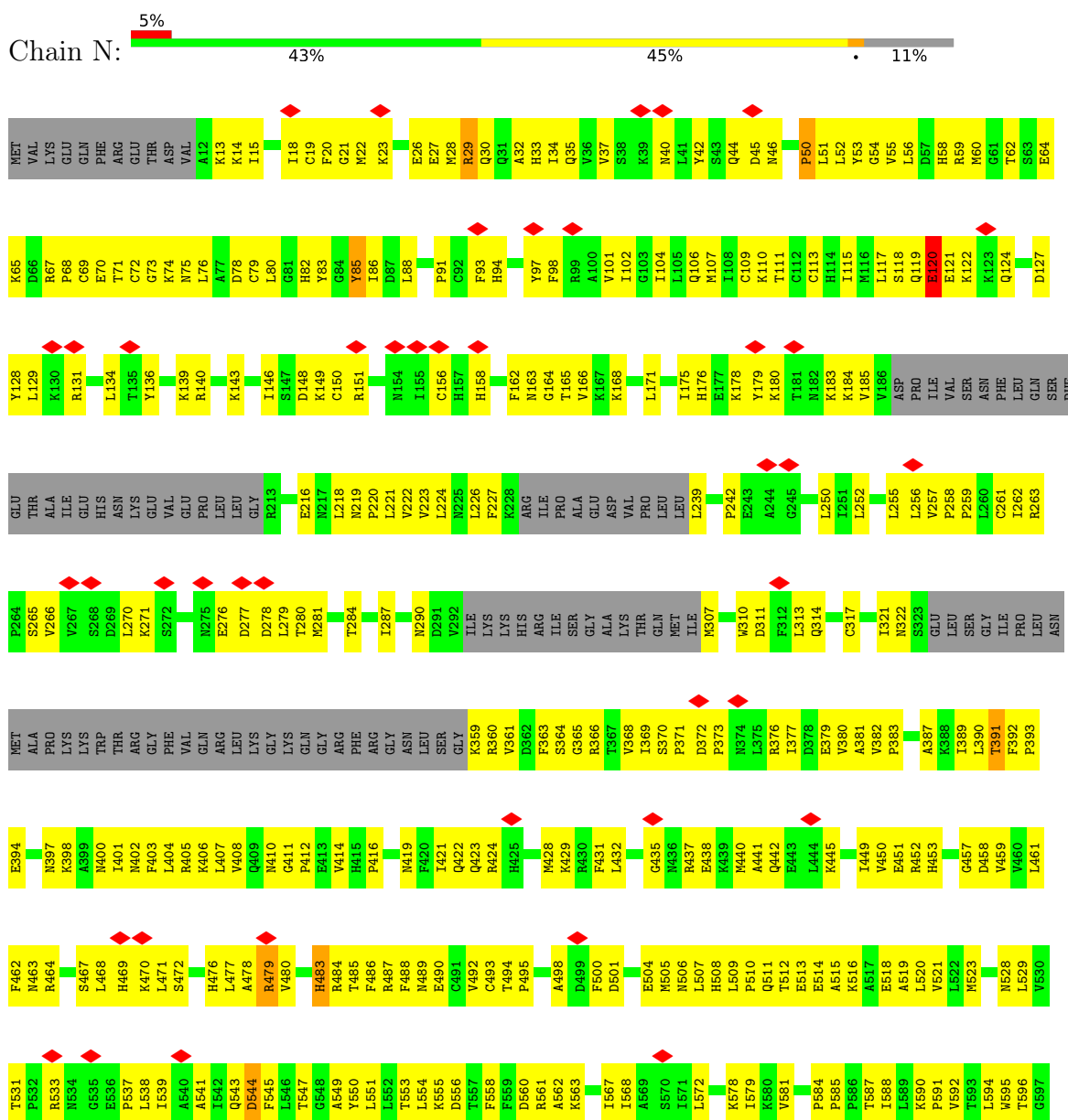
- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7-beta.

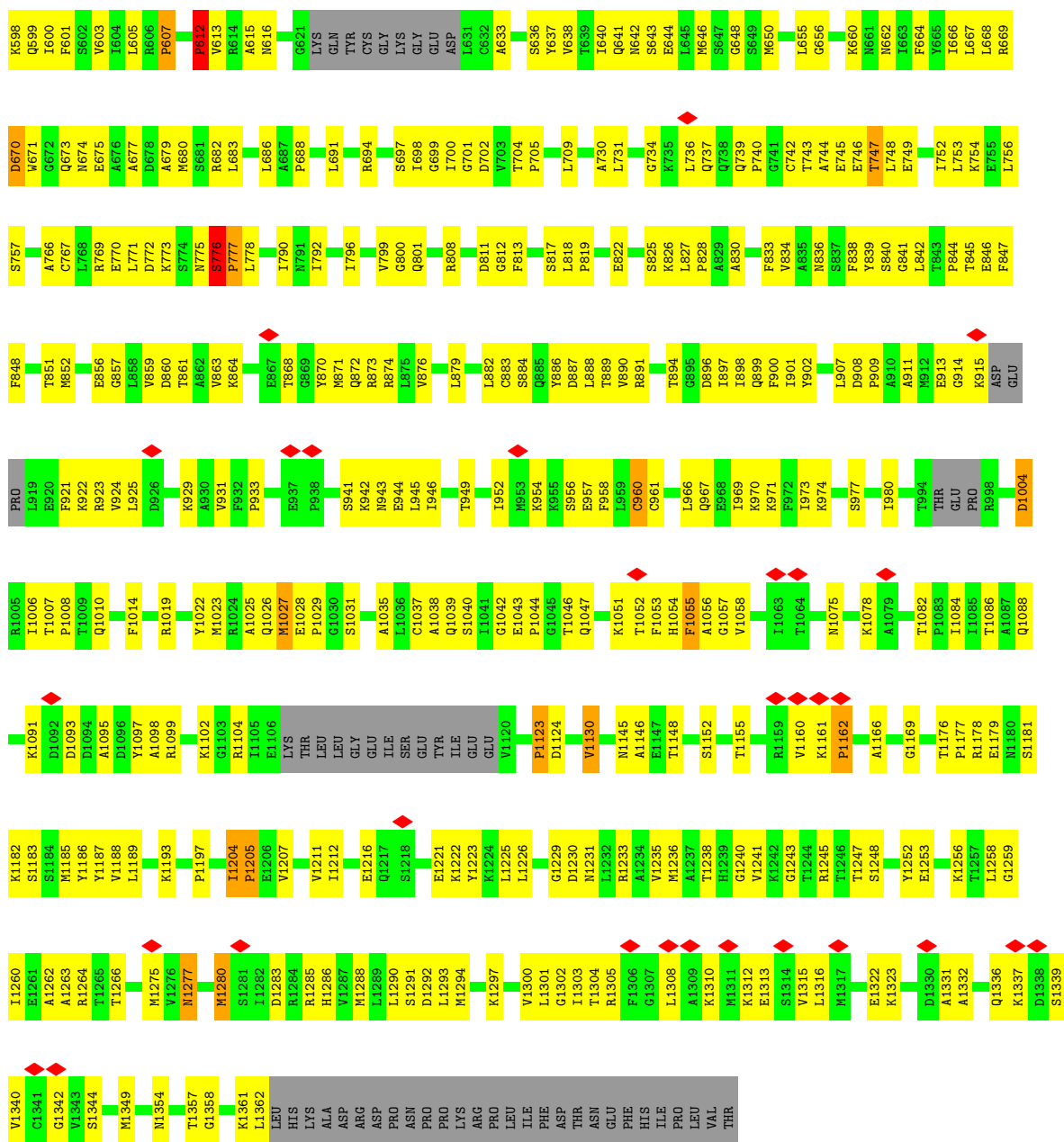
Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	36	Total	C	N	O	0	0
			180	108	36	36		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

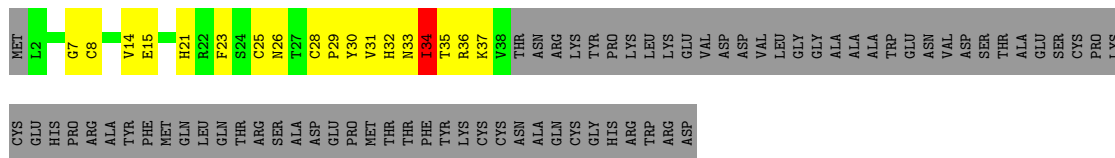
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1





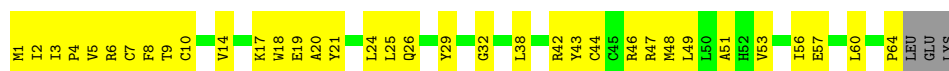
• Molecule 2: DNA-directed RNA polymerase III subunit RPC10

Chain A: 18% 16% 66%

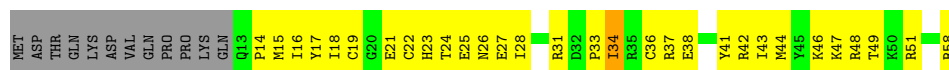


• Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC5

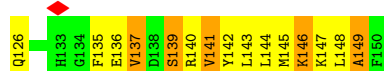
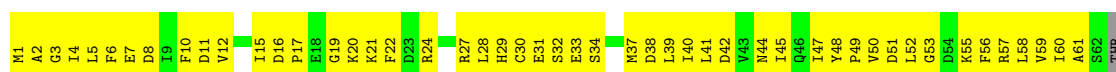
Chain B: 43% 52%



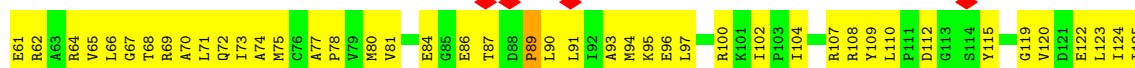
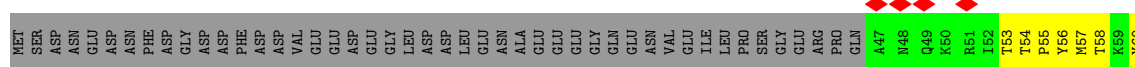
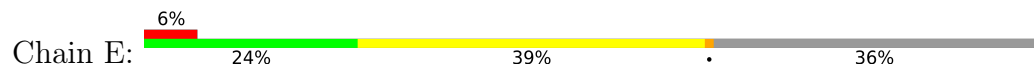
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



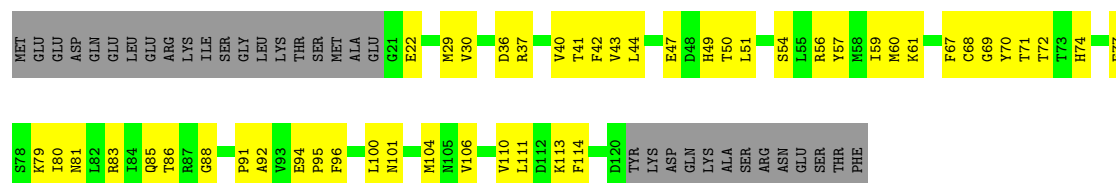
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1





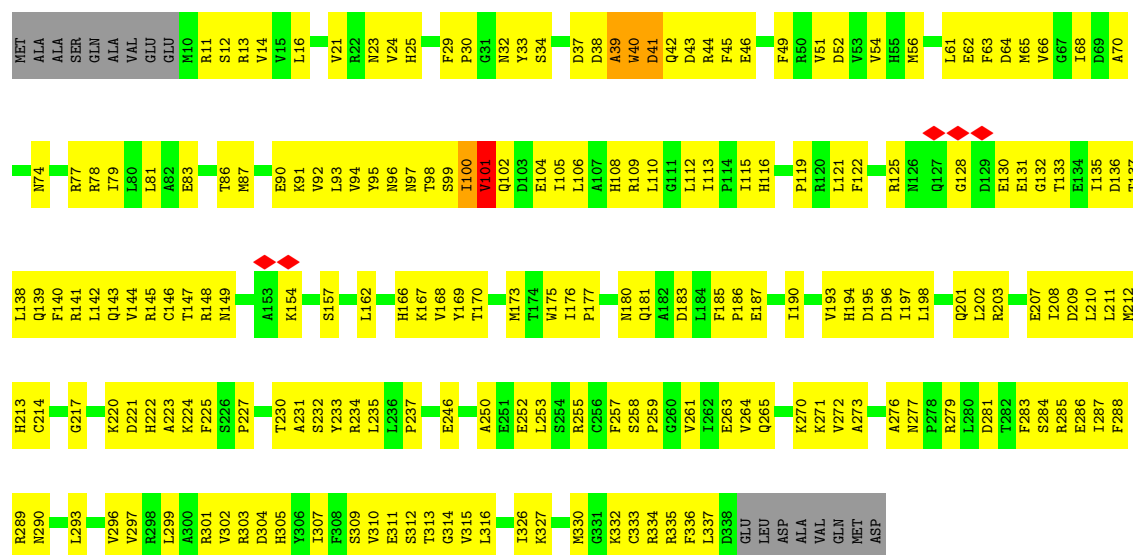
• Molecule 8: DNA-directed RNA polymerases I and III subunit RPAC2

Chain G: 39% 36% 25%



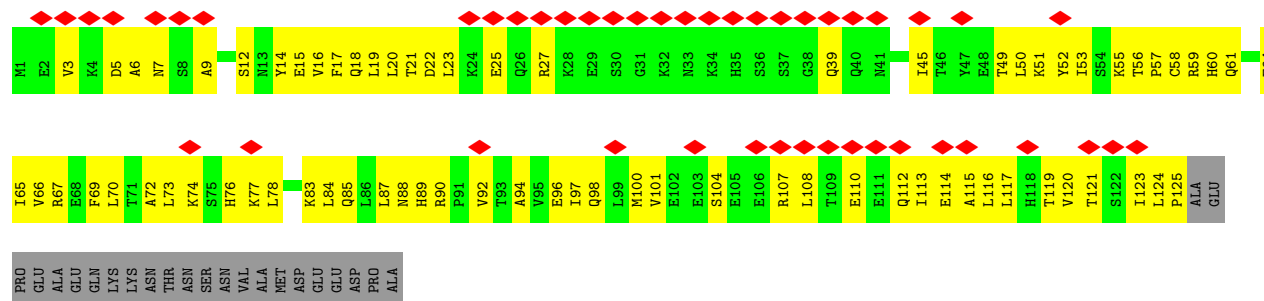
• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC1

Chain H: 38% 56% 5%



• Molecule 10: DNA-directed RNA polymerase III subunit RPC9

Chain I: 31% 34% 50% 16%

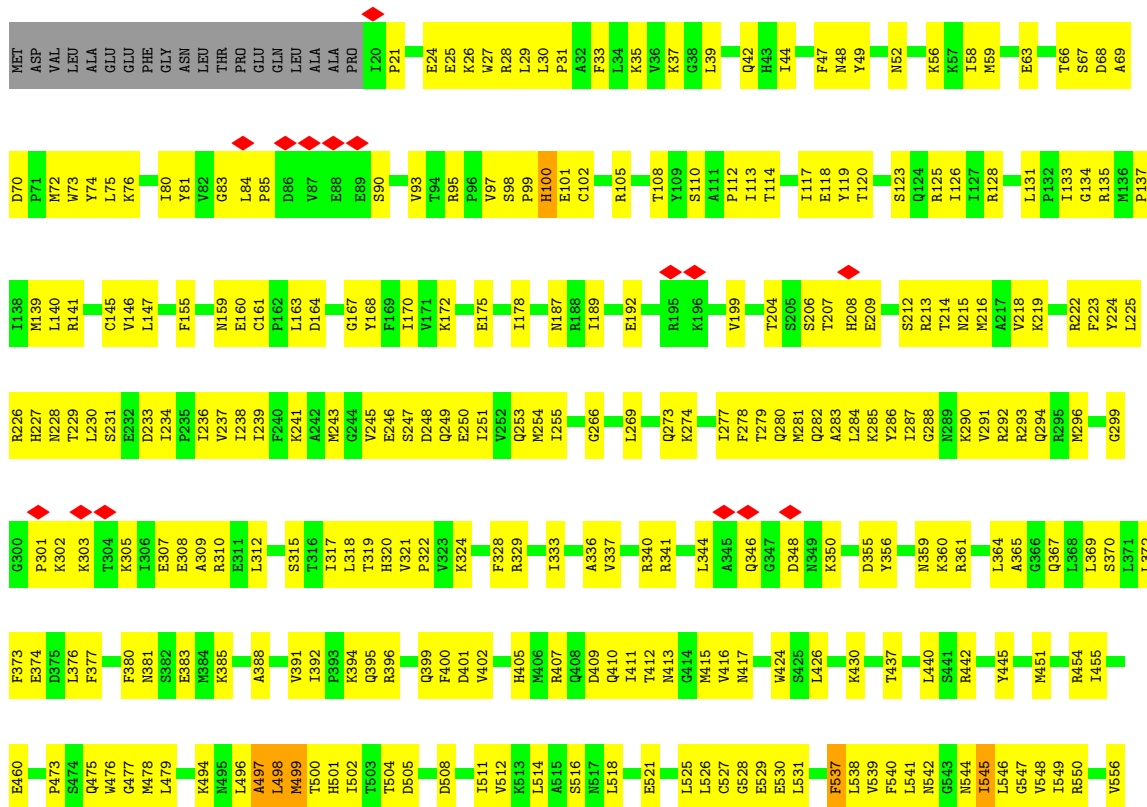


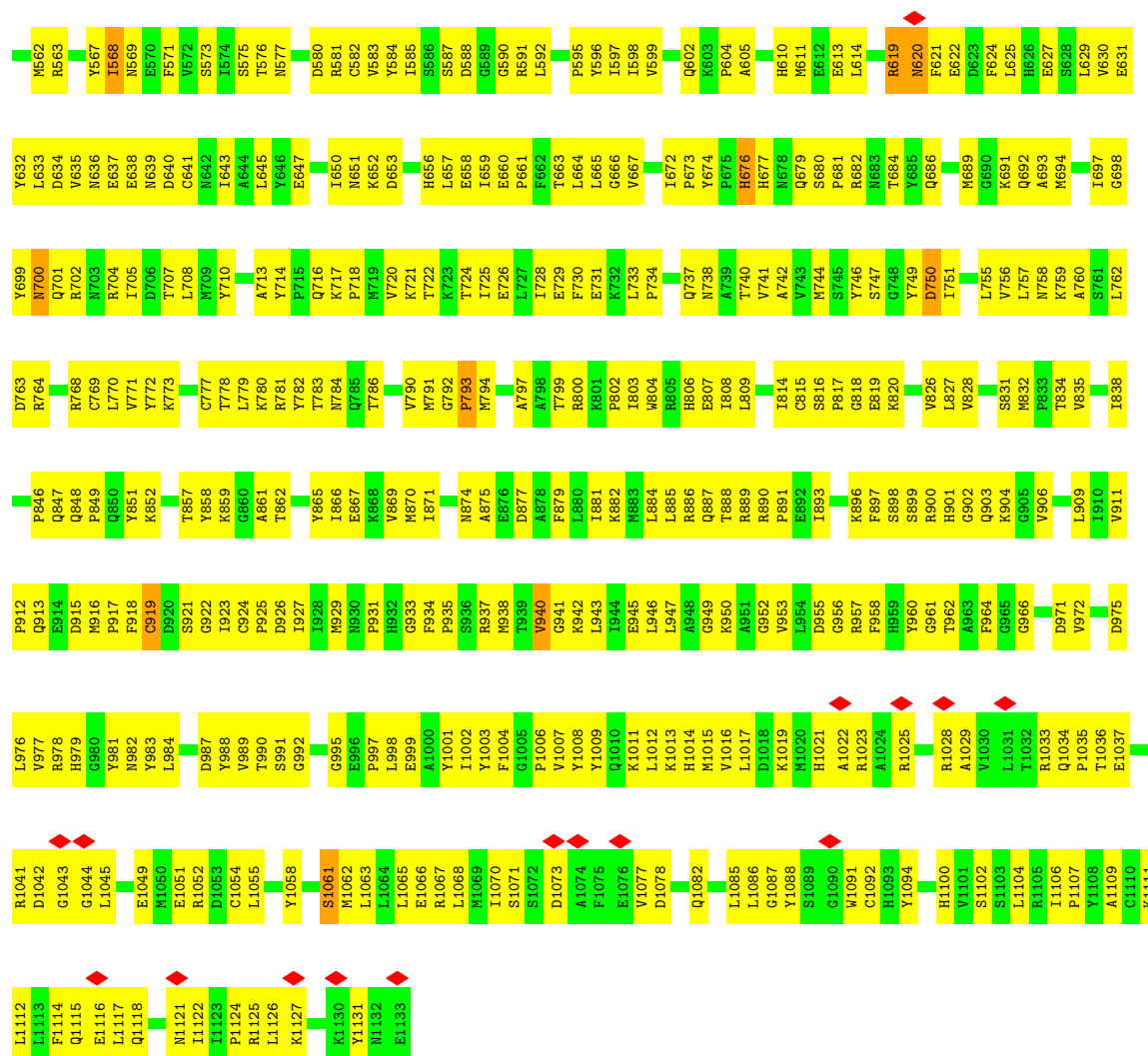
• Molecule 11: DNA-directed RNA polymerase III subunit RPC8



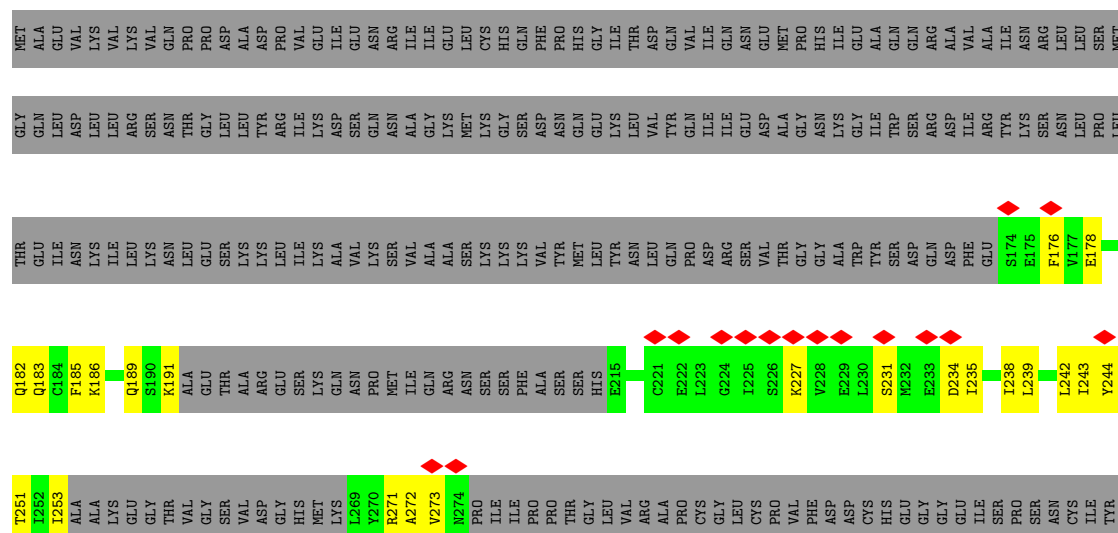
D367	GLN	LYS	PRO	GLY	ASN	MET
R368	GLU	THR	LEU	ASN	ASN	SER
R369	LYS	PRO	ALA	TRP	GLU	GLU
T370	ASP	GLY	HIS	ASP	GLY	GLY
G371	ARG	LEU	SER	LYS	ARG	ASN
E372	GLU	PRO	GLY	THR	LYS	ALA
M373	ALA	LYS	TRP	VAL	ILE	ALA
T374	LYS	ASP	LEU	ASP	LYS	GLY
V375	LEU	VAL	PHE	VAL	GLU	GLU
L376	ALA	SER	LYS	SER	GLU	PRO
G377	GLU	VAL	GLU	ASP	PRO	SER
H378	ASN	ALA	GLU	MET	LYS	THR
V379	ALA	GLU	ASN	GLY	GLU	PRO
K380	THR	LEU	ASP	PRO	GLU	GLY
H381	LYS	LEU	GLU	SER	VAL	GLY
K382	LEU	ARG	PRO	HIS	THR	PRO
L383	ALA	GLU	ASP	ILE	ARG	GLY
V384	ASP	LEU	VAL	ILE	LYS	PRO
C385	LEU	SER	LYS	ASN	LYS	PRO
S386	THR	L260	PRO	PRO	GLU	LEU
P387	GLU	T261	TRP	ILE	GLU	LEU
D388	GLY	K262	LEU	LYS	LYS	THR
F389	GLN	E263	ALA	GLU	ARG	GLY
GLU	V326		GLY	LYS	ARG	ALA
SER	G327	L266	PRO	ARG	ASP	GLY
LEU		L267	LYS	GLU	ARG	GLY
LEU	L330	F268	GLU	THR	ASP	ILE
ASP	I331	L269	GLU	ASP	GLY	GLY
HIS	R332	Q270	ASP	GLU	GLN	ARG
LYS		L271	MET	GLU	ARG	ARG
HIS	R336	P272	GLU	THR	GLU	PRO
ARG	V337		VAL	LYS	GLY	ALA
	Q338	L275	ASP	GLN	HIS	PRO
	L339	P276	ILE	ILE	GLY	PRO
	L340	G277	PRO	LEU	ARG	PRO
	L341		ALA	LEU	GLY	THR
	G342	GLN	VAL	MET	ARG	PRO
	K343	PRO	LYS	LEU	GLY	GLY
	V344	THR	VAL	GLU	ARG	ARG
	T345	GLN	LYS	LYS	PRO	LEU
	L346	ASP	GLU	ASP	GLU	PRO
	D347	ILE	GLU	ASP	VAL	SER
	V348	LYS	PRO	PHE	ILE	ILE
	T349	PRO	ARG	LEU	GLN	ARG
	M350	ILE	ASP	ASP	SER	ARG
		LYS	GLU	ASP	HIS	ARG
	A353	THR	GLU	PRO	SER	ASP
	C354	GLU	GLU	GLY	ILE	ASP
	S355	VAL	GLU	LEU	PHE	THR
	F356	GLN	ALA	ASN	GLU	THR
	L357	GLY	LYS	ARG	GLU	GLY
	Q358	GLU	MET	ASP	GLY	GLY
	F359	ASP	LYS	THR	PRO	VAL
	L360	GLY	ALA	ARG	ALA	LYS
	V361	GLN	PRO	ASN	GLU	LYS
	S362	VAL	PRO	MET	MET	LYS
	F363	VAL	LYS	PRO	MET	THR
	G364	LEU	ALA	VAL	LYS	PHE
	L365	ILE	ALA	GLN	THR	LYS
	C366	LYS	ARG	LEU	LYS	PRO

Chain M: 42% 55% ..





● Molecule 15: DNA-directed RNA polymerase III subunit RPC6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25369	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 ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.365	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	383.40002, 383.40002, 383.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	N	0.77	8/9535 (0.1%)	0.68	16/12862 (0.1%)
2	A	0.27	0/294	0.86	2/396 (0.5%)
3	B	0.37	0/516	0.70	0/696
4	C	0.25	0/394	0.69	0/524
5	D	2.20	7/988 (0.7%)	0.97	4/1323 (0.3%)
6	E	0.21	0/659	0.63	0/891
7	F	0.18	0/1745	0.53	1/2358 (0.0%)
8	G	0.30	0/808	0.57	0/1090
9	H	0.28	0/2689	0.67	0/3644
10	I	0.17	0/1021	0.46	0/1377
11	J	0.19	0/1481	0.46	0/2013
12	K	0.20	0/1146	0.57	0/1549
13	L	0.19	0/626	0.59	0/842
14	M	0.29	0/8982	0.65	5/12118 (0.0%)
15	Z	0.17	0/523	0.53	0/701
16	X	0.14	0/3534	0.41	0/4766
All	All	0.58	15/34941 (0.0%)	0.63	28/47150 (0.1%)

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	N	0	16
2	A	0	1
3	B	0	1
4	C	0	1
5	D	0	5
6	E	0	1
7	F	0	2
9	H	0	7
12	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	L	0	4
14	M	0	16
16	X	0	1
All	All	0	58

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	29	ARG	CB-CG	57.79	3.25	1.52
5	D	146	LYS	CD-CE	52.46	3.09	1.52
5	D	88	PHE	CD1-CE1	20.25	1.99	1.38
5	D	88	PHE	CD2-CE2	20.19	1.99	1.38
1	N	85	TYR	CD2-CE2	20.18	1.99	1.38
1	N	85	TYR	CD1-CE1	19.39	1.96	1.38
5	D	88	PHE	CE1-CZ	18.97	1.95	1.38
5	D	88	PHE	CE2-CZ	18.86	1.95	1.38
1	N	85	TYR	CE1-CZ	15.65	1.75	1.38
1	N	85	TYR	CE2-CZ	15.49	1.75	1.38
5	D	88	PHE	CG-CD2	14.34	1.69	1.38
5	D	88	PHE	CG-CD1	14.31	1.69	1.38
1	N	85	TYR	CG-CD2	13.56	1.67	1.39
1	N	85	TYR	CG-CD1	13.16	1.67	1.39
1	N	391	THR	C-N	6.12	1.46	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	146	LYS	CG-CD-CE	13.09	141.41	111.30
1	N	29	ARG	CA-CB-CG	10.35	134.80	114.10
1	N	29	ARG	CB-CG-CD	10.05	134.41	111.30
1	N	612	PRO	N-CA-CB	8.24	111.90	103.25
1	N	1123	PRO	N-CA-CB	7.59	110.40	103.34
1	N	1205	PRO	N-CA-CB	7.47	111.09	103.25
1	N	607	PRO	N-CA-CB	7.42	111.05	103.25
1	N	1188	VAL	N-CA-C	-6.89	104.88	112.80
14	M	940	VAL	N-CA-C	-6.78	105.91	112.29
14	M	477	GLY	CA-C-N	6.61	134.17	121.54
14	M	477	GLY	C-N-CA	6.61	134.17	121.54
1	N	1197	PRO	N-CA-CB	6.54	110.12	103.25
5	D	141	VAL	N-CA-C	-6.50	106.47	112.96
14	M	1061	SER	CA-C-N	-6.16	111.97	122.56
14	M	1061	SER	C-N-CA	-6.16	111.97	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	146	LYS	CD-CE-NZ	5.93	130.87	111.90
1	N	1162	PRO	N-CA-CB	5.86	109.41	103.25
7	F	72	MET	CA-CB-CG	5.67	125.43	114.10
1	N	1055	PHE	CA-C-N	5.53	131.66	121.70
1	N	1055	PHE	C-N-CA	5.53	131.66	121.70
1	N	120	GLU	CA-C-N	5.30	131.24	121.70
1	N	120	GLU	C-N-CA	5.30	131.24	121.70
1	N	1204	ILE	CA-C-N	5.16	126.28	119.84
1	N	1204	ILE	C-N-CA	5.16	126.28	119.84
5	D	146	LYS	CB-CG-CD	5.09	123.01	111.30
1	N	479	ARG	CA-CB-CG	5.02	124.14	114.10
2	A	32	HIS	CA-C-N	-5.01	111.97	121.54
2	A	32	HIS	C-N-CA	-5.01	111.97	121.54

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	34	ILE	Peptide
3	B	26	GLN	Peptide
4	C	34	ILE	Peptide
5	D	137	VAL	Peptide
5	D	139	SER	Peptide
5	D	149	ALA	Peptide
5	D	3	GLY	Peptide
5	D	88	PHE	Peptide
6	E	77	ALA	Peptide
7	F	28	VAL	Peptide
7	F	52	ARG	Peptide
9	H	100	ILE	Peptide
9	H	101	VAL	Peptide
9	H	37	ASP	Peptide
9	H	39	ALA	Peptide
9	H	40	TRP	Peptide
9	H	41	ASP	Peptide
9	H	56	MET	Peptide
12	K	113	ARG	Peptide
12	K	41	ASP	Peptide
12	K	43	PRO	Peptide
13	L	343	LYS	Peptide
13	L	349	THR	Peptide
13	L	356	PHE	Peptide

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Mol	Chain	Res	Type	Group
13	L	377	GLY	Peptide
14	M	100	HIS	Peptide
14	M	460	GLU	Peptide
14	M	497	ALA	Peptide
14	M	530	GLU	Peptide
14	M	537	PHE	Peptide
14	M	544	ASN	Peptide
14	M	568	ILE	Peptide
14	M	619	ARG	Peptide
14	M	620	ASN	Peptide
14	M	676	HIS	Peptide
14	M	700	ASN	Peptide
14	M	746	TYR	Peptide
14	M	750	ASP	Peptide
14	M	792	GLY	Peptide
14	M	857	THR	Peptide
14	M	95	ARG	Peptide
1	N	1004	ASP	Peptide
1	N	1027	MET	Peptide
1	N	1161	LYS	Peptide
1	N	120	GLU	Peptide
1	N	1277	ASN	Peptide
1	N	480	VAL	Peptide
1	N	483	HIS	Peptide
1	N	563	LYS	Peptide
1	N	572	LEU	Peptide
1	N	633	ALA	Peptide
1	N	670	ASP	Peptide
1	N	747	THR	Peptide
1	N	776	SER	Peptide
1	N	812	GLY	Peptide
1	N	840	SER	Peptide
1	N	960	CYS	Peptide
16	X	373	LYS	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	N	9385	0	9273	689	0
2	A	288	0	279	24	0
3	B	507	0	525	53	0
4	C	388	0	395	38	0
5	D	972	0	959	159	0
6	E	649	0	678	60	0
7	F	1715	0	1733	104	0
8	G	794	0	780	54	0
9	H	2635	0	2620	211	0
10	I	1008	0	1035	77	0
11	J	1442	0	1396	82	0
12	K	1119	0	1109	84	0
13	L	620	0	660	67	0
14	M	8811	0	8937	671	0
15	Z	518	0	525	26	0
16	X	3487	0	3523	139	0
17	Y	180	0	41	5	0
All	All	34518	0	34468	2263	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 33.

All (2263) 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:N:85:TYR:CZ	1:N:85:TYR:CE2	1.75	1.70
1:N:85:TYR:CZ	1:N:85:TYR:CE1	1.75	1.60
5:D:88:PHE:CE1	5:D:88:PHE:CZ	1.95	1.54
1:N:85:TYR:CE1	1:N:85:TYR:CD1	1.96	1.53
5:D:88:PHE:CZ	5:D:88:PHE:CE2	1.95	1.53
5:D:88:PHE:CE1	5:D:88:PHE:CD1	1.99	1.48
1:N:85:TYR:CE2	1:N:85:TYR:CD2	1.99	1.48
5:D:88:PHE:CE2	5:D:88:PHE:CD2	1.99	1.48
1:N:1275:MET:HB3	1:N:1280:MET:SD	1.61	1.40
1:N:1275:MET:CB	1:N:1280:MET:SD	2.27	1.17
5:D:88:PHE:CD1	5:D:146:LYS:CD	2.35	1.10
5:D:88:PHE:CE1	5:D:146:LYS:CD	2.35	1.10
5:D:88:PHE:CD1	5:D:146:LYS:HD3	1.88	1.09
1:N:29:ARG:CB	1:N:85:TYR:CE2	2.36	1.08
1:N:29:ARG:CB	1:N:85:TYR:CZ	2.36	1.08
5:D:88:PHE:CD2	5:D:146:LYS:CE	2.39	1.05
5:D:88:PHE:CE2	5:D:146:LYS:CE	2.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:ARG:CG	1:N:85:TYR:CD2	2.39	1.05
1:N:29:ARG:CG	1:N:85:TYR:CD1	2.40	1.04
1:N:29:ARG:CG	1:N:85:TYR:CE2	2.40	1.04
1:N:1275:MET:HA	1:N:1280:MET:SD	1.98	1.03
1:N:29:ARG:CB	1:N:85:TYR:CE1	2.42	1.02
5:D:88:PHE:CZ	5:D:146:LYS:CD	2.43	1.02
13:L:349:THR:HG21	13:L:386:SER:H	1.23	1.02
1:N:29:ARG:CG	1:N:85:TYR:CE1	2.44	1.01
5:D:88:PHE:CZ	5:D:146:LYS:CE	2.43	1.01
1:N:29:ARG:CB	1:N:85:TYR:CD2	2.43	1.01
5:D:88:PHE:CG	5:D:146:LYS:CE	2.44	1.00
1:N:29:ARG:CG	1:N:85:TYR:CZ	2.44	1.00
5:D:88:PHE:CE2	5:D:146:LYS:HE3	1.95	1.00
5:D:88:PHE:CE1	5:D:146:LYS:CE	2.46	0.99
1:N:29:ARG:CG	1:N:85:TYR:CG	2.45	0.99
1:N:29:ARG:HB2	1:N:85:TYR:CZ	1.97	0.98
1:N:1275:MET:CA	1:N:1280:MET:SD	2.51	0.98
5:D:88:PHE:CD1	5:D:146:LYS:CE	2.46	0.98
5:D:88:PHE:CE2	5:D:146:LYS:CD	2.48	0.97
5:D:88:PHE:CZ	5:D:146:LYS:HD2	2.00	0.96
5:D:88:PHE:CG	5:D:146:LYS:HE2	2.01	0.96
14:M:135:ARG:HB2	14:M:412:THR:HG22	1.47	0.96
5:D:88:PHE:CD2	5:D:146:LYS:CD	2.50	0.94
1:N:29:ARG:CB	1:N:85:TYR:CD1	2.51	0.93
5:D:88:PHE:CG	5:D:146:LYS:CD	2.52	0.93
14:M:497:ALA:HB1	14:M:666:GLY:HA3	1.51	0.92
1:N:29:ARG:HG3	1:N:85:TYR:CG	2.05	0.92
1:N:1052:THR:HB	1:N:1277:ASN:HB3	1.52	0.91
1:N:801:GLN:HE22	1:N:808:ARG:HD2	1.35	0.91
1:N:1053:PHE:CE1	1:N:1277:ASN:OD1	2.23	0.90
1:N:29:ARG:CB	1:N:85:TYR:CG	2.54	0.90
14:M:1049:GLU:HA	14:M:1052:ARG:HH12	1.31	0.90
5:D:96:VAL:HG22	5:D:141:VAL:HG23	1.55	0.89
12:K:110:ASN:HD22	13:L:270:GLN:HG2	1.38	0.89
14:M:213:ARG:HD2	14:M:320:HIS:HB2	1.54	0.89
9:H:232:SER:HB2	14:M:922:GLY:HA2	1.52	0.89
1:N:844:PRO:HG3	14:M:661:PRO:HB3	1.56	0.88
1:N:29:ARG:HB3	1:N:85:TYR:CD2	2.07	0.88
9:H:39:ALA:O	9:H:44:ARG:NH2	2.06	0.88
14:M:478:MET:HA	14:M:500:THR:HG21	1.55	0.88
14:M:521:GLU:HB2	14:M:549:ILE:HG13	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1361:LYS:H	6:E:109:TYR:HE2	1.21	0.87
1:N:1095:ALA:O	1:N:1099:ARG:HB2	1.73	0.87
14:M:946:LEU:HD11	14:M:1007:VAL:HG22	1.54	0.87
13:L:266:LEU:H	13:L:380:LYS:HG3	1.40	0.86
11:J:58:TYR:HB2	11:J:67:HIS:HB2	1.56	0.86
16:X:62:LEU:HD21	16:X:85:MET:HE3	1.55	0.86
5:D:4:ILE:HB	5:D:5:LEU:HA	1.57	0.86
7:F:36:THR:HG22	7:F:39:GLU:HG3	1.57	0.85
12:K:49:ILE:HG23	12:K:54:GLN:HG3	1.59	0.85
1:N:838:PHE:O	14:M:677:HIS:ND1	2.10	0.84
14:M:254:MET:HA	14:M:528:GLY:HA3	1.59	0.84
1:N:46:ASN:HD21	1:N:52:LEU:HD12	1.43	0.84
5:D:88:PHE:HB3	5:D:145:MET:O	1.78	0.84
3:B:9:THR:OG1	14:M:924:CYS:O	1.96	0.83
1:N:110:LYS:HG2	1:N:226:LEU:HD12	1.61	0.82
7:F:12:LYS:HD3	7:F:136:LEU:HD21	1.61	0.82
14:M:25:GLU:HG3	14:M:611:MET:HG2	1.60	0.82
1:N:656:GLY:O	1:N:662:ASN:ND2	2.10	0.82
1:N:874:ARG:HD3	1:N:1305:ARG:HD3	1.59	0.82
6:E:64:ARG:HD2	14:M:1062:MET:HE2	1.62	0.82
1:N:463:ASN:HB3	1:N:506:ASN:HB2	1.62	0.82
16:X:467:VAL:HG11	16:X:491:ILE:HD11	1.62	0.81
1:N:29:ARG:HG2	1:N:85:TYR:CE2	2.13	0.81
1:N:29:ARG:HG3	1:N:85:TYR:CD1	2.16	0.81
8:G:30:VAL:HG11	8:G:37:ARG:HE	1.43	0.81
5:D:32:SER:N	5:D:37:MET:O	2.13	0.81
3:B:10:CYS:SG	3:B:42:ARG:NH1	2.54	0.80
14:M:692:GLN:HG3	14:M:1013:LYS:HG2	1.62	0.80
14:M:307:GLU:H	14:M:310:ARG:HB2	1.46	0.80
14:M:758:ASN:HB3	14:M:916:MET:HE3	1.63	0.80
1:N:1053:PHE:HE1	1:N:1277:ASN:OD1	1.63	0.80
1:N:544:ASP:HA	1:N:547:THR:HG22	1.62	0.80
7:F:49:SER:HB2	7:F:55:ARG:HB3	1.64	0.80
16:X:433:ARG:HH22	16:X:531:MET:HE1	1.45	0.80
1:N:745:GLU:HG2	1:N:746:GLU:H	1.47	0.80
14:M:571:PHE:O	14:M:591:ARG:NH1	2.15	0.80
12:K:48:LYS:HB2	12:K:57:GLU:HB2	1.64	0.80
1:N:1233:ARG:HB3	1:N:1236:MET:HE3	1.65	0.79
14:M:975:ASP:OD1	14:M:978:ARG:NH2	2.16	0.79
1:N:28:MET:HG2	1:N:256:LEU:HD13	1.63	0.79
1:N:369:ILE:HD11	1:N:488:PHE:HE1	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:561:ARG:NH2	9:H:30:PRO:O	2.16	0.79
14:M:76:LYS:HB3	14:M:118:GLU:HB3	1.63	0.79
5:D:88:PHE:CE1	5:D:146:LYS:HD2	2.15	0.78
9:H:86:THR:HG21	9:H:227:PRO:HB3	1.64	0.78
1:N:1216:GLU:HG2	1:N:1221:GLU:HG2	1.64	0.78
5:D:28:LEU:HD13	5:D:52:LEU:HD22	1.65	0.78
5:D:12:VAL:HB	5:D:52:LEU:HB2	1.65	0.78
1:N:776:SER:O	1:N:778:LEU:N	2.17	0.78
14:M:760:ALA:O	14:M:764:ARG:NH1	2.18	0.77
1:N:590:LYS:NZ	5:D:89:GLU:OE1	2.17	0.77
9:H:263:GLU:HG3	9:H:276:ALA:HB2	1.66	0.77
14:M:1023:ARG:NH1	14:M:1036:THR:O	2.17	0.77
11:J:151:ARG:NH1	11:J:189:SER:OG	2.16	0.77
1:N:1084:ILE:HD11	1:N:1226:LEU:HD12	1.65	0.77
1:N:884:SER:HB3	1:N:1028:GLU:HG2	1.67	0.77
10:I:18:GLN:OE1	10:I:59:ARG:NH2	2.17	0.77
14:M:239:ILE:HG22	14:M:243:MET:HE1	1.65	0.77
1:N:664:PHE:O	1:N:668:LEU:N	2.17	0.76
1:N:261:CYS:HB3	14:M:1033:ARG:HE	1.50	0.76
9:H:16:LEU:O	9:H:285:ARG:NH2	2.17	0.76
5:D:88:PHE:CD2	5:D:146:LYS:HE2	2.16	0.76
14:M:508:ASP:HB3	14:M:541:LEU:HD21	1.66	0.76
14:M:514:LEU:HG	14:M:562:MET:HE1	1.66	0.76
7:F:61:LEU:HA	7:F:73:PHE:HB3	1.67	0.76
9:H:125:ARG:NH2	9:H:137:THR:OG1	2.18	0.76
2:A:25:CYS:O	12:K:73:LYS:NZ	2.18	0.76
14:M:714:TYR:O	14:M:737:GLN:NE2	2.17	0.76
14:M:682:ARG:HH21	14:M:937:ARG:HA	1.50	0.75
14:M:141:ARG:NH2	14:M:164:ASP:OD1	2.18	0.75
1:N:29:ARG:HG2	1:N:85:TYR:CD2	2.20	0.75
1:N:183:LYS:NZ	1:N:216:GLU:OE2	2.19	0.75
5:D:41:LEU:HD23	5:D:123:MET:HG3	1.68	0.75
5:D:24:ARG:HA	5:D:45:ILE:HG22	1.68	0.75
14:M:758:ASN:ND2	14:M:759:LYS:O	2.19	0.75
3:B:3:ILE:O	9:H:109:ARG:NH1	2.19	0.75
9:H:83:GLU:OE1	9:H:332:LYS:NZ	2.19	0.75
5:D:96:VAL:HG21	5:D:140:ARG:H	1.51	0.75
1:N:122:LYS:NZ	16:X:72:VAL:O	2.20	0.74
1:N:380:VAL:HG13	1:N:488:PHE:HB3	1.67	0.74
9:H:77:ARG:HE	9:H:233:TYR:HD2	1.34	0.74
11:J:115:GLN:HG3	11:J:198:LEU:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:61:GLN:NE2	10:I:123:ILE:O	2.20	0.74
14:M:955:ASP:OD1	14:M:979:HIS:ND1	2.20	0.74
9:H:201:GLN:OE1	9:H:203:ARG:NH2	2.20	0.74
9:H:74:ASN:ND2	14:M:992:GLY:O	2.20	0.74
14:M:454:ARG:HH22	14:M:691:LYS:HE2	1.53	0.74
1:N:884:SER:HB2	1:N:1031:SER:H	1.52	0.74
13:L:331:ILE:HG12	13:L:337:VAL:HG13	1.68	0.74
14:M:759:LYS:HG2	14:M:912:PRO:HA	1.69	0.74
1:N:59:ARG:NH1	1:N:69:CYS:SG	2.60	0.74
1:N:834:VAL:HG12	1:N:846:GLU:HB3	1.70	0.74
13:L:365:LEU:HA	13:L:373:MET:HG3	1.70	0.73
14:M:1049:GLU:HA	14:M:1052:ARG:NH1	2.02	0.73
4:C:34:ILE:HG21	4:C:42:ARG:HA	1.68	0.73
10:I:14:TYR:O	10:I:18:GLN:NE2	2.20	0.73
14:M:307:GLU:HB2	14:M:310:ARG:HH21	1.53	0.73
1:N:470:LYS:HG2	1:N:533:ARG:HH22	1.54	0.73
14:M:66:THR:HG22	14:M:385:LYS:HG3	1.70	0.73
16:X:362:CYS:SG	16:X:397:LYS:NZ	2.61	0.73
6:E:72:GLN:HB3	6:E:78:PRO:HG3	1.68	0.73
7:F:64:HIS:HB2	7:F:72:MET:HG3	1.70	0.73
1:N:553:THR:O	1:N:598:LYS:NZ	2.21	0.73
3:B:53:VAL:HG12	14:M:717:LYS:HE3	1.71	0.73
1:N:848:PHE:HE2	14:M:473:PRO:HA	1.52	0.73
5:D:45:ILE:HD11	5:D:48:TYR:HB2	1.71	0.72
5:D:98:ARG:NH2	5:D:99:ILE:O	2.22	0.72
5:D:56:PHE:O	5:D:58:LEU:N	2.21	0.72
1:N:817:SER:OG	1:N:830:ALA:O	2.04	0.72
5:D:93:TYR:HD1	5:D:142:TYR:HD1	1.37	0.72
14:M:913:GLN:NE2	14:M:924:CYS:SG	2.57	0.72
14:M:67:SER:HB3	14:M:70:ASP:HB3	1.71	0.72
14:M:595:PRO:HG3	14:M:632:TYR:HE1	1.54	0.72
12:K:24:LYS:O	13:L:365:LEU:N	2.20	0.72
13:L:361:VAL:HA	13:L:378:HIS:HA	1.72	0.72
1:N:122:LYS:HE2	16:X:68:HIS:HB2	1.71	0.72
14:M:234:ILE:HG21	14:M:287:ILE:HD12	1.71	0.72
9:H:261:VAL:HG21	9:H:281:ASP:HB3	1.71	0.72
7:F:193:ILE:HD13	7:F:207:ARG:HH11	1.55	0.72
12:K:15:VAL:HA	12:K:124:LEU:HB2	1.71	0.72
1:N:14:LYS:H	14:M:1131:TYR:HE2	1.36	0.71
1:N:70:GLU:O	1:N:82:HIS:ND1	2.21	0.71
1:N:844:PRO:HG2	14:M:645:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1263:ALA:HB3	1:N:1300:VAL:HG21	1.72	0.71
8:G:56:ARG:HG2	8:G:68:CYS:HB2	1.72	0.71
16:X:59:GLN:HG3	16:X:114:GLY:HA3	1.72	0.71
7:F:85:LYS:HA	7:F:88:LYS:HD2	1.72	0.71
10:I:65:ILE:HG21	10:I:124:LEU:HD21	1.72	0.71
14:M:445:TYR:HB3	14:M:730:PHE:CE2	2.26	0.71
1:N:615:ALA:H	1:N:637:TYR:HA	1.54	0.71
13:L:338:GLN:HG2	13:L:348:VAL:HG13	1.72	0.71
16:X:118:MET:SD	16:X:235:TRP:NE1	2.63	0.71
1:N:1262:ALA:HB2	7:F:145:VAL:HG22	1.72	0.71
1:N:122:LYS:HE3	16:X:70:ARG:H	1.56	0.71
1:N:730:ALA:O	1:N:734:GLY:N	2.23	0.71
14:M:319:THR:HG22	14:M:321:VAL:H	1.56	0.71
14:M:396:ARG:O	14:M:399:GLN:NE2	2.23	0.70
1:N:1037:CYS:SG	1:N:1286:HIS:ND1	2.61	0.70
14:M:610:HIS:O	14:M:614:LEU:N	2.20	0.70
1:N:1315:VAL:HG22	1:N:1339:SER:HB2	1.71	0.70
14:M:175:GLU:OE2	14:M:442:ARG:NH1	2.24	0.70
14:M:679:GLN:HB2	14:M:682:ARG:HD3	1.73	0.70
1:N:75:ASN:HB3	1:N:76:LEU:HD22	1.73	0.70
3:B:47:ARG:HB2	3:B:48:MET:HE2	1.72	0.70
8:G:49:HIS:ND1	8:G:70:TYR:OH	2.21	0.70
10:I:21:THR:HG22	10:I:50:LEU:HD11	1.74	0.70
14:M:478:MET:HB3	14:M:592:LEU:HD13	1.73	0.70
14:M:1033:ARG:HB2	14:M:1112:LEU:HD22	1.74	0.70
16:X:87:ARG:O	16:X:91:TYR:N	2.19	0.70
1:N:15:ILE:HG21	1:N:1349:MET:HE2	1.74	0.70
9:H:250:ALA:HB1	9:H:264:VAL:HG12	1.72	0.70
11:J:89:ILE:HD13	11:J:99:VAL:HG22	1.72	0.70
14:M:694:MET:HG2	14:M:710:TYR:HB3	1.73	0.70
16:X:443:ILE:HD12	16:X:520:ILE:HD12	1.73	0.70
5:D:24:ARG:O	5:D:44:ASN:HA	1.91	0.70
14:M:243:MET:HG3	14:M:328:PHE:HD1	1.56	0.70
1:N:242:PRO:HG3	16:X:30:ARG:HB3	1.72	0.69
1:N:879:LEU:HD23	1:N:1038:ALA:HB2	1.73	0.69
14:M:296:MET:HG2	14:M:299:GLY:HA3	1.73	0.69
1:N:1035:ALA:O	1:N:1039:GLN:NE2	2.25	0.69
14:M:917:PRO:HB2	14:M:989:VAL:HG11	1.74	0.69
1:N:567:ILE:HD11	1:N:600:ILE:HG23	1.74	0.69
4:C:58:ARG:NH1	9:H:221:ASP:OD1	2.25	0.69
1:N:587:THR:O	1:N:588:ILE:HG13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1297:LYS:HZ1	1:N:1312:LYS:HB2	1.57	0.69
14:M:602:GLN:HA	14:M:652:LYS:HD2	1.73	0.69
14:M:344:LEU:HD13	14:M:350:LYS:HB2	1.72	0.69
14:M:621:PHE:O	14:M:622:GLU:HG3	1.93	0.69
5:D:136:GLU:HB3	5:D:139:SER:HB3	1.75	0.69
14:M:781:ARG:HD3	14:M:877:ASP:HB3	1.73	0.69
16:X:493:ALA:O	16:X:497:GLN:NE2	2.24	0.69
5:D:10:PHE:HB2	5:D:56:PHE:HB2	1.75	0.69
10:I:94:ALA:HB1	10:I:117:LEU:HB3	1.74	0.69
11:J:190:ILE:HG22	11:J:191:SER:H	1.57	0.69
14:M:676:HIS:HB2	14:M:677:HIS:CD2	2.27	0.68
14:M:786:THR:O	14:M:848:GLN:NE2	2.26	0.68
11:J:4:LEU:HB3	11:J:73:ARG:HB2	1.73	0.68
1:N:366:ARG:HG2	14:M:1021:HIS:HB2	1.76	0.68
1:N:801:GLN:HG3	1:N:833:PHE:HA	1.76	0.68
1:N:1053:PHE:CD1	1:N:1277:ASN:OD1	2.45	0.68
1:N:1297:LYS:HG3	7:F:172:ARG:HD2	1.74	0.68
1:N:1301:LEU:HB3	1:N:1308:LEU:HD22	1.76	0.68
1:N:847:PHE:HE2	14:M:665:LEU:HD21	1.58	0.68
4:C:46:LYS:HD2	14:M:871:ILE:HD11	1.75	0.68
7:F:44:SER:HB3	7:F:48:PRO:HG3	1.74	0.68
9:H:105:ILE:HG13	9:H:106:LEU:H	1.56	0.68
14:M:376:LEU:HD22	14:M:415:MET:HE2	1.76	0.68
15:Z:248:VAL:HA	15:Z:273:VAL:H	1.57	0.68
1:N:470:LYS:H	1:N:533:ARG:NH2	1.91	0.68
6:E:64:ARG:HB2	14:M:1062:MET:HE2	1.74	0.68
14:M:777:CYS:HB3	14:M:881:ILE:HB	1.73	0.68
1:N:562:ALA:O	8:G:56:ARG:NH2	2.26	0.68
6:E:107:ARG:HD3	6:E:115:TYR:HB3	1.75	0.68
8:G:72:THR:HG22	8:G:80:ILE:HG22	1.74	0.68
14:M:511:ILE:HG21	14:M:585:ILE:HG21	1.75	0.68
15:Z:176:PHE:HB2	16:X:382:ASP:HB3	1.75	0.68
13:L:271:LEU:HA	13:L:385:CYS:HB2	1.76	0.68
14:M:896:LYS:HZ2	14:M:1014:HIS:HB3	1.58	0.68
1:N:541:ALA:HB1	1:N:545:PHE:HB2	1.76	0.68
1:N:560:ASP:HB3	9:H:32:ASN:HD21	1.59	0.68
1:N:15:ILE:HG13	14:M:1104:LEU:HB3	1.76	0.67
1:N:122:LYS:HE3	16:X:70:ARG:N	2.08	0.67
1:N:122:LYS:HZ2	16:X:72:VAL:H	1.42	0.67
7:F:130:PHE:HB3	7:F:132:GLN:HG2	1.75	0.67
11:J:151:ARG:NH1	11:J:189:SER:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:73:ILE:HA	6:E:78:PRO:HD2	1.77	0.67
14:M:750:ASP:OD1	14:M:756:VAL:HG23	1.94	0.67
14:M:943:LEU:O	14:M:1003:TYR:OH	2.11	0.67
1:N:371:PRO:HD3	1:N:500:PHE:CE1	2.29	0.67
1:N:432:LEU:O	1:N:435:GLY:N	2.28	0.67
1:N:698:ILE:HG21	14:M:934:PHE:HD2	1.59	0.67
14:M:1023:ARG:NH2	14:M:1045:LEU:O	2.28	0.67
1:N:359:LYS:HA	14:M:1071:SER:HB2	1.77	0.67
1:N:801:GLN:HB2	1:N:833:PHE:HD1	1.58	0.67
10:I:96:GLU:HA	10:I:100:MET:HB3	1.76	0.67
16:X:365:ILE:HA	16:X:368:LEU:HD12	1.74	0.67
14:M:514:LEU:O	14:M:518:LEU:HB2	1.95	0.67
6:E:97:LEU:O	6:E:100:ARG:NH1	2.28	0.67
14:M:140:LEU:HD11	14:M:147:LEU:HD12	1.77	0.67
16:X:290:SER:HB2	16:X:334:TYR:HE2	1.59	0.67
5:D:91:VAL:HG22	5:D:144:LEU:HA	1.77	0.67
9:H:285:ARG:HD3	14:M:988:TYR:CE2	2.30	0.67
14:M:213:ARG:NH2	14:M:318:LEU:O	2.28	0.67
16:X:27:HIS:NE2	16:X:34:GLN:OE1	2.28	0.67
5:D:38:ASP:OD2	5:D:124:ARG:NH2	2.27	0.66
9:H:12:SER:HA	9:H:303:ARG:HD2	1.76	0.66
1:N:412:PRO:HB3	1:N:432:LEU:HA	1.75	0.66
1:N:504:GLU:HB3	14:M:1019:LYS:HD3	1.78	0.66
3:B:4:PRO:HA	9:H:109:ARG:HH22	1.60	0.66
14:M:744:MET:HE1	14:M:998:LEU:HD11	1.78	0.66
1:N:848:PHE:CE2	14:M:473:PRO:HA	2.30	0.66
1:N:104:ILE:HB	1:N:107:MET:HE3	1.78	0.66
1:N:150:CYS:SG	1:N:151:ARG:N	2.67	0.66
1:N:400:ASN:HB3	1:N:404:LEU:HD23	1.76	0.66
1:N:519:ALA:HB1	1:N:523:MET:HE2	1.76	0.66
1:N:587:THR:HG21	1:N:599:GLN:HE22	1.59	0.66
1:N:641:GLN:NE2	5:D:96:VAL:O	2.28	0.66
14:M:901:HIS:CD2	14:M:942:LYS:HB2	2.31	0.66
1:N:612:PRO:HA	1:N:640:ILE:O	1.96	0.66
1:N:956:SER:OG	1:N:1019:ARG:NH2	2.29	0.66
14:M:273:GLN:HA	14:M:277:ILE:HG12	1.78	0.66
1:N:279:LEU:HD23	1:N:280:THR:H	1.60	0.66
1:N:407:LEU:HD12	1:N:452:ARG:HD2	1.77	0.66
10:I:97:ILE:HD11	10:I:120:VAL:HG21	1.78	0.66
12:K:27:LEU:HB2	12:K:132:ILE:HG12	1.77	0.66
5:D:96:VAL:HG11	5:D:140:ARG:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:143:LYS:HA	1:N:146:ILE:HG22	1.76	0.65
1:N:179:TYR:N	1:N:180:LYS:HA	2.11	0.65
6:E:57:MET:O	6:E:62:ARG:NH1	2.29	0.65
6:E:110:LEU:HD23	6:E:112:ASP:H	1.60	0.65
13:L:332:ARG:HH22	13:L:340:LEU:HD11	1.61	0.65
1:N:380:VAL:HG11	1:N:462:PHE:CE1	2.31	0.65
1:N:1104:ARG:O	1:N:1104:ARG:NH1	2.27	0.65
7:F:77:PRO:HD2	7:F:105:VAL:HB	1.79	0.65
12:K:16:TYR:N	12:K:124:LEU:O	2.27	0.65
14:M:526:LEU:HD12	14:M:548:VAL:HG11	1.78	0.65
14:M:741:VAL:HG22	14:M:927:ILE:HB	1.78	0.65
1:N:365:GLY:HA2	14:M:1022:ALA:HA	1.77	0.65
1:N:1166:ALA:HB1	1:N:1178:ARG:HH12	1.61	0.65
3:B:42:ARG:NH2	9:H:230:THR:HG22	2.12	0.65
4:C:49:THR:OG1	14:M:819:GLU:OE2	2.15	0.65
9:H:170:THR:OG1	9:H:194:HIS:O	2.14	0.65
14:M:44:ILE:HA	14:M:139:MET:HE1	1.78	0.65
14:M:478:MET:HE1	14:M:635:VAL:HG22	1.77	0.65
1:N:873:ARG:HD2	1:N:874:ARG:HG3	1.78	0.65
6:E:75:MET:HG3	11:J:15:PRO:HG2	1.78	0.65
12:K:113:ARG:HB3	13:L:271:LEU:H	1.61	0.65
13:L:355:SER:OG	13:L:356:PHE:N	2.30	0.65
14:M:545:ILE:HG23	14:M:546:LEU:H	1.60	0.65
1:N:371:PRO:HD3	1:N:500:PHE:HE1	1.60	0.65
5:D:98:ARG:HH12	5:D:112:LEU:HB2	1.62	0.65
9:H:108:HIS:NE2	14:M:763:ASP:O	2.27	0.65
14:M:44:ILE:HG22	14:M:48:ASN:HD21	1.62	0.65
14:M:1111:LYS:HG2	14:M:1115:GLN:HE21	1.60	0.65
3:B:3:ILE:HG12	3:B:18:TRP:CD1	2.32	0.65
3:B:47:ARG:CZ	14:M:1006:PRO:HG3	2.26	0.65
14:M:705:ILE:HG21	14:M:882:LYS:HB3	1.79	0.65
1:N:437:ARG:HG3	1:N:438:GLU:H	1.61	0.65
1:N:543:GLN:HB2	14:M:751:ILE:HG22	1.78	0.65
13:L:330:LEU:HD12	13:L:340:LEU:HD12	1.77	0.65
14:M:229:THR:HG21	14:M:293:ARG:HB3	1.78	0.65
1:N:588:ILE:HD12	1:N:594:LEU:HB2	1.78	0.64
5:D:28:LEU:HB2	5:D:41:LEU:HB2	1.79	0.64
6:E:84:GLU:O	6:E:87:THR:OG1	2.15	0.64
10:I:6:ALA:O	11:J:78:HIS:HE1	1.79	0.64
11:J:27:ALA:HA	11:J:30:LEU:HD12	1.80	0.64
14:M:218:VAL:HG12	14:M:219:LYS:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:86:ILE:HD12	1:N:257:VAL:HG11	1.77	0.64
1:N:470:LYS:H	1:N:533:ARG:HH22	1.45	0.64
14:M:900:ARG:O	14:M:901:HIS:ND1	2.30	0.64
16:X:61:ASN:O	16:X:81:ARG:NE	2.29	0.64
1:N:363:PHE:HB3	1:N:509:LEU:HB2	1.80	0.64
10:I:98:GLN:NE2	10:I:110:GLU:OE2	2.31	0.64
14:M:395:GLN:HG3	14:M:396:ARG:HH11	1.63	0.64
12:K:29:GLN:NE2	13:L:358:GLN:OE1	2.31	0.64
15:Z:182:GLN:OE1	16:X:364:ARG:NH2	2.29	0.64
15:Z:189:GLN:O	15:Z:191:LYS:NZ	2.30	0.64
1:N:376:ARG:HH12	1:N:479:ARG:HH22	1.45	0.64
16:X:401:GLU:O	16:X:434:MET:HE1	1.98	0.64
1:N:412:PRO:HA	1:N:419:ASN:HD21	1.61	0.64
11:J:107:ILE:HG12	11:J:186:LEU:HB2	1.80	0.64
13:L:349:THR:HG1	13:L:385:CYS:HG	1.39	0.64
14:M:478:MET:HA	14:M:500:THR:CG2	2.26	0.64
1:N:501:ASP:O	14:M:896:LYS:HG2	1.98	0.64
7:F:71:GLN:O	7:F:72:MET:HE2	1.97	0.64
14:M:496:LEU:HD11	14:M:502:ILE:HD11	1.78	0.64
14:M:797:ALA:H	14:M:802:PRO:HB3	1.63	0.64
1:N:397:ASN:ND2	6:E:74:ALA:O	2.28	0.64
7:F:24:ARG:NH1	7:F:182:TYR:O	2.31	0.64
14:M:1033:ARG:CZ	14:M:1115:GLN:HE22	2.11	0.64
1:N:514:GLU:HA	6:E:71:LEU:HD21	1.78	0.63
1:N:1253:GLU:OE1	1:N:1253:GLU:N	2.31	0.63
1:N:872:GLN:HE22	1:N:1042:GLY:HA3	1.61	0.63
14:M:305:LYS:HG2	14:M:310:ARG:HH11	1.63	0.63
1:N:29:ARG:HB2	1:N:85:TYR:CE2	2.31	0.63
1:N:380:VAL:HG11	1:N:462:PHE:HE1	1.63	0.63
14:M:741:VAL:HG21	14:M:1009:TYR:HE2	1.63	0.63
1:N:34:ILE:HG21	1:N:37:VAL:HB	1.80	0.63
1:N:394:GLU:HB3	6:E:90:LEU:HD11	1.80	0.63
1:N:478:ALA:O	1:N:479:ARG:HD3	1.99	0.63
9:H:12:SER:HB2	9:H:303:ARG:HB2	1.79	0.63
14:M:376:LEU:HD23	14:M:411:ILE:HG23	1.81	0.63
1:N:59:ARG:HB3	1:N:62:THR:H	1.63	0.63
1:N:64:GLU:HG3	1:N:65:LYS:H	1.64	0.63
12:K:116:ALA:H	13:L:269:LEU:H	1.45	0.63
14:M:901:HIS:HD2	14:M:942:LYS:HB2	1.64	0.63
1:N:29:ARG:HB3	1:N:85:TYR:CE2	2.33	0.63
1:N:1354:ASN:ND2	1:N:1358:GLY:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:61:GLU:OE1	6:E:108:ARG:NH2	2.32	0.63
10:I:64:GLU:OE2	10:I:67:ARG:NE	2.31	0.63
1:N:670:ASP:OD1	1:N:923:ARG:NH2	2.31	0.63
5:D:116:VAL:HG11	5:D:143:LEU:HD12	1.81	0.63
9:H:289:ARG:HH22	14:M:984:LEU:HG	1.64	0.63
14:M:1082:GLN:O	14:M:1100:HIS:ND1	2.31	0.63
1:N:26:GLU:HG2	1:N:27:GLU:H	1.64	0.63
1:N:888:LEU:HA	1:N:1028:GLU:HB2	1.81	0.63
8:G:41:THR:HG22	8:G:83:ARG:HG3	1.81	0.63
11:J:129:TRP:HB2	11:J:140:LEU:HB2	1.80	0.63
1:N:882:LEU:HD11	1:N:1293:LEU:HD21	1.81	0.62
8:G:80:ILE:O	8:G:80:ILE:HG13	1.99	0.62
14:M:756:VAL:HG22	14:M:909:LEU:HB2	1.81	0.62
9:H:93:LEU:HB2	9:H:211:LEU:HB2	1.80	0.62
14:M:59:MET:HB2	14:M:80:ILE:HG22	1.81	0.62
14:M:809:LEU:HD21	14:M:826:VAL:HG12	1.79	0.62
14:M:896:LYS:NZ	14:M:1014:HIS:HB3	2.14	0.62
1:N:1283:ASP:HB3	1:N:1286:HIS:CD2	2.35	0.62
9:H:77:ARG:HG2	9:H:233:TYR:HE2	1.64	0.62
9:H:284:SER:OG	9:H:286:GLU:OE2	2.16	0.62
5:D:4:ILE:HA	5:D:61:ALA:HA	1.81	0.62
14:M:708:LEU:HD22	14:M:710:TYR:HE2	1.64	0.62
1:N:543:GLN:HB2	14:M:751:ILE:CG2	2.29	0.62
1:N:828:PRO:O	1:N:833:PHE:HB3	1.99	0.62
1:N:1247:THR:HG22	1:N:1248:SER:H	1.64	0.62
8:G:83:ARG:NE	8:G:85:GLN:OE1	2.32	0.62
9:H:105:ILE:HG13	9:H:106:LEU:N	2.11	0.62
1:N:102:ILE:HG21	1:N:168:LYS:HD3	1.82	0.62
1:N:510:PRO:O	1:N:516:LYS:NZ	2.27	0.62
14:M:98:SER:OG	14:M:100:HIS:O	2.14	0.62
1:N:364:SER:OG	1:N:365:GLY:N	2.32	0.62
3:B:17:LYS:HB3	3:B:21:TYR:HE2	1.63	0.62
6:E:57:MET:HG3	6:E:108:ARG:HH22	1.64	0.62
7:F:41:LYS:HG2	7:F:46:ASP:HB2	1.80	0.62
1:N:379:GLU:HA	1:N:477:LEU:HB2	1.81	0.62
1:N:1152:SER:O	1:N:1155:THR:OG1	2.17	0.62
14:M:575:SER:HA	14:M:640:ASP:OD2	2.00	0.62
14:M:693:ALA:HB2	14:M:1012:LEU:HD23	1.82	0.62
14:M:726:GLU:OE2	14:M:960:TYR:OH	2.10	0.62
1:N:262:ILE:HD13	14:M:1116:GLU:HG2	1.82	0.62
5:D:91:VAL:HG11	5:D:93:TYR:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:145:CYS:SG	14:M:146:VAL:N	2.73	0.62
14:M:1015:MET:HG3	14:M:1017:LEU:H	1.65	0.62
9:H:283:PHE:HB3	14:M:988:TYR:CE2	2.35	0.61
12:K:22:ALA:HB2	12:K:127:THR:HB	1.81	0.61
14:M:901:HIS:NE2	14:M:941:GLY:O	2.32	0.61
1:N:59:ARG:H	1:N:60:MET:HA	1.65	0.61
1:N:739:GLN:N	1:N:740:PRO:O	2.33	0.61
5:D:32:SER:HB3	5:D:37:MET:N	2.15	0.61
5:D:116:VAL:HG12	5:D:118:TYR:HE1	1.65	0.61
7:F:21:CYS:HA	7:F:64:HIS:HE1	1.64	0.61
14:M:679:GLN:HB3	14:M:681:PRO:HD2	1.82	0.61
1:N:1093:ASP:HB3	1:N:1097:TYR:HB2	1.82	0.61
1:N:1221:GLU:OE1	1:N:1223:TYR:OH	2.18	0.61
7:F:48:PRO:HB2	7:F:55:ARG:HA	1.82	0.61
14:M:291:VAL:HG13	14:M:294:GLN:HB2	1.82	0.61
10:I:64:GLU:O	10:I:67:ARG:HG3	2.01	0.61
10:I:88:ASN:HD21	11:J:1:MET:HE3	1.65	0.61
14:M:204:THR:HG21	14:M:321:VAL:HG12	1.81	0.61
14:M:800:ARG:HG3	14:M:804:TRP:CD1	2.36	0.61
16:X:272:ARG:HH22	16:X:298:PRO:HB3	1.65	0.61
1:N:380:VAL:HG12	1:N:381:ALA:H	1.65	0.61
1:N:731:LEU:HD23	1:N:748:LEU:HD23	1.83	0.61
1:N:736:LEU:HB2	1:N:737:GLN:HA	1.83	0.61
9:H:170:THR:HG23	9:H:197:ILE:HB	1.83	0.61
9:H:246:GLU:HA	9:H:272:VAL:H	1.65	0.61
14:M:1067:ARG:HH21	14:M:1071:SER:HA	1.64	0.61
1:N:67:ARG:O	1:N:74:LYS:NZ	2.33	0.61
7:F:173:ILE:N	7:F:208:LEU:O	2.34	0.61
9:H:105:ILE:O	9:H:109:ARG:N	2.23	0.61
14:M:74:TYR:N	14:M:120:THR:OG1	2.34	0.61
1:N:185:VAL:HG13	1:N:216:GLU:CD	2.25	0.61
1:N:364:SER:HB2	14:M:1045:LEU:HD12	1.81	0.61
10:I:12:SER:HA	10:I:66:VAL:HG11	1.83	0.61
1:N:441:ALA:HB3	1:N:445:LYS:HG3	1.82	0.61
1:N:568:ILE:HD12	8:G:69:GLY:HA2	1.83	0.61
12:K:197:GLN:HA	12:K:201:ALA:HB3	1.83	0.61
1:N:80:LEU:HD23	14:M:1086:LEU:HB2	1.82	0.61
1:N:969:ILE:HG23	7:F:200:ALA:HB2	1.82	0.61
7:F:47:LYS:HG2	7:F:50:GLU:HB3	1.83	0.61
14:M:827:LEU:HD21	14:M:859:LYS:HE2	1.83	0.61
1:N:390:LEU:HD11	1:N:453:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2:ILE:HG22	3:B:3:ILE:H	1.66	0.60
3:B:19:GLU:OE2	9:H:167:LYS:NZ	2.34	0.60
12:K:50:LYS:HE2	12:K:55:LYS:HE3	1.82	0.60
1:N:250:LEU:HD22	14:M:1121:ASN:HD22	1.64	0.60
1:N:370:SER:N	1:N:485:THR:OG1	2.33	0.60
3:B:60:LEU:HB3	9:H:203:ARG:HG3	1.84	0.60
9:H:246:GLU:HB3	9:H:270:LYS:HB2	1.83	0.60
9:H:330:MET:HB3	9:H:334:ARG:HH12	1.66	0.60
1:N:369:ILE:HD13	1:N:498:ALA:HB1	1.83	0.60
3:B:51:ALA:O	14:M:717:LYS:N	2.23	0.60
6:E:61:GLU:HG2	6:E:64:ARG:NH2	2.16	0.60
9:H:144:VAL:HG21	9:H:168:VAL:HG13	1.82	0.60
14:M:1023:ARG:NH2	14:M:1043:GLY:O	2.34	0.60
1:N:129:LEU:HD22	16:X:38:VAL:HG21	1.82	0.60
1:N:258:PRO:HG2	1:N:279:LEU:HD21	1.83	0.60
9:H:77:ARG:HG2	9:H:233:TYR:CE2	2.35	0.60
9:H:110:LEU:HD23	9:H:212:MET:HE2	1.84	0.60
13:L:367:ASP:O	13:L:371:GLY:N	2.34	0.60
14:M:361:ARG:HB3	14:M:590:GLY:HA3	1.83	0.60
16:X:12:LEU:HD21	16:X:86:LEU:HD23	1.83	0.60
2:A:31:VAL:HG23	12:K:69:TYR:HA	1.84	0.60
9:H:284:SER:OG	14:M:981:TYR:O	2.17	0.60
14:M:580:ASP:OD2	14:M:581:ARG:N	2.34	0.60
16:X:265:GLU:HG2	16:X:301:TYR:CG	2.36	0.60
7:F:48:PRO:HG2	7:F:55:ARG:HB2	1.83	0.60
16:X:491:ILE:O	16:X:496:ARG:NH2	2.30	0.60
1:N:555:LYS:NZ	5:D:42:ASP:OD2	2.34	0.60
1:N:1007:THR:N	1:N:1010:GLN:OE1	2.34	0.60
1:N:1145:ASN:O	1:N:1148:THR:OG1	2.12	0.60
5:D:88:PHE:CZ	5:D:146:LYS:HE3	2.36	0.60
7:F:87:ILE:HD12	7:F:114:ALA:HB1	1.83	0.60
8:G:61:LYS:HZ1	9:H:40:TRP:CD1	2.19	0.60
8:G:104:MET:SD	9:H:334:ARG:HB3	2.42	0.60
1:N:852:MET:HE1	14:M:473:PRO:HD3	1.84	0.60
1:N:933:PRO:HD2	1:N:1010:GLN:HE21	1.67	0.60
3:B:43:TYR:O	3:B:47:ARG:HD2	2.02	0.60
10:I:77:LYS:O	10:I:107:ARG:NH1	2.34	0.60
13:L:268:PHE:HB2	13:L:382:LYS:HG2	1.82	0.60
14:M:123:SER:OG	14:M:125:ARG:NH1	2.34	0.60
15:Z:178:GLU:HA	15:Z:181:ASN:ND2	2.16	0.60
7:F:71:GLN:NE2	7:F:97:GLU:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:141:ARG:HG3	9:H:143:GLN:OE1	2.02	0.59
11:J:122:GLU:OE2	11:J:125:GLN:NE2	2.35	0.59
14:M:722:THR:OG1	14:M:725:ILE:HG13	2.02	0.59
16:X:58:VAL:O	16:X:115:LYS:NZ	2.35	0.59
1:N:122:LYS:HE2	16:X:68:HIS:CB	2.32	0.59
1:N:176:HIS:CE1	1:N:185:VAL:HG22	2.38	0.59
1:N:223:VAL:HG12	1:N:227:PHE:CZ	2.36	0.59
1:N:468:LEU:HD13	1:N:1047:GLN:HE21	1.67	0.59
9:H:65:MET:SD	9:H:68:ILE:HD11	2.42	0.59
14:M:772:TYR:HD1	14:M:884:LEU:HD22	1.67	0.59
4:C:48:ARG:HA	14:M:817:PRO:HB2	1.84	0.59
14:M:44:ILE:HG22	14:M:48:ASN:ND2	2.18	0.59
16:X:109:GLU:O	16:X:114:GLY:N	2.35	0.59
1:N:381:ALA:HB3	1:N:487:ARG:HG3	1.83	0.59
1:N:471:LEU:HD13	1:N:538:LEU:HD11	1.84	0.59
4:C:14:PRO:O	4:C:15:MET:HE2	2.01	0.59
9:H:193:VAL:HG11	9:H:314:GLY:HA3	1.85	0.59
13:L:343:LYS:O	13:L:345:THR:N	2.35	0.59
14:M:246:GLU:OE1	14:M:246:GLU:N	2.32	0.59
14:M:333:ILE:HD11	14:M:537:PHE:HZ	1.67	0.59
16:X:85:MET:HE1	16:X:88:TYR:CZ	2.37	0.59
16:X:126:ALA:HA	16:X:139:MET:HE1	1.83	0.59
14:M:539:VAL:HB	14:M:547:GLY:H	1.68	0.59
1:N:278:ASP:HB2	1:N:279:LEU:HA	1.85	0.59
1:N:414:VAL:HG12	1:N:416:PRO:HD2	1.85	0.59
1:N:845:THR:HG23	14:M:645:LEU:HD21	1.83	0.59
5:D:4:ILE:HD13	5:D:59:VAL:HG12	1.84	0.59
14:M:772:TYR:O	14:M:773:LYS:HG3	2.03	0.59
1:N:185:VAL:CG1	1:N:216:GLU:CD	2.76	0.59
1:N:753:LEU:HD13	1:N:1058:VAL:HB	1.84	0.59
1:N:1256:LYS:NZ	7:F:176:GLY:O	2.36	0.59
5:D:4:ILE:HG21	5:D:59:VAL:HG12	1.85	0.59
5:D:20:LYS:HG2	5:D:27:ARG:HH12	1.67	0.59
9:H:24:VAL:O	9:H:25:HIS:ND1	2.36	0.59
10:I:27:ARG:NH1	11:J:31:ASN:OD1	2.33	0.59
11:J:38:VAL:HG11	14:M:1091:TRP:HE1	1.68	0.59
12:K:206:VAL:HG13	13:L:373:MET:HE2	1.85	0.59
15:Z:239:LEU:O	15:Z:243:ILE:HG13	2.02	0.59
1:N:1145:ASN:OD1	1:N:1146:ALA:N	2.36	0.59
5:D:90:TYR:HB2	5:D:145:MET:SD	2.42	0.59
7:F:97:GLU:HB2	7:F:99:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:60:MET:HB2	12:K:100:GLN:HB3	1.83	0.59
14:M:44:ILE:O	14:M:48:ASN:ND2	2.36	0.59
14:M:498:LEU:C	14:M:500:THR:H	2.11	0.59
1:N:461:LEU:HB2	1:N:508:HIS:HB2	1.85	0.59
1:N:603:VAL:H	1:N:682:ARG:HH12	1.51	0.59
1:N:868:THR:HA	1:N:871:MET:HG2	1.85	0.59
3:B:43:TYR:HB3	3:B:47:ARG:HE	1.67	0.59
8:G:47:GLU:OE2	8:G:51:LEU:HB3	2.03	0.59
15:Z:251:THR:HG21	15:Z:271:ARG:HG2	1.85	0.59
1:N:476:HIS:NE2	1:N:528:ASN:OD1	2.31	0.59
2:A:35:THR:OG1	2:A:36:ARG:HG2	2.02	0.59
5:D:4:ILE:HG22	5:D:6:PHE:H	1.68	0.59
5:D:84:ARG:O	5:D:146:LYS:NZ	2.35	0.59
8:G:114:PHE:HD1	9:H:51:VAL:HG11	1.68	0.59
1:N:551:LEU:HD13	1:N:694:ARG:HD3	1.85	0.58
10:I:39:GLN:NE2	11:J:32:LYS:O	2.36	0.58
10:I:52:TYR:HA	10:I:55:LYS:HD2	1.84	0.58
14:M:1029:ALA:HB2	14:M:1041:ARG:HH22	1.68	0.58
16:X:92:ILE:O	16:X:96:LYS:HG3	2.03	0.58
1:N:401:ILE:HG22	1:N:405:ARG:HH12	1.67	0.58
9:H:42:GLN:O	9:H:46:GLU:N	2.24	0.58
14:M:762:LEU:O	14:M:890:ARG:NH1	2.35	0.58
1:N:94:HIS:HB2	1:N:97:TYR:HB2	1.84	0.58
1:N:113:CYS:HB2	1:N:226:LEU:HD13	1.84	0.58
1:N:492:VAL:HG23	1:N:539:ILE:HG12	1.85	0.58
1:N:966:LEU:HD22	1:N:1026:GLN:HG2	1.84	0.58
11:J:152:VAL:HA	11:J:188:GLY:HA2	1.83	0.58
14:M:710:TYR:CE2	14:M:771:VAL:HG13	2.38	0.58
1:N:140:ARG:HA	1:N:143:LYS:HG2	1.85	0.58
8:G:40:VAL:HG11	8:G:92:ALA:HB3	1.84	0.58
11:J:44:LEU:O	11:J:46:ILE:HG23	2.03	0.58
14:M:113:ILE:HB	14:M:133:ILE:HG22	1.85	0.58
14:M:216:MET:HB2	14:M:218:VAL:HG22	1.85	0.58
14:M:246:GLU:H	14:M:246:GLU:CD	2.12	0.58
1:N:533:ARG:HG2	1:N:1040:SER:OG	2.02	0.58
9:H:263:GLU:OE1	9:H:265:GLN:NE2	2.36	0.58
14:M:582:CYS:HB3	14:M:584:TYR:CE2	2.38	0.58
1:N:1361:LYS:N	6:E:109:TYR:HE2	1.98	0.58
5:D:88:PHE:CE1	5:D:146:LYS:NZ	2.72	0.58
5:D:116:VAL:HG22	5:D:140:ARG:HG3	1.85	0.58
11:J:114:LEU:HD22	11:J:127:TRP:HE3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:349:THR:HG21	13:L:386:SER:N	2.07	0.58
14:M:266:GLY:O	14:M:269:LEU:HG	2.03	0.58
14:M:597:ILE:HA	14:M:630:VAL:HG12	1.86	0.58
1:N:1207:VAL:HG23	1:N:1229:GLY:HA3	1.85	0.58
6:E:102:ILE:HG22	6:E:104:ILE:HG22	1.86	0.58
12:K:113:ARG:NH2	14:M:516:SER:O	2.37	0.58
14:M:537:PHE:CG	14:M:537:PHE:O	2.57	0.58
16:X:12:LEU:HD11	16:X:86:LEU:HG	1.85	0.58
9:H:234:ARG:NH1	9:H:279:ARG:O	2.37	0.58
1:N:766:ALA:HA	1:N:769:ARG:HH21	1.68	0.58
5:D:88:PHE:CE1	5:D:146:LYS:HD3	2.34	0.58
9:H:257:PHE:HZ	9:H:297:VAL:HG11	1.69	0.58
10:I:53:ILE:HG22	10:I:59:ARG:HD2	1.86	0.58
10:I:69:PHE:HZ	10:I:124:LEU:HD11	1.68	0.58
10:I:97:ILE:HD12	10:I:117:LEU:HD23	1.86	0.58
14:M:377:PHE:O	14:M:381:ASN:ND2	2.36	0.58
14:M:633:LEU:HD21	14:M:656:HIS:NE2	2.18	0.58
1:N:26:GLU:HG2	1:N:27:GLU:HG3	1.86	0.58
1:N:379:GLU:HG3	1:N:479:ARG:NH1	2.19	0.58
7:F:158:GLU:OE1	7:F:162:ARG:NH2	2.37	0.58
14:M:178:ILE:HG12	14:M:437:THR:HG22	1.85	0.58
14:M:779:LEU:HB3	14:M:879:PHE:HB2	1.86	0.58
1:N:101:VAL:HA	1:N:107:MET:HE1	1.84	0.57
1:N:641:GLN:O	1:N:643:SER:N	2.37	0.57
10:I:65:ILE:HD13	10:I:90:ARG:HH12	1.69	0.57
11:J:60:PHE:CG	11:J:63:ASP:HB2	2.38	0.57
14:M:160:GLU:HA	14:M:700:ASN:HD21	1.68	0.57
14:M:989:VAL:HG21	14:M:1004:PHE:HE2	1.69	0.57
1:N:46:ASN:ND2	1:N:52:LEU:HD12	2.18	0.57
1:N:59:ARG:HH12	1:N:75:ASN:HD21	1.50	0.57
1:N:80:LEU:HD21	14:M:1077:VAL:HB	1.85	0.57
1:N:438:GLU:HA	1:N:440:MET:HG2	1.86	0.57
1:N:894:THR:OG1	1:N:896:ASP:OD2	2.22	0.57
2:A:23:PHE:HE2	2:A:34:ILE:HB	1.69	0.57
5:D:58:LEU:HA	5:D:146:LYS:HB3	1.85	0.57
9:H:250:ALA:HA	9:H:272:VAL:HG23	1.86	0.57
15:Z:244:TYR:HD1	16:X:319:PRO:HB3	1.69	0.57
1:N:923:ARG:O	1:N:923:ARG:NH1	2.33	0.57
1:N:1043:GLU:O	1:N:1046:THR:N	2.31	0.57
4:C:46:LYS:HE2	14:M:815:CYS:SG	2.44	0.57
7:F:76:PHE:CE1	7:F:105:VAL:HG21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:54:VAL:HG21	9:H:279:ARG:HH22	1.69	0.57
9:H:286:GLU:OE2	14:M:977:VAL:HG13	2.05	0.57
14:M:159:ASN:O	14:M:700:ASN:ND2	2.37	0.57
14:M:527:CYS:O	14:M:529:GLU:N	2.35	0.57
14:M:725:ILE:HG22	14:M:731:GLU:HB2	1.87	0.57
14:M:742:ALA:HB2	14:M:925:PRO:HG3	1.86	0.57
1:N:508:HIS:CD2	14:M:1045:LEU:HD11	2.38	0.57
10:I:45:ILE:HG21	11:J:45:CYS:O	2.04	0.57
1:N:376:ARG:NH1	1:N:479:ARG:HH22	2.02	0.57
1:N:457:GLY:HA2	1:N:458:ASP:C	2.29	0.57
1:N:603:VAL:O	1:N:682:ARG:NH1	2.37	0.57
1:N:1362:LEU:HB2	11:J:58:TYR:HE1	1.68	0.57
6:E:124:ILE:HG22	6:E:125:ILE:H	1.70	0.57
13:L:266:LEU:N	13:L:380:LYS:HG3	2.16	0.57
14:M:636:ASN:O	14:M:639:ASN:N	2.38	0.57
15:Z:191:LYS:HG2	15:Z:271:ARG:HA	1.86	0.57
16:X:429:LEU:HD11	16:X:433:ARG:HH21	1.69	0.57
1:N:921:PHE:CZ	1:N:977:SER:HB2	2.40	0.57
9:H:231:ALA:HA	9:H:233:TYR:OH	2.05	0.57
14:M:140:LEU:HD23	14:M:168:TYR:CZ	2.40	0.57
15:Z:244:TYR:CD1	16:X:319:PRO:HB3	2.39	0.57
16:X:354:VAL:HA	16:X:358:PHE:HD1	1.70	0.57
1:N:45:ASP:OD2	1:N:53:TYR:OH	2.22	0.57
9:H:139:GLN:NE2	9:H:211:LEU:HD13	2.20	0.57
14:M:693:ALA:HA	14:M:1012:LEU:HA	1.86	0.57
1:N:117:LEU:HD12	1:N:120:GLU:HG3	1.87	0.57
1:N:677:ALA:HA	1:N:680:MET:HE2	1.86	0.57
5:D:48:TYR:CZ	5:D:147:LYS:HE2	2.40	0.57
14:M:405:HIS:ND1	14:M:405:HIS:O	2.38	0.57
14:M:903:GLN:HG2	14:M:929:MET:HE1	1.85	0.57
3:B:43:TYR:HB3	3:B:47:ARG:NE	2.19	0.57
14:M:563:ARG:NH1	14:M:637:GLU:OE2	2.37	0.57
1:N:165:THR:HB	1:N:178:LYS:HD2	1.86	0.56
1:N:558:PHE:HB3	1:N:594:LEU:HD13	1.87	0.56
7:F:18:MET:HE3	7:F:28:VAL:HB	1.87	0.56
13:L:337:VAL:HG11	13:L:350:MET:HE3	1.86	0.56
14:M:24:GLU:HG2	14:M:28:ARG:HD3	1.87	0.56
14:M:31:PRO:O	14:M:35:LYS:NZ	2.27	0.56
14:M:312:LEU:O	14:M:315:SER:OG	2.21	0.56
14:M:645:LEU:HA	14:M:658:GLU:CD	2.30	0.56
1:N:882:LEU:HD21	1:N:1293:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1331:ALA:HB1	1:N:1336:GLN:HB3	1.87	0.56
12:K:33:ARG:NH1	12:K:40:ASP:OD1	2.37	0.56
14:M:686:GLN:HB2	14:M:902:GLY:H	1.70	0.56
16:X:80:SER:HA	16:X:83:LEU:HD12	1.88	0.56
1:N:590:LYS:HE3	5:D:44:ASN:HB3	1.87	0.56
1:N:777:PRO:HG3	14:M:935:PRO:HB3	1.86	0.56
1:N:889:THR:HG22	1:N:900:PHE:HA	1.88	0.56
4:C:34:ILE:HG23	4:C:44:MET:HE2	1.87	0.56
5:D:24:ARG:HA	5:D:45:ILE:H	1.70	0.56
9:H:246:GLU:HG2	9:H:271:LYS:HA	1.87	0.56
13:L:353:ALA:HA	14:M:550:ARG:HH21	1.69	0.56
14:M:37:LYS:O	14:M:501:HIS:NE2	2.38	0.56
14:M:68:ASP:OD2	14:M:69:ALA:N	2.39	0.56
14:M:206:SER:O	14:M:207:THR:OG1	2.22	0.56
14:M:624:PHE:HB3	14:M:630:VAL:HG22	1.87	0.56
14:M:722:THR:HG22	14:M:961:GLY:O	2.06	0.56
14:M:848:GLN:HB3	14:M:851:TYR:OH	2.05	0.56
14:M:1088:TYR:HB2	14:M:1092:CYS:HA	1.87	0.56
15:Z:178:GLU:HB2	16:X:368:LEU:HD23	1.86	0.56
16:X:90:ARG:HD2	16:X:514:ILE:HG12	1.88	0.56
1:N:579:ILE:O	8:G:83:ARG:NH2	2.38	0.56
1:N:773:LYS:HB2	5:D:21:LYS:HD2	1.87	0.56
2:A:29:PRO:HB2	12:K:71:ARG:HH21	1.71	0.56
5:D:2:ALA:HA	5:D:61:ALA:HB1	1.86	0.56
9:H:43:ASP:OD1	9:H:44:ARG:NH1	2.39	0.56
9:H:154:LYS:O	9:H:157:SER:OG	2.22	0.56
11:J:5:VAL:H	11:J:74:CYS:H	1.53	0.56
11:J:89:ILE:HB	11:J:145:GLY:H	1.71	0.56
14:M:75:LEU:HD21	14:M:400:PHE:HB3	1.88	0.56
14:M:990:THR:HA	14:M:997:PRO:HA	1.87	0.56
16:X:449:ARG:HA	16:X:452:PHE:CD2	2.40	0.56
1:N:549:ALA:O	1:N:553:THR:HG23	2.05	0.56
1:N:915:LYS:O	1:N:922:LYS:N	2.30	0.56
1:N:1264:ARG:HG3	1:N:1291:SER:HB2	1.86	0.56
9:H:97:ASN:HB3	9:H:102:GLN:NE2	2.20	0.56
14:M:285:LYS:N	14:M:308:GLU:OE1	2.39	0.56
14:M:919:CYS:HA	14:M:989:VAL:HG22	1.87	0.56
16:X:122:VAL:HG22	16:X:144:VAL:HG12	1.87	0.56
1:N:149:LYS:HE3	1:N:180:LYS:HD3	1.87	0.56
2:A:8:CYS:SG	2:A:30:TYR:OH	2.58	0.56
3:B:6:ARG:HD2	9:H:112:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:1065:LEU:HA	14:M:1068:LEU:HD12	1.88	0.56
1:N:18:ILE:HG23	14:M:1126:LEU:HD23	1.88	0.56
1:N:23:LYS:HB3	14:M:1118:GLN:HE21	1.70	0.56
1:N:411:GLY:O	1:N:419:ASN:ND2	2.38	0.56
1:N:698:ILE:HG22	14:M:931:PRO:HB3	1.86	0.56
1:N:822:GLU:OE1	1:N:822:GLU:N	2.38	0.56
1:N:899:GLN:NE2	1:N:1292:ASP:OD2	2.35	0.56
6:E:54:THR:O	6:E:56:TYR:N	2.35	0.56
14:M:222:ARG:HB3	14:M:224:TYR:HE2	1.71	0.56
14:M:401:ASP:OD1	14:M:402:VAL:N	2.39	0.56
1:N:32:ALA:HB2	1:N:85:TYR:HB2	1.86	0.56
7:F:176:GLY:HA2	7:F:181:ARG:HH21	1.71	0.56
8:G:106:VAL:HG13	9:H:45:PHE:CZ	2.41	0.56
10:I:94:ALA:HB2	10:I:121:THR:HG23	1.88	0.56
16:X:90:ARG:HD2	16:X:514:ILE:HG23	1.87	0.56
1:N:387:ALA:O	1:N:453:HIS:ND1	2.37	0.56
3:B:21:TYR:O	3:B:25:LEU:N	2.36	0.56
10:I:120:VAL:HG13	10:I:124:LEU:HD12	1.87	0.56
12:K:43:PRO:HA	12:K:44:HIS:C	2.31	0.56
14:M:81:TYR:HB3	14:M:84:LEU:HG	1.88	0.56
14:M:721:LYS:O	14:M:960:TYR:HA	2.06	0.56
16:X:436:LEU:HA	16:X:523:LEU:HD13	1.86	0.56
8:G:111:LEU:HD12	9:H:326:ILE:HG23	1.88	0.56
9:H:106:LEU:HD21	9:H:210:LEU:HD11	1.88	0.56
9:H:283:PHE:HB3	14:M:988:TYR:HE2	1.71	0.56
16:X:261:GLN:OE1	16:X:264:SER:OG	2.23	0.56
1:N:270:LEU:HD21	14:M:852:LYS:HB3	1.89	0.55
1:N:391:THR:O	14:M:1025:ARG:NH1	2.40	0.55
3:B:9:THR:HG23	3:B:44:CYS:SG	2.46	0.55
1:N:23:LYS:HD2	1:N:256:LEU:HD12	1.88	0.55
1:N:33:HIS:NE2	1:N:70:GLU:OE2	2.34	0.55
1:N:83:TYR:HE2	14:M:1085:LEU:HD13	1.71	0.55
12:K:126:LEU:HD21	13:L:269:LEU:HD12	1.88	0.55
14:M:160:GLU:HA	14:M:700:ASN:ND2	2.20	0.55
14:M:537:PHE:CZ	14:M:546:LEU:HD22	2.41	0.55
1:N:163:ASN:O	1:N:178:LYS:N	2.38	0.55
7:F:21:CYS:HA	7:F:64:HIS:CE1	2.40	0.55
9:H:144:VAL:HG11	9:H:168:VAL:HG22	1.88	0.55
11:J:80:PHE:HB2	11:J:83:GLU:HG2	1.88	0.55
14:M:47:PHE:HE1	14:M:369:LEU:HG	1.72	0.55
1:N:60:MET:O	1:N:82:HIS:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:391:THR:HA	1:N:451:GLU:OE1	2.06	0.55
5:D:44:ASN:H	5:D:90:TYR:HH	1.48	0.55
7:F:146:PRO:HG3	7:F:196:PRO:HD3	1.88	0.55
10:I:6:ALA:HA	11:J:5:VAL:HG13	1.87	0.55
14:M:697:ILE:N	14:M:701:GLN:HE21	2.04	0.55
14:M:772:TYR:HE1	14:M:884:LEU:HD13	1.70	0.55
14:M:971:ASP:OD1	14:M:972:VAL:N	2.39	0.55
1:N:19:CYS:SG	1:N:20:PHE:N	2.79	0.55
1:N:1055:PHE:HA	1:N:1057:GLY:N	2.21	0.55
8:G:51:LEU:HD22	9:H:332:LYS:HB3	1.89	0.55
10:I:6:ALA:O	11:J:78:HIS:CE1	2.58	0.55
14:M:81:TYR:HB2	14:M:85:PRO:HD3	1.88	0.55
14:M:777:CYS:HB2	14:M:828:VAL:HG11	1.88	0.55
14:M:870:MET:HB2	14:M:882:LYS:HB2	1.88	0.55
1:N:94:HIS:HE1	1:N:224:LEU:HD21	1.72	0.55
9:H:232:SER:HB3	14:M:918:PHE:CD1	2.41	0.55
14:M:611:MET:HA	14:M:614:LEU:HB2	1.89	0.55
16:X:251:ILE:O	16:X:255:VAL:HG23	2.06	0.55
1:N:1187:TYR:HB2	1:N:1189:LEU:HB2	1.88	0.55
11:J:101:LEU:HD23	11:J:107:ILE:HD13	1.88	0.55
12:K:46:SER:HB2	12:K:59:GLU:HB2	1.88	0.55
14:M:947:LEU:HB3	14:M:972:VAL:HG11	1.89	0.55
16:X:394:MET:O	16:X:398:MET:HG2	2.07	0.55
5:D:44:ASN:N	5:D:90:TYR:OH	2.25	0.55
9:H:70:ALA:HB1	14:M:995:GLY:O	2.06	0.55
11:J:60:PHE:HE2	11:J:65:ALA:HB3	1.72	0.55
11:J:118:ALA:HA	11:J:130:GLU:HG2	1.88	0.55
14:M:102:CYS:HB3	14:M:170:ILE:HG21	1.88	0.55
14:M:542:ASN:OD1	14:M:587:SER:N	2.39	0.55
1:N:642:ASN:O	1:N:643:SER:OG	2.23	0.55
8:G:57:TYR:O	8:G:61:LYS:HG3	2.07	0.55
9:H:100:ILE:HG13	9:H:101:VAL:H	1.71	0.55
1:N:29:ARG:CD	1:N:85:TYR:CE1	2.90	0.55
1:N:163:ASN:HA	1:N:180:LYS:HZ2	1.71	0.55
1:N:709:LEU:HD13	1:N:769:ARG:HH22	1.72	0.55
7:F:131:LEU:HB3	7:F:134:GLU:HB2	1.89	0.55
7:F:171:PRO:O	7:F:208:LEU:N	2.25	0.55
9:H:23:ASN:O	9:H:303:ARG:NH1	2.35	0.55
9:H:78:ARG:NH1	14:M:915:ASP:OD2	2.39	0.55
14:M:372:LEU:HD21	14:M:424:TRP:HB3	1.89	0.55
1:N:107:MET:O	1:N:143:LYS:NZ	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:148:ASP:O	1:N:180:LYS:NZ	2.36	0.54
1:N:494:THR:OG1	1:N:538:LEU:O	2.23	0.54
1:N:551:LEU:HD23	1:N:554:LEU:HD12	1.89	0.54
1:N:682:ARG:O	1:N:686:LEU:HB2	2.08	0.54
3:B:42:ARG:HH22	9:H:230:THR:HG22	1.72	0.54
9:H:285:ARG:NH2	14:M:1001:TYR:OH	2.39	0.54
1:N:528:ASN:HB2	1:N:529:LEU:HD12	1.90	0.54
1:N:766:ALA:HA	1:N:769:ARG:HE	1.72	0.54
14:M:759:LYS:N	14:M:911:VAL:O	2.38	0.54
1:N:185:VAL:HG13	1:N:216:GLU:OE1	2.06	0.54
1:N:638:VAL:HG12	1:N:648:GLY:HA3	1.88	0.54
1:N:901:ILE:HG22	1:N:902:TYR:H	1.72	0.54
1:N:1297:LYS:HD3	1:N:1310:LYS:HG2	1.90	0.54
5:D:2:ALA:HB1	5:D:4:ILE:HD11	1.89	0.54
9:H:79:ILE:HA	9:H:83:GLU:HB2	1.90	0.54
13:L:269:LEU:HD23	13:L:383:LEU:HB2	1.90	0.54
14:M:117:ILE:HD12	14:M:131:LEU:HD12	1.87	0.54
14:M:708:LEU:HD22	14:M:710:TYR:CE2	2.42	0.54
14:M:1111:LYS:HG2	14:M:1115:GLN:NE2	2.23	0.54
1:N:109:CYS:SG	1:N:143:LYS:NZ	2.67	0.54
1:N:359:LYS:N	1:N:360:ARG:HH21	2.05	0.54
14:M:218:VAL:HG21	14:M:224:TYR:HD2	1.72	0.54
14:M:769:CYS:O	14:M:770:LEU:HD23	2.06	0.54
14:M:800:ARG:HG3	14:M:804:TRP:HD1	1.71	0.54
5:D:31:GLU:HA	5:D:38:ASP:HA	1.90	0.54
16:X:448:GLU:HG2	16:X:452:PHE:CZ	2.43	0.54
1:N:429:LYS:HD3	1:N:437:ARG:HH12	1.73	0.54
1:N:773:LYS:NZ	5:D:19:GLY:O	2.27	0.54
1:N:1181:SER:O	1:N:1183:SER:N	2.40	0.54
7:F:35:GLN:CD	7:F:43:GLN:HE21	2.15	0.54
14:M:133:ILE:HD11	14:M:380:PHE:CE1	2.43	0.54
14:M:770:LEU:O	14:M:772:TYR:HD2	1.91	0.54
14:M:831:SER:HB3	14:M:851:TYR:HB3	1.89	0.54
1:N:71:THR:HG22	14:M:1088:TYR:H	1.72	0.54
1:N:279:LEU:HD23	1:N:280:THR:N	2.21	0.54
3:B:5:VAL:HG23	9:H:109:ARG:NH1	2.22	0.54
7:F:26:TYR:HA	7:F:65:ASN:HB2	1.90	0.54
16:X:13:LEU:HD13	16:X:22:GLU:HA	1.89	0.54
1:N:175:ILE:HD13	1:N:218:LEU:HB3	1.89	0.54
1:N:483:HIS:O	1:N:485:THR:N	2.40	0.54
6:E:86:GLU:HG2	6:E:86:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:107:ARG:HG2	6:E:109:TYR:HE1	1.72	0.54
7:F:87:ILE:HG12	7:F:104:ILE:HD13	1.88	0.54
12:K:25:LEU:HA	13:L:364:GLY:HA2	1.90	0.54
12:K:52:LYS:HG3	12:K:53:GLN:OE1	2.08	0.54
14:M:236:ILE:O	14:M:239:ILE:N	2.41	0.54
16:X:28:LEU:HD21	16:X:39:ILE:HD11	1.88	0.54
1:N:366:ARG:HH21	1:N:504:GLU:HG3	1.73	0.54
1:N:1357:THR:HB	6:E:64:ARG:NH2	2.23	0.54
8:G:22:GLU:HG2	9:H:336:PHE:HA	1.90	0.54
11:J:60:PHE:HB3	11:J:63:ASP:H	1.73	0.54
14:M:1007:VAL:HG12	14:M:1008:TYR:H	1.73	0.54
1:N:29:ARG:CA	1:N:85:TYR:CD1	2.91	0.54
12:K:42:ILE:H	12:K:42:ILE:HD12	1.73	0.54
14:M:49:TYR:CD2	14:M:504:THR:HG21	2.43	0.54
16:X:68:HIS:CE1	16:X:74:GLU:HB2	2.43	0.54
1:N:102:ILE:HA	1:N:166:VAL:HG11	1.90	0.53
1:N:469:HIS:CE1	1:N:533:ARG:HD2	2.43	0.53
4:C:36:CYS:HB2	4:C:41:TYR:HB2	1.90	0.53
4:C:51:ARG:NH2	14:M:819:GLU:OE2	2.41	0.53
5:D:15:ILE:HG13	5:D:51:ASP:O	2.08	0.53
9:H:138:LEU:HB2	9:H:214:CYS:HB2	1.90	0.53
1:N:402:ASN:O	1:N:406:LYS:HG2	2.08	0.53
1:N:752:ILE:O	1:N:756:LEU:HG	2.08	0.53
1:N:801:GLN:HE21	1:N:833:PHE:HB2	1.72	0.53
12:K:49:ILE:HG12	12:K:56:VAL:HG23	1.89	0.53
14:M:394:LYS:O	14:M:399:GLN:NE2	2.38	0.53
4:C:26:ASN:HB3	4:C:28:ILE:HG13	1.91	0.53
14:M:595:PRO:HB2	14:M:659:ILE:HD11	1.89	0.53
14:M:1023:ARG:HD3	14:M:1042:ASP:HB3	1.90	0.53
16:X:434:MET:HE3	16:X:438:ARG:HE	1.72	0.53
1:N:120:GLU:HB2	1:N:121:GLU:O	2.09	0.53
5:D:1:MET:HE2	5:D:144:LEU:HD12	1.89	0.53
9:H:90:GLU:OE1	9:H:224:LYS:NZ	2.30	0.53
10:I:20:LEU:HD21	10:I:49:THR:HB	1.90	0.53
14:M:498:LEU:O	14:M:500:THR:N	2.41	0.53
1:N:601:PHE:CE1	1:N:683:LEU:HD21	2.43	0.53
4:C:48:ARG:HH21	9:H:96:ASN:CG	2.16	0.53
11:J:4:LEU:HD13	11:J:73:ARG:HD3	1.90	0.53
14:M:887:GLN:OE1	14:M:889:ARG:NH2	2.34	0.53
1:N:59:ARG:N	1:N:60:MET:HA	2.24	0.53
7:F:72:MET:SD	7:F:101:ARG:NH2	2.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:360:LEU:HB2	13:L:379:VAL:HB	1.90	0.53
14:M:794:MET:HE3	14:M:809:LEU:HB2	1.89	0.53
16:X:24:ILE:HG23	16:X:57:LEU:HD11	1.91	0.53
1:N:790:ILE:HD11	1:N:1051:LYS:NZ	2.24	0.53
10:I:92:VAL:N	10:I:96:GLU:OE1	2.41	0.53
13:L:368:SER:HA	13:L:371:GLY:C	2.34	0.53
14:M:47:PHE:HB3	14:M:139:MET:CE	2.39	0.53
14:M:278:PHE:HB2	14:M:283:ALA:CB	2.39	0.53
14:M:815:CYS:HB2	14:M:817:PRO:HD3	1.90	0.53
14:M:921:SER:OG	14:M:923:ILE:HG12	2.09	0.53
14:M:946:LEU:CD1	14:M:1007:VAL:HG22	2.35	0.53
1:N:555:LYS:HB3	5:D:20:LYS:HD2	1.90	0.53
5:D:4:ILE:HG22	5:D:6:PHE:N	2.24	0.53
9:H:94:VAL:HG13	9:H:97:ASN:ND2	2.23	0.53
9:H:198:LEU:HD23	9:H:198:LEU:O	2.08	0.53
10:I:17:PHE:O	10:I:21:THR:HG23	2.08	0.53
14:M:1034:GLN:HB2	14:M:1037:GLU:OE1	2.08	0.53
1:N:59:ARG:NH1	1:N:67:ARG:O	2.42	0.53
11:J:97:VAL:HB	11:J:127:TRP:CE2	2.44	0.53
14:M:134:GLY:HA2	14:M:409:ASP:HA	1.91	0.53
15:Z:249:GLU:H	15:Z:272:ALA:HA	1.73	0.53
1:N:464:ARG:HG2	1:N:505:MET:HE3	1.91	0.53
1:N:945:LEU:HD11	1:N:1008:PRO:HG3	1.90	0.53
5:D:96:VAL:HG12	5:D:97:TYR:N	2.24	0.53
1:N:19:CYS:HB3	14:M:1125:ARG:HB2	1.90	0.52
1:N:679:ALA:O	1:N:682:ARG:HG2	2.07	0.52
1:N:856:GLU:O	1:N:860:ASP:N	2.24	0.52
6:E:57:MET:SD	6:E:123:LEU:HB3	2.49	0.52
14:M:440:LEU:HA	14:M:451:MET:HG2	1.90	0.52
5:D:48:TYR:HB3	5:D:53:GLY:HA2	1.90	0.52
8:G:49:HIS:NE2	8:G:77:GLU:OE2	2.41	0.52
15:Z:185:PHE:HE2	15:Z:242:LEU:HD23	1.73	0.52
1:N:1053:PHE:HE1	1:N:1277:ASN:CG	2.17	0.52
1:N:1303:ILE:HA	1:N:1308:LEU:HD11	1.91	0.52
9:H:166:HIS:CD2	9:H:167:LYS:HG3	2.44	0.52
10:I:12:SER:HB3	10:I:15:GLU:HB3	1.91	0.52
1:N:64:GLU:HB3	1:N:67:ARG:HH22	1.74	0.52
1:N:148:ASP:HB3	1:N:164:GLY:H	1.75	0.52
1:N:371:PRO:HA	1:N:487:ARG:HA	1.90	0.52
8:G:60:MET:HB2	8:G:68:CYS:HB3	1.92	0.52
9:H:125:ARG:HH21	9:H:136:ASP:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:10:THR:HG22	11:J:69:LYS:HZ3	1.74	0.52
11:J:111:PRO:HA	11:J:127:TRP:HZ3	1.73	0.52
13:L:338:GLN:HA	13:L:348:VAL:HA	1.91	0.52
5:D:4:ILE:CB	5:D:5:LEU:HA	2.34	0.52
5:D:29:HIS:H	5:D:52:LEU:CD1	2.23	0.52
5:D:141:VAL:O	5:D:143:LEU:N	2.43	0.52
7:F:139:ILE:H	7:F:182:TYR:HE2	1.56	0.52
8:G:74:HIS:CE1	8:G:79:LYS:HD2	2.45	0.52
11:J:110:PRO:O	11:J:113:SER:OG	2.27	0.52
14:M:63:GLU:OE1	14:M:66:THR:HG21	2.09	0.52
14:M:168:TYR:CG	14:M:440:LEU:HD11	2.45	0.52
14:M:402:VAL:HA	14:M:405:HIS:HB3	1.91	0.52
14:M:575:SER:HB2	14:M:636:ASN:HB3	1.91	0.52
14:M:639:ASN:ND2	14:M:639:ASN:O	2.42	0.52
14:M:760:ALA:N	14:M:763:ASP:OD2	2.33	0.52
14:M:820:LYS:HB3	14:M:865:TYR:CE1	2.44	0.52
16:X:102:THR:O	16:X:106:ILE:HG12	2.09	0.52
16:X:260:ASP:OD1	16:X:311:TYR:OH	2.23	0.52
16:X:265:GLU:OE2	16:X:272:ARG:NH2	2.42	0.52
1:N:1258:LEU:HD12	7:F:139:ILE:HG12	1.92	0.52
5:D:10:PHE:CB	5:D:56:PHE:HB2	2.39	0.52
5:D:135:PHE:HB2	5:D:140:ARG:NH2	2.25	0.52
10:I:73:LEU:HD12	10:I:83:LYS:HB3	1.92	0.52
14:M:222:ARG:HB3	14:M:224:TYR:CE2	2.44	0.52
1:N:94:HIS:O	1:N:98:PHE:N	2.39	0.52
3:B:44:CYS:O	3:B:48:MET:HG2	2.09	0.52
9:H:104:GLU:OE1	14:M:886:ARG:NH2	2.41	0.52
10:I:84:LEU:HD11	11:J:1:MET:HE2	1.90	0.52
14:M:67:SER:H	14:M:74:TYR:HE1	1.57	0.52
15:Z:176:PHE:O	15:Z:227:LYS:NZ	2.43	0.52
5:D:12:VAL:HG21	5:D:52:LEU:C	2.35	0.52
5:D:147:LYS:HG2	5:D:148:LEU:H	1.75	0.52
7:F:187:ARG:HA	7:F:209:VAL:HG11	1.92	0.52
12:K:59:GLU:O	12:K:61:ALA:N	2.40	0.52
14:M:163:LEU:HD11	14:M:733:LEU:HD11	1.91	0.52
14:M:577:ASN:HB2	14:M:582:CYS:HB2	1.91	0.52
15:Z:250:MET:H	16:X:259:MET:HE1	1.73	0.52
1:N:1316:LEU:HB2	1:N:1342:GLY:HA3	1.92	0.52
9:H:125:ARG:HD2	9:H:132:GLY:HA3	1.92	0.52
9:H:327:LYS:HD2	9:H:330:MET:HG3	1.92	0.52
1:N:598:LYS:HE2	5:D:120:GLY:HA2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:697:SER:HB2	14:M:1003:TYR:H	1.75	0.52
1:N:859:VAL:O	1:N:863:VAL:HG22	2.10	0.52
1:N:861:THR:HA	1:N:864:LYS:HD2	1.91	0.52
5:D:140:ARG:CD	5:D:143:LEU:HD11	2.39	0.52
9:H:12:SER:O	9:H:13:ARG:HD2	2.10	0.52
9:H:169:TYR:HA	9:H:197:ILE:O	2.09	0.52
1:N:122:LYS:NZ	16:X:72:VAL:H	2.06	0.51
2:A:26:ASN:OD1	14:M:273:GLN:NE2	2.43	0.51
3:B:44:CYS:SG	14:M:923:ILE:HD12	2.50	0.51
5:D:120:GLY:O	5:D:121:LEU:HD23	2.10	0.51
8:G:36:ASP:O	8:G:37:ARG:HD2	2.10	0.51
10:I:39:GLN:HG3	11:J:32:LYS:HA	1.91	0.51
14:M:619:ARG:NH1	14:M:627:GLU:OE1	2.43	0.51
14:M:982:ASN:ND2	14:M:988:TYR:OH	2.43	0.51
1:N:422:GLN:HA	1:N:428:MET:HB3	1.92	0.51
1:N:704:THR:HG22	1:N:839:TYR:CZ	2.44	0.51
7:F:130:PHE:HZ	7:F:181:ARG:HB3	1.75	0.51
9:H:285:ARG:HE	9:H:288:PHE:HE2	1.56	0.51
10:I:70:LEU:HD23	10:I:83:LYS:HD3	1.92	0.51
14:M:372:LEU:HB3	14:M:415:MET:HE1	1.93	0.51
14:M:933:GLY:HA2	14:M:937:ARG:NH1	2.24	0.51
17:Y:-12:UNK:N	17:Y:-11:UNK:HA	2.25	0.51
1:N:277:ASP:OD1	1:N:278:ASP:HA	2.11	0.51
1:N:380:VAL:HG12	1:N:381:ALA:N	2.26	0.51
1:N:913:GLU:CD	1:N:914:GLY:H	2.18	0.51
9:H:94:VAL:HG13	9:H:97:ASN:CG	2.35	0.51
9:H:96:ASN:OD1	9:H:98:THR:OG1	2.28	0.51
9:H:109:ARG:NE	14:M:714:TYR:OH	2.44	0.51
12:K:58:LEU:H	12:K:101:THR:HG22	1.74	0.51
14:M:588:ASP:O	14:M:591:ARG:NE	2.41	0.51
14:M:638:GLU:HA	14:M:641:CYS:SG	2.51	0.51
1:N:110:LYS:HD2	1:N:222:VAL:HG13	1.92	0.51
1:N:857:GLY:O	1:N:861:THR:OG1	2.28	0.51
1:N:971:LYS:HA	1:N:974:LYS:HD2	1.92	0.51
1:N:1182:LYS:HE3	1:N:1185:MET:HA	1.92	0.51
1:N:1312:LYS:NZ	7:F:170:LEU:O	2.39	0.51
5:D:4:ILE:HD13	5:D:59:VAL:CG1	2.40	0.51
8:G:40:VAL:HG12	8:G:42:PHE:CE1	2.45	0.51
8:G:49:HIS:CG	8:G:70:TYR:HH	2.24	0.51
9:H:143:GLN:OE1	9:H:143:GLN:N	2.44	0.51
11:J:1:MET:SD	11:J:2:PHE:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:56:ASP:HB3	11:J:58:TYR:CE1	2.45	0.51
14:M:455:ILE:O	14:M:494:LYS:N	2.35	0.51
14:M:755:LEU:N	14:M:906:VAL:O	2.39	0.51
14:M:889:ARG:HD3	14:M:1017:LEU:HD13	1.92	0.51
1:N:127:ASP:OD1	1:N:131:ARG:NE	2.43	0.51
1:N:467:SER:OG	14:M:1054:CYS:SG	2.49	0.51
4:C:22:CYS:HB2	4:C:41:TYR:CD1	2.44	0.51
7:F:129:GLN:OE1	7:F:129:GLN:N	2.43	0.51
12:K:32:VAL:HG23	12:K:33:ARG:HG2	1.93	0.51
1:N:115:ILE:O	1:N:158:HIS:HB2	2.11	0.51
1:N:219:ASN:O	1:N:222:VAL:HG12	2.10	0.51
1:N:1145:ASN:HB3	1:N:1148:THR:HG23	1.91	0.51
1:N:1235:VAL:HA	1:N:1238:THR:HG23	1.92	0.51
5:D:12:VAL:HG12	5:D:30:CYS:HB3	1.92	0.51
7:F:73:PHE:CD2	7:F:99:ILE:HD12	2.45	0.51
9:H:49:PHE:HE2	9:H:68:ILE:HG12	1.75	0.51
10:I:19:LEU:HB3	11:J:49:PHE:CE1	2.45	0.51
14:M:831:SER:HB3	14:M:851:TYR:CG	2.46	0.51
1:N:585:PRO:HG2	5:D:93:TYR:HB2	1.92	0.51
1:N:697:SER:OG	14:M:1001:TYR:O	2.13	0.51
1:N:1054:HIS:C	1:N:1056:ALA:HB3	2.36	0.51
4:C:18:ILE:HD11	4:C:47:LYS:HG2	1.92	0.51
9:H:130:GLU:O	9:H:131:GLU:HB3	2.09	0.51
10:I:90:ARG:HG2	10:I:124:LEU:HD13	1.93	0.51
1:N:120:GLU:OE1	1:N:156:CYS:HA	2.10	0.51
1:N:705:PRO:HB3	1:N:796:ILE:HG23	1.93	0.51
1:N:901:ILE:HG22	1:N:902:TYR:N	2.26	0.51
1:N:911:ALA:HB3	1:N:1025:ALA:HB2	1.92	0.51
1:N:1297:LYS:NZ	1:N:1310:LYS:HB3	2.26	0.51
3:B:47:ARG:NH1	14:M:740:THR:OG1	2.44	0.51
6:E:94:MET:HA	6:E:97:LEU:HD12	1.92	0.51
9:H:108:HIS:HB3	14:M:768:ARG:HH22	1.76	0.51
14:M:633:LEU:HD21	14:M:656:HIS:CD2	2.46	0.51
14:M:898:SER:OG	14:M:899:SER:N	2.44	0.51
1:N:942:LYS:O	1:N:946:ILE:N	2.36	0.51
4:C:31:ARG:HH11	4:C:31:ARG:HG3	1.76	0.51
7:F:61:LEU:HD23	7:F:73:PHE:HB3	1.92	0.51
9:H:38:ASP:O	9:H:40:TRP:CD1	2.64	0.51
11:J:89:ILE:HG13	11:J:146:GLU:HB2	1.92	0.51
11:J:140:LEU:HB3	11:J:142:MET:HE2	1.93	0.51
14:M:380:PHE:O	14:M:383:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:679:GLN:HE21	14:M:938:MET:CE	2.24	0.51
14:M:701:GLN:O	14:M:704:ARG:HG2	2.10	0.51
14:M:722:THR:H	14:M:725:ILE:HD12	1.76	0.51
1:N:307:MET:HA	1:N:310:TRP:CD1	2.46	0.51
1:N:360:ARG:HH22	14:M:1052:ARG:HD2	1.75	0.51
1:N:364:SER:HG	1:N:365:GLY:H	1.59	0.51
3:B:56:ILE:HG13	3:B:57:GLU:N	2.26	0.51
7:F:50:GLU:OE1	7:F:50:GLU:N	2.26	0.51
8:G:94:GLU:HB2	8:G:95:PRO:HD3	1.92	0.51
10:I:85:GLN:NE2	11:J:81:LEU:O	2.44	0.51
12:K:136:ARG:NH2	14:M:250:GLU:OE2	2.44	0.51
14:M:539:VAL:O	14:M:546:LEU:HA	2.11	0.51
14:M:1078:ASP:OD2	14:M:1102:SER:N	2.36	0.51
1:N:72:CYS:HB2	1:N:82:HIS:HE1	1.74	0.50
1:N:567:ILE:CD1	1:N:600:ILE:HG23	2.40	0.50
1:N:745:GLU:HG2	1:N:746:GLU:N	2.18	0.50
1:N:1290:LEU:HG	1:N:1294:MET:HE3	1.93	0.50
4:C:19:CYS:HB2	4:C:22:CYS:O	2.11	0.50
5:D:15:ILE:HG12	5:D:52:LEU:HD23	1.93	0.50
8:G:50:THR:HG22	9:H:78:ARG:HE	1.77	0.50
9:H:99:SER:OG	9:H:100:ILE:N	2.44	0.50
10:I:9:ALA:HB2	11:J:4:LEU:H	1.76	0.50
10:I:66:VAL:HG22	10:I:87:LEU:HD22	1.91	0.50
12:K:49:ILE:N	12:K:206:VAL:HG21	2.26	0.50
14:M:224:TYR:CG	14:M:233:ASP:HB3	2.45	0.50
14:M:651:ASN:O	14:M:653:ASP:N	2.39	0.50
14:M:1106:ILE:HD12	14:M:1107:PRO:HD2	1.92	0.50
1:N:550:TYR:CZ	1:N:554:LEU:HD21	2.46	0.50
1:N:747:THR:C	1:N:749:GLU:H	2.19	0.50
1:N:883:CYS:SG	1:N:884:SER:N	2.84	0.50
7:F:160:LEU:HD22	7:F:165:LEU:HB3	1.93	0.50
14:M:321:VAL:HB	14:M:322:PRO:HD2	1.92	0.50
14:M:575:SER:O	14:M:583:VAL:HA	2.11	0.50
14:M:597:ILE:HB	14:M:657:LEU:HB3	1.93	0.50
16:X:237:ALA:HB1	16:X:242:PHE:HE2	1.76	0.50
17:Y:9:UNK:C	17:Y:11:UNK:H	2.24	0.50
1:N:479:ARG:O	1:N:479:ARG:HG2	2.11	0.50
1:N:699:GLY:O	14:M:943:LEU:HD13	2.11	0.50
1:N:1028:GLU:HA	1:N:1029:PRO:C	2.36	0.50
5:D:87:GLN:C	5:D:88:PHE:HD1	2.19	0.50
6:E:65:VAL:HA	6:E:68:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:87:ILE:HA	7:F:90:TYR:CD2	2.46	0.50
11:J:17:GLN:HB3	11:J:20:ARG:HB2	1.93	0.50
14:M:215:ASN:OD1	14:M:216:MET:N	2.44	0.50
14:M:538:LEU:HD22	14:M:582:CYS:HA	1.92	0.50
14:M:620:ASN:O	14:M:621:PHE:CD2	2.63	0.50
16:X:239:LEU:O	16:X:243:HIS:ND1	2.27	0.50
16:X:398:MET:HA	16:X:398:MET:HE3	1.92	0.50
1:N:870:TYR:O	1:N:873:ARG:HG3	2.11	0.50
1:N:945:LEU:HD21	1:N:1008:PRO:HG3	1.94	0.50
1:N:1044:PRO:HB2	1:N:1275:MET:HE3	1.94	0.50
7:F:41:LYS:O	7:F:45:GLY:N	2.40	0.50
7:F:94:MET:O	7:F:99:ILE:HG12	2.12	0.50
9:H:217:GLY:HA3	9:H:225:PHE:CE2	2.46	0.50
11:J:195:LEU:HD13	11:J:201:TRP:NE1	2.26	0.50
14:M:847:GLN:C	14:M:849:PRO:HD3	2.36	0.50
1:N:363:PHE:CZ	14:M:1025:ARG:HG2	2.46	0.50
1:N:421:ILE:HG23	1:N:450:VAL:HA	1.93	0.50
2:A:14:VAL:H	2:A:23:PHE:HE1	1.58	0.50
8:G:101:ASN:CG	9:H:337:LEU:HD21	2.37	0.50
10:I:76:HIS:O	10:I:78:LEU:HD12	2.11	0.50
12:K:48:LYS:N	12:K:57:GLU:O	2.44	0.50
14:M:307:GLU:CB	14:M:310:ARG:HH21	2.24	0.50
14:M:337:VAL:HG22	14:M:341:ARG:HH12	1.75	0.50
1:N:380:VAL:HG23	1:N:476:HIS:HB3	1.93	0.50
12:K:50:LYS:HD2	12:K:204:PRO:HG3	1.93	0.50
14:M:225:LEU:HB3	14:M:227:HIS:CD2	2.47	0.50
14:M:790:VAL:HG11	14:M:831:SER:HB2	1.93	0.50
1:N:553:THR:HG21	1:N:650:MET:HG2	1.92	0.50
1:N:660:LYS:HE2	1:N:922:LYS:NZ	2.27	0.50
1:N:884:SER:HB2	1:N:1031:SER:N	2.25	0.50
6:E:62:ARG:NH2	6:E:124:ILE:O	2.37	0.50
16:X:354:VAL:O	16:X:359:GLY:N	2.44	0.50
4:C:41:TYR:C	4:C:43:ILE:HD12	2.37	0.50
5:D:93:TYR:CD1	5:D:142:TYR:HD1	2.24	0.50
10:I:119:THR:O	10:I:123:ILE:HG22	2.12	0.50
12:K:32:VAL:C	12:K:34:PRO:HD3	2.37	0.50
12:K:50:LYS:HD3	12:K:55:LYS:HB2	1.92	0.50
14:M:47:PHE:HB3	14:M:139:MET:HE1	1.94	0.50
14:M:126:ILE:O	14:M:128:ARG:NE	2.44	0.50
14:M:284:LEU:O	14:M:288:GLY:N	2.44	0.50
14:M:308:GLU:HG3	14:M:309:ALA:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:356:TYR:HB3	14:M:359:ASN:ND2	2.26	0.50
14:M:912:PRO:HD2	14:M:915:ASP:OD1	2.11	0.50
1:N:393:PRO:HD2	1:N:511:GLN:HB2	1.94	0.50
1:N:587:THR:HA	5:D:91:VAL:O	2.12	0.50
1:N:822:GLU:HG2	1:N:825:SER:HB3	1.94	0.50
10:I:96:GLU:O	10:I:101:VAL:N	2.44	0.50
10:I:97:ILE:O	10:I:104:SER:OG	2.30	0.50
14:M:407:ARG:HG2	14:M:410:GLN:HB2	1.93	0.50
1:N:29:ARG:HD3	1:N:256:LEU:HD21	1.93	0.49
1:N:185:VAL:CG2	1:N:216:GLU:HB2	2.41	0.49
5:D:98:ARG:HG2	5:D:135:PHE:CZ	2.47	0.49
10:I:73:LEU:HB2	10:I:83:LYS:HE3	1.92	0.49
14:M:26:LYS:HG3	14:M:27:TRP:HD1	1.77	0.49
14:M:98:SER:HB2	14:M:99:PRO:HD2	1.93	0.49
14:M:108:THR:HG22	14:M:172:LYS:H	1.76	0.49
16:X:285:THR:HG23	16:X:338:LEU:HD11	1.94	0.49
16:X:330:GLY:HA2	16:X:332:GLY:H	1.77	0.49
1:N:33:HIS:HE2	1:N:70:GLU:CD	2.17	0.49
4:C:17:TYR:HE1	4:C:46:LYS:HE3	1.78	0.49
7:F:49:SER:OG	7:F:52:ARG:HA	2.11	0.49
9:H:108:HIS:HB3	14:M:768:ARG:NH2	2.27	0.49
12:K:66:ASN:HB2	12:K:69:TYR:CE2	2.47	0.49
14:M:807:GLU:HG2	14:M:808:ILE:HG12	1.94	0.49
1:N:924:VAL:HG23	1:N:1014:PHE:HE1	1.77	0.49
1:N:1169:GLY:HA2	1:N:1178:ARG:HE	1.77	0.49
4:C:16:ILE:O	4:C:16:ILE:HG22	2.12	0.49
5:D:116:VAL:HG12	5:D:118:TYR:CE1	2.45	0.49
9:H:145:ARG:HA	9:H:207:GLU:HG3	1.95	0.49
14:M:278:PHE:HB2	14:M:283:ALA:HB2	1.94	0.49
14:M:545:ILE:O	14:M:546:LEU:HD12	2.11	0.49
14:M:846:PRO:O	14:M:848:GLN:N	2.40	0.49
15:Z:191:LYS:HD2	15:Z:271:ARG:HH11	1.77	0.49
16:X:394:MET:O	16:X:397:LYS:HG3	2.13	0.49
1:N:111:THR:H	1:N:162:PHE:HD2	1.59	0.49
1:N:514:GLU:HA	6:E:71:LEU:CD2	2.42	0.49
1:N:568:ILE:HD11	8:G:67:PHE:CD2	2.47	0.49
1:N:1189:LEU:HB3	1:N:1193:LYS:NZ	2.26	0.49
14:M:475:GLN:HG3	14:M:479:LEU:HB2	1.94	0.49
1:N:640:ILE:HG23	1:N:644:GLU:O	2.11	0.49
9:H:106:LEU:HD11	9:H:208:ILE:HD13	1.94	0.49
14:M:29:LEU:HD22	14:M:33:PHE:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:291:VAL:CG2	14:M:293:ARG:HG2	2.42	0.49
14:M:803:ILE:O	14:M:807:GLU:N	2.46	0.49
14:M:950:LYS:N	14:M:1006:PRO:HD2	2.27	0.49
1:N:88:LEU:HB2	1:N:255:LEU:HD21	1.93	0.49
1:N:545:PHE:HD1	1:N:688:PRO:HD3	1.76	0.49
7:F:13:ILE:O	7:F:17:ILE:HG12	2.11	0.49
9:H:87:MET:HA	9:H:87:MET:HE3	1.95	0.49
11:J:82:ASP:HB3	11:J:151:ARG:HG2	1.95	0.49
12:K:55:LYS:HA	12:K:103:CYS:HA	1.95	0.49
14:M:37:LYS:HE3	14:M:501:HIS:HB3	1.94	0.49
14:M:307:GLU:O	14:M:310:ARG:N	2.35	0.49
14:M:1028:ARG:NH1	14:M:1109:ALA:HB2	2.27	0.49
16:X:117:THR:HA	16:X:233:ILE:C	2.36	0.49
1:N:373:PRO:HD3	14:M:749:TYR:CE1	2.48	0.49
1:N:468:LEU:HA	1:N:1043:GLU:HG2	1.94	0.49
1:N:669:ARG:NH2	1:N:911:ALA:HA	2.28	0.49
1:N:883:CYS:O	1:N:890:VAL:HG13	2.12	0.49
1:N:1241:VAL:HB	1:N:1243:GLY:H	1.77	0.49
6:E:89:PRO:O	6:E:91:LEU:N	2.43	0.49
7:F:76:PHE:CD1	7:F:105:VAL:HG21	2.48	0.49
7:F:102:ALA:HB3	7:F:127:LEU:HD21	1.94	0.49
12:K:113:ARG:CB	13:L:271:LEU:H	2.26	0.49
14:M:30:LEU:HD11	14:M:660:GLU:OE1	2.12	0.49
14:M:230:LEU:HD13	14:M:287:ILE:HD11	1.94	0.49
14:M:538:LEU:HB2	14:M:582:CYS:HA	1.93	0.49
14:M:762:LEU:HD22	14:M:891:PRO:HD2	1.95	0.49
1:N:51:LEU:HB3	1:N:58:HIS:HE1	1.78	0.49
1:N:673:GLN:CD	1:N:674:ASN:H	2.16	0.49
1:N:1264:ARG:NH1	1:N:1292:ASP:OD1	2.46	0.49
11:J:116:GLN:H	11:J:116:GLN:CD	2.20	0.49
12:K:43:PRO:HB3	12:K:45:LEU:HG	1.94	0.49
12:K:203:GLU:O	12:K:205:TRP:N	2.43	0.49
14:M:455:ILE:N	14:M:494:LYS:O	2.24	0.49
14:M:674:TYR:HB3	14:M:677:HIS:HD2	1.78	0.49
1:N:13:LYS:HA	14:M:1131:TYR:HD2	1.76	0.49
1:N:495:PRO:HB3	1:N:538:LEU:HD13	1.94	0.49
1:N:595:TRP:HD1	1:N:600:ILE:HD11	1.77	0.49
1:N:1078:LYS:HZ2	1:N:1252:TYR:HB3	1.77	0.49
2:A:34:ILE:O	2:A:35:THR:HB	2.13	0.49
3:B:1:MET:N	14:M:713:ALA:O	2.43	0.49
3:B:42:ARG:O	3:B:46:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:115:ILE:O	9:H:315:VAL:HG22	2.13	0.49
9:H:196:ASP:N	9:H:196:ASP:OD1	2.46	0.49
11:J:90:LYS:HE3	11:J:100:SER:HB3	1.95	0.49
14:M:596:TYR:CE1	14:M:643:ILE:HD13	2.47	0.49
14:M:676:HIS:CE1	14:M:964:PHE:H	2.30	0.49
14:M:1055:LEU:HD12	14:M:1067:ARG:HG2	1.94	0.49
1:N:767:CYS:SG	1:N:796:ILE:HB	2.53	0.49
5:D:93:TYR:HD1	5:D:142:TYR:CD1	2.24	0.49
7:F:105:VAL:HG13	7:F:132:GLN:HB2	1.95	0.49
10:I:58:CYS:HA	10:I:90:ARG:HE	1.78	0.49
14:M:139:MET:SD	14:M:167:GLY:HA2	2.53	0.49
14:M:527:CYS:SG	14:M:528:GLY:N	2.84	0.49
14:M:539:VAL:HB	14:M:547:GLY:N	2.27	0.49
1:N:93:PHE:HB2	1:N:98:PHE:CE2	2.47	0.48
1:N:450:VAL:HG22	1:N:451:GLU:H	1.78	0.48
1:N:1301:LEU:HB2	1:N:1310:LYS:HD2	1.95	0.48
2:A:30:TYR:HA	12:K:69:TYR:HD1	1.77	0.48
9:H:104:GLU:HG2	14:M:888:THR:HG21	1.94	0.48
12:K:54:GLN:HB3	12:K:104:SER:HB3	1.94	0.48
1:N:29:ARG:HB2	1:N:85:TYR:CE1	2.45	0.48
1:N:88:LEU:HD21	1:N:284:THR:HG22	1.95	0.48
8:G:44:LEU:HD12	8:G:80:ILE:HD11	1.95	0.48
9:H:263:GLU:C	9:H:273:ALA:HB3	2.39	0.48
14:M:307:GLU:HG3	14:M:308:GLU:H	1.77	0.48
14:M:772:TYR:CD1	14:M:884:LEU:HD22	2.47	0.48
1:N:136:TYR:HB3	1:N:239:LEU:HA	1.95	0.48
1:N:581:VAL:HA	1:N:605:LEU:CB	2.43	0.48
1:N:1238:THR:O	1:N:1240:GLY:N	2.45	0.48
1:N:1297:LYS:HZ3	1:N:1310:LYS:HB3	1.78	0.48
3:B:20:ALA:O	3:B:24:LEU:N	2.46	0.48
6:E:119:GLY:O	6:E:122:GLU:HG2	2.12	0.48
9:H:81:LEU:CD2	9:H:231:ALA:HB3	2.43	0.48
9:H:95:TYR:O	9:H:209:ASP:HB2	2.13	0.48
12:K:56:VAL:HG13	12:K:102:PHE:HD2	1.79	0.48
14:M:208:HIS:HB3	14:M:209:GLU:CD	2.38	0.48
16:X:86:LEU:O	16:X:90:ARG:NH2	2.47	0.48
1:N:119:GLN:H	1:N:120:GLU:HA	1.78	0.48
1:N:219:ASN:ND2	1:N:221:LEU:HD13	2.27	0.48
1:N:902:TYR:CE2	1:N:1028:GLU:HG3	2.48	0.48
6:E:86:GLU:HG2	6:E:95:LYS:HD3	1.95	0.48
14:M:70:ASP:OD1	14:M:73:TRP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:337:VAL:HG23	14:M:581:ARG:HH22	1.77	0.48
14:M:672:ILE:H	14:M:672:ILE:HD12	1.79	0.48
16:X:351:GLU:HG2	16:X:363:ALA:HB1	1.95	0.48
16:X:380:VAL:HG21	16:X:395:LEU:HD12	1.95	0.48
5:D:6:PHE:HB2	5:D:60:ILE:H	1.78	0.48
7:F:94:MET:SD	7:F:99:ILE:HG13	2.53	0.48
8:G:54:SER:O	8:G:57:TYR:HB3	2.13	0.48
14:M:30:LEU:HD11	14:M:660:GLU:CD	2.38	0.48
14:M:355:ASP:OD1	14:M:360:LYS:HD2	2.13	0.48
14:M:818:GLY:N	14:M:866:ILE:O	2.47	0.48
15:Z:186:LYS:HA	15:Z:189:GLN:OE1	2.13	0.48
16:X:434:MET:O	16:X:438:ARG:HG3	2.13	0.48
1:N:34:ILE:HD13	1:N:54:GLY:HA3	1.95	0.48
1:N:512:THR:HB	1:N:514:GLU:OE1	2.13	0.48
1:N:1124:ASP:O	2:A:37:LYS:NZ	2.40	0.48
5:D:15:ILE:HG22	5:D:17:PRO:HD3	1.95	0.48
6:E:61:GLU:HG2	6:E:64:ARG:CZ	2.44	0.48
7:F:73:PHE:CE2	7:F:99:ILE:HD12	2.49	0.48
14:M:81:TYR:CD2	14:M:84:LEU:HD12	2.48	0.48
14:M:504:THR:HG23	14:M:505:ASP:H	1.77	0.48
14:M:1007:VAL:HG12	14:M:1008:TYR:N	2.29	0.48
16:X:376:GLU:OE1	16:X:378:LYS:NZ	2.43	0.48
1:N:261:CYS:HB3	14:M:1033:ARG:NE	2.24	0.48
1:N:400:ASN:HB3	1:N:404:LEU:CD2	2.44	0.48
1:N:1123:PRO:HA	1:N:1130:VAL:HA	1.95	0.48
12:K:136:ARG:NE	14:M:250:GLU:OE1	2.47	0.48
14:M:192:GLU:HG2	14:M:199:VAL:HB	1.95	0.48
14:M:243:MET:HG3	14:M:328:PHE:CD1	2.43	0.48
14:M:786:THR:OG1	14:M:848:GLN:NE2	2.47	0.48
14:M:802:PRO:HD2	14:M:806:HIS:HB2	1.94	0.48
16:X:86:LEU:HB2	16:X:87:ARG:HD2	1.96	0.48
1:N:27:GLU:HB3	14:M:1094:TYR:CD1	2.48	0.48
1:N:799:VAL:HG13	1:N:834:VAL:CG2	2.44	0.48
1:N:970:LYS:HB2	1:N:974:LYS:HZ2	1.78	0.48
3:B:1:MET:O	3:B:56:ILE:HG23	2.13	0.48
9:H:289:ARG:CZ	14:M:983:TYR:HB2	2.43	0.48
14:M:39:LEU:HD23	14:M:39:LEU:H	1.78	0.48
14:M:707:THR:HG22	14:M:708:LEU:HG	1.96	0.48
1:N:410:ASN:ND2	1:N:416:PRO:O	2.47	0.48
1:N:519:ALA:HB2	14:M:1063:LEU:HD13	1.95	0.48
1:N:556:ASP:OD2	5:D:21:LYS:HE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:88:PHE:CE1	5:D:149:ALA:HB2	2.49	0.48
5:D:135:PHE:CG	5:D:136:GLU:N	2.82	0.48
6:E:69:ARG:HH21	6:E:104:ILE:HB	1.78	0.48
7:F:20:LEU:O	7:F:23:ASP:HB3	2.14	0.48
9:H:121:LEU:HD22	9:H:185:PHE:CZ	2.48	0.48
10:I:12:SER:O	10:I:16:VAL:HG23	2.13	0.48
10:I:76:HIS:NE2	10:I:112:GLN:OE1	2.46	0.48
12:K:66:ASN:HB2	12:K:69:TYR:CZ	2.48	0.48
14:M:689:MET:HE3	14:M:904:LYS:HE2	1.96	0.48
14:M:870:MET:O	14:M:881:ILE:HA	2.14	0.48
3:B:8:PHE:HD2	3:B:48:MET:SD	2.36	0.48
4:C:34:ILE:CG2	4:C:42:ARG:HA	2.41	0.48
5:D:94:GLY:H	5:D:141:VAL:CG1	2.27	0.48
9:H:108:HIS:CB	14:M:768:ARG:HH22	2.27	0.48
9:H:211:LEU:HA	9:H:211:LEU:HD23	1.74	0.48
12:K:53:GLN:NE2	12:K:106:GLN:OE1	2.47	0.48
12:K:206:VAL:HA	13:L:368:SER:HB2	1.96	0.48
14:M:93:VAL:HG11	14:M:112:PRO:HD3	1.94	0.48
14:M:223:PHE:HB3	14:M:236:ILE:HG13	1.96	0.48
14:M:251:ILE:O	14:M:255:ILE:HG12	2.13	0.48
14:M:647:GLU:HA	14:M:650:ILE:HG13	1.96	0.48
14:M:1102:SER:HB3	14:M:1104:LEU:HD21	1.96	0.48
1:N:27:GLU:HA	1:N:30:GLN:OE1	2.14	0.47
1:N:368:VAL:H	14:M:1016:VAL:HG23	1.78	0.47
1:N:404:LEU:CD1	1:N:450:VAL:HG11	2.43	0.47
1:N:1283:ASP:OD2	1:N:1285:ARG:HB2	2.14	0.47
1:N:1340:VAL:O	1:N:1340:VAL:HG12	2.13	0.47
3:B:43:TYR:CE1	14:M:950:LYS:HD3	2.49	0.47
4:C:26:ASN:HD21	4:C:37:ARG:H	1.62	0.47
5:D:22:PHE:HE1	5:D:24:ARG:HH21	1.61	0.47
5:D:32:SER:HG	5:D:34:SER:HG	1.52	0.47
12:K:206:VAL:HG13	13:L:373:MET:CE	2.44	0.47
14:M:991:SER:HB3	14:M:998:LEU:HD22	1.95	0.47
15:Z:185:PHE:CE2	15:Z:242:LEU:HB2	2.48	0.47
16:X:316:ALA:HA	16:X:324:GLY:HA2	1.95	0.47
1:N:360:ARG:HH22	14:M:1052:ARG:CD	2.28	0.47
1:N:404:LEU:O	1:N:408:VAL:HG23	2.14	0.47
1:N:682:ARG:O	1:N:686:LEU:CB	2.62	0.47
1:N:961:CYS:SG	1:N:967:GLN:NE2	2.87	0.47
1:N:1189:LEU:HB3	1:N:1193:LYS:HZ2	1.79	0.47
1:N:1258:LEU:HG	1:N:1259:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1297:LYS:N	1:N:1297:LYS:HD2	2.29	0.47
3:B:9:THR:HB	14:M:926:ASP:OD1	2.14	0.47
7:F:35:GLN:HB3	7:F:39:GLU:HB2	1.96	0.47
9:H:122:PHE:HD1	9:H:136:ASP:HA	1.79	0.47
12:K:56:VAL:HG12	12:K:135:LEU:HD22	1.95	0.47
14:M:161:CYS:SG	14:M:699:TYR:HB2	2.54	0.47
14:M:247:SER:O	14:M:250:GLU:N	2.40	0.47
14:M:790:VAL:CG1	14:M:831:SER:HB2	2.44	0.47
1:N:129:LEU:HD13	16:X:38:VAL:HG11	1.96	0.47
1:N:175:ILE:HB	1:N:218:LEU:HB2	1.95	0.47
7:F:12:LYS:O	7:F:16:THR:HG23	2.14	0.47
10:I:113:ILE:O	10:I:117:LEU:HG	2.14	0.47
14:M:721:LYS:HD2	14:M:958:PHE:CE2	2.48	0.47
16:X:491:ILE:HG23	16:X:495:GLU:OE1	2.14	0.47
1:N:180:LYS:N	1:N:180:LYS:HD2	2.30	0.47
5:D:20:LYS:HE2	5:D:20:LYS:HA	1.97	0.47
6:E:66:LEU:HD13	6:E:97:LEU:HD23	1.96	0.47
7:F:107:GLN:O	7:F:133:GLN:NE2	2.47	0.47
9:H:91:LYS:HB3	9:H:213:HIS:HB2	1.95	0.47
14:M:234:ILE:HG23	14:M:290:LYS:HZ1	1.78	0.47
14:M:755:LEU:HD13	14:M:897:PHE:HD2	1.80	0.47
14:M:1052:ARG:HA	14:M:1055:LEU:HB2	1.96	0.47
16:X:329:SER:OG	16:X:330:GLY:N	2.46	0.47
16:X:362:CYS:HA	16:X:365:ILE:HG22	1.96	0.47
1:N:404:LEU:HD11	6:E:90:LEU:HD12	1.96	0.47
1:N:531:THR:HG22	1:N:533:ARG:H	1.79	0.47
1:N:773:LYS:CB	5:D:21:LYS:HD2	2.45	0.47
1:N:1322:GLU:N	1:N:1323:LYS:HA	2.28	0.47
5:D:11:ASP:HB2	5:D:33:GLU:OE2	2.14	0.47
12:K:52:LYS:HE3	12:K:106:GLN:HE22	1.78	0.47
14:M:1028:ARG:CZ	14:M:1035:PRO:HD3	2.44	0.47
1:N:122:LYS:HG2	16:X:70:ARG:H	1.78	0.47
1:N:772:ASP:O	1:N:775:ASN:HB2	2.14	0.47
5:D:146:LYS:HD3	5:D:147:LYS:H	1.80	0.47
14:M:134:GLY:HA3	14:M:411:ILE:HB	1.96	0.47
14:M:204:THR:OG1	14:M:320:HIS:O	2.30	0.47
14:M:496:LEU:HD23	14:M:496:LEU:O	2.14	0.47
14:M:686:GLN:OE1	14:M:900:ARG:HA	2.15	0.47
15:Z:235:ILE:HD13	15:Z:238:ILE:HD12	1.96	0.47
16:X:80:SER:O	16:X:84:ARG:NH1	2.47	0.47
1:N:13:LYS:HA	14:M:1131:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:TYR:HE2	1:N:250:LEU:HD12	1.80	0.47
1:N:360:ARG:HG3	14:M:1037:GLU:HG2	1.97	0.47
1:N:533:ARG:HE	1:N:1039:GLN:CB	2.28	0.47
3:B:3:ILE:H	3:B:3:ILE:HD12	1.79	0.47
4:C:37:ARG:HG2	4:C:38:GLU:CD	2.39	0.47
7:F:3:ASP:HA	7:F:6:GLU:HB2	1.97	0.47
7:F:49:SER:C	7:F:53:PRO:HD2	2.40	0.47
9:H:231:ALA:O	9:H:232:SER:OG	2.29	0.47
9:H:315:VAL:HG12	9:H:316:LEU:HG	1.95	0.47
10:I:51:LYS:HG3	10:I:55:LYS:HZ2	1.80	0.47
14:M:218:VAL:HG13	14:M:226:ARG:HH22	1.79	0.47
14:M:312:LEU:HA	14:M:315:SER:HB3	1.96	0.47
14:M:413:ASN:O	14:M:417:ASN:ND2	2.38	0.47
14:M:797:ALA:H	14:M:802:PRO:CB	2.28	0.47
15:Z:250:MET:HE3	15:Z:251:THR:O	2.15	0.47
1:N:1241:VAL:HB	1:N:1243:GLY:N	2.30	0.47
6:E:55:PRO:HA	6:E:123:LEU:HD11	1.96	0.47
11:J:129:TRP:CD1	11:J:142:MET:HE3	2.50	0.47
12:K:42:ILE:HB	12:K:43:PRO:HD3	1.97	0.47
12:K:42:ILE:HG12	13:L:375:VAL:HG11	1.97	0.47
12:K:50:LYS:O	12:K:54:GLN:HA	2.15	0.47
14:M:231:SER:HA	14:M:292:ARG:HD3	1.97	0.47
14:M:333:ILE:HD11	14:M:537:PHE:CZ	2.50	0.47
14:M:573:SER:OG	14:M:637:GLU:HB2	2.15	0.47
14:M:778:THR:O	14:M:780:LYS:HD2	2.14	0.47
14:M:982:ASN:HB3	14:M:984:LEU:H	1.80	0.47
1:N:176:HIS:CE1	1:N:185:VAL:H	2.32	0.47
1:N:1091:LYS:NZ	1:N:1222:LYS:HE2	2.30	0.47
9:H:41:ASP:HB3	9:H:42:GLN:H	1.55	0.47
10:I:67:ARG:HA	10:I:70:LEU:HD12	1.97	0.47
14:M:48:ASN:O	14:M:52:ASN:HB2	2.14	0.47
14:M:168:TYR:CE2	14:M:175:GLU:HG2	2.50	0.47
14:M:231:SER:OG	14:M:290:LYS:O	2.18	0.47
14:M:364:LEU:O	14:M:367:GLN:N	2.48	0.47
14:M:782:TYR:CZ	14:M:835:VAL:HG22	2.49	0.47
1:N:183:LYS:H	1:N:184:LYS:HZ3	1.63	0.47
1:N:377:ILE:HG23	1:N:489:ASN:ND2	2.30	0.47
5:D:45:ILE:CD1	5:D:48:TYR:HB2	2.43	0.47
10:I:73:LEU:HB3	10:I:78:LEU:HD22	1.96	0.47
12:K:29:GLN:HA	13:L:360:LEU:HG	1.97	0.47
14:M:30:LEU:N	14:M:30:LEU:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:897:PHE:HE1	14:M:1011:LYS:NZ	2.13	0.47
1:N:94:HIS:CB	1:N:97:TYR:HB2	2.45	0.46
1:N:405:ARG:NH1	1:N:442:GLN:O	2.48	0.46
1:N:931:VAL:O	1:N:933:PRO:HD3	2.15	0.46
2:A:23:PHE:CE2	2:A:34:ILE:HB	2.49	0.46
3:B:3:ILE:HD13	9:H:198:LEU:HD13	1.97	0.46
5:D:28:LEU:HD13	5:D:52:LEU:HB3	1.97	0.46
8:G:44:LEU:HD22	9:H:336:PHE:CD1	2.49	0.46
9:H:43:ASP:OD1	9:H:43:ASP:N	2.46	0.46
10:I:22:ASP:O	10:I:25:GLU:HG3	2.15	0.46
11:J:115:GLN:CG	11:J:198:LEU:HB2	2.44	0.46
14:M:917:PRO:HB2	14:M:989:VAL:CG1	2.42	0.46
14:M:942:LYS:HZ1	14:M:1007:VAL:HG11	1.79	0.46
1:N:407:LEU:HG	1:N:452:ARG:HH11	1.80	0.46
1:N:601:PHE:HE1	1:N:683:LEU:HD21	1.79	0.46
2:A:8:CYS:HG	2:A:30:TYR:HH	1.50	0.46
6:E:53:THR:HG21	6:E:108:ARG:NH1	2.29	0.46
7:F:54:ARG:HA	7:F:78:GLU:OE1	2.15	0.46
7:F:61:LEU:HD21	7:F:75:PHE:CE1	2.50	0.46
8:G:57:TYR:CD1	8:G:61:LYS:HD2	2.50	0.46
11:J:48:LEU:HD22	11:J:72:PHE:CD1	2.50	0.46
14:M:308:GLU:HG3	14:M:309:ALA:H	1.80	0.46
14:M:1117:LEU:HD13	14:M:1122:ILE:HG21	1.95	0.46
16:X:312:LEU:HD13	16:X:334:TYR:CD2	2.49	0.46
1:N:514:GLU:HG3	6:E:71:LEU:HD21	1.96	0.46
1:N:591:PRO:HA	9:H:34:SER:OG	2.16	0.46
1:N:1310:LYS:NZ	1:N:1313:GLU:OE2	2.39	0.46
2:A:28:CYS:SG	2:A:28:CYS:O	2.72	0.46
7:F:91:CYS:O	7:F:95:GLN:HG3	2.14	0.46
9:H:230:THR:HG23	9:H:311:GLU:CD	2.40	0.46
9:H:287:ILE:HD12	9:H:290:ASN:HD22	1.80	0.46
12:K:42:ILE:O	12:K:44:HIS:HB2	2.16	0.46
14:M:209:GLU:HB3	14:M:430:LYS:HD2	1.96	0.46
14:M:597:ILE:HG12	14:M:630:VAL:HG12	1.98	0.46
14:M:645:LEU:HD23	14:M:658:GLU:OE2	2.15	0.46
14:M:1033:ARG:HD3	14:M:1112:LEU:HB2	1.97	0.46
1:N:40:ASN:ND2	1:N:44:GLN:OE1	2.48	0.46
1:N:263:ARG:HH22	1:N:281:MET:HE2	1.80	0.46
1:N:311:ASP:HA	1:N:314:GLN:HG2	1.97	0.46
1:N:391:THR:HA	1:N:451:GLU:CD	2.40	0.46
1:N:709:LEU:HD12	1:N:770:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4:PRO:HA	9:H:109:ARG:HH12	1.79	0.46
3:B:56:ILE:HD12	9:H:201:GLN:NE2	2.30	0.46
9:H:16:LEU:HB2	9:H:299:LEU:HB2	1.97	0.46
14:M:1033:ARG:HH22	14:M:1111:LYS:HD2	1.80	0.46
1:N:50:PRO:O	1:N:51:LEU:HG	2.15	0.46
1:N:588:ILE:HG22	1:N:590:LYS:H	1.80	0.46
1:N:592:VAL:HG12	9:H:33:TYR:CE1	2.50	0.46
4:C:17:TYR:O	4:C:25:GLU:HA	2.15	0.46
6:E:53:THR:HG21	6:E:108:ARG:HH11	1.81	0.46
6:E:62:ARG:O	6:E:66:LEU:HG	2.16	0.46
8:G:49:HIS:CE1	8:G:70:TYR:HH	2.25	0.46
9:H:21:VAL:O	14:M:999:GLU:HG3	2.15	0.46
9:H:222:HIS:O	9:H:224:LYS:N	2.49	0.46
10:I:70:LEU:O	10:I:74:LYS:HG2	2.15	0.46
12:K:30:TYR:O	13:L:358:GLN:HA	2.14	0.46
12:K:106:GLN:HG3	12:K:133:LEU:HG	1.97	0.46
13:L:338:GLN:HB3	13:L:348:VAL:HG22	1.97	0.46
14:M:305:LYS:C	14:M:310:ARG:HG2	2.41	0.46
14:M:686:GLN:O	14:M:686:GLN:NE2	2.49	0.46
16:X:272:ARG:O	16:X:273:MET:HE2	2.16	0.46
16:X:526:TYR:O	16:X:530:THR:N	2.41	0.46
1:N:163:ASN:HA	1:N:180:LYS:NZ	2.31	0.46
1:N:371:PRO:HG2	1:N:490:GLU:CD	2.40	0.46
1:N:470:LYS:CG	1:N:533:ARG:HH22	2.26	0.46
1:N:486:PHE:CD2	1:N:505:MET:HB3	2.51	0.46
9:H:54:VAL:HB	9:H:62:GLU:HG2	1.96	0.46
9:H:92:VAL:CG1	9:H:210:LEU:HD13	2.45	0.46
9:H:237:PRO:HA	9:H:301:ARG:HA	1.97	0.46
11:J:92:CYS:HG	11:J:144:THR:HG1	1.63	0.46
14:M:394:LYS:HG3	14:M:396:ARG:NH2	2.30	0.46
14:M:580:ASP:HB3	14:M:582:CYS:SG	2.56	0.46
14:M:950:LYS:HG2	14:M:976:LEU:HD22	1.98	0.46
1:N:71:THR:HG22	1:N:71:THR:O	2.15	0.46
1:N:890:VAL:HG12	1:N:898:ILE:HD12	1.98	0.46
4:C:48:ARG:HB2	14:M:817:PRO:O	2.15	0.46
9:H:135:ILE:HD13	9:H:180:ASN:HD21	1.81	0.46
9:H:330:MET:HB3	9:H:334:ARG:NH1	2.30	0.46
11:J:90:LYS:N	11:J:98:HIS:O	2.47	0.46
14:M:212:SER:O	14:M:214:THR:HG23	2.16	0.46
1:N:107:MET:SD	1:N:107:MET:N	2.88	0.46
1:N:391:THR:HG22	14:M:1025:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:744:ALA:HA	1:N:747:THR:HB	1.97	0.46
5:D:88:PHE:HE1	5:D:149:ALA:HB2	1.81	0.46
5:D:96:VAL:HG12	5:D:97:TYR:H	1.80	0.46
9:H:233:TYR:HE1	9:H:309:SER:O	1.98	0.46
9:H:302:VAL:HG12	9:H:304:ASP:H	1.81	0.46
14:M:563:ARG:HH12	14:M:637:GLU:CD	2.23	0.46
14:M:569:ASN:O	14:M:571:PHE:N	2.49	0.46
14:M:816:SER:O	14:M:818:GLY:N	2.48	0.46
14:M:1001:TYR:O	14:M:1002:ILE:HD13	2.16	0.46
1:N:844:PRO:HB2	14:M:476:TRP:HZ2	1.81	0.46
3:B:4:PRO:HA	9:H:109:ARG:NH2	2.29	0.46
9:H:41:ASP:H	9:H:44:ARG:NH2	2.14	0.46
14:M:372:LEU:HG	14:M:424:TRP:HE3	1.81	0.46
16:X:80:SER:HB2	16:X:84:ARG:HH12	1.81	0.46
1:N:977:SER:O	1:N:980:ILE:HG22	2.16	0.46
5:D:98:ARG:NH2	5:D:113:SER:O	2.49	0.46
7:F:19:GLN:NE2	7:F:141:GLU:OE2	2.49	0.46
14:M:249:GLN:O	14:M:253:GLN:HG2	2.16	0.46
14:M:319:THR:O	14:M:321:VAL:HG22	2.15	0.46
14:M:778:THR:OG1	14:M:780:LYS:NZ	2.32	0.46
14:M:989:VAL:HG21	14:M:1004:PHE:CE2	2.50	0.46
1:N:321:ILE:HG13	1:N:322:ASN:N	2.31	0.45
1:N:558:PHE:CE1	1:N:596:THR:HG22	2.51	0.45
1:N:584:PRO:HA	1:N:585:PRO:HD3	1.79	0.45
1:N:1240:GLY:H	1:N:1241:VAL:HA	1.81	0.45
3:B:43:TYR:HD2	14:M:923:ILE:HG13	1.81	0.45
5:D:8:ASP:O	5:D:57:ARG:NH1	2.47	0.45
5:D:28:LEU:CB	5:D:41:LEU:HB2	2.46	0.45
7:F:104:ILE:CD1	7:F:127:LEU:HD13	2.46	0.45
10:I:23:LEU:O	10:I:27:ARG:HG2	2.16	0.45
14:M:322:PRO:O	14:M:324:LYS:HG2	2.16	0.45
14:M:364:LEU:H	14:M:367:GLN:HB2	1.81	0.45
14:M:933:GLY:O	14:M:937:ARG:HB2	2.15	0.45
14:M:1055:LEU:HD13	14:M:1058:TYR:OH	2.15	0.45
16:X:156:PHE:O	16:X:238:ASN:N	2.48	0.45
1:N:53:TYR:O	1:N:55:VAL:N	2.49	0.45
1:N:578:LYS:HE3	8:G:29:MET:HE1	1.98	0.45
1:N:941:SER:O	1:N:943:ASN:N	2.49	0.45
1:N:1099:ARG:HA	1:N:1102:LYS:HD2	1.98	0.45
9:H:304:ASP:HB2	9:H:305:HIS:HD2	1.81	0.45
9:H:330:MET:HB3	9:H:330:MET:HE3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:1028:ARG:NH1	14:M:1035:PRO:HD3	2.32	0.45
1:N:35:GLN:HA	1:N:86:ILE:HA	1.96	0.45
1:N:558:PHE:HE1	1:N:596:THR:HG22	1.81	0.45
2:A:29:PRO:O	12:K:71:ARG:NH2	2.49	0.45
5:D:50:VAL:HB	5:D:53:GLY:O	2.16	0.45
7:F:90:TYR:HA	7:F:93:ARG:HD2	1.98	0.45
7:F:170:LEU:HB2	7:F:208:LEU:HG	1.98	0.45
9:H:140:PHE:HB2	9:H:212:MET:HB3	1.98	0.45
10:I:69:PHE:HD2	10:I:87:LEU:HD23	1.81	0.45
13:L:343:LYS:O	13:L:345:THR:HG22	2.16	0.45
14:M:540:PHE:HE1	14:M:546:LEU:HG	1.81	0.45
14:M:605:ALA:O	14:M:629:LEU:HD22	2.16	0.45
14:M:835:VAL:HG12	14:M:835:VAL:O	2.16	0.45
16:X:496:ARG:O	16:X:500:GLU:HG2	2.16	0.45
1:N:970:LYS:O	1:N:974:LYS:HG3	2.16	0.45
5:D:96:VAL:HG21	5:D:140:ARG:N	2.28	0.45
5:D:98:ARG:NH2	5:D:113:SER:H	2.15	0.45
7:F:88:LYS:HA	7:F:91:CYS:SG	2.57	0.45
11:J:99:VAL:HG21	11:J:150:PHE:CZ	2.52	0.45
13:L:275:LEU:O	13:L:277:GLY:N	2.48	0.45
14:M:97:VAL:HG13	14:M:101:GLU:HB3	1.99	0.45
14:M:563:ARG:HB2	14:M:568:ILE:O	2.16	0.45
14:M:676:HIS:HE1	14:M:964:PHE:HA	1.82	0.45
16:X:52:LYS:O	16:X:56:VAL:HG23	2.15	0.45
1:N:72:CYS:SG	14:M:1087:GLY:HA2	2.57	0.45
1:N:1264:ARG:NH2	1:N:1292:ASP:HA	2.31	0.45
5:D:61:ALA:O	5:D:143:LEU:HA	2.17	0.45
6:E:67:GLY:O	6:E:70:ALA:HB3	2.17	0.45
7:F:85:LYS:O	7:F:89:VAL:HG23	2.17	0.45
9:H:309:SER:O	9:H:309:SER:OG	2.31	0.45
12:K:113:ARG:O	12:K:114:TYR:CD1	2.69	0.45
14:M:946:LEU:HD23	14:M:1004:PHE:O	2.16	0.45
16:X:4:ALA:HB2	16:X:441:LYS:HE3	1.98	0.45
1:N:134:LEU:HD23	1:N:1337:LYS:HE3	1.98	0.45
1:N:841:GLY:HA3	14:M:676:HIS:HB3	1.98	0.45
1:N:908:ASP:OD2	1:N:1027:MET:HG3	2.16	0.45
1:N:1233:ARG:O	1:N:1236:MET:HG3	2.16	0.45
9:H:252:GLU:HA	9:H:255:ARG:NH2	2.32	0.45
9:H:335:ARG:HG3	9:H:335:ARG:O	2.17	0.45
12:K:120:ARG:NH2	12:K:123:GLU:OE1	2.50	0.45
14:M:49:TYR:HD2	14:M:504:THR:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:305:LYS:HG2	14:M:310:ARG:HG2	1.98	0.45
16:X:443:ILE:HD11	16:X:516:VAL:C	2.41	0.45
1:N:23:LYS:HB3	14:M:1118:GLN:NE2	2.32	0.45
1:N:23:LYS:HD3	1:N:256:LEU:HB2	1.99	0.45
1:N:60:MET:HE3	1:N:86:ILE:HD11	1.97	0.45
1:N:106:GLN:NE2	1:N:110:LYS:O	2.50	0.45
1:N:393:PRO:O	1:N:449:ILE:HG23	2.16	0.45
1:N:646:MET:HE1	5:D:97:TYR:HB3	1.99	0.45
1:N:753:LEU:HD21	1:N:808:ARG:CG	2.46	0.45
7:F:194:ILE:HG21	7:F:202:ARG:HG2	1.98	0.45
8:G:60:MET:O	8:G:60:MET:HE3	2.16	0.45
9:H:263:GLU:HG3	9:H:276:ALA:CB	2.40	0.45
14:M:498:LEU:HD12	14:M:663:THR:HA	1.98	0.45
14:M:556:VAL:HG21	14:M:576:THR:HG22	1.99	0.45
14:M:672:ILE:HG13	14:M:686:GLN:HG2	1.97	0.45
14:M:791:MET:HE2	14:M:814:ILE:HG12	1.98	0.45
14:M:896:LYS:HD2	14:M:1014:HIS:O	2.16	0.45
16:X:106:ILE:HD11	16:X:125:VAL:HG21	1.99	0.45
16:X:290:SER:HA	16:X:293:ILE:HD12	1.99	0.45
1:N:219:ASN:OD1	1:N:220:PRO:HD2	2.16	0.45
1:N:464:ARG:HB2	1:N:472:SER:OG	2.17	0.45
1:N:468:LEU:HD22	1:N:1047:GLN:NE2	2.32	0.45
1:N:513:GLU:HG3	1:N:516:LYS:HD2	1.99	0.45
1:N:1055:PHE:HA	1:N:1057:GLY:H	1.81	0.45
11:J:87:GLY:HA3	11:J:150:PHE:HB2	1.98	0.45
13:L:272:PRO:HG2	13:L:387:PRO:HD3	1.99	0.45
13:L:327:GLY:HA2	13:L:341:LEU:HD22	1.98	0.45
14:M:760:ALA:HB3	14:M:913:GLN:HB2	1.99	0.45
16:X:289:SER:O	16:X:293:ILE:HG13	2.16	0.45
1:N:27:GLU:HB3	14:M:1094:TYR:HD1	1.81	0.45
1:N:949:THR:HA	1:N:952:ILE:HG22	1.99	0.45
1:N:1130:VAL:H	1:N:1177:PRO:HD2	1.81	0.45
4:C:17:TYR:CD2	4:C:27:GLU:HA	2.52	0.45
8:G:111:LEU:HD13	9:H:327:LYS:HD3	1.98	0.45
11:J:197:LEU:HB2	11:J:201:TRP:CE3	2.51	0.45
14:M:155:PHE:HB3	14:M:160:GLU:O	2.17	0.45
14:M:318:LEU:HA	14:M:320:HIS:ND1	2.32	0.45
14:M:598:ILE:HD11	14:M:631:GLU:HB2	1.99	0.45
14:M:815:CYS:HB3	14:M:869:VAL:HG11	1.98	0.45
14:M:834:THR:HG22	14:M:835:VAL:HG23	1.97	0.45
15:Z:178:GLU:CB	16:X:368:LEU:HD23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:80:SER:O	16:X:84:ARG:HG2	2.17	0.45
1:N:369:ILE:HD11	1:N:488:PHE:CE1	2.39	0.45
1:N:412:PRO:HA	1:N:419:ASN:ND2	2.31	0.45
1:N:533:ARG:HE	1:N:1039:GLN:HB2	1.81	0.45
1:N:551:LEU:HD23	1:N:551:LEU:HA	1.86	0.45
1:N:886:TYR:OH	6:E:61:GLU:OE2	2.11	0.45
1:N:1055:PHE:N	1:N:1056:ALA:HB3	2.32	0.45
3:B:47:ARG:NH2	14:M:1006:PRO:HG3	2.31	0.45
4:C:22:CYS:O	4:C:24:THR:N	2.49	0.45
7:F:105:VAL:HG22	7:F:132:GLN:HB2	1.99	0.45
7:F:167:GLU:OE1	7:F:167:GLU:N	2.49	0.45
8:G:29:MET:SD	8:G:41:THR:OG1	2.74	0.45
9:H:232:SER:C	9:H:233:TYR:CG	2.95	0.45
14:M:281:MET:HB2	14:M:282:GLN:NE2	2.32	0.45
14:M:677:HIS:HB3	14:M:940:VAL:HB	1.98	0.45
16:X:312:LEU:HB3	16:X:334:TYR:CE1	2.52	0.45
1:N:372:ASP:OD2	1:N:487:ARG:NH1	2.49	0.44
1:N:421:ILE:HA	1:N:451:GLU:HG2	1.99	0.44
1:N:688:PRO:O	14:M:747:SER:HA	2.16	0.44
1:N:742:CYS:N	1:N:743:THR:O	2.49	0.44
1:N:1023:MET:SD	1:N:1026:GLN:NE2	2.90	0.44
3:B:14:VAL:HG13	3:B:49:LEU:HD11	1.98	0.44
7:F:37:LEU:O	7:F:41:LYS:HG3	2.17	0.44
7:F:178:PRO:HA	7:F:181:ARG:HG3	1.98	0.44
10:I:14:TYR:CD2	10:I:66:VAL:HG23	2.52	0.44
10:I:108:LEU:HD13	10:I:113:ILE:HD13	1.98	0.44
14:M:254:MET:SD	14:M:329:ARG:NH2	2.77	0.44
14:M:412:THR:O	14:M:416:VAL:HG23	2.16	0.44
1:N:83:TYR:HE1	1:N:259:PRO:HD3	1.82	0.44
1:N:872:GLN:O	1:N:876:VAL:HG23	2.17	0.44
3:B:7:CYS:O	3:B:9:THR:N	2.50	0.44
9:H:38:ASP:O	9:H:40:TRP:N	2.51	0.44
10:I:57:PRO:O	10:I:90:ARG:HD2	2.17	0.44
10:I:90:ARG:HD3	10:I:124:LEU:HD22	1.99	0.44
10:I:114:GLU:HA	10:I:117:LEU:HD12	1.99	0.44
14:M:241:LYS:NZ	14:M:246:GLU:O	2.50	0.44
14:M:521:GLU:HB3	14:M:548:VAL:HB	1.99	0.44
16:X:88:TYR:CD1	16:X:111:LEU:HD13	2.52	0.44
1:N:69:CYS:H	1:N:74:LYS:NZ	2.15	0.44
1:N:91:PRO:HB2	1:N:313:LEU:HD13	1.98	0.44
1:N:185:VAL:HG21	1:N:216:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:483:HIS:CG	14:M:893:ILE:HD13	2.52	0.44
1:N:836:ASN:HD22	1:N:846:GLU:CD	2.23	0.44
5:D:113:SER:HB3	5:D:126:GLN:HG2	2.00	0.44
5:D:140:ARG:HD3	5:D:143:LEU:HD11	1.99	0.44
7:F:22:HIS:C	7:F:25:GLY:H	2.26	0.44
9:H:65:MET:O	9:H:305:HIS:HA	2.18	0.44
9:H:222:HIS:ND1	9:H:224:LYS:HG2	2.33	0.44
9:H:258:SER:HB3	9:H:259:PRO:HD2	2.00	0.44
10:I:7:ASN:HA	11:J:3:VAL:HG13	1.98	0.44
14:M:110:SER:HB3	14:M:135:ARG:HG2	1.98	0.44
14:M:224:TYR:HA	14:M:234:ILE:O	2.17	0.44
14:M:498:LEU:HG	14:M:666:GLY:HA2	1.99	0.44
1:N:106:GLN:HG3	1:N:110:LYS:HZ3	1.83	0.44
1:N:363:PHE:O	1:N:509:LEU:N	2.50	0.44
1:N:528:ASN:HB3	1:N:539:ILE:HD11	1.98	0.44
1:N:590:LYS:HG2	5:D:89:GLU:CD	2.42	0.44
1:N:792:ILE:O	1:N:792:ILE:HG22	2.17	0.44
1:N:1179:GLU:HG2	1:N:1179:GLU:O	2.17	0.44
1:N:1290:LEU:O	1:N:1294:MET:HG2	2.18	0.44
1:N:1332:ALA:HB1	14:M:1121:ASN:O	2.17	0.44
5:D:4:ILE:HG12	5:D:61:ALA:HB2	2.00	0.44
9:H:186:PRO:HB3	9:H:190:ILE:HD13	1.98	0.44
10:I:61:GLN:HE22	10:I:125:PRO:HD3	1.83	0.44
10:I:66:VAL:HA	10:I:87:LEU:HD21	2.00	0.44
12:K:74:GLY:O	12:K:78:ALA:N	2.50	0.44
13:L:332:ARG:HG3	13:L:338:GLN:NE2	2.31	0.44
14:M:344:LEU:HB3	14:M:350:LYS:HG3	1.99	0.44
14:M:1066:GLU:O	14:M:1070:ILE:HG12	2.18	0.44
16:X:35:PRO:HA	16:X:74:GLU:HA	1.98	0.44
1:N:398:LYS:HE2	1:N:401:ILE:HD11	1.99	0.44
1:N:515:ALA:HB1	1:N:518:GLU:OE1	2.17	0.44
1:N:811:ASP:HB2	1:N:813:PHE:O	2.18	0.44
1:N:942:LYS:O	1:N:946:ILE:HG13	2.16	0.44
1:N:1297:LYS:HA	7:F:172:ARG:HB2	1.99	0.44
13:L:268:PHE:HZ	13:L:362:SER:HB2	1.82	0.44
14:M:228:ASN:HD21	14:M:320:HIS:CE1	2.35	0.44
14:M:676:HIS:HE1	14:M:964:PHE:CA	2.30	0.44
14:M:682:ARG:HD2	14:M:682:ARG:N	2.32	0.44
16:X:449:ARG:O	16:X:453:GLU:HG2	2.16	0.44
1:N:72:CYS:HB2	1:N:79:CYS:HA	1.99	0.44
1:N:560:ASP:HB3	9:H:32:ASN:ND2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1075:ASN:HA	1:N:1304:THR:HG23	1.99	0.44
2:A:14:VAL:HG22	2:A:15:GLU:H	1.83	0.44
6:E:124:ILE:HG22	6:E:125:ILE:N	2.33	0.44
8:G:69:GLY:O	8:G:71:THR:HG23	2.17	0.44
9:H:235:LEU:O	9:H:307:ILE:HG22	2.18	0.44
9:H:253:LEU:HD21	9:H:293:LEU:HD13	2.00	0.44
11:J:89:ILE:HB	11:J:146:GLU:H	1.83	0.44
14:M:58:ILE:HG21	14:M:374:GLU:HA	1.98	0.44
14:M:768:ARG:HG2	14:M:890:ARG:HE	1.83	0.44
14:M:816:SER:N	14:M:817:PRO:HD3	2.32	0.44
14:M:1051:GLU:O	14:M:1055:LEU:HD23	2.17	0.44
16:X:66:GLN:O	16:X:68:HIS:ND1	2.48	0.44
16:X:290:SER:OG	16:X:309:ASP:OD1	2.20	0.44
1:N:392:PHE:O	1:N:451:GLU:HB3	2.18	0.44
1:N:925:LEU:O	1:N:929:LYS:HG3	2.18	0.44
3:B:4:PRO:CA	9:H:109:ARG:HH12	2.31	0.44
5:D:55:LYS:HB2	5:D:148:LEU:CD2	2.48	0.44
5:D:140:ARG:HD2	5:D:143:LEU:HD11	1.99	0.44
9:H:91:LYS:HE3	9:H:91:LYS:HB2	1.66	0.44
14:M:309:ALA:HB3	14:M:310:ARG:HD3	1.99	0.44
14:M:478:MET:O	14:M:479:LEU:HD23	2.18	0.44
14:M:529:GLU:O	14:M:531:LEU:N	2.48	0.44
14:M:897:PHE:CE1	14:M:1011:LYS:HG2	2.53	0.44
16:X:255:VAL:HG22	16:X:322:PHE:CD2	2.53	0.44
1:N:265:SER:HB2	1:N:276:GLU:OE2	2.18	0.44
1:N:944:GLU:OE1	1:N:944:GLU:N	2.48	0.44
2:A:21:HIS:ND1	2:A:33:ASN:HB3	2.32	0.44
3:B:53:VAL:O	3:B:53:VAL:HG23	2.18	0.44
7:F:171:PRO:HB2	7:F:207:ARG:HG2	2.00	0.44
9:H:11:ARG:HD2	9:H:33:TYR:CE2	2.53	0.44
10:I:89:HIS:HB2	11:J:84:ILE:HG23	1.98	0.44
11:J:51:ILE:HG22	11:J:72:PHE:CE1	2.53	0.44
13:L:270:GLN:HB2	13:L:384:VAL:HA	2.00	0.44
14:M:187:ASN:ND2	14:M:322:PRO:HB3	2.32	0.44
14:M:282:GLN:C	14:M:284:LEU:H	2.26	0.44
14:M:1028:ARG:N	14:M:1073:ASP:OD2	2.39	0.44
14:M:1086:LEU:HD12	14:M:1111:LYS:HD3	2.00	0.44
1:N:555:LYS:HE2	5:D:120:GLY:O	2.17	0.44
1:N:699:GLY:N	1:N:702:ASP:OD2	2.48	0.44
1:N:1035:ALA:HB1	1:N:1039:GLN:HE22	1.81	0.44
2:A:28:CYS:HB2	2:A:30:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:172:ARG:HA	7:F:208:LEU:N	2.33	0.44
8:G:37:ARG:CB	8:G:91:PRO:HA	2.48	0.44
10:I:5:ASP:H	11:J:6:GLU:HB3	1.82	0.44
11:J:5:VAL:HB	11:J:74:CYS:HB3	2.00	0.44
14:M:392:ILE:H	14:M:392:ILE:HD12	1.83	0.44
14:M:625:LEU:HD23	14:M:630:VAL:O	2.17	0.44
16:X:81:ARG:NH1	16:X:84:ARG:HB2	2.33	0.44
1:N:369:ILE:HG13	1:N:486:PHE:O	2.17	0.43
1:N:521:VAL:O	1:N:521:VAL:HG12	2.17	0.43
2:A:35:THR:OG1	2:A:36:ARG:NH1	2.50	0.43
2:A:36:ARG:NE	2:A:36:ARG:HA	2.33	0.43
5:D:98:ARG:HH22	5:D:113:SER:H	1.64	0.43
14:M:163:LEU:HD12	14:M:163:LEU:O	2.18	0.43
14:M:302:LYS:HG2	14:M:303:LYS:H	1.82	0.43
14:M:832:MET:HE3	14:M:834:THR:OG1	2.18	0.43
1:N:106:GLN:NE2	1:N:110:LYS:HB2	2.33	0.43
1:N:421:ILE:HD13	1:N:450:VAL:HG23	2.00	0.43
1:N:700:ILE:HB	14:M:984:LEU:HD22	1.99	0.43
1:N:974:LYS:HE3	1:N:1022:TYR:CE2	2.53	0.43
1:N:974:LYS:O	1:N:977:SER:OG	2.26	0.43
7:F:7:THR:O	7:F:11:TRP:HD1	2.00	0.43
9:H:147:THR:OG1	9:H:148:ARG:N	2.51	0.43
13:L:272:PRO:CG	13:L:387:PRO:HD3	2.48	0.43
1:N:69:CYS:H	1:N:74:LYS:HZ3	1.65	0.43
1:N:377:ILE:HG21	1:N:680:MET:CE	2.48	0.43
5:D:4:ILE:H	5:D:5:LEU:HD23	1.82	0.43
5:D:135:PHE:HB2	5:D:140:ARG:HH21	1.82	0.43
10:I:58:CYS:C	10:I:90:ARG:HE	2.26	0.43
14:M:99:PRO:HG3	14:M:160:GLU:OE1	2.19	0.43
14:M:317:ILE:C	14:M:319:THR:N	2.77	0.43
14:M:504:THR:HG23	14:M:505:ASP:N	2.34	0.43
14:M:595:PRO:HG3	14:M:632:TYR:CE1	2.44	0.43
14:M:673:PRO:HG3	14:M:945:GLU:CD	2.42	0.43
14:M:893:ILE:H	14:M:893:ILE:HD12	1.83	0.43
14:M:1016:VAL:HG22	14:M:1016:VAL:O	2.19	0.43
16:X:160:CYS:HB2	16:X:234:TYR:CD2	2.54	0.43
16:X:255:VAL:HG21	16:X:267:VAL:HG21	1.99	0.43
16:X:373:LYS:HE2	16:X:379:GLN:HB2	1.99	0.43
1:N:598:LYS:HE2	5:D:120:GLY:CA	2.48	0.43
5:D:87:GLN:HB2	5:D:88:PHE:CD1	2.53	0.43
8:G:56:ARG:HG2	8:G:68:CYS:CB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:97:ASN:HB3	9:H:102:GLN:CD	2.44	0.43
9:H:139:GLN:HG2	9:H:211:LEU:HD22	2.01	0.43
12:K:17:LEU:O	12:K:19:LYS:HD3	2.17	0.43
12:K:207:HIS:HB2	13:L:372:GLU:HG2	2.00	0.43
13:L:270:GLN:HE22	14:M:521:GLU:HG3	1.83	0.43
1:N:691:LEU:HD23	1:N:691:LEU:HA	1.81	0.43
1:N:771:LEU:HD22	1:N:775:ASN:ND2	2.32	0.43
1:N:907:LEU:O	1:N:1285:ARG:NE	2.45	0.43
1:N:970:LYS:O	1:N:973:ILE:HG22	2.18	0.43
7:F:71:GLN:NE2	7:F:98:ASN:O	2.52	0.43
9:H:45:PHE:O	9:H:49:PHE:HB2	2.19	0.43
9:H:119:PRO:HD2	9:H:316:LEU:HD11	2.00	0.43
10:I:72:ALA:HB3	10:I:116:LEU:HD12	1.99	0.43
12:K:50:LYS:HG3	12:K:201:ALA:HA	1.99	0.43
14:M:299:GLY:C	14:M:301:PRO:HD3	2.43	0.43
14:M:498:LEU:HB3	14:M:499:MET:H	1.44	0.43
14:M:949:GLY:O	14:M:953:VAL:HG22	2.17	0.43
16:X:385:MET:O	16:X:385:MET:HG2	2.19	0.43
1:N:106:GLN:HG3	1:N:110:LYS:NZ	2.34	0.43
1:N:377:ILE:HG21	1:N:680:MET:HE1	1.99	0.43
1:N:463:ASN:OD1	1:N:464:ARG:N	2.51	0.43
1:N:670:ASP:HA	1:N:671:TRP:HA	1.63	0.43
1:N:1054:HIS:O	1:N:1055:PHE:HD1	2.02	0.43
1:N:1166:ALA:CB	1:N:1178:ARG:HH22	2.32	0.43
1:N:1305:ARG:HB3	1:N:1322:GLU:OE2	2.18	0.43
5:D:47:ILE:O	5:D:49:PRO:HD3	2.18	0.43
7:F:93:ARG:HA	7:F:96:GLU:CD	2.43	0.43
9:H:146:CYS:SG	9:H:202:LEU:HB3	2.59	0.43
12:K:20:SER:OG	12:K:214:ARG:NH1	2.52	0.43
12:K:25:LEU:HB3	12:K:129:LEU:HD22	2.00	0.43
12:K:74:GLY:HA3	12:K:79:LEU:HD12	2.01	0.43
13:L:346:LEU:HB3	13:L:348:VAL:HG23	2.01	0.43
14:M:21:PRO:HG2	14:M:24:GLU:H	1.82	0.43
14:M:105:ARG:HD3	14:M:874:ASN:HA	2.01	0.43
14:M:279:THR:OG1	14:M:280:GLN:N	2.48	0.43
16:X:63:VAL:HG22	16:X:77:ALA:HB2	1.99	0.43
16:X:436:LEU:HB2	16:X:523:LEU:HB3	2.01	0.43
1:N:64:GLU:HB3	1:N:67:ARG:HH12	1.83	0.43
1:N:513:GLU:HA	1:N:516:LYS:HB3	2.01	0.43
5:D:92:MET:SD	5:D:119:GLY:N	2.91	0.43
11:J:129:TRP:HE1	11:J:146:GLU:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:697:ILE:H	14:M:701:GLN:HE21	1.66	0.43
14:M:728:ILE:O	14:M:729:GLU:HB2	2.19	0.43
14:M:816:SER:HB2	14:M:866:ILE:HD12	2.01	0.43
14:M:1085:LEU:HD23	14:M:1085:LEU:HA	1.90	0.43
1:N:94:HIS:HA	1:N:252:LEU:HD13	2.00	0.43
1:N:709:LEU:HD23	1:N:709:LEU:HA	1.90	0.43
6:E:61:GLU:HG2	6:E:64:ARG:HH22	1.84	0.43
7:F:30:GLN:OE1	7:F:33:LEU:HB3	2.18	0.43
11:J:197:LEU:HB2	11:J:201:TRP:CZ3	2.54	0.43
12:K:15:VAL:HG22	12:K:124:LEU:HD13	2.00	0.43
14:M:108:THR:HA	14:M:170:ILE:HG22	2.01	0.43
14:M:698:GLY:HA2	14:M:733:LEU:HD22	2.00	0.43
14:M:1033:ARG:HH12	14:M:1111:LYS:HB3	1.83	0.43
1:N:26:GLU:HG2	1:N:27:GLU:N	2.31	0.43
1:N:139:LYS:HE3	1:N:239:LEU:N	2.33	0.43
1:N:317:CYS:O	1:N:321:ILE:HG12	2.18	0.43
1:N:698:ILE:HG23	1:N:698:ILE:O	2.19	0.43
1:N:1078:LYS:NZ	1:N:1252:TYR:HB3	2.33	0.43
1:N:1176:THR:O	1:N:1176:THR:HG23	2.19	0.43
7:F:45:GLY:C	7:F:47:LYS:H	2.26	0.43
7:F:74:VAL:HG13	7:F:103:LEU:HD22	2.00	0.43
7:F:121:MET:C	7:F:123:PRO:HD2	2.43	0.43
8:G:106:VAL:O	8:G:110:VAL:HG23	2.18	0.43
9:H:14:VAL:HB	9:H:301:ARG:O	2.19	0.43
12:K:71:ARG:NE	12:K:71:ARG:HA	2.34	0.43
14:M:108:THR:CG2	14:M:172:LYS:H	2.31	0.43
14:M:595:PRO:HB2	14:M:659:ILE:CD1	2.49	0.43
14:M:718:PRO:HD3	14:M:734:PRO:HB3	2.01	0.43
14:M:859:LYS:NZ	14:M:885:LEU:HD22	2.33	0.43
16:X:361:ARG:HD2	16:X:364:ARG:HH11	1.84	0.43
1:N:22:MET:HG2	14:M:1124:PRO:HB3	2.01	0.43
1:N:102:ILE:HA	1:N:166:VAL:CG1	2.48	0.43
1:N:897:ILE:HG13	7:F:165:LEU:HD22	2.00	0.43
5:D:6:PHE:O	5:D:7:GLU:HG3	2.19	0.43
5:D:113:SER:CB	5:D:126:GLN:HG2	2.49	0.43
9:H:142:LEU:HD23	9:H:144:VAL:HG23	2.01	0.43
10:I:100:MET:SD	11:J:201:TRP:HZ2	2.42	0.43
11:J:41:ASN:HA	11:J:42:VAL:HA	1.59	0.43
11:J:150:PHE:CD1	11:J:190:ILE:HD11	2.54	0.43
13:L:368:SER:HA	13:L:371:GLY:O	2.19	0.43
1:N:423:GLN:HG2	1:N:424:ARG:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:701:GLY:H	14:M:984:LEU:HD22	1.84	0.42
2:A:7:GLY:HA3	2:A:30:TYR:CD2	2.54	0.42
4:C:22:CYS:HB2	4:C:41:TYR:HD1	1.82	0.42
5:D:28:LEU:O	5:D:40:ILE:HA	2.19	0.42
6:E:80:MET:HB3	6:E:81:VAL:H	1.71	0.42
7:F:149:VAL:O	7:F:192:LYS:N	2.36	0.42
8:G:57:TYR:CE1	8:G:61:LYS:HD2	2.54	0.42
8:G:92:ALA:C	8:G:95:PRO:HD2	2.44	0.42
14:M:39:LEU:HD12	14:M:667:VAL:HG11	2.01	0.42
14:M:70:ASP:C	14:M:72:MET:H	2.28	0.42
14:M:100:HIS:HD2	14:M:159:ASN:HB3	1.84	0.42
14:M:254:MET:HG2	14:M:336:ALA:HB1	2.01	0.42
14:M:391:VAL:HG22	14:M:394:LYS:HB2	2.01	0.42
14:M:757:LEU:HD12	14:M:897:PHE:CE2	2.54	0.42
14:M:783:THR:OG1	14:M:784:ASN:N	2.52	0.42
16:X:15:GLU:OE1	16:X:450:ARG:NH2	2.52	0.42
16:X:361:ARG:HD2	16:X:364:ARG:NH1	2.34	0.42
17:Y:1:UNK:HA	17:Y:2:UNK:HA	1.64	0.42
1:N:32:ALA:CB	1:N:85:TYR:HB2	2.49	0.42
1:N:595:TRP:CD1	1:N:600:ILE:HD11	2.54	0.42
1:N:596:THR:OG1	1:N:599:GLN:OE1	2.37	0.42
1:N:1088:GLN:NE2	1:N:1245:ARG:HD2	2.34	0.42
3:B:6:ARG:CD	9:H:112:LEU:HD22	2.49	0.42
5:D:98:ARG:NH1	5:D:112:LEU:HD12	2.35	0.42
7:F:55:ARG:N	7:F:78:GLU:OE2	2.51	0.42
7:F:72:MET:HE1	7:F:101:ARG:HE	1.83	0.42
9:H:170:THR:O	9:H:195:ASP:HA	2.19	0.42
9:H:196:ASP:O	9:H:197:ILE:HG13	2.19	0.42
11:J:42:VAL:HG13	11:J:157:PHE:CZ	2.53	0.42
14:M:224:TYR:CB	14:M:233:ASP:HB3	2.49	0.42
14:M:861:ALA:O	14:M:862:THR:OG1	2.34	0.42
1:N:53:TYR:C	1:N:55:VAL:H	2.27	0.42
1:N:391:THR:CG2	14:M:1025:ARG:HD2	2.50	0.42
1:N:421:ILE:HG13	1:N:431:PHE:HE2	1.83	0.42
1:N:486:PHE:CE1	1:N:507:LEU:HB3	2.54	0.42
1:N:698:ILE:HA	1:N:702:ASP:OD2	2.19	0.42
1:N:1288:MET:HE2	1:N:1288:MET:HB3	1.97	0.42
4:C:26:ASN:HD21	4:C:37:ARG:N	2.18	0.42
5:D:135:PHE:CZ	5:D:137:VAL:HG13	2.55	0.42
5:D:139:SER:CB	5:D:142:TYR:HD2	2.32	0.42
9:H:130:GLU:C	9:H:132:GLY:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:173:MET:HE3	9:H:212:MET:SD	2.59	0.42
14:M:199:VAL:HG22	14:M:216:MET:SD	2.59	0.42
14:M:760:ALA:CB	14:M:913:GLN:HB2	2.49	0.42
14:M:793:PRO:O	14:M:794:MET:HB2	2.19	0.42
14:M:947:LEU:HD23	14:M:947:LEU:HA	1.81	0.42
16:X:81:ARG:NH1	16:X:81:ARG:O	2.52	0.42
1:N:71:THR:HG21	14:M:1094:TYR:CD2	2.55	0.42
1:N:390:LEU:CD1	1:N:419:ASN:HB2	2.49	0.42
1:N:801:GLN:HB2	1:N:833:PHE:CD1	2.46	0.42
1:N:957:GLU:HB3	1:N:1019:ARG:HE	1.84	0.42
5:D:55:LYS:C	5:D:56:PHE:HD1	2.28	0.42
5:D:88:PHE:CD1	5:D:88:PHE:N	2.87	0.42
6:E:102:ILE:HB	6:E:120:VAL:HG11	2.00	0.42
9:H:62:GLU:HA	9:H:309:SER:HA	2.01	0.42
14:M:285:LYS:HA	14:M:308:GLU:HB3	2.01	0.42
14:M:991:SER:HB3	14:M:998:LEU:CD2	2.49	0.42
1:N:42:TYR:CE1	1:N:56:LEU:HD13	2.55	0.42
1:N:459:VAL:HB	1:N:520:LEU:HD12	2.01	0.42
1:N:748:LEU:HD12	1:N:748:LEU:HA	1.72	0.42
1:N:800:GLY:HA2	1:N:801:GLN:HA	1.70	0.42
1:N:908:ASP:HB3	1:N:909:PRO:HD2	2.00	0.42
1:N:1362:LEU:HD23	6:E:107:ARG:HD2	2.00	0.42
6:E:86:GLU:OE1	6:E:95:LYS:HB3	2.19	0.42
8:G:43:VAL:HG13	8:G:81:ASN:OD1	2.19	0.42
10:I:115:ALA:O	10:I:119:THR:HG23	2.20	0.42
11:J:191:SER:OG	11:J:198:LEU:HD21	2.19	0.42
13:L:336:ARG:CZ	13:L:348:VAL:HG11	2.49	0.42
14:M:58:ILE:HG13	14:M:374:GLU:HG2	2.01	0.42
14:M:508:ASP:O	14:M:512:VAL:HG23	2.20	0.42
14:M:758:ASN:CB	14:M:916:MET:HE3	2.41	0.42
16:X:10:SER:O	16:X:22:GLU:HG3	2.20	0.42
16:X:451:GLN:O	16:X:455:LYS:HB2	2.19	0.42
17:Y:-14:UNK:HA	17:Y:-13:UNK:HA	1.58	0.42
1:N:59:ARG:HB2	1:N:60:MET:C	2.45	0.42
1:N:171:LEU:HB3	1:N:314:GLN:NE2	2.35	0.42
1:N:429:LYS:HD3	1:N:437:ARG:NH1	2.34	0.42
1:N:562:ALA:HB1	8:G:56:ARG:HH22	1.84	0.42
1:N:746:GLU:N	1:N:746:GLU:OE1	2.52	0.42
2:A:23:PHE:O	2:A:31:VAL:HG22	2.19	0.42
5:D:15:ILE:HG22	5:D:16:ASP:N	2.34	0.42
9:H:64:ASP:OD1	9:H:305:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:128:GLY:H	9:H:131:GLU:C	2.26	0.42
9:H:176:ILE:HD12	9:H:211:LEU:HD21	2.02	0.42
9:H:283:PHE:HB3	14:M:988:TYR:CD2	2.54	0.42
11:J:44:LEU:O	11:J:44:LEU:HG	2.19	0.42
12:K:12:GLU:HB3	13:L:330:LEU:HD22	2.00	0.42
13:L:367:ASP:O	13:L:370:THR:N	2.41	0.42
14:M:56:LYS:HD3	14:M:81:TYR:CE1	2.55	0.42
14:M:858:TYR:O	14:M:859:LYS:HG3	2.19	0.42
14:M:903:GLN:OE1	14:M:934:PHE:HE1	2.00	0.42
16:X:86:LEU:O	16:X:89:PRO:HD2	2.20	0.42
1:N:263:ARG:HH12	1:N:281:MET:CE	2.33	0.42
1:N:543:GLN:O	1:N:545:PHE:N	2.52	0.42
1:N:887:ASP:O	1:N:889:THR:HG23	2.19	0.42
1:N:1230:ASP:OD1	1:N:1230:ASP:N	2.53	0.42
9:H:175:TRP:CZ3	9:H:177:PRO:HA	2.54	0.42
11:J:12:ARG:O	11:J:14:PRO:HD3	2.20	0.42
13:L:266:LEU:HD12	13:L:377:GLY:HA2	2.01	0.42
14:M:591:ARG:HD2	14:M:634:ASP:OD2	2.19	0.42
14:M:867:GLU:OE1	14:M:886:ARG:HD3	2.19	0.42
14:M:899:SER:HB3	14:M:903:GLN:HB3	2.00	0.42
14:M:911:VAL:HB	14:M:916:MET:HE2	2.02	0.42
16:X:84:ARG:NH2	16:X:524:GLU:OE1	2.52	0.42
1:N:1294:MET:HE1	1:N:1303:ILE:HB	2.01	0.42
3:B:38:LEU:HD23	3:B:38:LEU:HA	1.93	0.42
4:C:16:ILE:H	4:C:27:GLU:HG3	1.84	0.42
4:C:42:ARG:HH12	14:M:875:ALA:HA	1.85	0.42
8:G:86:THR:HG23	8:G:88:GLY:H	1.85	0.42
9:H:141:ARG:HB2	9:H:176:ILE:HG13	2.01	0.42
12:K:28:PHE:HZ	13:L:365:LEU:HD21	1.85	0.42
13:L:272:PRO:HD3	13:L:385:CYS:CB	2.50	0.42
13:L:349:THR:OG1	13:L:385:CYS:SG	2.57	0.42
14:M:100:HIS:O	14:M:101:GLU:HB2	2.18	0.42
14:M:237:VAL:HG21	14:M:269:LEU:HA	2.00	0.42
14:M:537:PHE:CD1	14:M:548:VAL:HA	2.55	0.42
14:M:716:GLN:OE1	14:M:738:ASN:HB3	2.20	0.42
14:M:900:ARG:HA	14:M:900:ARG:HD3	1.87	0.42
15:Z:231:SER:H	15:Z:234:ASP:HB2	1.85	0.42
16:X:262:THR:HA	16:X:301:TYR:CE2	2.55	0.42
16:X:312:LEU:HB3	16:X:334:TYR:CD1	2.54	0.42
1:N:966:LEU:HB2	1:N:1026:GLN:HE21	1.85	0.42
1:N:1186:TYR:HA	14:M:274:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:25:GLU:HG2	4:C:47:LYS:HE3	2.00	0.42
5:D:88:PHE:CD2	5:D:146:LYS:CG	3.03	0.42
8:G:113:LYS:HE2	9:H:49:PHE:O	2.20	0.42
10:I:3:VAL:HG11	11:J:40:TYR:CE2	2.55	0.42
14:M:426:LEU:HD23	14:M:426:LEU:HA	1.85	0.42
14:M:602:GLN:O	14:M:652:LYS:NZ	2.26	0.42
1:N:106:GLN:NE2	1:N:148:ASP:OD1	2.53	0.42
1:N:490:GLU:HG3	1:N:493:CYS:SG	2.59	0.42
3:B:64:PRO:HB2	4:C:23:HIS:NE2	2.35	0.42
5:D:12:VAL:HG23	5:D:51:ASP:OD2	2.20	0.42
5:D:30:CYS:SG	5:D:39:LEU:HB2	2.60	0.42
5:D:92:MET:HG2	5:D:93:TYR:N	2.34	0.42
9:H:233:TYR:OH	9:H:310:VAL:HG22	2.20	0.42
12:K:111:THR:HG21	12:K:131:GLY:HA2	2.01	0.42
13:L:337:VAL:CG1	13:L:350:MET:HE3	2.49	0.42
14:M:445:TYR:HB3	14:M:730:PHE:CD2	2.55	0.42
14:M:498:LEU:HA	14:M:498:LEU:HD23	1.63	0.42
14:M:680:SER:O	14:M:684:THR:HG23	2.19	0.42
15:Z:178:GLU:H	16:X:383:PHE:HE1	1.66	0.42
16:X:92:ILE:HG22	16:X:96:LYS:NZ	2.35	0.42
16:X:98:LEU:HD12	16:X:99:TYR:CG	2.55	0.42
1:N:29:ARG:CD	1:N:85:TYR:CZ	3.03	0.41
1:N:390:LEU:HD13	1:N:419:ASN:HB2	2.02	0.41
1:N:404:LEU:HD12	1:N:450:VAL:HG11	2.02	0.41
1:N:655:LEU:HD23	1:N:655:LEU:O	2.20	0.41
1:N:790:ILE:HD11	1:N:1051:LYS:HZ1	1.85	0.41
1:N:902:TYR:HE2	1:N:1028:GLU:HG3	1.84	0.41
5:D:116:VAL:HG13	5:D:140:ARG:O	2.20	0.41
7:F:176:GLY:O	7:F:181:ARG:NE	2.52	0.41
9:H:169:TYR:CD1	9:H:196:ASP:HA	2.55	0.41
11:J:7:MET:HE3	11:J:7:MET:HB2	1.84	0.41
11:J:94:PRO:HD3	11:J:125:GLN:HE22	1.85	0.41
12:K:27:LEU:HD22	13:L:360:LEU:HD23	2.02	0.41
12:K:99:LYS:HB3	12:K:101:THR:HG23	2.02	0.41
12:K:211:TYR:OH	13:L:372:GLU:OE1	2.22	0.41
14:M:93:VAL:HG22	14:M:110:SER:O	2.20	0.41
14:M:245:VAL:O	14:M:247:SER:N	2.54	0.41
14:M:373:PHE:HB3	14:M:377:PHE:CE2	2.54	0.41
14:M:758:ASN:OD1	14:M:926:ASP:HA	2.20	0.41
14:M:952:GLY:O	14:M:957:ARG:N	2.53	0.41
16:X:265:GLU:OE1	16:X:268:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:499:LEU:O	16:X:502:LEU:HG	2.20	0.41
1:N:110:LYS:CD	1:N:223:VAL:HG22	2.50	0.41
1:N:185:VAL:HG11	1:N:216:GLU:CD	2.44	0.41
1:N:492:VAL:O	1:N:495:PRO:HD2	2.20	0.41
1:N:554:LEU:HA	1:N:554:LEU:HD23	1.61	0.41
1:N:562:ALA:HB2	9:H:29:PHE:CD2	2.54	0.41
1:N:666:ILE:O	1:N:667:LEU:HD23	2.19	0.41
1:N:766:ALA:CA	1:N:769:ARG:HH21	2.34	0.41
1:N:1225:LEU:HD23	1:N:1225:LEU:HA	1.93	0.41
3:B:47:ARG:HD2	3:B:47:ARG:H	1.85	0.41
4:C:42:ARG:NH1	14:M:875:ALA:HA	2.34	0.41
5:D:57:ARG:O	5:D:146:LYS:HG2	2.20	0.41
6:E:53:THR:HG22	6:E:54:THR:O	2.20	0.41
6:E:54:THR:C	6:E:56:TYR:H	2.23	0.41
7:F:64:HIS:H	7:F:72:MET:HB2	1.85	0.41
7:F:84:ILE:HD11	7:F:113:SER:HB2	2.02	0.41
9:H:185:PHE:O	9:H:187:GLU:N	2.44	0.41
12:K:121:GLN:NE2	13:L:263:GLU:HA	2.35	0.41
14:M:652:LYS:HA	14:M:652:LYS:HD3	1.82	0.41
16:X:254:ALA:HB2	16:X:345:LEU:HD21	2.01	0.41
1:N:72:CYS:HB3	1:N:78:ASP:O	2.20	0.41
1:N:391:THR:HG21	14:M:1025:ARG:HD2	2.03	0.41
1:N:537:PRO:HB3	1:N:664:PHE:CD2	2.55	0.41
1:N:638:VAL:HA	1:N:648:GLY:HA3	2.02	0.41
1:N:1322:GLU:HA	1:N:1323:LYS:HG3	2.02	0.41
4:C:34:ILE:CG2	4:C:44:MET:HE2	2.50	0.41
9:H:110:LEU:HA	9:H:113:ILE:CD1	2.50	0.41
9:H:181:GLN:O	9:H:183:ASP:N	2.53	0.41
10:I:9:ALA:CB	11:J:4:LEU:H	2.33	0.41
14:M:475:GLN:HG2	14:M:475:GLN:O	2.19	0.41
14:M:599:VAL:HA	14:M:604:PRO:HA	2.01	0.41
14:M:664:LEU:HD23	14:M:664:LEU:H	1.85	0.41
14:M:938:MET:HE3	14:M:938:MET:HB2	1.78	0.41
14:M:962:THR:H	14:M:966:GLY:HA2	1.85	0.41
14:M:1021:HIS:HB3	14:M:1044:GLY:H	1.84	0.41
16:X:447:ILE:O	16:X:451:GLN:HG2	2.19	0.41
1:N:1238:THR:O	1:N:1238:THR:OG1	2.38	0.41
3:B:42:ARG:HB3	14:M:923:ILE:HD11	2.02	0.41
4:C:44:MET:HB2	14:M:871:ILE:HD12	2.01	0.41
8:G:104:MET:HG2	9:H:333:CYS:SG	2.60	0.41
9:H:105:ILE:O	9:H:109:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:121:LEU:HD22	9:H:185:PHE:CE1	2.55	0.41
9:H:149:ASN:N	9:H:162:LEU:O	2.48	0.41
9:H:223:ALA:C	9:H:225:PHE:H	2.28	0.41
14:M:189:ILE:HG21	14:M:341:ARG:HH21	1.84	0.41
14:M:312:LEU:HA	14:M:312:LEU:HD23	1.90	0.41
14:M:407:ARG:HG2	14:M:407:ARG:O	2.21	0.41
14:M:720:VAL:HG21	14:M:945:GLU:O	2.21	0.41
14:M:799:THR:OG1	14:M:800:ARG:N	2.52	0.41
16:X:374:HIS:HB3	16:X:375:ILE:H	1.53	0.41
1:N:59:ARG:HD3	1:N:68:PRO:C	2.46	0.41
1:N:71:THR:CG2	14:M:1094:TYR:H	2.34	0.41
1:N:128:TYR:HB3	1:N:136:TYR:HE1	1.85	0.41
1:N:389:ILE:HG13	14:M:1022:ALA:CB	2.51	0.41
1:N:868:THR:HG21	1:N:1046:THR:HA	2.01	0.41
5:D:135:PHE:HZ	5:D:137:VAL:HG13	1.86	0.41
6:E:93:ALA:HA	6:E:96:GLU:OE2	2.21	0.41
12:K:50:LYS:HD3	12:K:54:GLN:O	2.20	0.41
13:L:270:GLN:O	13:L:385:CYS:N	2.54	0.41
14:M:1036:THR:HA	14:M:1041:ARG:HG3	2.03	0.41
14:M:1062:MET:HB3	14:M:1065:LEU:HB3	2.02	0.41
14:M:1111:LYS:HE2	14:M:1111:LYS:HB2	1.87	0.41
15:Z:253:ILE:HD12	15:Z:253:ILE:H	1.85	0.41
16:X:117:THR:HB	16:X:232:GLY:C	2.45	0.41
16:X:269:THR:HG23	16:X:272:ARG:NH1	2.35	0.41
4:C:43:ILE:HG22	4:C:43:ILE:O	2.20	0.41
5:D:39:LEU:HD21	5:D:125:LEU:HD12	2.02	0.41
6:E:64:ARG:HB2	14:M:1062:MET:CE	2.47	0.41
6:E:71:LEU:O	6:E:75:MET:HG2	2.21	0.41
7:F:95:GLN:HA	7:F:125:TYR:OH	2.21	0.41
9:H:104:GLU:CD	14:M:886:ARG:HH22	2.28	0.41
9:H:327:LYS:HD2	9:H:327:LYS:HA	1.73	0.41
10:I:52:TYR:O	10:I:56:THR:HG23	2.21	0.41
12:K:11:GLN:CD	13:L:262:LYS:HD2	2.45	0.41
14:M:749:TYR:CD2	14:M:909:LEU:HG	2.55	0.41
16:X:48:ASP:OD1	16:X:48:ASP:N	2.52	0.41
16:X:99:TYR:OH	16:X:154:THR:HG21	2.20	0.41
16:X:106:ILE:HD13	16:X:125:VAL:HG11	2.01	0.41
1:N:271:LYS:HD3	14:M:838:ILE:HD11	2.02	0.41
1:N:361:VAL:HG11	14:M:1023:ARG:CZ	2.51	0.41
1:N:641:GLN:OE1	5:D:95:LYS:HB3	2.20	0.41
1:N:842:LEU:CD1	1:N:847:PHE:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:8:PHE:CD2	3:B:48:MET:SD	3.13	0.41
3:B:32:GLY:CA	14:M:956:GLY:HA3	2.51	0.41
5:D:15:ILE:HA	5:D:52:LEU:HD21	2.03	0.41
6:E:58:THR:HG23	6:E:61:GLU:H	1.85	0.41
7:F:115:LYS:O	7:F:129:GLN:NE2	2.54	0.41
10:I:73:LEU:HD22	10:I:78:LEU:HD22	2.02	0.41
14:M:33:PHE:HB2	14:M:499:MET:CE	2.51	0.41
14:M:365:ALA:O	14:M:369:LEU:HD23	2.20	0.41
14:M:545:ILE:C	14:M:546:LEU:HD12	2.46	0.41
14:M:899:SER:O	14:M:900:ARG:HB2	2.21	0.41
1:N:110:LYS:HD3	1:N:223:VAL:HG22	2.02	0.41
1:N:818:LEU:HD22	1:N:819:PRO:HD2	2.02	0.41
1:N:954:LYS:HE2	1:N:954:LYS:HB2	1.85	0.41
1:N:1230:ASP:HA	1:N:1231:ASN:HA	1.63	0.41
3:B:24:LEU:HG	3:B:29:TYR:HE2	1.86	0.41
4:C:49:THR:HG1	4:C:51:ARG:HH21	1.68	0.41
7:F:23:ASP:OD2	7:F:183:PHE:HA	2.19	0.41
12:K:213:LEU:HB3	12:K:214:ARG:HH21	1.85	0.41
14:M:870:MET:CB	14:M:882:LYS:HB2	2.51	0.41
1:N:266:VAL:HG13	1:N:266:VAL:O	2.20	0.41
1:N:277:ASP:HA	1:N:278:ASP:HA	1.71	0.41
1:N:390:LEU:HB3	1:N:391:THR:H	1.64	0.41
1:N:464:ARG:HD2	1:N:464:ARG:HA	1.88	0.41
1:N:616:ASN:CB	1:N:636:SER:HA	2.51	0.41
1:N:671:TRP:HB2	1:N:675:GLU:OE1	2.21	0.41
1:N:754:LYS:HA	1:N:757:SER:HB3	2.02	0.41
1:N:891:ARG:CZ	6:E:110:LEU:HD21	2.51	0.41
1:N:1044:PRO:HA	1:N:1047:GLN:OE1	2.20	0.41
5:D:48:TYR:HB3	5:D:53:GLY:CA	2.51	0.41
5:D:55:LYS:HB2	5:D:148:LEU:HD23	2.03	0.41
6:E:54:THR:OG1	6:E:55:PRO:HD2	2.20	0.41
6:E:107:ARG:HG2	6:E:109:TYR:CE1	2.55	0.41
7:F:2:ASP:N	7:F:6:GLU:OE1	2.54	0.41
8:G:22:GLU:CG	9:H:336:PHE:HA	2.50	0.41
8:G:59:ILE:C	8:G:61:LYS:H	2.29	0.41
9:H:293:LEU:O	9:H:296:VAL:N	2.54	0.41
12:K:17:LEU:HD22	13:L:326:VAL:N	2.36	0.41
12:K:119:TYR:HD2	12:K:124:LEU:HA	1.85	0.41
13:L:344:VAL:O	13:L:345:THR:C	2.64	0.41
13:L:348:VAL:C	13:L:349:THR:HG23	2.46	0.41
14:M:83:GLY:O	14:M:90:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:225:LEU:HD13	14:M:227:HIS:NE2	2.35	0.41
14:M:694:MET:HE2	14:M:1012:LEU:O	2.21	0.41
14:M:730:PHE:N	14:M:730:PHE:CD1	2.88	0.41
14:M:751:ILE:HG21	14:M:751:ILE:HD13	1.81	0.41
14:M:831:SER:HB3	14:M:851:TYR:CB	2.51	0.41
14:M:881:ILE:HA	14:M:881:ILE:HD13	1.95	0.41
17:Y:-1:UNK:HA	17:Y:0:UNK:HA	1.49	0.41
1:N:18:ILE:HD13	14:M:1127:LYS:H	1.86	0.41
1:N:118:SER:N	1:N:120:GLU:OE2	2.47	0.41
1:N:382:VAL:HG23	1:N:383:PRO:O	2.21	0.41
1:N:1098:ALA:O	1:N:1102:LYS:HG3	2.21	0.41
5:D:84:ARG:C	5:D:86:ASP:H	2.29	0.41
7:F:122:ALA:N	7:F:123:PRO:HD2	2.36	0.41
9:H:220:LYS:HB3	9:H:220:LYS:HE3	1.86	0.41
12:K:109:SER:HB3	14:M:525:LEU:HD21	2.03	0.41
14:M:135:ARG:O	14:M:137:PRO:HD3	2.21	0.41
14:M:370:SER:HA	14:M:373:PHE:CD2	2.56	0.41
14:M:538:LEU:O	14:M:583:VAL:HB	2.21	0.41
14:M:708:LEU:O	14:M:710:TYR:N	2.54	0.41
14:M:1061:SER:OG	14:M:1062:MET:N	2.53	0.41
15:Z:183:GLN:HA	15:Z:186:LYS:NZ	2.36	0.41
16:X:88:TYR:CZ	16:X:111:LEU:HB3	2.56	0.41
16:X:330:GLY:HA3	16:X:331:GLY:HA2	1.81	0.41
16:X:354:VAL:CG1	16:X:362:CYS:HB3	2.51	0.41
1:N:42:TYR:CD1	1:N:56:LEU:HD13	2.56	0.40
1:N:403:PHE:O	1:N:452:ARG:NH1	2.54	0.40
1:N:1004:ASP:O	1:N:1006:ILE:N	2.53	0.40
1:N:1082:THR:O	1:N:1082:THR:HG23	2.21	0.40
1:N:1302:GLY:O	1:N:1308:LEU:HD21	2.21	0.40
7:F:40:PHE:O	7:F:43:GLN:HB2	2.21	0.40
8:G:42:PHE:CE2	8:G:96:PHE:HB2	2.57	0.40
9:H:61:LEU:HD23	9:H:62:GLU:N	2.35	0.40
9:H:133:THR:HG22	9:H:133:THR:O	2.21	0.40
9:H:231:ALA:HA	9:H:233:TYR:CZ	2.56	0.40
9:H:277:ASN:O	9:H:279:ARG:N	2.47	0.40
9:H:285:ARG:HD3	14:M:988:TYR:CZ	2.55	0.40
11:J:128:VAL:HG13	11:J:141:TYR:HA	2.03	0.40
14:M:56:LYS:O	14:M:59:MET:HB3	2.21	0.40
14:M:238:ILE:HD13	14:M:286:TYR:CE2	2.56	0.40
14:M:329:ARG:O	14:M:333:ILE:HG22	2.21	0.40
14:M:340:ARG:HE	14:M:531:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:1052:ARG:HG2	14:M:1052:ARG:HH11	1.86	0.40
1:N:26:GLU:H	1:N:26:GLU:CD	2.30	0.40
1:N:73:GLY:HA2	1:N:74:LYS:HA	1.53	0.40
1:N:365:GLY:O	1:N:507:LEU:HG	2.21	0.40
1:N:826:LYS:O	1:N:827:LEU:HG	2.21	0.40
3:B:32:GLY:HA3	14:M:956:GLY:HA3	2.04	0.40
5:D:2:ALA:HB1	5:D:4:ILE:CG1	2.51	0.40
9:H:209:ASP:O	9:H:210:LEU:HD23	2.20	0.40
14:M:315:SER:HA	14:M:318:LEU:CB	2.52	0.40
14:M:318:LEU:O	14:M:318:LEU:HD23	2.22	0.40
14:M:346:GLN:O	14:M:348:ASP:N	2.47	0.40
14:M:567:TYR:HB3	14:M:568:ILE:H	1.72	0.40
16:X:87:ARG:HD2	16:X:87:ARG:N	2.36	0.40
16:X:289:SER:HA	16:X:332:GLY:O	2.21	0.40
1:N:18:ILE:HB	1:N:1349:MET:CE	2.52	0.40
1:N:220:PRO:HA	1:N:223:VAL:HG23	2.03	0.40
1:N:958:PHE:C	1:N:960:CYS:H	2.29	0.40
1:N:1211:VAL:HG12	1:N:1212:ILE:N	2.36	0.40
9:H:49:PHE:HA	9:H:66:VAL:O	2.21	0.40
9:H:116:HIS:O	9:H:116:HIS:CG	2.74	0.40
14:M:388:ALA:O	14:M:391:VAL:HG12	2.21	0.40
14:M:596:TYR:N	14:M:631:GLU:O	2.54	0.40
14:M:610:HIS:HA	14:M:613:GLU:OE1	2.21	0.40
14:M:679:GLN:HB2	14:M:682:ARG:CD	2.46	0.40
14:M:757:LEU:HD23	14:M:758:ASN:O	2.21	0.40
14:M:901:HIS:HD2	14:M:942:LYS:CB	2.31	0.40
15:Z:185:PHE:HE1	15:Z:239:LEU:HA	1.86	0.40
1:N:851:THR:HG22	14:M:680:SER:OG	2.22	0.40
1:N:1262:ALA:O	1:N:1266:THR:HG23	2.22	0.40
1:N:1312:LYS:HB2	1:N:1312:LYS:HE3	1.82	0.40
2:A:7:GLY:HA3	2:A:30:TYR:CE2	2.57	0.40
6:E:60:TYR:O	6:E:64:ARG:HG2	2.21	0.40
6:E:62:ARG:O	6:E:65:VAL:HG12	2.21	0.40
7:F:84:ILE:HG12	7:F:114:ALA:HB2	2.04	0.40
8:G:100:LEU:HD23	8:G:100:LEU:HA	1.86	0.40
9:H:52:ASP:O	9:H:63:PHE:HB2	2.22	0.40
10:I:9:ALA:HB3	11:J:3:VAL:HA	2.02	0.40
10:I:88:ASN:ND2	11:J:1:MET:HE3	2.31	0.40
11:J:117:PRO:HG2	11:J:130:GLU:O	2.22	0.40
13:L:260:LEU:HB3	13:L:261:THR:H	1.54	0.40
13:L:366:GLY:H	13:L:373:MET:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:42:GLN:NE2	14:M:496:LEU:HD22	2.36	0.40
14:M:75:LEU:HD22	14:M:119:TYR:CD1	2.57	0.40
14:M:396:ARG:HD3	14:M:396:ARG:N	2.36	0.40
14:M:498:LEU:C	14:M:500:THR:N	2.78	0.40
14:M:897:PHE:HE2	14:M:927:ILE:HD12	1.87	0.40
16:X:237:ALA:HB1	16:X:242:PHE:CE2	2.55	0.40
16:X:492:THR:HG23	16:X:495:GLU:H	1.85	0.40
1:N:21:GLY:HA3	14:M:1114:PHE:CD1	2.57	0.40
1:N:58:HIS:H	1:N:67:ARG:HE	1.70	0.40
1:N:124:GLN:H	1:N:124:GLN:HG3	1.70	0.40
1:N:183:LYS:H	1:N:184:LYS:NZ	2.18	0.40
1:N:287:ILE:HA	1:N:290:ASN:HB2	2.04	0.40
1:N:494:THR:OG1	1:N:495:PRO:HD3	2.21	0.40
1:N:1086:THR:HG23	1:N:1247:THR:HB	2.02	0.40
1:N:1256:LYS:HD2	1:N:1256:LYS:HA	1.74	0.40
1:N:1260:ILE:HD13	7:F:173:ILE:HG12	2.04	0.40
1:N:1316:LEU:HD21	1:N:1344:SER:HB3	2.04	0.40
2:A:28:CYS:O	2:A:30:TYR:N	2.55	0.40
4:C:21:GLU:CD	4:C:43:ILE:HD13	2.45	0.40
7:F:21:CYS:SG	7:F:26:TYR:HB3	2.62	0.40
9:H:16:LEU:HD22	9:H:285:ARG:NH1	2.37	0.40
9:H:312:SER:OG	9:H:313:THR:N	2.55	0.40
10:I:60:HIS:C	10:I:61:GLN:HG3	2.46	0.40
12:K:49:ILE:HG23	12:K:54:GLN:CG	2.42	0.40
14:M:80:ILE:HG13	14:M:114:THR:O	2.22	0.40
14:M:213:ARG:HD3	14:M:321:VAL:HG13	2.03	0.40
14:M:241:LYS:NZ	14:M:248:ASP:OD1	2.52	0.40
14:M:702:ARG:HD2	14:M:702:ARG:HA	1.79	0.40
14:M:724:THR:O	14:M:728:ILE:HG13	2.21	0.40
14:M:987:ASP:C	14:M:988:TYR:CD1	3.00	0.40
14:M:1055:LEU:HA	14:M:1058:TYR:CZ	2.57	0.40
16:X:386:ILE:HB	16:X:387:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	N	1220/1390 (88%)	948 (78%)	258 (21%)	14 (1%)	11	44
2	A	35/108 (32%)	23 (66%)	11 (31%)	1 (3%)	3	26
3	B	62/67 (92%)	54 (87%)	8 (13%)	0	100	100
4	C	44/58 (76%)	32 (73%)	11 (25%)	1 (2%)	5	31
5	D	115/150 (77%)	77 (67%)	38 (33%)	0	100	100
6	E	79/127 (62%)	56 (71%)	22 (28%)	1 (1%)	9	41
7	F	207/210 (99%)	182 (88%)	24 (12%)	1 (0%)	24	60
8	G	98/133 (74%)	71 (72%)	27 (28%)	0	100	100
9	H	327/346 (94%)	246 (75%)	80 (24%)	1 (0%)	36	70
10	I	123/148 (83%)	113 (92%)	10 (8%)	0	100	100
11	J	175/204 (86%)	138 (79%)	37 (21%)	0	100	100
12	K	131/708 (18%)	92 (70%)	38 (29%)	1 (1%)	16	52
13	L	78/398 (20%)	60 (77%)	17 (22%)	1 (1%)	9	41
14	M	1112/1133 (98%)	831 (75%)	276 (25%)	5 (0%)	30	65
15	Z	57/316 (18%)	50 (88%)	7 (12%)	0	100	100
16	X	434/534 (81%)	405 (93%)	29 (7%)	0	100	100
All	All	4297/6030 (71%)	3378 (79%)	893 (21%)	26 (1%)	23	57

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	607	PRO
1	N	612	PRO
1	N	777	PRO
1	N	1162	PRO
1	N	1205	PRO
2	A	34	ILE
7	F	29	THR
14	M	498	LEU
14	M	499	MET
14	M	545	ILE
1	N	484	ARG
1	N	544	ASP

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Mol	Chain	Res	Type
1	N	776	SER
1	N	1130	VAL
1	N	1160	VAL
13	L	344	VAL
1	N	1204	ILE
1	N	1280	MET
14	M	793	PRO
14	M	919	CYS
1	N	50	PRO
4	C	33	PRO
1	N	613	VAL
9	H	101	VAL
6	E	89	PRO
12	K	204	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	N	983/1212 (81%)	983 (100%)	0	100	100
2	A	33/94 (35%)	33 (100%)	0	100	100
3	B	53/56 (95%)	53 (100%)	0	100	100
4	C	43/55 (78%)	43 (100%)	0	100	100
5	D	103/131 (79%)	103 (100%)	0	100	100
6	E	70/111 (63%)	70 (100%)	0	100	100
7	F	191/192 (100%)	191 (100%)	0	100	100
8	G	89/119 (75%)	89 (100%)	0	100	100
9	H	289/302 (96%)	289 (100%)	0	100	100
10	I	117/136 (86%)	117 (100%)	0	100	100
11	J	160/181 (88%)	160 (100%)	0	100	100
12	K	122/622 (20%)	122 (100%)	0	100	100
13	L	72/347 (21%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	973/988 (98%)	973 (100%)	0	100	100
15	Z	60/280 (21%)	60 (100%)	0	100	100
16	X	386/476 (81%)	386 (100%)	0	100	100
All	All	3744/5302 (71%)	3744 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	31	GLN
1	N	40	ASN
1	N	46	ASN
1	N	58	HIS
1	N	106	GLN
1	N	217	ASN
1	N	225	ASN
1	N	419	ASN
1	N	528	ASN
1	N	801	GLN
1	N	836	ASN
1	N	872	GLN
1	N	1026	GLN
1	N	1039	GLN
1	N	1075	ASN
1	N	1088	GLN
1	N	1213	HIS
1	N	1272	GLN
1	N	1277	ASN
7	F	43	GLN
7	F	108	GLN
9	H	32	ASN
9	H	42	GLN
9	H	97	ASN
9	H	149	ASN
9	H	180	ASN
9	H	290	ASN
9	H	305	HIS
10	I	7	ASN
10	I	39	GLN
10	I	60	HIS

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Mol	Chain	Res	Type
11	J	78	HIS
12	K	29	GLN
12	K	110	ASN
12	K	121	GLN
14	M	62	ASN
14	M	79	ASN
14	M	92	ASN
14	M	227	HIS
14	M	253	GLN
14	M	282	GLN
14	M	359	ASN
14	M	408	GLN
14	M	651	ASN
14	M	676	HIS
14	M	686	GLN
14	M	701	GLN
14	M	848	GLN
14	M	913	GLN
14	M	1034	GLN
14	M	1093	HIS
14	M	1115	GLN
14	M	1121	ASN
15	Z	183	GLN
16	X	14	GLN
16	X	244	GLN
16	X	445	ASN
16	X	483	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

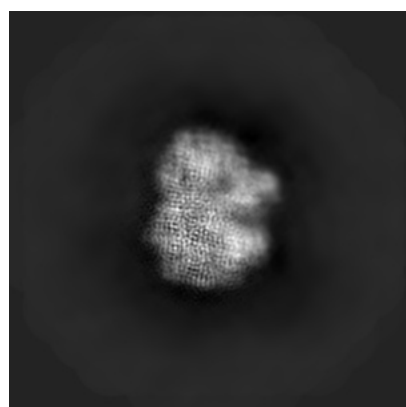
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11904. These allow visual inspection of the internal detail of the map and identification of artifacts.

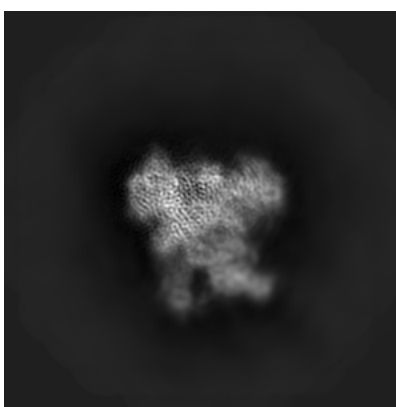
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

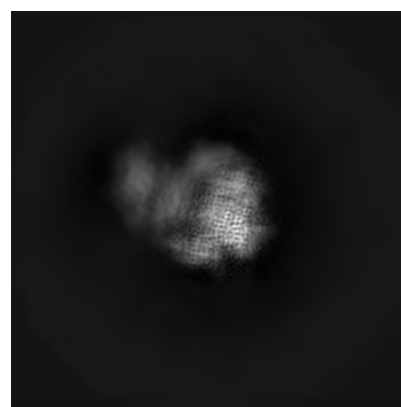
6.1.1 Primary map



X



Y

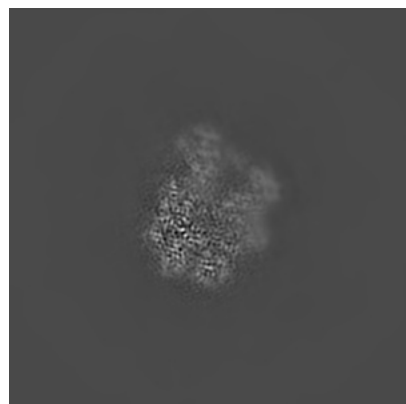


Z

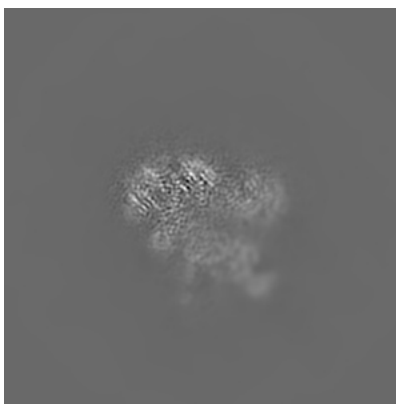
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

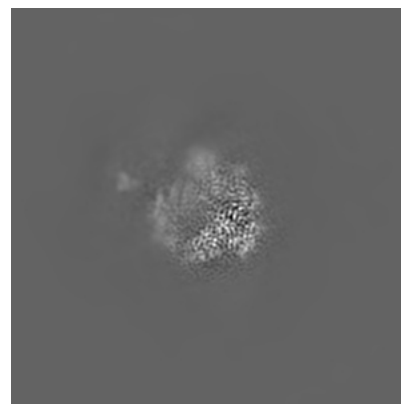
6.2.1 Primary map



X Index: 180



Y Index: 180

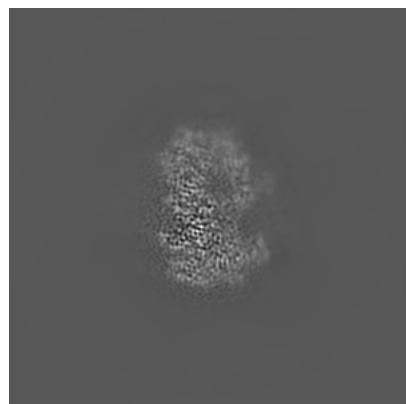


Z Index: 180

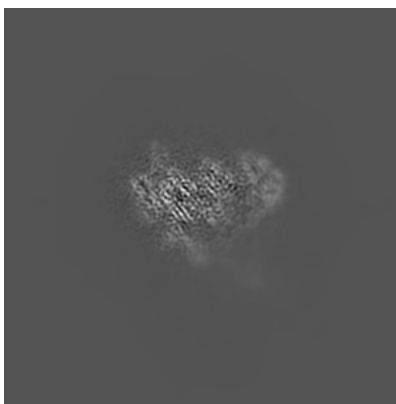
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

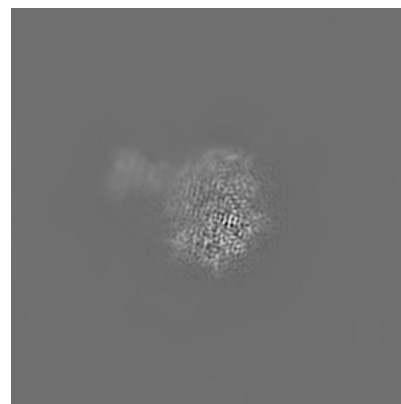
6.3.1 Primary map



X Index: 202



Y Index: 157

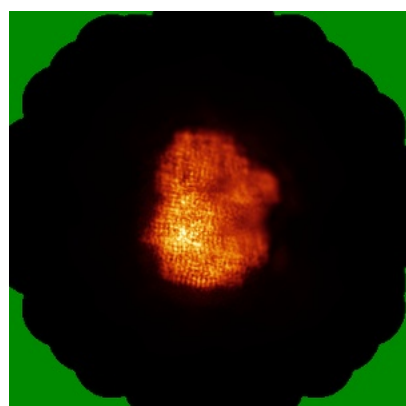


Z Index: 150

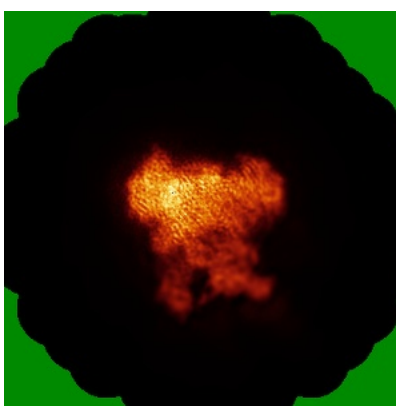
The images above show the largest variance slices of the map in three orthogonal directions.

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

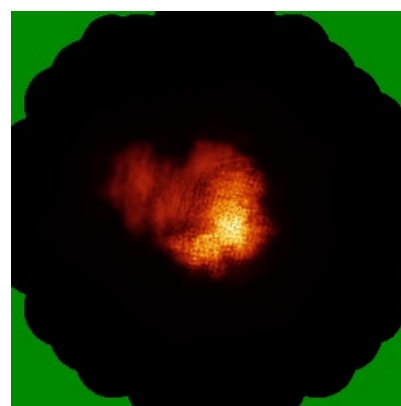
6.4.1 Primary map



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

This section was not generated.

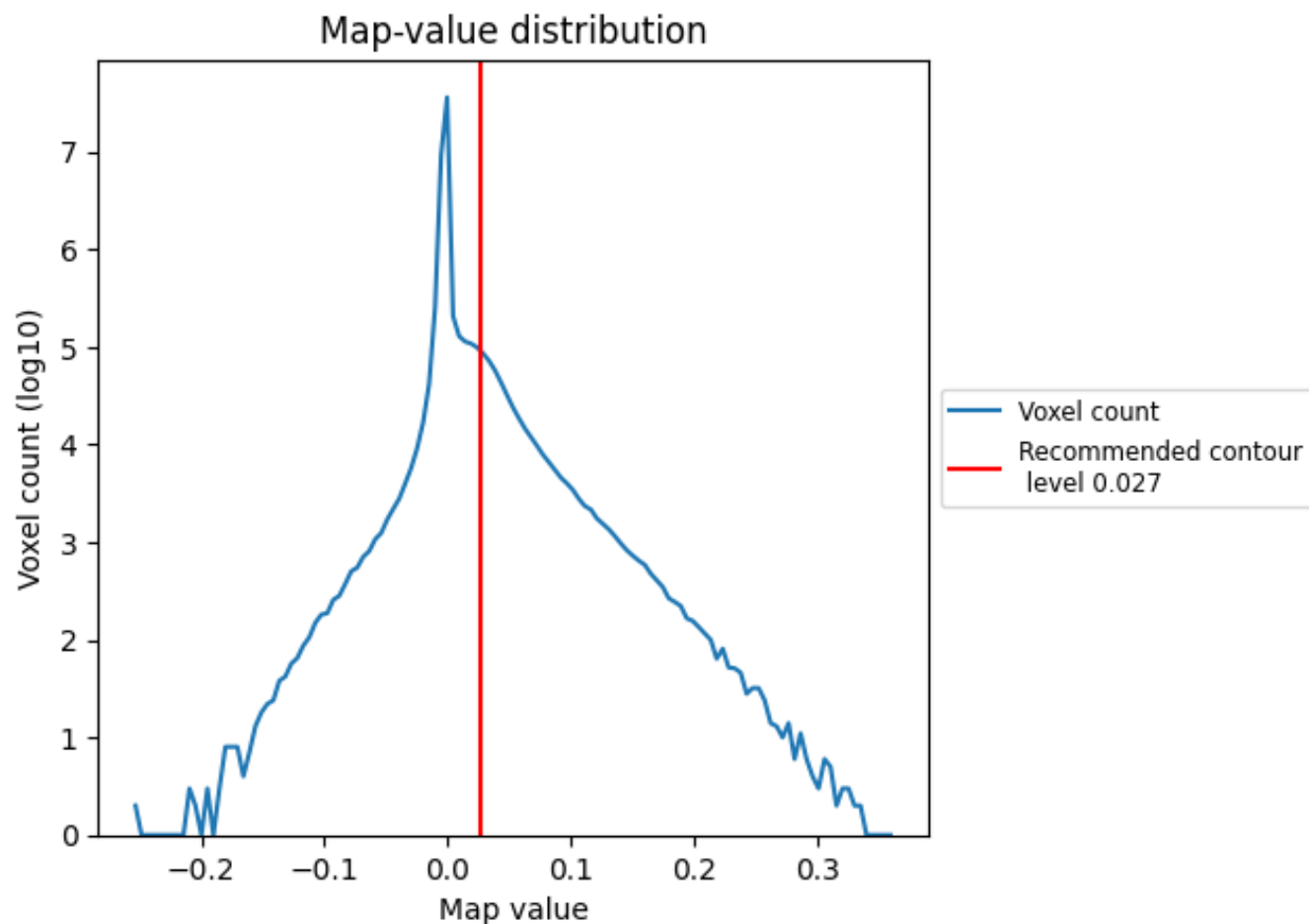
6.6 Mask visualisation

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

7 Map analysis [i](#)

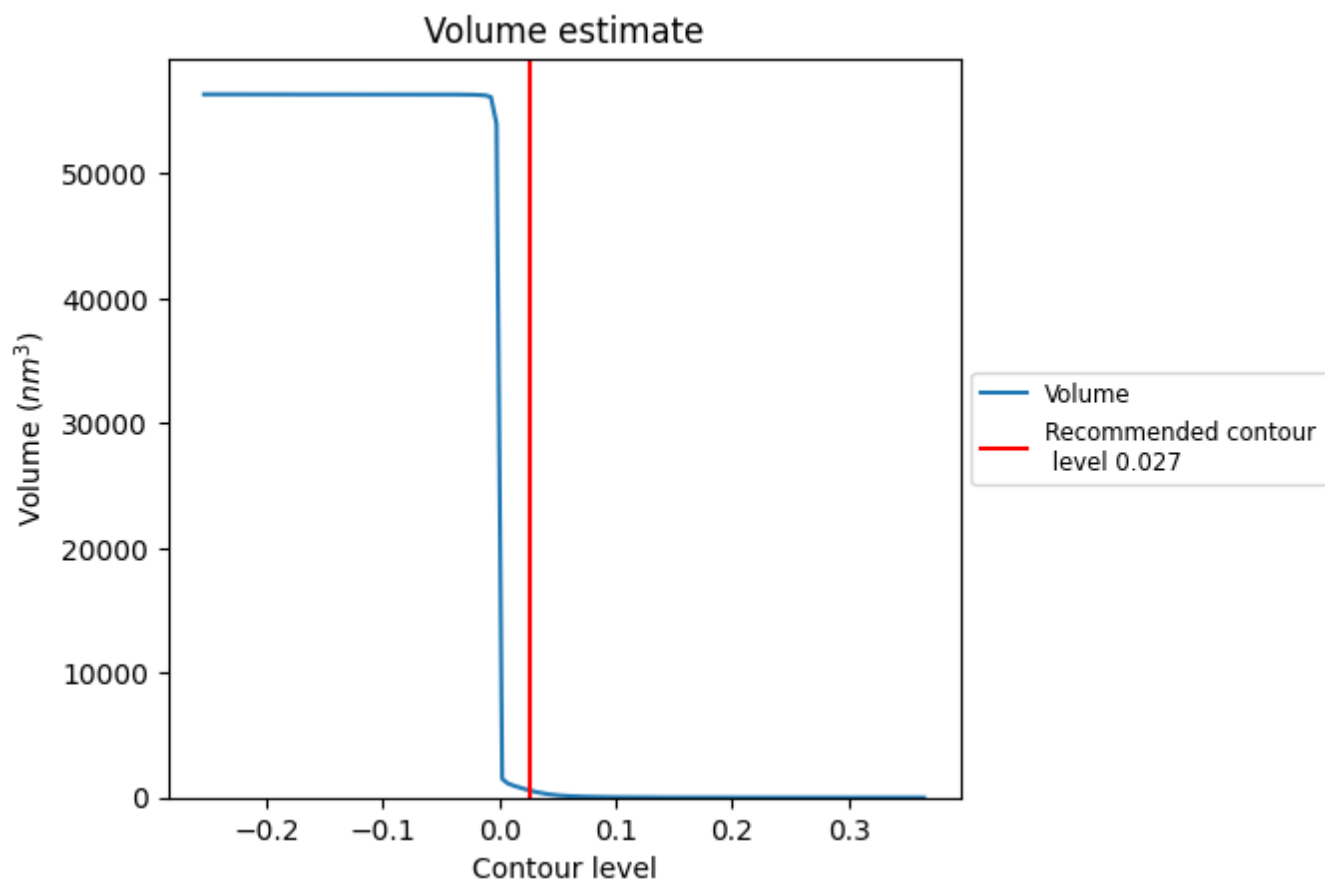
This section contains the results of statistical analysis of the map.

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.

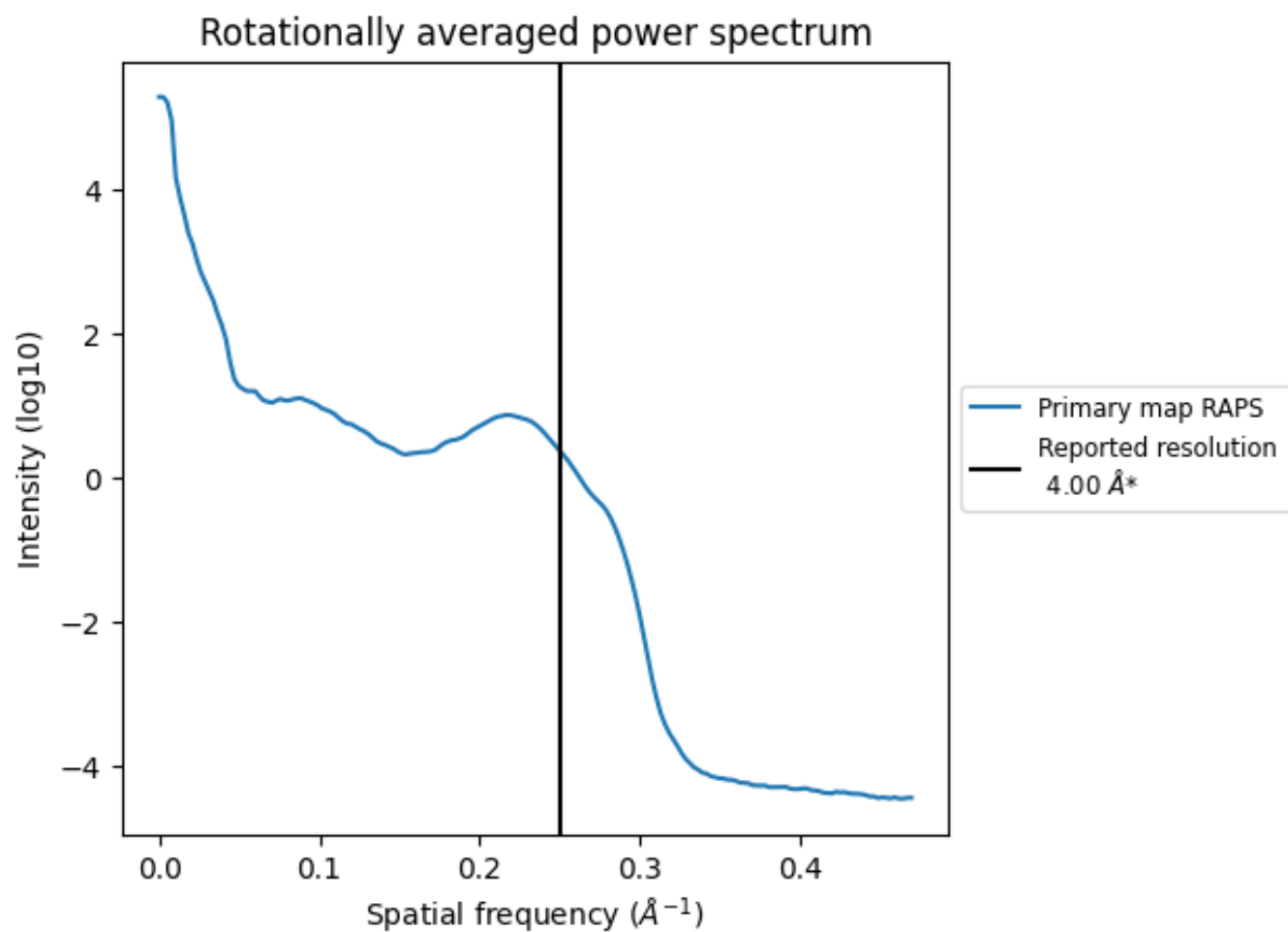
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 555 nm³; this corresponds to an approximate mass of 501 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 ⓘ

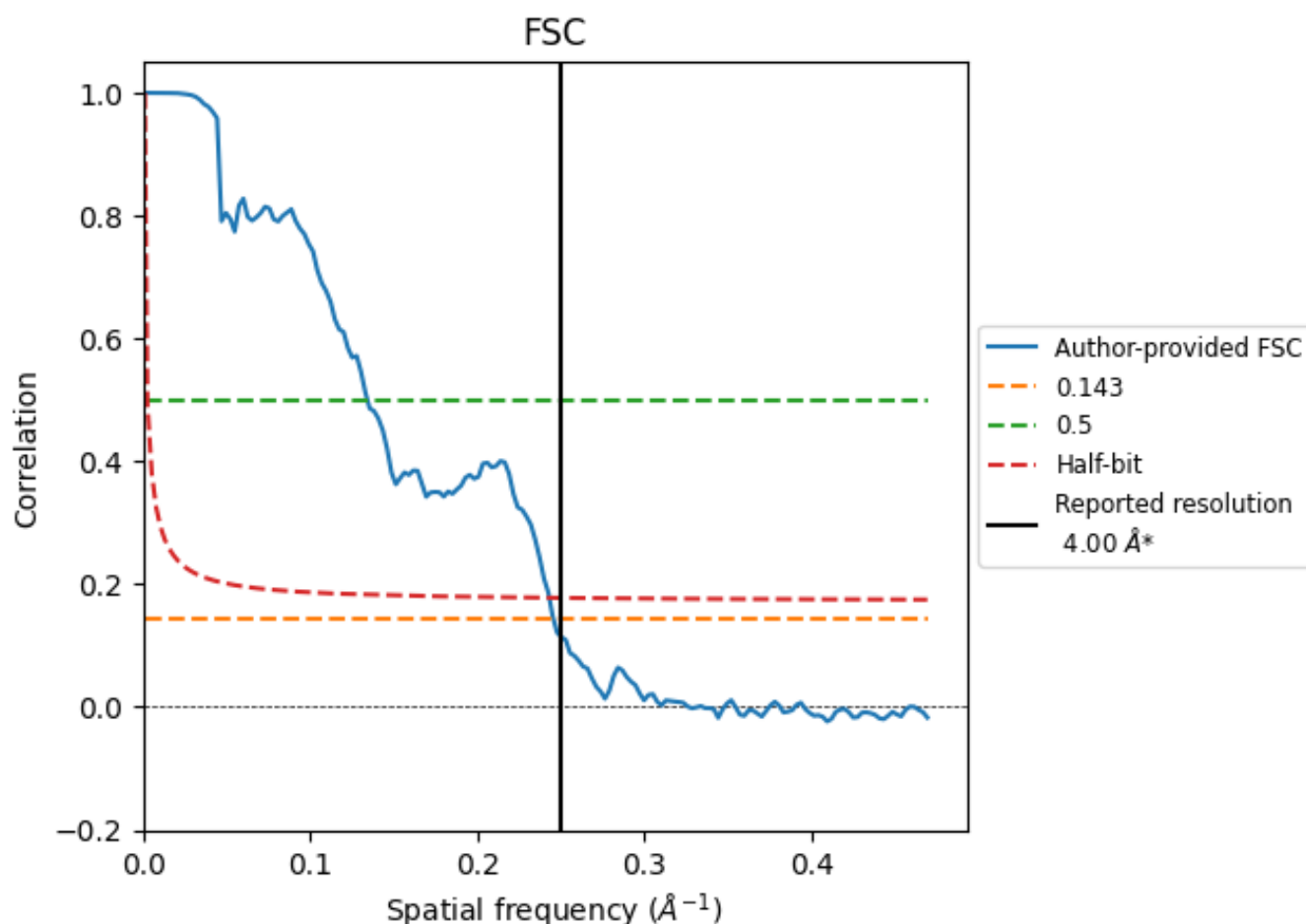


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.07	7.45	4.11
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-11904 and PDB model 7AST. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

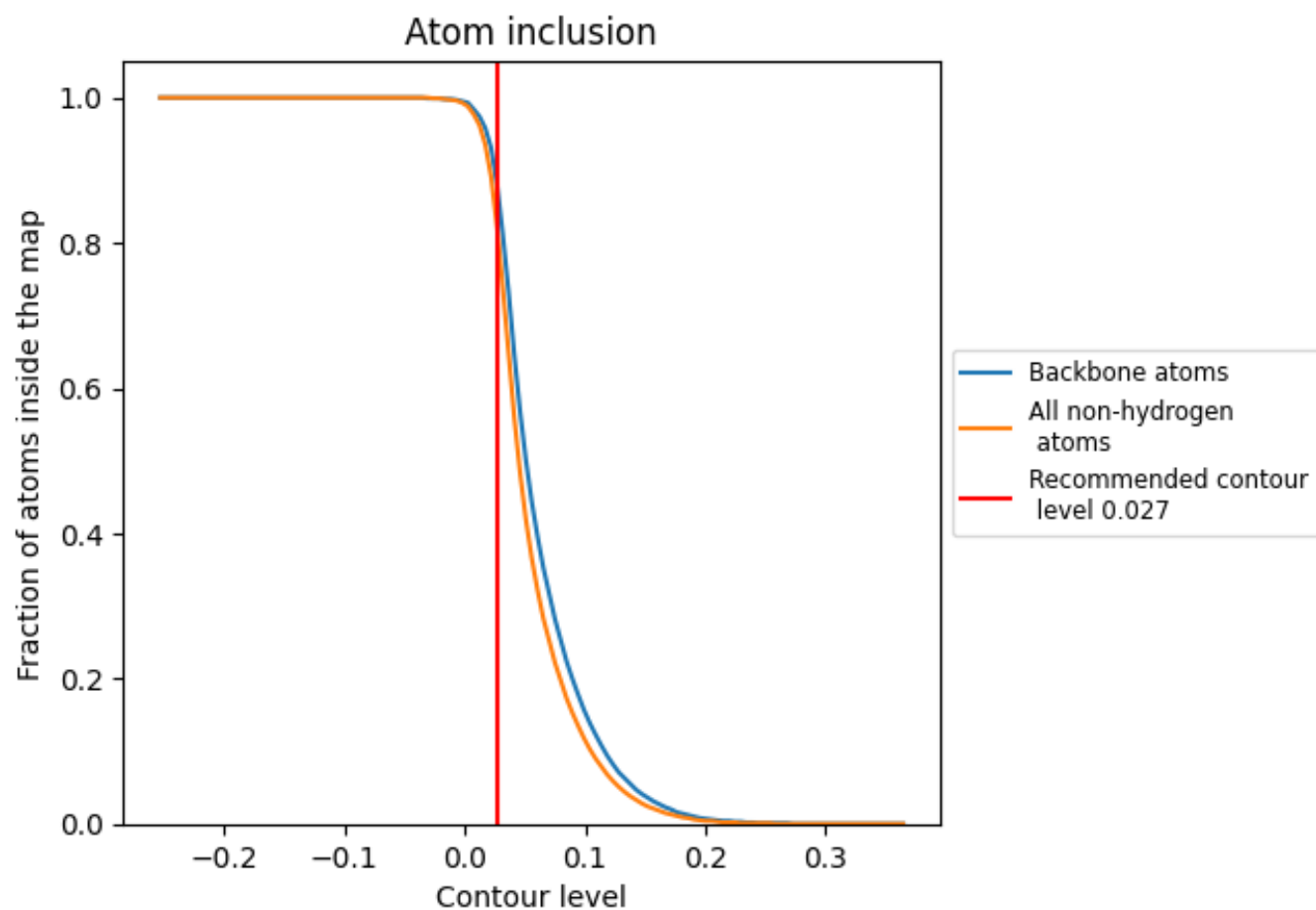


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.2400
A	 0.9960	 0.2280
B	 0.9190	 0.3890
C	 0.9270	 0.2890
D	 0.8980	 0.2860
E	 0.8180	 0.2110
F	 0.8750	 0.1970
G	 0.9240	 0.3620
H	 0.9170	 0.3520
I	 0.5670	 0.1330
J	 0.6800	 0.1370
K	 0.9380	 0.2130
L	 0.9480	 0.2860
M	 0.8720	 0.3090
N	 0.8270	 0.2280
X	 0.5860	 0.0820
Y	 0.5280	 0.0640
Z	 0.7230	 0.0750

