



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:50 PM UTC

PDB ID : 7VBC / pdb\_00007vbc  
EMDB ID : EMD-31878  
Title : Back track state of human RNA Polymerase I Elongation Complex  
Authors : Zhao, D.; Liu, W.; Chen, K.; Yang, H.; Xu, Y.  
Deposited on : 2021-08-31  
Resolution : 3.01 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](mailto: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>.

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

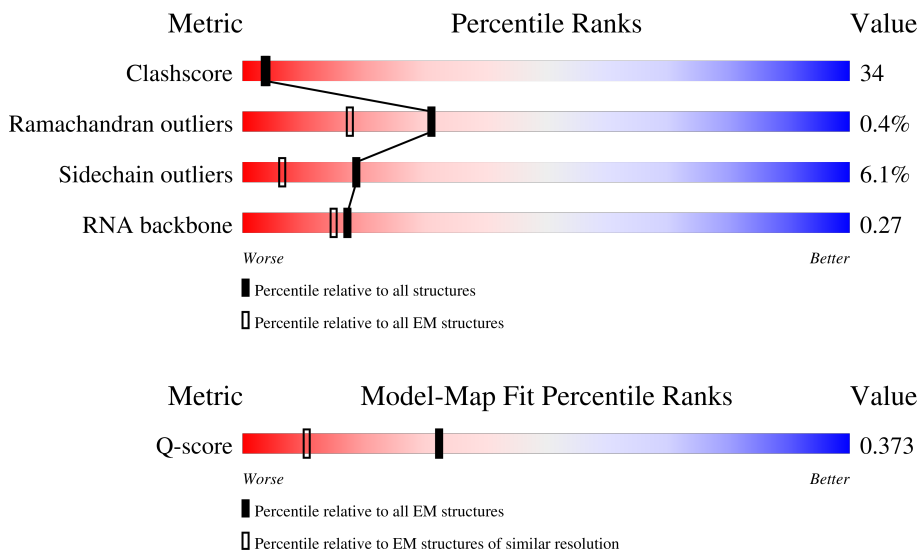
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.01 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13882 ( 2.51 - 3.51 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1719	
2	B	1135	
3	C	346	

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Mol	Chain	Length	Quality of chain
4	E	210	
5	F	127	
6	H	150	
7	J	67	
8	K	133	
9	L	58	
10	N	510	
11	G	338	
12	M	419	
13	I	126	
14	R	6	
15	T	20	
16	U	14	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 33414 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 I subunit RPA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1477	11775	7488	2067	2142	78	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1123	8912	5710	1517	1614	71	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	337	2697	1701	480	505	11	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	199	1641	1042	286	305	8	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	76	610	392	103	110	5	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	146	1176	744	192	235	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	K	108	863	535	156	165	7	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	45	379	236	73	64	6	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	151	1105	698	198	204	5	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	157	1229	775	215	232	7	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	110	867	539	159	163	6	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	107	822	501	148	162	11	0	0

- Molecule 14 is a RNA chain called RNA (5'-R(P\*UP\*GP\*CP\*UP\*GP\*A)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
14	R	6	128	57	22	43	6	0	0

- Molecule 15 is a DNA chain called DNA (5'-D(P\*AP\*GP\*GP\*AP\*CP\*AP\*GP\*CP\*GP\*TP\*GP\*TP\*CP\*AP\*GP\*CP\*AP\*AP\*TP\*A)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
15	T	20	415	196	83	116	20	0	0

- Molecule 16 is a DNA chain called DNA (5'-D(\*GP\*TP\*AP\*CP\*TP\*GP\*TP\*CP\*CP\*TP\*CP\*TP\*GP\*G)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
16	U	14	282	136	47	86	13	0	0

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

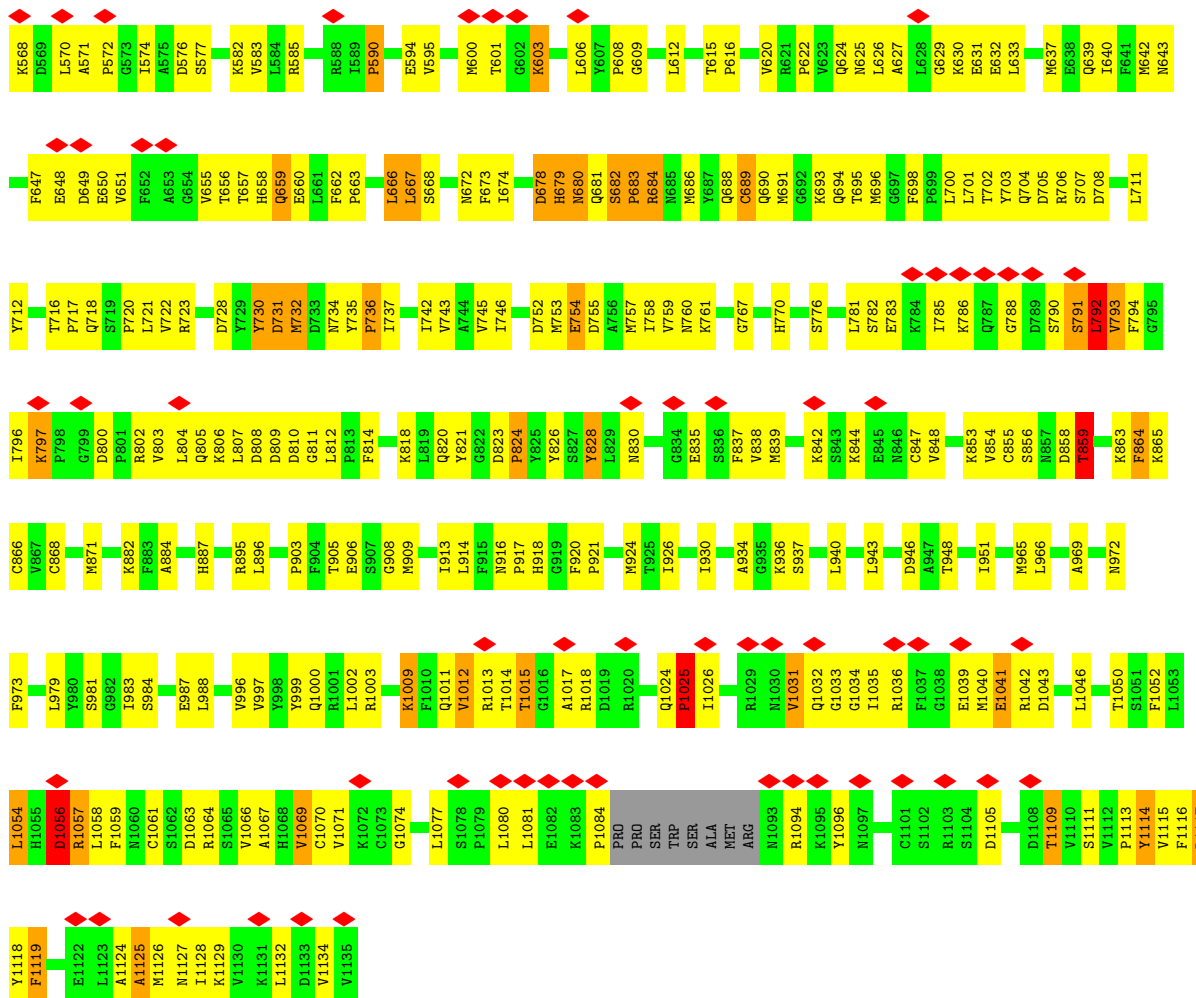
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

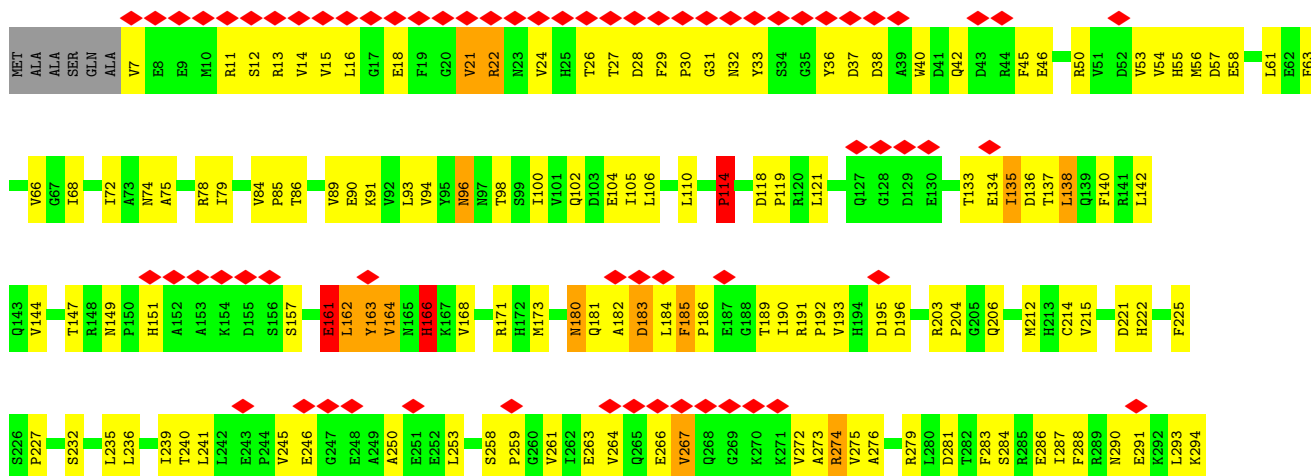


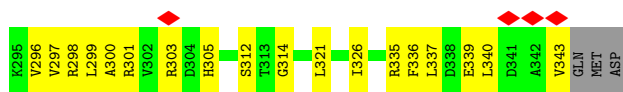




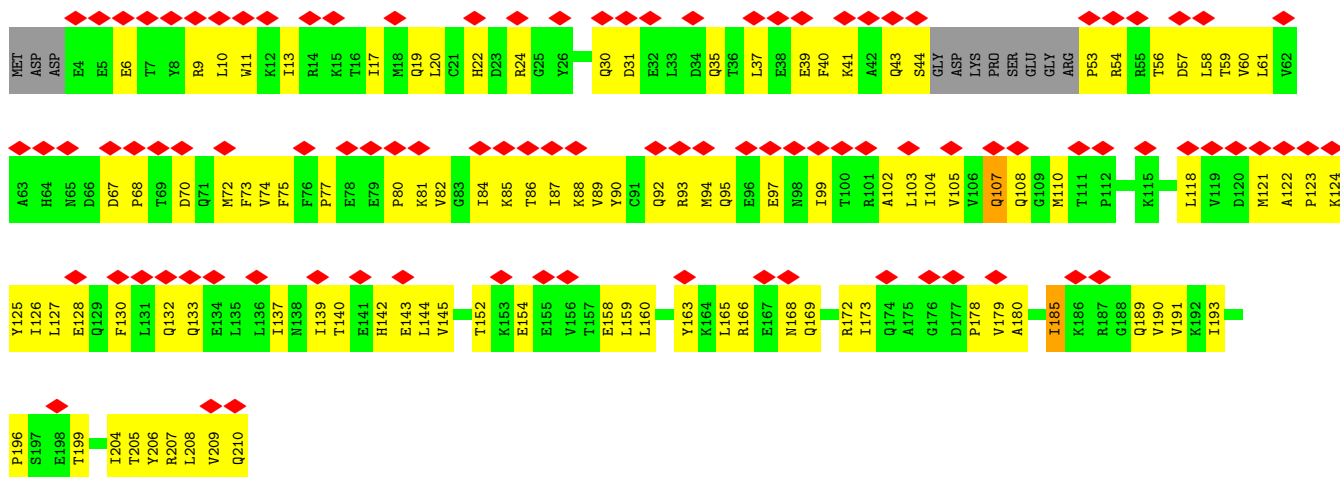
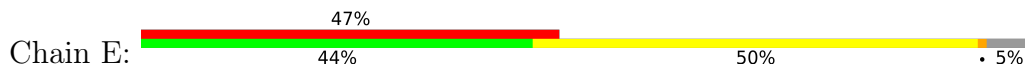


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

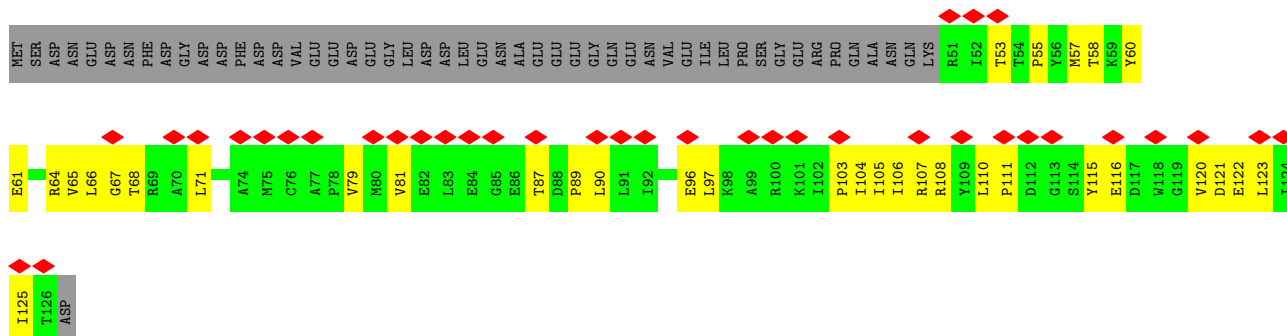
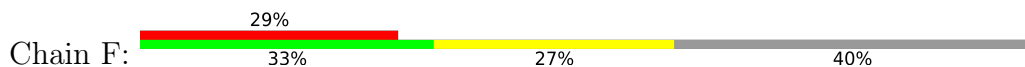




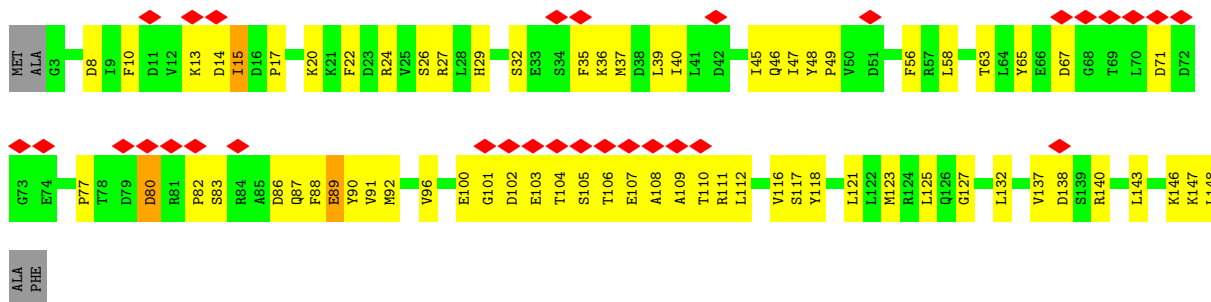
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



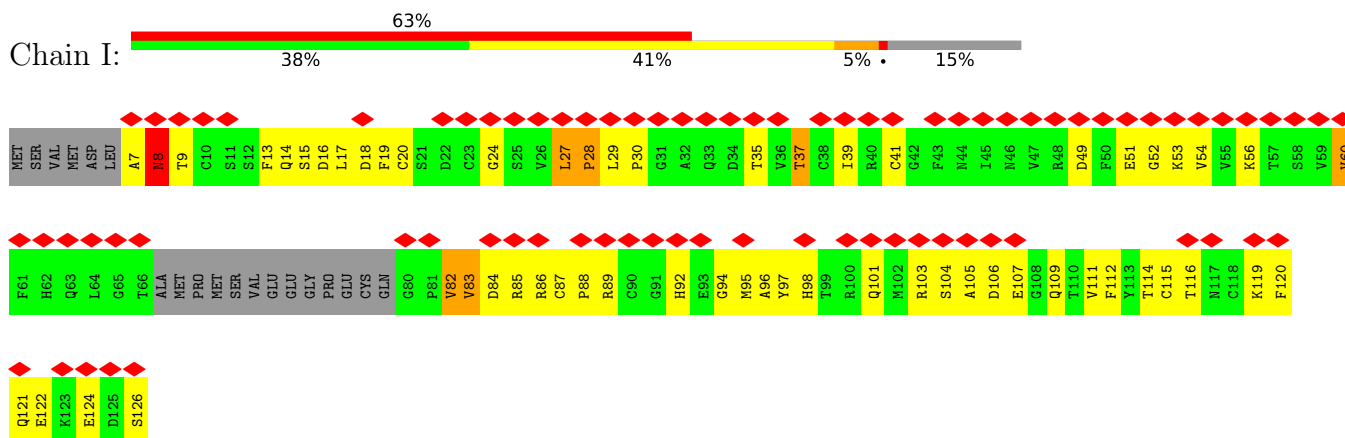
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



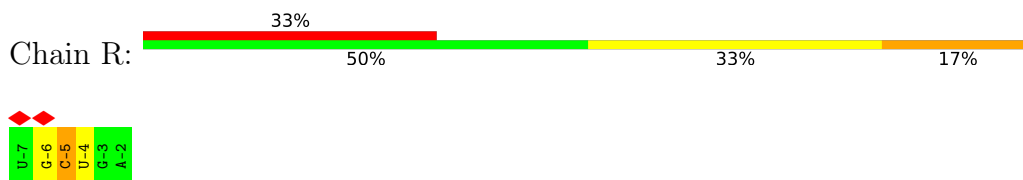




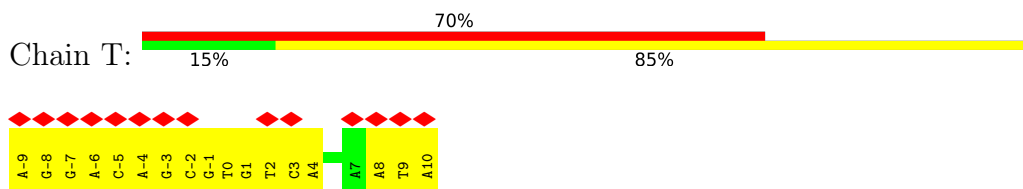
- Molecule 13: DNA-directed RNA polymerase I subunit RPA12



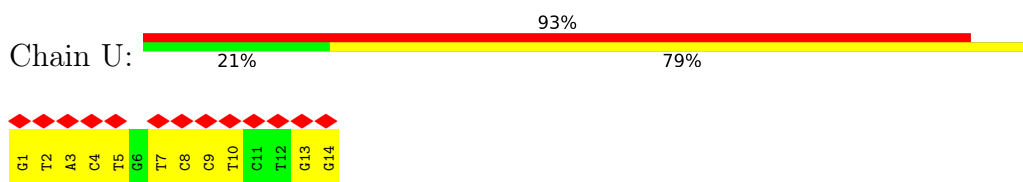
- Molecule 14: RNA (5'-R(P\*UP\*GP\*CP\*UP\*GP\*A)-3')



- Molecule 15: DNA (5'-D(P\*AP\*GP\*GP\*AP\*CP\*AP\*GP\*CP\*GP\*TP\*GP\*TP\*CP\*AP\*GP\*CP\*AP\*AP\*TP\*A)-3')



- Molecule 16: DNA (5'-D(\*GP\*TP\*AP\*CP\*TP\*GP\*TP\*CP\*CP\*TP\*CP\*TP\*GP\*G)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152653	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.977	Depositor
Minimum map value	-2.344	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.112	Depositor
Recommended contour level	0.575	Depositor
Map size ( $\text{\AA}$ )	337.28, 337.28, 337.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.054, 1.054, 1.054	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.67	9/12014 (0.1%)	1.02	63/16219 (0.4%)
2	B	0.76	8/9127 (0.1%)	1.18	80/12350 (0.6%)
3	C	0.74	2/2751 (0.1%)	1.18	28/3729 (0.8%)
4	E	0.35	0/1669	0.58	1/2254 (0.0%)
5	F	0.29	0/620	0.46	0/839
6	H	0.47	0/1197	0.83	3/1614 (0.2%)
7	J	0.66	0/516	1.18	5/696 (0.7%)
8	K	0.39	0/878	0.82	1/1182 (0.1%)
9	L	0.35	0/385	0.66	0/511
10	N	1.10	9/1140 (0.8%)	1.43	21/1560 (1.3%)
11	G	0.38	0/1252	0.64	1/1691 (0.1%)
12	M	1.06	6/884 (0.7%)	1.29	13/1192 (1.1%)
13	I	0.43	0/836	0.93	3/1126 (0.3%)
14	R	0.37	0/142	0.45	0/219
15	T	0.34	0/467	0.48	0/719
16	U	0.29	0/314	0.53	0/483
All	All	0.68	34/34192 (0.1%)	1.04	219/46384 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
All	All	0	5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	66	ARG	C-N	-9.01	1.22	1.33
2	B	590	PRO	C-O	-8.24	1.18	1.25
12	M	61	ALA	C-N	-7.76	1.23	1.33
10	N	155	ASN	C-N	7.58	1.42	1.33
10	N	100	GLU	C-N	-7.53	1.24	1.33
1	A	1498	MET	C-O	7.13	1.32	1.24
10	N	57	ASN	C-N	7.00	1.44	1.33
1	A	1503	GLN	C-O	-6.50	1.16	1.24
2	B	143	SER	CA-CB	-6.42	1.44	1.53
2	B	682	SER	CA-CB	-6.37	1.45	1.53
10	N	58	GLY	C-N	-6.26	1.24	1.33
12	M	32	LYS	C-N	-6.12	1.24	1.33
12	M	57	GLN	C-N	-6.02	1.25	1.33
10	N	69	VAL	C-N	-6.00	1.25	1.33
12	M	39	MET	C-N	-5.97	1.25	1.33
1	A	629	GLY	C-O	-5.93	1.17	1.24
10	N	38	PRO	N-CD	5.83	1.55	1.47
1	A	632	GLN	C-O	-5.81	1.19	1.24
10	N	14	CYS	C-N	-5.66	1.28	1.33
2	B	507	PRO	C-O	-5.59	1.18	1.23
2	B	283	SER	CA-CB	-5.46	1.44	1.53
2	B	683	PRO	C-O	-5.40	1.17	1.24
10	N	91	GLU	C-N	-5.39	1.26	1.33
1	A	674	SER	CA-CB	-5.35	1.44	1.53
12	M	33	LEU	C-N	-5.34	1.26	1.34
1	A	447	PRO	C-O	-5.27	1.18	1.23
1	A	673	PRO	C-O	-5.23	1.17	1.23
1	A	581	ASN	C-O	-5.21	1.16	1.24
2	B	260	SER	CA-CB	-5.14	1.45	1.53
1	A	57	PRO	C-O	-5.12	1.18	1.23
10	N	90	GLY	C-N	-5.11	1.26	1.33
2	B	1041	GLU	N-CA	5.11	1.52	1.46
3	C	114	PRO	C-O	-5.04	1.18	1.23
3	C	284	SER	CA-CB	-5.01	1.46	1.54

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	164	VAL	N-CA-C	-16.04	98.64	112.12
7	J	10	CYS	CB-CA-C	-12.82	90.65	110.90
1	A	875	GLU	CA-C-N	-11.41	102.85	121.34
1	A	875	GLU	C-N-CA	-11.41	102.85	121.34
1	A	1507	GLU	N-CA-C	-10.94	99.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	25	THR	N-CA-C	-10.14	100.91	113.18
2	B	19	LEU	N-CA-C	-9.87	97.50	110.53
2	B	159	HIS	N-CA-C	-9.45	95.30	110.32
13	I	60	VAL	N-CA-C	-9.36	103.81	112.43
1	A	1598	ARG	N-CA-C	-9.20	95.36	110.17
10	N	121	PRO	CA-N-CD	-8.98	99.42	112.00
10	N	155	ASN	CA-C-N	8.89	129.53	120.38
10	N	155	ASN	C-N-CA	8.89	129.53	120.38
2	B	1009	LYS	CB-CA-C	-8.85	98.84	111.85
2	B	1040	MET	O-C-N	-8.61	112.99	122.12
3	C	163	TYR	CB-CA-C	-8.57	100.19	111.42
1	A	1606	HIS	N-CA-C	-8.38	103.57	113.88
2	B	734	ASN	N-CA-C	-8.31	102.18	111.82
1	A	1505	VAL	CA-C-O	-8.18	112.44	120.95
3	C	166	HIS	CA-CB-CG	8.03	121.83	113.80
2	B	791	SER	N-CA-C	-7.98	103.63	112.72
1	A	634	HIS	N-CA-C	-7.85	103.73	113.38
3	C	191	ARG	CB-CA-C	-7.78	99.96	110.22
1	A	57	PRO	CB-CA-C	-7.65	104.44	111.40
7	J	27	ALA	N-CA-C	-7.61	99.77	110.50
3	C	191	ARG	N-CA-CB	-7.59	103.13	111.10
2	B	291	GLU	N-CA-C	-7.57	104.02	113.18
12	M	111	PRO	N-CA-C	7.57	123.24	111.21
2	B	662	PHE	CA-CB-CG	7.43	121.23	113.80
1	A	313	SER	CA-C-O	-7.38	115.57	119.77
10	N	155	ASN	CA-C-O	-7.34	110.10	120.16
1	A	1268	VAL	N-CA-C	7.32	119.17	112.29
2	B	288	ILE	CA-C-N	-7.29	111.83	122.69
2	B	288	ILE	C-N-CA	-7.29	111.83	122.69
1	A	313	SER	O-C-N	7.22	126.17	120.83
2	B	730	TYR	CB-CA-C	-7.16	99.29	111.31
2	B	736	PRO	CB-CA-C	7.14	122.00	111.22
2	B	544	GLY	N-CA-C	7.09	120.77	110.63
2	B	791	SER	CA-C-N	-7.07	112.82	122.86
2	B	791	SER	C-N-CA	-7.07	112.82	122.86
7	J	4	PRO	CB-CA-C	7.04	120.54	111.46
3	C	163	TYR	CA-C-N	-6.98	115.44	122.77
3	C	163	TYR	C-N-CA	-6.98	115.44	122.77
12	M	14	CYS	N-CA-C	-6.97	103.62	111.07
1	A	412	ASP	N-CA-C	-6.96	104.73	113.23
2	B	34	ALA	N-CA-C	-6.96	104.41	113.12
1	A	871	HIS	N-CA-C	-6.93	103.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	284	SER	N-CA-C	-6.92	105.77	114.56
2	B	839	MET	CA-C-O	-6.90	113.48	122.45
10	N	138	PRO	N-CA-C	6.88	119.10	110.70
1	A	680	PRO	N-CA-CB	-6.84	97.11	103.27
3	C	183	ASP	N-CA-C	-6.83	101.72	110.53
2	B	732	MET	N-CA-C	-6.83	104.07	112.88
1	A	1676	THR	CB-CA-C	6.82	121.57	111.89
10	N	25	SER	N-CA-C	-6.79	105.00	113.28
12	M	19	GLY	N-CA-C	-6.75	106.49	115.40
3	C	114	PRO	N-CA-CB	-6.71	97.79	103.36
2	B	1114	TYR	O-C-N	6.70	131.87	122.36
10	N	134	PRO	N-CA-C	6.69	121.74	111.57
1	A	470	GLN	CB-CA-C	-6.64	99.18	109.08
1	A	874	ASN	N-CA-C	-6.59	104.02	111.07
2	B	75	PHE	CA-CB-CG	-6.58	107.22	113.80
12	M	110	GLN	CA-C-N	6.54	126.52	119.78
12	M	110	GLN	C-N-CA	6.54	126.52	119.78
6	H	77	PRO	N-CA-C	-6.53	106.19	114.35
3	C	22	ARG	N-CA-C	6.50	118.45	111.36
1	A	553	GLN	N-CA-C	6.46	122.48	113.57
3	C	258	SER	N-CA-C	-6.46	101.44	109.64
2	B	339	ASN	N-CA-C	-6.42	105.61	113.50
2	B	443	THR	CB-CA-C	-6.41	98.63	109.72
2	B	730	TYR	CA-C-O	-6.39	113.94	120.84
1	A	678	PRO	N-CA-C	-6.38	103.44	113.78
6	H	87	GLN	N-CA-C	-6.35	105.63	113.19
2	B	259	PHE	CA-CB-CG	6.34	120.14	113.80
2	B	547	HIS	CB-CA-C	6.33	119.60	110.04
4	E	180	ALA	N-CA-C	-6.33	105.69	113.41
1	A	1267	PRO	CB-CA-C	6.30	119.25	111.12
2	B	106	ARG	N-CA-C	-6.29	102.41	110.53
2	B	590	PRO	N-CA-CB	-6.29	99.67	103.19
2	B	145	LEU	N-CA-C	-6.26	103.04	111.87
1	A	447	PRO	CB-CA-C	-6.26	102.89	111.21
3	C	225	PHE	CA-CB-CG	6.26	120.06	113.80
2	B	32	LYS	N-CA-C	6.25	118.10	111.28
3	C	166	HIS	CB-CA-C	6.24	121.46	110.85
2	B	279	ARG	N-CA-C	-6.21	104.51	111.28
10	N	78	HIS	CA-C-N	-6.21	114.24	122.99
10	N	78	HIS	C-N-CA	-6.21	114.24	122.99
2	B	351	ARG	N-CA-C	-6.18	104.60	111.71
2	B	1043	ASP	CB-CA-C	-6.18	101.18	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1115	VAL	N-CA-C	-6.18	103.16	111.44
1	A	1177	GLN	N-CA-C	-6.17	106.39	114.04
2	B	794	PHE	CB-CA-C	6.15	120.16	109.65
2	B	216	ARG	CB-CA-C	-6.13	100.13	110.19
1	A	55	LEU	N-CA-C	-6.13	105.67	113.02
3	C	259	PRO	N-CA-C	6.13	122.88	113.75
2	B	585	ARG	CB-CA-C	6.09	120.37	111.73
2	B	265	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	1319	PHE	CB-CA-C	6.04	121.12	110.85
11	G	168	THR	N-CA-C	6.00	117.49	111.07
2	B	500	VAL	N-CA-C	5.98	116.76	110.72
2	B	1056	ASP	CA-C-O	-5.97	114.55	120.82
2	B	603	LYS	CB-CA-C	5.96	120.24	109.45
1	A	1182	TYR	CB-CA-C	5.96	120.63	110.56
1	A	1503	GLN	CA-C-O	-5.93	114.60	120.82
7	J	8	PHE	CA-CB-CG	5.91	119.71	113.80
12	M	110	GLN	CB-CA-C	-5.89	100.30	109.55
12	M	77	GLY	CA-C-N	-5.86	112.74	120.95
12	M	77	GLY	C-N-CA	-5.86	112.74	120.95
2	B	824	PRO	N-CA-CB	-5.84	98.11	103.31
1	A	1049	LYS	CB-CA-C	-5.83	101.72	110.88
7	J	10	CYS	N-CA-C	5.83	117.44	111.14
6	H	15	ILE	CA-C-O	-5.81	114.49	120.71
3	C	96	ASN	CA-C-N	-5.81	112.77	121.72
3	C	96	ASN	C-N-CA	-5.81	112.77	121.72
10	N	141	ILE	N-CA-C	5.81	114.64	108.95
3	C	180	ASN	N-CA-C	-5.80	106.06	113.02
1	A	88	TYR	CA-C-O	-5.75	114.72	121.16
2	B	731	ASP	CB-CA-C	5.72	118.01	110.06
2	B	826	TYR	CB-CA-C	5.71	122.37	111.17
13	I	8	ASN	CA-C-N	-5.71	110.62	121.54
13	I	8	ASN	C-N-CA	-5.71	110.62	121.54
1	A	890	PRO	N-CA-C	-5.71	105.59	113.53
1	A	1263	MET	CA-C-O	-5.71	115.34	121.45
2	B	464	ARG	N-CA-C	-5.70	103.83	112.04
2	B	318	TYR	CB-CA-C	-5.69	100.60	109.08
2	B	32	LYS	CA-C-O	-5.69	114.52	120.55
2	B	266	GLN	CB-CA-C	5.69	121.15	110.63
3	C	183	ASP	CA-C-O	-5.69	115.40	121.94
2	B	147	ASN	CB-CA-C	5.68	120.90	110.11
1	A	678	PRO	CB-CA-C	5.64	122.73	113.20
2	B	859	THR	CB-CA-C	5.64	120.34	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASN	N-CA-C	-5.63	103.06	110.39
3	C	164	VAL	CB-CA-C	5.62	116.42	110.91
1	A	832	ASN	CB-CA-C	5.62	120.00	111.80
3	C	161	GLU	CA-C-O	-5.62	115.05	121.68
2	B	609	GLY	CA-C-O	-5.62	116.25	122.14
10	N	26	GLU	N-CA-C	-5.62	106.20	113.16
1	A	90	PRO	N-CA-C	5.60	121.12	113.84
2	B	594	GLU	CB-CA-C	-5.59	101.92	111.31
2	B	287	ARG	CB-CA-C	-5.57	100.93	110.24
2	B	461	ASN	N-CA-C	-5.57	100.66	108.96
3	C	118	ASP	CA-CB-CG	5.54	118.14	112.60
2	B	1056	ASP	N-CA-C	-5.54	105.14	111.07
3	C	162	LEU	N-CA-C	-5.52	105.18	112.24
1	A	1059	ARG	N-CA-C	-5.51	106.44	112.72
3	C	192	PRO	CB-CA-C	5.51	118.19	110.98
1	A	718	LYS	CA-C-O	-5.49	114.44	120.43
2	B	1025	PRO	N-CA-CB	-5.46	98.73	103.32
10	N	130	LEU	N-CA-CB	-5.45	102.11	110.01
1	A	1145	PRO	N-CA-CB	-5.44	98.75	103.32
12	M	69	TYR	CA-C-N	-5.44	115.43	122.99
12	M	69	TYR	C-N-CA	-5.44	115.43	122.99
3	C	185	PHE	CB-CA-C	5.41	116.37	110.15
1	A	54	ALA	N-CA-C	-5.41	107.05	113.97
2	B	19	LEU	CA-C-O	-5.39	115.61	121.87
2	B	279	ARG	CB-CA-C	5.39	119.74	110.79
1	A	1257	ALA	N-CA-C	-5.39	106.55	113.23
2	B	754	GLU	CA-C-O	-5.38	115.36	121.65
12	M	111	PRO	CB-CA-C	-5.36	104.37	111.23
2	B	351	ARG	CB-CA-C	5.36	120.54	110.63
1	A	875	GLU	N-CA-C	-5.36	106.01	112.54
1	A	452	ASN	CA-CB-CG	5.35	117.95	112.60
2	B	342	LYS	CB-CA-C	5.34	119.66	110.79
3	C	164	VAL	N-CA-CB	5.34	119.22	111.90
2	B	792	LEU	N-CA-CB	-5.34	102.73	110.84
2	B	689	CYS	CA-C-O	-5.33	114.07	120.10
10	N	79	ARG	CB-CA-C	5.33	119.47	109.71
10	N	37	GLY	CA-C-N	5.30	124.97	119.56
10	N	37	GLY	C-N-CA	5.30	124.97	119.56
1	A	452	ASN	CB-CA-C	5.30	119.29	109.54
1	A	575	LEU	CA-C-O	-5.28	115.05	120.54
2	B	106	ARG	CA-C-N	-5.25	114.99	123.23
2	B	106	ARG	C-N-CA	-5.25	114.99	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	TYR	N-CA-C	-5.24	106.28	113.30
1	A	579	TYR	CB-CA-C	-5.24	99.52	109.95
2	B	1117	ARG	CB-CA-C	5.23	119.47	110.79
1	A	664	LYS	N-CA-C	-5.22	107.56	114.04
10	N	23	PRO	CB-CA-C	-5.22	103.33	111.22
2	B	1061	CYS	N-CA-C	-5.22	106.14	112.88
12	M	82	ASN	CB-CA-C	5.21	120.68	110.67
1	A	770	GLY	CA-C-O	-5.20	117.20	122.56
2	B	107	ARG	CB-CA-C	5.19	120.24	111.41
1	A	874	ASN	CB-CA-C	-5.19	102.74	110.88
2	B	679	HIS	CA-CB-CG	5.18	118.98	113.80
10	N	23	PRO	CA-C-N	-5.18	115.89	122.77
10	N	23	PRO	C-N-CA	-5.18	115.89	122.77
2	B	793	VAL	N-CA-C	-5.17	98.59	109.34
2	B	1054	LEU	N-CA-C	-5.16	106.24	112.54
3	C	283	PHE	CB-CA-C	5.14	119.35	110.77
10	N	142	PRO	N-CA-C	-5.14	104.43	110.70
1	A	572	GLU	CA-C-O	-5.13	115.94	121.38
2	B	335	HIS	CA-CB-CG	5.13	118.93	113.80
2	B	1119	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	651	GLU	N-CA-CB	-5.12	102.42	110.30
2	B	1119	PHE	CB-CA-C	5.12	119.55	110.85
3	C	57	ASP	CB-CA-C	-5.12	101.76	113.33
1	A	840	ASP	CA-C-N	-5.12	112.53	120.31
1	A	840	ASP	C-N-CA	-5.12	112.53	120.31
1	A	1598	ARG	CA-C-O	-5.11	115.25	121.28
1	A	451	ILE	N-CA-C	-5.10	100.55	108.86
1	A	682	TRP	CA-C-O	-5.09	114.69	121.46
1	A	67	CYS	CA-C-N	-5.09	113.55	121.18
1	A	67	CYS	C-N-CA	-5.09	113.55	121.18
1	A	557	HIS	CA-CB-CG	5.09	118.89	113.80
2	B	249	LEU	N-CA-C	-5.09	103.82	110.53
10	N	140	GLN	N-CA-C	5.08	116.52	108.96
1	A	573	LYS	N-CA-C	-5.07	104.88	112.54
1	A	335	VAL	N-CA-C	-5.07	105.45	110.62
1	A	1340	ARG	N-CA-C	-5.06	105.89	111.71
1	A	21	SER	CA-C-O	-5.05	115.20	120.55
12	M	81	CYS	CB-CA-C	-5.04	101.31	110.63
10	N	130	LEU	N-CA-C	5.04	116.46	111.07
1	A	206	PRO	CB-CA-C	-5.03	103.26	111.56
2	B	826	TYR	CA-C-O	-5.03	116.05	121.38
2	B	503	PRO	CB-CA-C	5.02	117.66	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	683	PRO	CA-C-N	5.01	127.25	120.44
2	B	683	PRO	C-N-CA	5.01	127.25	120.44
2	B	499	PRO	CA-C-N	5.01	127.53	120.42
2	B	499	PRO	C-N-CA	5.01	127.53	120.42

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	721	PRO	Mainchain
2	B	1056	ASP	Mainchain
2	B	1057	ARG	Mainchain
2	B	1058	LEU	Mainchain
2	B	684	ARG	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11775	0	11912	982	0
2	B	8912	0	8896	775	0
3	C	2697	0	2676	162	0
4	E	1641	0	1671	136	0
5	F	610	0	642	59	0
6	H	1176	0	1137	73	0
7	J	507	0	523	27	0
8	K	863	0	850	61	0
9	L	379	0	387	29	0
10	N	1105	0	1098	94	0
11	G	1229	0	1212	0	0
12	M	867	0	844	156	0
13	I	822	0	774	169	0
14	R	128	0	64	2	0
15	T	415	0	224	39	0
16	U	282	0	161	12	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	33414	0	33071	2149	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 34.

All (2149) 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)
12:M:33:LEU:CD2	12:M:39:MET:HE1	1.31	1.59
1:A:972:ARG:NH2	2:B:509:GLY:HA2	1.17	1.46
12:M:33:LEU:HD22	12:M:39:MET:CE	1.47	1.44
10:N:142:PRO:CG	10:N:145:LEU:HD21	1.50	1.42
1:A:975:LEU:CD2	13:I:104:SER:HA	1.49	1.41
10:N:142:PRO:HG2	10:N:145:LEU:CD2	1.54	1.35
1:A:408:LYS:NZ	1:A:409:LEU:HD22	1.46	1.30
2:B:570:LEU:CD2	10:N:81:ARG:NH1	1.98	1.27
2:B:570:LEU:HD23	10:N:81:ARG:NH1	1.47	1.27
2:B:260:SER:HB2	12:M:30:ASN:OD1	1.34	1.27
1:A:934:SER:O	2:B:491:PRO:CB	1.87	1.23
12:M:33:LEU:CD2	12:M:39:MET:CE	2.10	1.23
12:M:28:PHE:CZ	12:M:33:LEU:HD11	1.73	1.22
1:A:429:ARG:NH1	15:T:1:DG:OP1	1.73	1.22
2:B:260:SER:CB	12:M:30:ASN:OD1	1.87	1.20
1:A:972:ARG:NH2	2:B:509:GLY:CA	2.05	1.20
1:A:408:LYS:NZ	1:A:409:LEU:CD2	2.06	1.18
1:A:408:LYS:HZ3	1:A:409:LEU:CD2	1.56	1.17
12:M:111:PRO:HG2	13:I:18:ASP:CG	1.68	1.17
1:A:407:ASP:OD2	1:A:410:MET:HG3	1.40	1.17
2:B:792:LEU:HB2	2:B:865:LYS:HD3	1.24	1.16
12:M:66:ARG:HD3	13:I:37:THR:CB	1.74	1.16
2:B:540:THR:HG23	10:N:116:ARG:NH2	1.62	1.15
2:B:785:ILE:HG21	2:B:792:LEU:HD21	1.27	1.14
1:A:929:MET:HE2	2:B:492:GLU:HA	1.25	1.13
2:B:684:ARG:HH22	13:I:106:ASP:C	1.56	1.13
1:A:936:PRO:HG2	2:B:494:TRP:CB	1.79	1.13
2:B:543:ASP:OD2	12:M:81:CYS:N	1.81	1.12
1:A:975:LEU:HD23	13:I:104:SER:HA	1.15	1.11
12:M:67:LEU:HD21	12:M:69:TYR:CZ	1.84	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:ASN:O	10:N:119:GLU:N	1.84	1.10
1:A:430:LYS:HA	2:B:1036:ARG:HH21	0.94	1.10
12:M:67:LEU:HB3	13:I:17:LEU:HD23	1.24	1.09
12:M:67:LEU:HB3	13:I:17:LEU:CD2	1.83	1.09
1:A:851:LEU:CD2	2:B:362:MET:HE2	1.80	1.09
12:M:33:LEU:HD22	12:M:39:MET:HE3	1.27	1.08
1:A:972:ARG:CZ	2:B:509:GLY:HA2	1.82	1.08
2:B:262:TYR:CE2	13:I:9:THR:OG1	2.06	1.07
12:M:33:LEU:HD21	12:M:39:MET:HE1	1.16	1.07
12:M:33:LEU:HD13	12:M:39:MET:SD	1.94	1.07
12:M:67:LEU:HD22	13:I:17:LEU:HA	1.07	1.07
1:A:521:GLN:HA	1:A:524:THR:HB	1.36	1.06
1:A:975:LEU:CD2	13:I:104:SER:CA	2.33	1.06
12:M:69:TYR:OH	13:I:16:ASP:O	1.72	1.06
1:A:1615:GLU:HG3	4:E:193:ILE:HD13	1.37	1.06
2:B:543:ASP:HB2	12:M:81:CYS:SG	1.95	1.06
2:B:259:PHE:HA	12:M:110:GLN:NE2	1.70	1.06
2:B:262:TYR:HB3	12:M:30:ASN:HA	1.30	1.06
1:A:1326:TYR:O	13:I:60:VAL:HG11	1.56	1.05
3:C:267:VAL:HG12	3:C:272:VAL:CG1	1.86	1.05
1:A:312:VAL:HG21	1:A:320:PHE:HB3	1.34	1.05
2:B:73:ILE:HB	2:B:75:PHE:CZ	1.91	1.05
1:A:929:MET:HE2	2:B:492:GLU:CA	1.86	1.04
2:B:14:PRO:HD3	2:B:946:ASP:HB3	1.36	1.04
7:J:1:MET:HE3	7:J:56:ILE:HD13	1.37	1.04
12:M:67:LEU:CD2	13:I:17:LEU:HA	1.88	1.03
1:A:936:PRO:CG	2:B:494:TRP:HB3	1.89	1.03
1:A:881:MET:HG3	1:A:910:MET:HG2	1.39	1.02
2:B:684:ARG:NH2	13:I:106:ASP:C	2.16	1.02
3:C:291:GLU:HA	3:C:294:LYS:HE3	1.36	1.02
1:A:430:LYS:HA	2:B:1036:ARG:NH2	1.73	1.02
2:B:262:TYR:CD2	12:M:30:ASN:O	2.12	1.01
12:M:111:PRO:CG	13:I:18:ASP:OD2	2.09	1.01
1:A:1619:ARG:HH22	4:E:196:PRO:HD2	1.21	1.01
2:B:262:TYR:HE2	13:I:9:THR:OG1	1.43	1.01
1:A:181:VAL:HG11	4:E:166:ARG:NH2	1.75	1.01
1:A:754:TYR:CE1	1:A:781:LEU:HD13	1.95	1.01
1:A:934:SER:O	2:B:491:PRO:HB3	1.61	1.01
12:M:67:LEU:HD21	12:M:69:TYR:OH	1.59	1.00
3:C:267:VAL:HG12	3:C:272:VAL:HG12	1.36	1.00
12:M:111:PRO:HG2	13:I:18:ASP:OD2	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:66:ARG:HD3	13:I:37:THR:CG2	1.92	1.00
2:B:540:THR:HG22	10:N:116:ARG:NE	1.76	1.00
2:B:263:GLN:HB2	12:M:29:SER:O	1.60	0.99
12:M:34:GLN:HG3	13:I:7:ALA:C	1.87	0.99
2:B:570:LEU:HD11	10:N:83:LEU:HD11	1.41	0.99
12:M:28:PHE:CZ	12:M:33:LEU:CD1	2.44	0.99
2:B:110:TYR:CE2	2:B:146:CYS:SG	2.56	0.99
1:A:316:GLY:N	15:T:10:DA:H2'	1.78	0.99
1:A:408:LYS:HZ3	1:A:409:LEU:HD22	0.91	0.99
2:B:110:TYR:HE2	2:B:146:CYS:SG	1.86	0.99
1:A:658:TYR:HB2	8:K:67:PHE:HZ	1.27	0.98
12:M:111:PRO:HG2	13:I:18:ASP:CB	1.92	0.98
1:A:972:ARG:HH21	2:B:509:GLY:CA	1.70	0.98
1:A:1014:VAL:CG2	4:E:165:LEU:HD21	1.92	0.98
1:A:851:LEU:HD22	2:B:362:MET:HE2	1.43	0.98
2:B:568:LYS:HE2	2:B:600:MET:HE3	1.47	0.97
1:A:912:ILE:HD11	2:B:924:MET:HG2	1.43	0.97
2:B:785:ILE:CG2	2:B:792:LEU:HD21	1.95	0.96
2:B:856:SER:HB3	9:L:42:ARG:HB3	1.46	0.95
1:A:912:ILE:CG1	2:B:924:MET:HG2	1.95	0.95
1:A:936:PRO:HD3	2:B:491:PRO:O	1.65	0.95
1:A:316:GLY:H	15:T:10:DA:H2'	1.28	0.95
1:A:1512:ILE:HG21	1:A:1515:TYR:HE1	1.28	0.94
4:E:110:MET:HE1	4:E:118:LEU:HD11	1.49	0.94
1:A:1326:TYR:O	13:I:60:VAL:CG1	2.15	0.94
1:A:972:ARG:HH21	2:B:509:GLY:HA2	1.18	0.94
4:E:72:MET:HE2	4:E:103:LEU:HB2	1.49	0.94
1:A:745:LEU:HD22	6:H:117:SER:OG	1.67	0.94
12:M:12:GLN:OE1	12:M:98:GLN:NE2	2.01	0.94
1:A:1282:LYS:HE3	1:A:1564:LEU:HD13	1.49	0.93
12:M:66:ARG:HD3	13:I:37:THR:HG21	1.50	0.93
1:A:931:SER:OG	2:B:640:ILE:CG2	2.16	0.93
2:B:10:LEU:HD12	2:B:11:PRO:HD2	1.48	0.93
1:A:299:LEU:HD21	2:B:1127:ASN:OD1	1.67	0.93
1:A:912:ILE:CD1	2:B:924:MET:HG2	1.98	0.93
12:M:66:ARG:HD3	13:I:37:THR:OG1	1.67	0.93
13:I:7:ALA:C	13:I:9:THR:H	1.74	0.93
10:N:35:LEU:HD22	10:N:42:LEU:HD21	1.50	0.93
2:B:396:ILE:HG22	2:B:422:MET:HB2	1.48	0.93
1:A:1326:TYR:HB3	13:I:60:VAL:HG12	1.48	0.93
1:A:424:LYS:HZ3	15:T:1:DG:P	1.91	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:THR:HG23	10:N:116:ARG:HH21	1.24	0.92
2:B:88:PRO:HD2	2:B:92:ILE:HD12	1.51	0.92
1:A:424:LYS:NZ	15:T:1:DG:P	2.41	0.92
1:A:316:GLY:H	15:T:10:DA:C2'	1.81	0.92
1:A:430:LYS:CA	2:B:1036:ARG:HH21	1.80	0.92
1:A:936:PRO:HG2	2:B:494:TRP:HB3	0.94	0.92
1:A:754:TYR:HE1	1:A:781:LEU:HD13	1.32	0.92
2:B:540:THR:CG2	10:N:116:ARG:NE	2.33	0.92
1:A:678:PRO:HB2	6:H:47:ILE:HG23	1.52	0.91
1:A:882:PRO:HG3	13:I:85:ARG:HH12	1.35	0.91
1:A:934:SER:O	2:B:491:PRO:CG	2.18	0.91
10:N:146:ARG:HH12	10:N:148:ARG:HH22	1.17	0.91
1:A:939:GLU:HG2	1:A:940:PRO:HD2	1.49	0.91
1:A:964:PHE:HZ	2:B:500:VAL:HG21	1.35	0.91
1:A:316:GLY:CA	15:T:10:DA:H3'	2.00	0.91
13:I:27:LEU:HB3	13:I:28:PRO:HD3	1.53	0.90
1:A:423:LYS:NZ	15:T:0:DT:OP2	2.03	0.90
6:H:104:THR:HG22	6:H:107:GLU:HB3	1.54	0.90
2:B:570:LEU:CD2	10:N:81:ARG:CZ	2.49	0.90
2:B:259:PHE:HA	12:M:110:GLN:HE22	1.34	0.90
1:A:1313:GLN:HE22	1:A:1535:LYS:HB2	1.37	0.89
2:B:540:THR:CG2	10:N:116:ARG:CZ	2.50	0.89
1:A:882:PRO:HD3	13:I:85:ARG:HH22	1.37	0.89
2:B:600:MET:HB3	2:B:608:PRO:HB3	1.54	0.89
12:M:67:LEU:HD21	12:M:69:TYR:CE1	2.05	0.89
1:A:929:MET:HG2	2:B:492:GLU:CD	1.98	0.89
1:A:1714:GLU:HB2	5:F:107:ARG:HB3	1.53	0.89
1:A:122:CYS:HB3	1:A:165:THR:HG21	1.53	0.89
2:B:547:HIS:CE1	10:N:83:LEU:HD13	2.08	0.89
2:B:543:ASP:CB	12:M:81:CYS:HB2	2.03	0.89
1:A:1580:THR:HG22	1:A:1582:GLY:H	1.35	0.89
2:B:73:ILE:HB	2:B:75:PHE:HZ	1.39	0.88
5:F:79:VAL:HG12	5:F:81:VAL:HG12	1.53	0.88
1:A:407:ASP:OD2	1:A:410:MET:CG	2.22	0.88
1:A:929:MET:HG2	2:B:492:GLU:OE2	1.74	0.88
2:B:792:LEU:HB2	2:B:865:LYS:CD	2.04	0.87
1:A:1326:TYR:HD2	13:I:60:VAL:CG1	1.86	0.87
2:B:408:SER:HA	2:B:411:MET:HB2	1.56	0.87
12:M:34:GLN:H	13:I:7:ALA:HB3	1.39	0.87
2:B:403:LYS:HB2	2:B:418:ARG:HH12	1.40	0.87
1:A:658:TYR:HB2	8:K:67:PHE:CZ	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:THR:HG23	10:N:116:ARG:CZ	2.05	0.87
1:A:969:MET:HG3	2:B:489:LEU:HD22	1.54	0.86
1:A:316:GLY:HA3	15:T:10:DA:H3'	1.55	0.86
1:A:929:MET:CE	2:B:492:GLU:HA	2.03	0.86
1:A:1296:LYS:NZ	13:I:52:GLY:HA3	1.89	0.86
1:A:1713:PHE:CZ	5:F:61:GLU:HA	2.11	0.86
1:A:1718:PRO:HD2	5:F:103:PRO:O	1.74	0.86
2:B:216:ARG:HB2	2:B:334:ILE:HG22	1.54	0.86
1:A:965:PHE:CE2	2:B:489:LEU:HD23	2.11	0.86
12:M:33:LEU:CD1	12:M:39:MET:SD	2.64	0.85
1:A:965:PHE:CE2	2:B:489:LEU:CD2	2.59	0.85
2:B:392:TRP:HE1	2:B:423:GLY:HA2	1.39	0.85
2:B:940:LEU:HD12	7:J:43:TYR:HB3	1.58	0.85
12:M:66:ARG:NH1	13:I:37:THR:OG1	2.08	0.85
1:A:975:LEU:HD21	13:I:104:SER:C	2.01	0.85
1:A:1619:ARG:NH2	4:E:196:PRO:HD2	1.91	0.85
2:B:262:TYR:HB3	12:M:30:ASN:CA	2.07	0.85
1:A:877:ASN:ND2	13:I:83:VAL:HG21	1.92	0.85
1:A:911:GLN:CD	13:I:109:GLN:HE22	1.84	0.85
2:B:117:ASP:HB3	2:B:131:LYS:HE2	1.56	0.84
1:A:1326:TYR:HD2	13:I:60:VAL:HG13	1.41	0.84
1:A:964:PHE:CE1	2:B:500:VAL:HG23	2.11	0.84
2:B:68:PHE:HA	2:B:405:GLN:HE22	1.42	0.84
2:B:538:GLY:HA2	10:N:118:LEU:HB3	1.59	0.84
1:A:308:ARG:NH1	2:B:1114:TYR:OH	2.10	0.84
1:A:433:MET:HB2	2:B:1039:GLU:HG2	1.57	0.84
12:M:34:GLN:HG3	13:I:8:ASN:N	1.92	0.84
2:B:178:VAL:HB	2:B:457:ALA:HB2	1.60	0.84
2:B:781:LEU:HD22	2:B:792:LEU:HB3	1.60	0.84
2:B:570:LEU:HD21	10:N:81:ARG:CZ	2.08	0.83
4:E:94:MET:HG2	4:E:99:ILE:HD11	1.58	0.83
1:A:975:LEU:HD22	13:I:104:SER:HA	1.56	0.83
2:B:570:LEU:CD2	10:N:81:ARG:HH11	1.88	0.83
2:B:810:ASP:OD2	9:L:17:TYR:OH	1.94	0.83
4:E:85:LYS:O	4:E:89:VAL:HG13	1.78	0.83
1:A:678:PRO:HB2	6:H:47:ILE:CG2	2.07	0.83
1:A:929:MET:HA	2:B:492:GLU:OE2	1.78	0.83
1:A:860:MET:HE2	1:A:864:LYS:HE3	1.60	0.83
2:B:260:SER:HB3	12:M:30:ASN:HD21	1.44	0.82
2:B:538:GLY:HA2	10:N:118:LEU:CB	2.09	0.82
2:B:854:VAL:HG12	9:L:34:ILE:HG21	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:7:ALA:C	13:I:9:THR:N	2.37	0.82
1:A:1334:ARG:HG3	1:A:1335:PRO:HD2	1.58	0.82
2:B:400:PHE:HA	2:B:418:ARG:CZ	2.09	0.82
2:B:792:LEU:HD12	2:B:865:LYS:HD2	1.61	0.82
1:A:1597:LEU:HD12	4:E:137:ILE:HG21	1.60	0.82
1:A:964:PHE:CZ	2:B:500:VAL:HG21	2.14	0.82
2:B:856:SER:CB	9:L:42:ARG:HB3	2.09	0.82
1:A:316:GLY:HA3	15:T:10:DA:C3'	2.10	0.82
2:B:965:MET:HE1	10:N:142:PRO:HD3	1.62	0.82
1:A:312:VAL:CG2	1:A:320:PHE:HB3	2.10	0.82
3:C:91:LYS:HE2	9:L:54:VAL:HG11	1.62	0.81
1:A:1590:LYS:NZ	4:E:133:GLN:NE2	2.28	0.81
2:B:758:ILE:HB	2:B:914:LEU:HB2	1.62	0.81
2:B:965:MET:HE1	10:N:142:PRO:CD	2.10	0.81
1:A:975:LEU:HD23	13:I:104:SER:CA	2.04	0.81
2:B:482:ARG:HB2	16:U:1:DG:O5'	1.80	0.81
2:B:708:ASP:O	2:B:776:SER:HB3	1.80	0.81
2:B:796:ILE:HD11	2:B:807:LEU:HB2	1.61	0.81
1:A:929:MET:CE	2:B:491:PRO:O	2.28	0.81
2:B:631:GLU:HG3	2:B:631:GLU:O	1.80	0.81
12:M:66:ARG:CD	13:I:37:THR:HG21	2.11	0.81
1:A:1097:GLN:O	1:A:1101:LYS:HG2	1.81	0.81
1:A:1153:ASP:OD1	1:A:1154:ILE:N	2.12	0.81
3:C:104:GLU:HG2	3:C:105:ILE:HD12	1.61	0.80
12:M:66:ARG:CD	13:I:37:THR:CB	2.57	0.80
1:A:1145:PRO:HD2	4:E:204:ILE:HD11	1.63	0.80
1:A:1512:ILE:HG21	1:A:1515:TYR:CE1	2.15	0.80
8:K:22:GLU:HG3	8:K:25:THR:H	1.44	0.80
12:M:34:GLN:HG2	13:I:8:ASN:HA	1.62	0.80
2:B:700:LEU:HD11	2:B:706:ARG:HG3	1.63	0.80
2:B:14:PRO:CD	2:B:946:ASP:HB3	2.10	0.80
2:B:540:THR:CG2	10:N:116:ARG:NH2	2.45	0.80
1:A:309:TYR:HE1	2:B:1114:TYR:CE1	2.00	0.80
2:B:73:ILE:CB	2:B:75:PHE:CZ	2.65	0.80
2:B:567:ASP:OD1	2:B:568:LYS:N	2.15	0.80
7:J:40:LEU:HD11	7:J:49:LEU:HD12	1.64	0.80
2:B:543:ASP:OD2	12:M:81:CYS:HB2	1.80	0.80
1:A:8:PRO:HB3	2:B:1109:THR:HB	1.62	0.79
2:B:783:GLU:OE1	2:B:783:GLU:N	2.15	0.79
1:A:935:LEU:HA	2:B:491:PRO:HB2	1.64	0.79
2:B:396:ILE:HA	2:B:422:MET:HG3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:66:ARG:CG	13:I:37:THR:HG21	2.12	0.79
1:A:929:MET:HG2	2:B:492:GLU:HG3	1.63	0.79
3:C:33:TYR:HB3	3:C:36:TYR:HB3	1.63	0.79
3:C:102:GLN:HB2	3:C:105:ILE:HD13	1.65	0.79
1:A:934:SER:O	2:B:491:PRO:HB2	1.83	0.79
1:A:1354:ILE:O	1:A:1357:LYS:HG2	1.81	0.79
1:A:929:MET:HE3	2:B:491:PRO:O	1.82	0.79
2:B:259:PHE:CA	12:M:110:GLN:HE22	1.96	0.79
3:C:53:VAL:HG21	8:K:118:ILE:HD13	1.64	0.79
1:A:310:ARG:HE	1:A:325:THR:HG22	1.47	0.78
1:A:1531:LEU:HB3	1:A:1535:LYS:HE2	1.64	0.78
1:A:1014:VAL:HG23	4:E:165:LEU:HD21	1.64	0.78
1:A:404:SER:HB2	1:A:415:PRO:HA	1.65	0.78
1:A:659:ARG:HH22	1:A:790:GLN:NE2	1.81	0.78
3:C:163:TYR:HD1	3:C:166:HIS:HB3	1.49	0.78
1:A:181:VAL:HG11	4:E:166:ARG:HH21	1.45	0.78
1:A:606:ALA:HB2	5:F:90:LEU:HD11	1.64	0.78
2:B:92:ILE:HD11	2:B:859:THR:HA	1.66	0.78
1:A:914:CYS:H	1:A:954:ARG:HD3	1.48	0.78
2:B:536:ASN:HA	10:N:48:PRO:CG	2.13	0.78
1:A:1715:LEU:O	5:F:105:ILE:N	2.15	0.78
2:B:548:ARG:O	10:N:88:GLN:NE2	2.16	0.77
1:A:403:ASP:HB3	1:A:406:MET:HE2	1.66	0.77
15:T:-2:DC:H42	16:U:3:DA:H61	1.32	0.77
1:A:964:PHE:CZ	2:B:500:VAL:CG2	2.66	0.77
1:A:425:GLU:HG3	1:A:426:GLY:H	1.48	0.77
1:A:929:MET:HG2	2:B:492:GLU:CG	2.13	0.77
1:A:429:ARG:HH12	15:T:1:DG:P	2.07	0.77
1:A:1531:LEU:HB3	1:A:1535:LYS:CE	2.15	0.77
5:F:81:VAL:HB	5:F:96:GLU:HG2	1.66	0.77
12:M:66:ARG:HB3	13:I:37:THR:HG21	1.64	0.77
1:A:1350:LEU:O	1:A:1354:ILE:HG12	1.83	0.77
2:B:758:ILE:CD1	2:B:895:ARG:HB2	2.13	0.77
13:I:82:VAL:HG23	13:I:96:ALA:HB1	1.67	0.77
1:A:934:SER:O	2:B:491:PRO:HG3	1.82	0.77
8:K:90:LEU:HD23	8:K:90:LEU:H	1.50	0.77
1:A:1716:LYS:HB2	5:F:105:ILE:HB	1.67	0.77
4:E:86:THR:O	4:E:89:VAL:HG22	1.84	0.77
1:A:430:LYS:HE3	1:A:431:HIS:HE1	1.51	0.76
1:A:1515:TYR:O	1:A:1516:GLN:HG2	1.85	0.76
2:B:75:PHE:CD2	2:B:397:LYS:HE3	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:916:ASN:OD1	2:B:917:PRO:HD2	1.86	0.76
2:B:262:TYR:CZ	13:I:9:THR:OG1	2.38	0.76
12:M:28:PHE:CE1	12:M:33:LEU:HD12	2.19	0.76
1:A:122:CYS:CB	1:A:165:THR:HG21	2.16	0.76
1:A:1111:ASN:ND2	4:E:61:LEU:HD23	2.00	0.76
2:B:651:VAL:HG21	10:N:130:LEU:HD23	1.67	0.76
4:E:168:ASN:O	4:E:169:GLN:HB3	1.84	0.76
1:A:874:ASN:HA	13:I:83:VAL:HG23	1.67	0.76
1:A:433:MET:CB	2:B:1039:GLU:HG2	2.14	0.76
1:A:1288:VAL:HG21	1:A:1333:LEU:HD22	1.67	0.76
3:C:147:THR:H	3:C:164:VAL:HG22	1.50	0.76
12:M:67:LEU:CB	13:I:17:LEU:HD23	2.10	0.76
1:A:316:GLY:N	15:T:10:DA:C2'	2.46	0.76
2:B:543:ASP:HB2	12:M:81:CYS:CB	2.16	0.76
2:B:68:PHE:HA	2:B:405:GLN:NE2	1.99	0.76
2:B:73:ILE:CB	2:B:75:PHE:HZ	1.99	0.76
12:M:67:LEU:HD12	12:M:68:SER:O	1.86	0.76
2:B:540:THR:HG22	10:N:116:ARG:HE	1.47	0.75
4:E:110:MET:CE	4:E:118:LEU:HD11	2.16	0.75
1:A:911:GLN:OE1	13:I:109:GLN:NE2	2.16	0.75
3:C:267:VAL:CG1	3:C:272:VAL:CG1	2.62	0.75
1:A:316:GLY:CA	15:T:10:DA:C3'	2.64	0.75
1:A:939:GLU:HG2	1:A:940:PRO:CD	2.17	0.75
1:A:1296:LYS:HE3	13:I:53:LYS:H	1.51	0.75
1:A:793:ARG:HG3	1:A:794:GLY:N	2.02	0.75
3:C:186:PRO:HG2	3:C:189:THR:OG1	1.86	0.75
2:B:684:ARG:HH22	13:I:106:ASP:CA	1.99	0.74
1:A:429:ARG:O	2:B:1036:ARG:NH2	2.19	0.74
2:B:1003:ARG:HD2	2:B:1003:ARG:O	1.87	0.74
10:N:88:GLN:O	10:N:91:GLU:HG3	1.86	0.74
1:A:31:LYS:NZ	1:A:48:ASN:OD1	2.21	0.74
1:A:797:LEU:HD12	1:A:897:MET:HE1	1.69	0.74
2:B:260:SER:CB	12:M:30:ASN:CG	2.60	0.74
12:M:67:LEU:HD22	13:I:17:LEU:CA	2.03	0.74
15:T:-5:DC:H2''	15:T:-4:DA:N7	2.03	0.74
2:B:170:PHE:O	2:B:176:GLU:HA	1.87	0.74
2:B:88:PRO:HD2	2:B:92:ILE:CD1	2.17	0.74
6:H:37:MET:HE3	6:H:127:GLY:HA3	1.70	0.74
1:A:877:ASN:ND2	13:I:97:TYR:OH	2.21	0.74
1:A:312:VAL:HG23	1:A:320:PHE:HA	1.70	0.73
3:C:267:VAL:HG12	3:C:272:VAL:HG11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:743:VAL:HG21	2:B:999:TYR:HE2	1.53	0.73
1:A:1225:GLN:O	1:A:1226:MET:HB2	1.87	0.73
1:A:1013:SER:HA	4:E:169:GLN:HG3	1.71	0.73
1:A:1014:VAL:HG21	4:E:165:LEU:HD21	1.70	0.73
3:C:27:THR:HA	3:C:32:ASN:ND2	2.03	0.73
12:M:67:LEU:CD2	13:I:17:LEU:HD23	2.19	0.73
1:A:134:ALA:O	1:A:138:LEU:HD23	1.89	0.73
1:A:424:LYS:NZ	15:T:1:DG:O5'	2.21	0.73
1:A:1289:CYS:HA	1:A:1552:VAL:HA	1.71	0.73
2:B:260:SER:OG	12:M:30:ASN:OD1	2.05	0.73
12:M:28:PHE:CE1	12:M:33:LEU:CD1	2.71	0.73
1:A:125:ARG:O	1:A:128:GLU:HG2	1.88	0.73
1:A:677:LYS:HG2	6:H:89:GLU:O	1.88	0.73
2:B:64:PHE:HE2	2:B:397:LYS:HB2	1.54	0.73
1:A:911:GLN:HA	1:A:915:LEU:O	1.89	0.73
1:A:1334:ARG:CG	1:A:1335:PRO:HD2	2.19	0.72
1:A:1349:LEU:HD21	1:A:1547:LEU:HD11	1.71	0.72
2:B:92:ILE:HG22	2:B:93:CYS:H	1.52	0.72
1:A:1328:GLN:NE2	1:A:1333:LEU:O	2.22	0.72
1:A:1590:LYS:NZ	4:E:133:GLN:HE22	1.87	0.72
2:B:181:MET:HE1	2:B:514:LEU:HD11	1.72	0.72
2:B:403:LYS:HB3	2:B:418:ARG:HH22	1.53	0.72
1:A:967:HIS:CD2	2:B:682:SER:HB2	2.25	0.72
2:B:73:ILE:HB	2:B:75:PHE:CE2	2.23	0.72
2:B:396:ILE:HA	2:B:422:MET:CG	2.19	0.72
8:K:30:VAL:HG23	8:K:41:THR:HB	1.70	0.72
1:A:749:LEU:HB3	1:A:754:TYR:HE2	1.53	0.72
2:B:538:GLY:HA3	10:N:118:LEU:HD13	1.72	0.72
4:E:61:LEU:HD13	4:E:73:PHE:HD1	1.55	0.72
7:J:57:GLU:O	7:J:61:ASN:ND2	2.21	0.72
1:A:429:ARG:CZ	15:T:1:DG:OP1	2.36	0.72
2:B:262:TYR:CB	12:M:30:ASN:HA	2.15	0.72
1:A:1335:PRO:O	1:A:1338:ILE:HG22	1.90	0.72
2:B:193:MET:SD	2:B:195:ARG:NH2	2.63	0.71
1:A:927:PRO:HG3	2:B:488:ARG:NH2	2.05	0.71
1:A:19:MET:HE1	1:A:91:LEU:HD11	1.72	0.71
1:A:1593:GLU:OE1	1:A:1593:GLU:N	2.21	0.71
2:B:73:ILE:CG2	2:B:75:PHE:CZ	2.74	0.71
1:A:749:LEU:HD23	1:A:754:TYR:OH	1.90	0.71
1:A:104:CYS:SG	1:A:211:GLY:HA3	2.30	0.71
1:A:138:LEU:HD11	1:A:165:THR:HG23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:ARG:NH2	13:I:106:ASP:CA	2.53	0.71
1:A:882:PRO:CG	13:I:85:ARG:HH12	2.02	0.71
2:B:622:PRO:HB3	2:B:631:GLU:OE2	1.91	0.71
3:C:287:ILE:HD11	3:C:299:LEU:HD22	1.71	0.71
12:M:28:PHE:CE2	12:M:33:LEU:HD11	2.24	0.71
1:A:650:ARG:HG2	1:A:654:MET:HE2	1.72	0.71
1:A:850:HIS:O	1:A:855:GLN:NE2	2.24	0.71
1:A:929:MET:SD	2:B:492:GLU:HG3	2.31	0.71
2:B:543:ASP:HB2	12:M:81:CYS:HB2	1.73	0.71
2:B:691:MET:HE3	2:B:884:ALA:HB1	1.73	0.71
6:H:104:THR:CG2	6:H:107:GLU:HB3	2.21	0.71
1:A:929:MET:CG	2:B:492:GLU:HG3	2.21	0.70
1:A:430:LYS:HE3	1:A:431:HIS:CE1	2.25	0.70
1:A:686:GLN:O	1:A:690:THR:HG22	1.92	0.70
1:A:1713:PHE:HZ	5:F:61:GLU:HA	1.52	0.70
1:A:512:MET:SD	1:A:515:ARG:NH2	2.65	0.70
1:A:1686:MET:HG3	1:A:1687:LEU:HD12	1.74	0.70
2:B:570:LEU:HD23	10:N:81:ARG:HH12	1.50	0.70
2:B:717:PRO:HB2	2:B:736:PRO:HB2	1.74	0.70
4:E:13:ILE:O	4:E:17:ILE:HG13	1.91	0.70
2:B:576:ASP:OD1	2:B:577:SER:N	2.25	0.70
2:B:394:VAL:O	2:B:398:ILE:HG12	1.91	0.70
3:C:54:VAL:HG21	3:C:279:ARG:NH2	2.07	0.70
4:E:159:LEU:HD23	4:E:160:LEU:HD23	1.74	0.70
6:H:104:THR:HB	6:H:109:ALA:HB2	1.74	0.70
6:H:96:VAL:HG22	6:H:116:VAL:HG22	1.73	0.70
1:A:1024:LEU:HA	1:A:1203:SER:O	1.92	0.70
2:B:46:PHE:O	2:B:50:VAL:HG22	1.92	0.70
4:E:190:VAL:HG22	4:E:208:LEU:HD12	1.73	0.70
1:A:793:ARG:HG3	1:A:794:GLY:H	1.57	0.70
3:C:184:LEU:HD23	3:C:185:PHE:CE2	2.27	0.70
2:B:58:VAL:HA	2:B:61:ILE:HG13	1.71	0.69
12:M:33:LEU:CG	12:M:39:MET:HE1	2.21	0.69
1:A:258:PRO:HD2	1:A:391:TRP:CZ3	2.27	0.69
2:B:543:ASP:CG	12:M:81:CYS:HB2	2.17	0.69
2:B:781:LEU:HD23	2:B:781:LEU:O	1.92	0.69
4:E:92:GLN:O	4:E:95:GLN:HG2	1.92	0.69
15:T:-1:DG:H2'	15:T:0:DT:C2	2.27	0.69
1:A:691:LEU:HD22	1:A:784:LEU:HD22	1.74	0.69
2:B:140:MET:CE	2:B:168:GLY:HA2	2.21	0.69
2:B:909:MET:HG2	7:J:42:ARG:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:93:ARG:NH1	4:E:97:GLU:OE2	2.26	0.69
1:A:1715:LEU:HD22	5:F:104:ILE:HG21	1.73	0.69
2:B:392:TRP:O	2:B:396:ILE:HG23	1.93	0.69
2:B:541:PRO:HD2	10:N:46:GLN:NE2	2.07	0.69
2:B:570:LEU:HD22	10:N:81:ARG:HH11	1.57	0.69
6:H:101:GLY:HA2	6:H:112:LEU:HD23	1.74	0.69
1:A:1097:GLN:HA	1:A:1100:VAL:HG22	1.75	0.69
2:B:263:GLN:CB	12:M:29:SER:O	2.38	0.69
2:B:541:PRO:HG2	12:M:85:CYS:SG	2.33	0.69
1:A:312:VAL:HG23	1:A:320:PHE:CA	2.22	0.69
1:A:754:TYR:HE1	1:A:781:LEU:CD1	2.05	0.69
4:E:54:ARG:HD2	4:E:57:ASP:HB3	1.72	0.69
12:M:111:PRO:CB	13:I:18:ASP:OD2	2.40	0.69
1:A:965:PHE:CZ	2:B:489:LEU:CD2	2.76	0.69
1:A:1326:TYR:CD2	13:I:60:VAL:CG1	2.74	0.69
1:A:851:LEU:HD21	2:B:362:MET:HE2	1.72	0.69
1:A:1296:LYS:CE	13:I:52:GLY:HA3	2.23	0.69
1:A:181:VAL:CG1	4:E:166:ARG:NH2	2.55	0.68
1:A:309:TYR:HE1	2:B:1114:TYR:HE1	1.40	0.68
1:A:964:PHE:HE1	2:B:500:VAL:HG23	1.53	0.68
1:A:929:MET:HE3	2:B:491:PRO:C	2.18	0.68
1:A:1516:GLN:HG3	1:A:1526:GLN:HG3	1.76	0.68
1:A:1715:LEU:O	5:F:104:ILE:HG23	1.94	0.68
2:B:651:VAL:HG13	2:B:656:THR:HG21	1.75	0.68
3:C:267:VAL:CG1	3:C:272:VAL:HG11	2.22	0.68
15:T:-9:DA:N6	16:U:10:DT:O2	2.27	0.68
1:A:908:ASN:ND2	13:I:126:SER:OG	2.26	0.68
1:A:1710:THR:HG23	5:F:64:ARG:HB2	1.73	0.68
12:M:66:ARG:CB	13:I:37:THR:HG21	2.22	0.68
1:A:20:TYR:CG	2:B:1129:LYS:HB2	2.29	0.68
1:A:1326:TYR:CB	13:I:60:VAL:HG12	2.22	0.68
1:A:1702:VAL:HG23	1:A:1704:LYS:HG3	1.76	0.68
3:C:138:LEU:HD12	3:C:181:GLN:HE22	1.58	0.68
2:B:400:PHE:CD1	2:B:418:ARG:HG2	2.29	0.68
1:A:316:GLY:HA3	15:T:10:DA:O3'	1.94	0.68
1:A:929:MET:HE2	2:B:492:GLU:HG3	1.76	0.68
2:B:392:TRP:NE1	2:B:423:GLY:HA2	2.09	0.68
2:B:568:LYS:HG3	2:B:600:MET:HE2	1.75	0.68
12:M:66:ARG:CZ	13:I:37:THR:HB	2.23	0.68
1:A:408:LYS:HZ2	1:A:409:LEU:HD22	1.54	0.68
1:A:860:MET:CE	1:A:864:LYS:HE3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:PRO:HA	1:A:1603:ASN:HD21	1.58	0.68
3:C:291:GLU:CA	3:C:294:LYS:HE3	2.21	0.68
15:T:-2:DC:H42	16:U:3:DA:N6	1.92	0.68
1:A:713:GLY:O	6:H:20:LYS:HE3	1.93	0.67
1:A:929:MET:CE	2:B:491:PRO:C	2.66	0.67
12:M:111:PRO:CG	13:I:18:ASP:CB	2.72	0.67
2:B:75:PHE:CE1	2:B:120:TRP:HB2	2.29	0.67
10:N:48:PRO:HD3	10:N:117:ILE:O	1.95	0.67
1:A:140:ARG:HH11	1:A:144:ARG:HH12	1.42	0.67
1:A:690:THR:O	1:A:694:ASN:ND2	2.27	0.67
1:A:806:PRO:O	1:A:807:LYS:HB3	1.93	0.67
3:C:16:LEU:HD12	3:C:21:VAL:HG23	1.77	0.67
1:A:44:ASN:HB2	1:A:45:PRO:HD2	1.74	0.67
1:A:911:GLN:NE2	13:I:109:GLN:OE1	2.27	0.67
1:A:965:PHE:CZ	2:B:489:LEU:HD21	2.29	0.67
1:A:1515:TYR:CD1	1:A:1527:VAL:HG23	2.30	0.67
1:A:1590:LYS:HZ2	4:E:133:GLN:NE2	1.93	0.67
7:J:3:ILE:HD12	7:J:4:PRO:HD2	1.75	0.67
10:N:70:LYS:HG2	10:N:79:ARG:HG2	1.74	0.67
1:A:1512:ILE:HD13	1:A:1529:VAL:HG22	1.77	0.67
1:A:1534:MET:C	1:A:1535:LYS:HD2	2.19	0.67
1:A:166:THR:HA	1:A:169:VAL:HG22	1.77	0.67
1:A:843:ARG:NH1	1:A:939:GLU:OE2	2.27	0.67
1:A:910:MET:O	1:A:911:GLN:HB3	1.94	0.67
2:B:260:SER:HB3	12:M:30:ASN:ND2	2.10	0.67
2:B:690:GLN:OE1	2:B:694:GLN:NE2	2.27	0.67
2:B:110:TYR:OH	2:B:146:CYS:SG	2.48	0.67
2:B:187:ARG:HD2	2:B:615:THR:HB	1.77	0.67
1:A:338:ILE:HG12	1:A:390:ILE:HD12	1.77	0.66
1:A:911:GLN:CD	13:I:109:GLN:NE2	2.53	0.66
2:B:785:ILE:HG21	2:B:792:LEU:CD2	2.17	0.66
12:M:111:PRO:HB2	13:I:18:ASP:OD2	1.95	0.66
1:A:979:ALA:O	1:A:982:THR:HG22	1.95	0.66
1:A:1566:GLU:HA	1:A:1576:LEU:HD13	1.75	0.66
2:B:1013:ARG:HD2	2:B:1034:GLY:N	2.10	0.66
1:A:430:LYS:HG2	1:A:431:HIS:ND1	2.10	0.66
1:A:916:LEU:HB2	1:A:953:GLY:O	1.96	0.66
4:E:84:ILE:O	4:E:88:LYS:HG2	1.95	0.66
1:A:299:LEU:CD2	2:B:1127:ASN:OD1	2.42	0.66
1:A:929:MET:CG	2:B:492:GLU:OE2	2.43	0.66
2:B:536:ASN:HA	10:N:48:PRO:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:LEU:HB2	3:C:301:ARG:HD3	1.76	0.66
4:E:77:PRO:HD2	4:E:105:VAL:O	1.96	0.66
1:A:603:LEU:O	1:A:603:LEU:HD23	1.96	0.66
12:M:34:GLN:HG2	13:I:8:ASN:CA	2.25	0.66
12:M:67:LEU:HD21	12:M:69:TYR:HH	1.58	0.66
1:A:181:VAL:HG11	4:E:166:ARG:HH22	1.58	0.65
1:A:874:ASN:CA	13:I:83:VAL:HG23	2.25	0.65
1:A:961:PRO:HB3	2:B:666:LEU:HD22	1.77	0.65
1:A:1034:PRO:HD3	1:A:1166:LYS:HD3	1.78	0.65
4:E:127:LEU:O	4:E:128:GLU:HG3	1.95	0.65
8:K:42:PHE:CE1	8:K:84:ILE:HD12	2.31	0.65
3:C:245:VAL:CG2	3:C:273:ALA:HB3	2.26	0.65
1:A:1296:LYS:HZ2	13:I:52:GLY:HA3	1.60	0.65
1:A:1566:GLU:HA	1:A:1576:LEU:CD1	2.26	0.65
2:B:194:ILE:HG23	2:B:207:GLN:OE1	1.97	0.65
2:B:233:THR:HG23	2:B:285:MET:HG2	1.78	0.65
2:B:566:VAL:HG21	2:B:574:ILE:HD12	1.78	0.65
2:B:757:MET:HE3	2:B:759:VAL:CG2	2.26	0.65
4:E:94:MET:SD	4:E:102:ALA:HB2	2.37	0.65
6:H:102:ASP:OD2	6:H:111:ARG:HB2	1.96	0.65
1:A:1104:LYS:CB	1:A:1116:GLY:HA2	2.27	0.65
1:A:1349:LEU:CD2	1:A:1547:LEU:HD11	2.26	0.65
2:B:403:LYS:HE2	2:B:418:ARG:NH2	2.11	0.65
5:F:79:VAL:CG1	5:F:81:VAL:HG12	2.25	0.65
10:N:112:GLN:OE1	10:N:112:GLN:N	2.30	0.65
1:A:173:LEU:O	1:A:174:LEU:HB3	1.96	0.65
1:A:651:GLU:HG2	3:C:29:PHE:HD2	1.61	0.65
2:B:806:LYS:HG2	2:B:824:PRO:HD2	1.78	0.65
6:H:48:TYR:OH	6:H:147:LYS:HG3	1.96	0.65
1:A:642:THR:O	1:A:685:LYS:HE2	1.96	0.65
2:B:540:THR:CG2	10:N:116:ARG:HE	2.04	0.65
1:A:1006:THR:HG21	1:A:1008:ARG:HE	1.62	0.65
2:B:1013:ARG:NE	2:B:1025:PRO:HB3	2.12	0.65
1:A:137:GLU:HG2	1:A:164:TYR:OH	1.97	0.65
1:A:8:PRO:HG3	2:B:1066:VAL:HG13	1.77	0.65
1:A:1096:ILE:O	1:A:1100:VAL:HG13	1.97	0.65
1:A:1133:ARG:HG2	1:A:1133:ARG:O	1.97	0.65
1:A:1296:LYS:HE3	13:I:52:GLY:CA	2.27	0.65
1:A:1334:ARG:CD	1:A:1335:PRO:HD2	2.27	0.65
12:M:32:LYS:O	13:I:8:ASN:N	2.30	0.65
1:A:807:LYS:HG3	1:A:807:LYS:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:21:GLU:OE1	9:L:21:GLU:N	2.31	0.64
1:A:812:ARG:HD2	1:A:914:CYS:HA	1.77	0.64
1:A:1104:LYS:HB2	1:A:1116:GLY:HA2	1.78	0.64
1:A:1516:GLN:HG3	1:A:1526:GLN:H	1.62	0.64
2:B:504:ASP:OD2	13:I:105:ALA:HB2	1.97	0.64
2:B:936:LYS:HG2	2:B:966:LEU:HD21	1.79	0.64
4:E:110:MET:SD	4:E:118:LEU:HD11	2.37	0.64
2:B:346:LEU:O	2:B:350:THR:HG23	1.97	0.64
3:C:11:ARG:O	3:C:303:ARG:HD3	1.97	0.64
1:A:316:GLY:N	15:T:10:DA:C3'	2.61	0.64
1:A:440:ALA:HB1	2:B:1035:ILE:HD11	1.80	0.64
1:A:677:LYS:CG	6:H:89:GLU:O	2.44	0.64
1:A:1008:ARG:NH1	5:F:111:PRO:HG2	2.13	0.64
2:B:856:SER:HB3	9:L:42:ARG:CB	2.26	0.64
12:M:111:PRO:CD	13:I:18:ASP:OD2	2.45	0.64
1:A:607:GLU:OE2	1:A:1710:THR:HG21	1.98	0.64
1:A:1313:GLN:HG2	1:A:1537:ASN:HD21	1.63	0.64
1:A:749:LEU:HD23	1:A:754:TYR:CZ	2.32	0.64
1:A:791:LEU:HD22	2:B:984:SER:HB3	1.79	0.64
1:A:877:ASN:HD21	13:I:83:VAL:HG21	1.62	0.64
1:A:882:PRO:HG3	13:I:85:ARG:NH1	2.09	0.64
1:A:1718:PRO:CD	5:F:103:PRO:O	2.44	0.64
3:C:274:ARG:HB3	3:C:274:ARG:HH11	1.61	0.64
4:E:20:LEU:HD11	4:E:24:ARG:HE	1.61	0.64
1:A:1145:PRO:HD2	4:E:204:ILE:CD1	2.28	0.64
2:B:684:ARG:NH2	13:I:106:ASP:HA	2.12	0.64
7:J:1:MET:HE3	7:J:56:ILE:CD1	2.22	0.64
1:A:408:LYS:HZ1	1:A:409:LEU:CD2	2.11	0.64
1:A:873:SER:C	1:A:876:ILE:H	2.06	0.64
1:A:1296:LYS:HB2	13:I:53:LYS:H	1.62	0.64
9:L:34:ILE:O	9:L:34:ILE:HG22	1.98	0.64
1:A:85:LEU:HD22	1:A:391:TRP:HE1	1.63	0.64
1:A:606:ALA:CB	5:F:90:LEU:HD11	2.28	0.64
1:A:674:SER:HB2	6:H:118:TYR:O	1.97	0.64
4:E:90:TYR:OH	4:E:104:ILE:HD13	1.97	0.64
1:A:964:PHE:CE1	2:B:500:VAL:CG2	2.80	0.64
2:B:842:LYS:O	2:B:844:LYS:HE2	1.97	0.64
4:E:185:ILE:HD12	4:E:191:VAL:HG11	1.80	0.64
1:A:1090:LEU:HD12	4:E:22:HIS:NE2	2.13	0.63
2:B:75:PHE:CD1	2:B:120:TRP:HB2	2.33	0.63
2:B:216:ARG:HB2	2:B:334:ILE:CG2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LYS:HG2	1:A:431:HIS:CE1	2.34	0.63
1:A:868:GLU:H	1:A:868:GLU:CD	2.06	0.63
1:A:936:PRO:CG	2:B:494:TRP:CB	2.63	0.63
2:B:73:ILE:CG2	2:B:75:PHE:HZ	2.09	0.63
2:B:146:CYS:O	2:B:149:ARG:HG2	1.97	0.63
2:B:566:VAL:CG2	2:B:574:ILE:HD12	2.28	0.63
4:E:9:ARG:HD2	4:E:132:GLN:HE21	1.64	0.63
1:A:929:MET:HE2	2:B:492:GLU:N	2.12	0.63
1:A:1119:GLU:OE1	1:A:1122:ARG:NH1	2.22	0.63
1:A:1293:VAL:O	1:A:1294:LEU:HG	1.99	0.63
2:B:190:PRO:HB3	2:B:349:MET:HG2	1.79	0.63
1:A:460:MET:HG3	1:A:570:PRO:HA	1.81	0.63
2:B:229:LEU:HD11	2:B:235:MET:HE3	1.79	0.63
2:B:400:PHE:HD1	2:B:418:ARG:HG2	1.61	0.63
6:H:39:LEU:HD13	6:H:125:LEU:HD13	1.80	0.63
3:C:7:VAL:N	6:H:49:PRO:HD2	2.13	0.63
13:I:87:CYS:O	13:I:95:MET:HG3	1.99	0.63
1:A:21:SER:HB3	1:A:24:GLU:HG2	1.81	0.63
1:A:679:PHE:CD1	6:H:47:ILE:HG12	2.33	0.63
1:A:823:GLY:HA2	1:A:865:PHE:HE1	1.64	0.63
1:A:1113:ARG:HD3	4:E:61:LEU:O	1.99	0.63
1:A:1338:ILE:HG23	1:A:1339:LEU:HD12	1.81	0.63
2:B:538:GLY:CA	10:N:118:LEU:HD13	2.27	0.63
1:A:897:MET:SD	2:B:918:HIS:ND1	2.72	0.63
10:N:146:ARG:HH12	10:N:148:ARG:NH2	1.92	0.63
1:A:414:TYR:HB3	1:A:415:PRO:HD2	1.81	0.63
2:B:171:ILE:HG23	2:B:174:GLY:HA2	1.81	0.63
12:M:32:LYS:O	13:I:7:ALA:N	2.32	0.63
1:A:1282:LYS:CE	1:A:1564:LEU:HD13	2.27	0.62
2:B:721:LEU:CD2	7:J:50:LEU:HD23	2.29	0.62
3:C:15:VAL:HA	3:C:300:ALA:HB2	1.81	0.62
12:M:66:ARG:CD	13:I:37:THR:OG1	2.45	0.62
1:A:20:TYR:HB2	2:B:1127:ASN:O	1.99	0.62
1:A:1223:SER:HB2	1:A:1245:ILE:CD1	2.29	0.62
1:A:1289:CYS:N	1:A:1292:GLU:OE2	2.31	0.62
2:B:791:SER:HB3	2:B:792:LEU:HD23	1.81	0.62
2:B:936:LYS:HE3	2:B:966:LEU:CD2	2.29	0.62
4:E:59:THR:HG23	4:E:74:VAL:O	1.99	0.62
1:A:1619:ARG:HH12	4:E:196:PRO:HG2	1.63	0.62
2:B:791:SER:HA	2:B:830:ASN:HA	1.81	0.62
1:A:632:GLN:HE22	2:B:754:GLU:H	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:LEU:HD22	4:E:30:GLN:HG2	1.80	0.62
2:B:743:VAL:HG22	2:B:913:ILE:HB	1.81	0.62
8:K:55:LEU:HD21	8:K:96:PHE:CE1	2.34	0.62
1:A:423:LYS:HG3	1:A:424:LYS:H	1.63	0.62
1:A:1569:ASN:O	1:A:1573:GLU:HA	2.00	0.62
12:M:66:ARG:NE	13:I:37:THR:HB	2.14	0.62
12:M:67:LEU:CD2	12:M:69:TYR:CE1	2.81	0.62
13:I:54:VAL:HG22	13:I:56:LYS:H	1.64	0.62
1:A:122:CYS:SG	1:A:165:THR:HG21	2.40	0.62
1:A:127:LEU:HD21	1:A:135:VAL:CG2	2.30	0.62
1:A:677:LYS:O	1:A:678:PRO:C	2.42	0.62
1:A:846:TRP:HE1	1:A:858:PHE:HE1	1.48	0.62
2:B:1013:ARG:HG3	2:B:1032:GLN:HB3	1.81	0.62
6:H:39:LEU:CD1	6:H:125:LEU:HD13	2.28	0.62
15:T:3:DC:H2'	15:T:4:DA:C8	2.34	0.62
1:A:1326:TYR:CD2	13:I:60:VAL:HG12	2.35	0.62
1:A:1670:GLN:O	1:A:1671:GLN:HB3	2.00	0.62
2:B:113:LYS:HG3	2:B:133:PHE:HE1	1.65	0.62
2:B:647:PHE:O	2:B:650:GLU:HB2	1.99	0.62
2:B:742:ILE:HD13	2:B:996:VAL:HG22	1.81	0.62
2:B:791:SER:HA	2:B:830:ASN:OD1	2.00	0.62
3:C:241:LEU:HD23	3:C:297:VAL:HG22	1.80	0.62
3:C:326:ILE:HG21	8:K:111:LEU:HB2	1.82	0.62
1:A:225:ILE:HG23	1:A:256:LEU:CD1	2.30	0.62
1:A:677:LYS:HB3	6:H:91:VAL:H	1.65	0.62
2:B:583:VAL:HG13	2:B:630:LYS:HB3	1.81	0.62
1:A:974:GLY:HA3	13:I:101:GLN:O	1.99	0.61
2:B:237:ASN:HD21	2:B:244:LEU:HD22	1.65	0.61
4:E:173:ILE:HG23	4:E:209:VAL:HA	1.81	0.61
1:A:668:VAL:H	8:K:85:GLN:HE22	1.49	0.61
1:A:975:LEU:CD2	13:I:104:SER:C	2.67	0.61
1:A:1008:ARG:CZ	5:F:111:PRO:HG2	2.31	0.61
1:A:1583:ILE:HD11	1:A:1607:ALA:CB	2.30	0.61
1:A:1619:ARG:HH22	4:E:196:PRO:CD	2.04	0.61
2:B:64:PHE:CE2	2:B:397:LYS:HB2	2.35	0.61
2:B:312:LEU:HD21	2:B:327:LEU:HD12	1.82	0.61
2:B:392:TRP:HE1	2:B:423:GLY:CA	2.13	0.61
2:B:936:LYS:HE3	2:B:966:LEU:HD22	1.80	0.61
8:K:25:THR:HB	8:K:46:GLU:OE1	2.00	0.61
1:A:433:MET:HB2	2:B:1039:GLU:CG	2.29	0.61
1:A:1024:LEU:HD12	1:A:1204:LEU:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1615:GLU:OE2	4:E:207:ARG:NE	2.31	0.61
3:C:33:TYR:CB	3:C:36:TYR:HB3	2.29	0.61
1:A:743:GLU:CD	6:H:140:ARG:HH22	2.09	0.61
2:B:695:THR:HG21	2:B:737:ILE:HG12	1.81	0.61
1:A:1004:ASP:OD1	1:A:1006:THR:HG22	2.00	0.61
2:B:262:TYR:OH	13:I:9:THR:OG1	2.18	0.61
1:A:223:LEU:O	1:A:256:LEU:HB2	2.00	0.61
1:A:895:GLN:O	1:A:896:MET:HB3	2.01	0.61
1:A:967:HIS:CD2	2:B:682:SER:H	2.18	0.61
1:A:970:ALA:O	1:A:973:GLU:HG2	2.00	0.61
1:A:424:LYS:NZ	15:T:1:DG:OP2	2.28	0.61
1:A:926:PRO:HD2	1:A:948:GLY:O	2.01	0.61
1:A:939:GLU:CG	1:A:940:PRO:HD2	2.26	0.61
3:C:53:VAL:O	10:N:157:PRO:HD3	2.01	0.61
1:A:397:HIS:CE1	1:A:410:MET:HE1	2.35	0.61
2:B:262:TYR:CD2	12:M:30:ASN:C	2.77	0.61
2:B:1069:VAL:HG21	2:B:1134:VAL:HG21	1.83	0.61
9:L:16:ILE:HG23	9:L:25:GLU:HB3	1.81	0.61
10:N:142:PRO:HG2	10:N:145:LEU:HD21	0.70	0.61
1:A:438:ASP:HB3	2:B:1014:THR:O	2.00	0.61
1:A:812:ARG:HG3	1:A:876:ILE:HG23	1.81	0.61
1:A:1111:ASN:ND2	4:E:61:LEU:CD2	2.64	0.61
1:A:1335:PRO:HA	1:A:1338:ILE:HG22	1.82	0.61
1:A:1498:MET:HA	1:A:1501:ARG:HH12	1.65	0.61
2:B:752:ASP:O	2:B:916:ASN:HB2	2.00	0.61
12:M:34:GLN:CG	13:I:8:ASN:N	2.63	0.61
3:C:264:VAL:HG13	3:C:264:VAL:O	2.00	0.61
4:E:126:ILE:O	4:E:126:ILE:HG13	1.99	0.61
1:A:919:ILE:HG12	1:A:949:GLY:O	2.01	0.60
2:B:92:ILE:HG22	2:B:93:CYS:N	2.15	0.60
3:C:12:SER:O	3:C:303:ARG:N	2.34	0.60
6:H:63:THR:HA	6:H:71:ASP:OD1	2.01	0.60
7:J:40:LEU:CD1	7:J:49:LEU:HD12	2.31	0.60
1:A:408:LYS:NZ	1:A:409:LEU:HD21	2.12	0.60
1:A:651:GLU:HG2	3:C:29:PHE:CD2	2.37	0.60
1:A:732:MET:HE2	6:H:27:ARG:HH12	1.66	0.60
1:A:790:GLN:NE2	2:B:983:ILE:HD13	2.16	0.60
1:A:865:PHE:C	1:A:867:GLU:H	2.09	0.60
2:B:691:MET:HE3	2:B:884:ALA:CB	2.31	0.60
3:C:18:GLU:HB2	3:C:288:PHE:CD2	2.37	0.60
13:I:29:LEU:HD21	13:I:39:ILE:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:THR:HG21	2:B:1041:GLU:HG3	1.81	0.60
1:A:976:VAL:CG1	2:B:484:THR:HG21	2.31	0.60
2:B:680:ASN:HD21	2:B:887:HIS:HD2	1.46	0.60
3:C:30:PRO:CG	8:K:61:LYS:HA	2.31	0.60
10:N:61:VAL:HG11	12:M:11:TRP:CE3	2.35	0.60
1:A:137:GLU:OE1	1:A:140:ARG:NH2	2.34	0.60
2:B:648:GLU:HG3	10:N:130:LEU:HD22	1.83	0.60
2:B:185:PRO:O	2:B:372:GLN:HA	2.02	0.60
2:B:536:ASN:HA	10:N:48:PRO:HG3	1.83	0.60
1:A:975:LEU:HD23	13:I:103:ARG:O	2.02	0.60
1:A:975:LEU:HD21	13:I:105:ALA:N	2.15	0.60
2:B:263:GLN:HB2	12:M:29:SER:C	2.26	0.60
2:B:547:HIS:NE2	10:N:83:LEU:HD13	2.17	0.60
13:I:14:GLN:NE2	13:I:35:THR:O	2.34	0.60
1:A:37:ARG:HH11	1:A:40:ASP:HA	1.67	0.60
1:A:1170:TYR:HE2	1:A:1192:LEU:HD21	1.67	0.60
1:A:1541:SER:HA	1:A:1544:VAL:HG22	1.83	0.60
2:B:201:ARG:HB2	2:B:205:TYR:HD2	1.67	0.60
2:B:526:TYR:CE2	2:B:528:ALA:HB3	2.37	0.60
1:A:898:VAL:HG21	1:A:909:THR:HG21	1.83	0.60
1:A:967:HIS:CD2	2:B:682:SER:CB	2.84	0.60
2:B:498:CYS:HB2	2:B:668:SER:HB2	1.84	0.60
2:B:943:LEU:HD11	10:N:142:PRO:HG3	1.84	0.60
3:C:337:LEU:HD12	8:K:104:MET:HE1	1.84	0.60
8:K:83:ARG:HH11	8:K:85:GLN:HE21	1.48	0.60
1:A:468:TYR:CE2	1:A:605:ARG:HD2	2.37	0.60
1:A:877:ASN:ND2	13:I:83:VAL:CG2	2.64	0.60
1:A:309:TYR:CE1	2:B:1114:TYR:HE1	2.20	0.59
1:A:951:VAL:HG22	1:A:963:GLU:OE1	2.02	0.59
1:A:1037:PHE:N	1:A:1038:PRO:HD2	2.16	0.59
2:B:543:ASP:OD2	12:M:81:CYS:CB	2.49	0.59
3:C:337:LEU:HD12	8:K:104:MET:CE	2.32	0.59
8:K:22:GLU:HG2	8:K:25:THR:OG1	2.02	0.59
1:A:873:SER:HB2	13:I:83:VAL:HB	1.82	0.59
1:A:1318:ARG:HD2	1:A:1524:TRP:HE3	1.67	0.59
2:B:562:MET:HE2	2:B:564:GLY:HA2	1.83	0.59
2:B:758:ILE:HD13	2:B:895:ARG:HB2	1.84	0.59
1:A:826:ALA:HB2	1:A:868:GLU:CD	2.26	0.59
2:B:703:TYR:HE1	2:B:711:LEU:HD22	1.67	0.59
2:B:965:MET:HE1	10:N:142:PRO:HD2	1.85	0.59
4:E:37:LEU:O	4:E:41:LYS:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:66:GLU:HB3	8:K:87:ARG:HE	1.67	0.59
1:A:316:GLY:H	15:T:10:DA:C3'	2.16	0.59
1:A:968:CYS:CB	2:B:686:MET:CE	2.80	0.59
3:C:245:VAL:HG21	3:C:253:LEU:CD2	2.32	0.59
1:A:1565:ASN:HD22	1:A:1579:ASN:ND2	2.01	0.59
6:H:24:ARG:HG2	6:H:46:GLN:OE1	2.02	0.59
6:H:14:ASP:HB2	6:H:29:HIS:HB2	1.84	0.59
7:J:10:CYS:SG	7:J:42:ARG:HD2	2.42	0.59
1:A:1523:LEU:HD12	1:A:1524:TRP:N	2.17	0.59
4:E:60:VAL:HG22	4:E:74:VAL:HB	1.84	0.59
1:A:632:GLN:HB2	2:B:753:MET:HE3	1.82	0.59
1:A:865:PHE:O	1:A:867:GLU:N	2.36	0.59
1:A:1006:THR:HG23	1:A:1008:ARG:HG3	1.83	0.59
2:B:42:HIS:O	2:B:140:MET:HE1	2.03	0.59
2:B:235:MET:HE2	2:B:248:PRO:HA	1.85	0.59
2:B:549:SER:O	2:B:550:TYR:HB2	2.02	0.59
10:N:142:PRO:HG2	10:N:145:LEU:CG	2.27	0.59
2:B:139:ILE:HG22	2:B:140:MET:O	2.03	0.59
2:B:500:VAL:HA	2:B:686:MET:HG2	1.85	0.59
4:E:35:GLN:HA	4:E:39:GLU:OE2	2.03	0.59
12:M:68:SER:O	12:M:111:PRO:HA	2.02	0.59
1:A:39:LEU:HD12	1:A:39:LEU:O	2.03	0.59
1:A:404:SER:O	1:A:413:LYS:HD2	2.03	0.59
2:B:75:PHE:CE2	2:B:397:LYS:HE3	2.37	0.59
2:B:500:VAL:HG13	2:B:686:MET:HA	1.84	0.59
1:A:654:MET:HE1	8:K:60:MET:HE1	1.84	0.58
1:A:754:TYR:CD1	1:A:781:LEU:HD13	2.37	0.58
1:A:1505:VAL:HG22	1:A:1509:HIS:CE1	2.38	0.58
2:B:39:THR:HG22	2:B:469:PHE:CG	2.38	0.58
2:B:229:LEU:HD21	2:B:235:MET:HB2	1.85	0.58
2:B:414:ASP:CB	2:B:417:MET:HE3	2.33	0.58
2:B:882:LYS:HD2	2:B:1002:LEU:HD23	1.85	0.58
12:M:111:PRO:CG	13:I:18:ASP:CG	2.56	0.58
1:A:1590:LYS:HZ1	4:E:133:GLN:HE22	1.49	0.58
1:A:1669:LEU:HB2	1:A:1691:ASP:OD2	2.03	0.58
2:B:92:ILE:HD11	2:B:858:ASP:O	2.03	0.58
2:B:239:ILE:HD11	2:B:242:LYS:HA	1.85	0.58
2:B:781:LEU:CD2	2:B:792:LEU:HB3	2.31	0.58
3:C:42:GLN:O	3:C:46:GLU:HG3	2.03	0.58
3:C:245:VAL:HG23	3:C:273:ALA:HB3	1.85	0.58
1:A:122:CYS:HB3	1:A:165:THR:CG2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLN:HA	1:A:524:THR:CB	2.23	0.58
1:A:959:ILE:O	2:B:678:ASP:OD1	2.20	0.58
1:A:1117:THR:O	1:A:1121:LEU:HD23	2.03	0.58
2:B:403:LYS:HB2	2:B:418:ARG:NH1	2.14	0.58
2:B:753:MET:HA	2:B:916:ASN:HD22	1.68	0.58
1:A:91:LEU:H	1:A:91:LEU:HD23	1.68	0.58
1:A:929:MET:CA	2:B:492:GLU:OE2	2.51	0.58
1:A:1296:LYS:CE	13:I:52:GLY:CA	2.82	0.58
3:C:290:ASN:ND2	3:C:293:LEU:HD12	2.18	0.58
8:K:44:LEU:HD12	8:K:80:ILE:HD11	1.84	0.58
1:A:654:MET:CE	8:K:60:MET:HE1	2.33	0.58
2:B:68:PHE:HB3	2:B:73:ILE:HD11	1.83	0.58
2:B:106:ARG:HG2	2:B:855:CYS:HB3	1.84	0.58
2:B:162:GLU:C	2:B:164:GLU:H	2.11	0.58
12:M:11:TRP:CE2	12:M:101:VAL:HG21	2.39	0.58
1:A:33:ILE:CD1	1:A:50:LEU:HD13	2.34	0.58
1:A:912:ILE:HG12	2:B:924:MET:HG2	1.83	0.58
2:B:66:PHE:HZ	2:B:400:PHE:CD2	2.21	0.58
2:B:703:TYR:HE1	2:B:711:LEU:CD2	2.17	0.58
1:A:678:PRO:CB	6:H:47:ILE:CG2	2.81	0.58
1:A:678:PRO:CB	6:H:47:ILE:HG23	2.30	0.58
1:A:1296:LYS:HE3	13:I:53:LYS:N	2.17	0.58
2:B:648:GLU:O	2:B:649:ASP:HB2	2.03	0.58
3:C:30:PRO:HG2	8:K:60:MET:O	2.03	0.58
1:A:112:CYS:HB2	1:A:117:ILE:HD11	1.85	0.58
4:E:73:PHE:HB2	4:E:99:ILE:CD1	2.34	0.58
12:M:72:ASN:ND2	12:M:74:PHE:O	2.36	0.58
3:C:91:LYS:HE2	9:L:54:VAL:CG1	2.32	0.58
3:C:93:LEU:HD22	9:L:54:VAL:HG22	1.84	0.58
6:H:100:GLU:HG3	6:H:100:GLU:O	2.02	0.58
1:A:42:LEU:O	1:A:42:LEU:HD23	2.03	0.58
1:A:225:ILE:HG23	1:A:256:LEU:HG	1.85	0.58
1:A:912:ILE:HD11	2:B:924:MET:CG	2.26	0.58
1:A:929:MET:CE	2:B:492:GLU:HG3	2.34	0.58
1:A:1318:ARG:HA	1:A:1526:GLN:HA	1.85	0.58
10:N:142:PRO:HG3	10:N:145:LEU:HD21	1.72	0.58
1:A:76:GLY:HA3	1:A:306:PRO:HB3	1.86	0.57
1:A:652:HIS:HE1	3:C:24:VAL:O	1.87	0.57
1:A:797:LEU:HD12	1:A:897:MET:CE	2.34	0.57
1:A:1110:ARG:HB3	1:A:1118:GLN:HE22	1.69	0.57
2:B:416:LEU:HA	2:B:419:ILE:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:147:LYS:O	6:H:148:LEU:HD23	2.04	0.57
1:A:969:MET:CG	2:B:489:LEU:HB3	2.34	0.57
1:A:972:ARG:HG3	2:B:508:CYS:SG	2.43	0.57
1:A:1710:THR:HA	5:F:60:TYR:HB3	1.86	0.57
2:B:130:ILE:HG21	2:B:419:ILE:HD13	1.86	0.57
2:B:543:ASP:OD2	12:M:81:CYS:CA	2.52	0.57
2:B:684:ARG:HH22	13:I:106:ASP:HA	1.67	0.57
3:C:245:VAL:CG1	3:C:296:VAL:HG11	2.35	0.57
6:H:90:TYR:HH	6:H:92:MET:HE3	1.69	0.57
8:K:25:THR:HB	8:K:46:GLU:CD	2.29	0.57
12:M:66:ARG:NH1	13:I:37:THR:CB	2.67	0.57
13:I:7:ALA:HA	13:I:15:SER:HB2	1.85	0.57
1:A:488:PRO:HG3	1:A:508:SER:HA	1.86	0.57
3:C:54:VAL:HA	10:N:157:PRO:HD3	1.86	0.57
3:C:86:THR:CG2	3:C:227:PRO:HB3	2.34	0.57
1:A:137:GLU:HG2	1:A:164:TYR:CZ	2.39	0.57
1:A:965:PHE:CZ	2:B:489:LEU:HD23	2.39	0.57
1:A:1008:ARG:CZ	5:F:111:PRO:CG	2.81	0.57
1:A:1110:ARG:HB3	1:A:1118:GLN:NE2	2.19	0.57
1:A:1117:THR:HG22	1:A:1121:LEU:HD23	1.86	0.57
2:B:568:LYS:HE2	2:B:600:MET:CE	2.29	0.57
2:B:821:TYR:HB2	2:B:844:LYS:NZ	2.18	0.57
1:A:602:GLU:OE1	5:F:89:PRO:HG2	2.05	0.57
1:A:654:MET:O	1:A:655:GLU:HB3	2.05	0.57
1:A:1585:LEU:HB2	1:A:1586:PRO:HD3	1.87	0.57
1:A:1585:LEU:HD12	1:A:1600:LEU:HD21	1.87	0.57
2:B:104:ARG:O	2:B:707:SER:OG	2.22	0.57
2:B:554:TYR:O	2:B:565:TRP:HA	2.05	0.57
2:B:700:LEU:HD21	2:B:711:LEU:HD11	1.86	0.57
4:E:142:HIS:HB3	4:E:145:VAL:HG23	1.85	0.57
13:I:86:ARG:HA	13:I:94:GLY:HA2	1.86	0.57
1:A:651:GLU:CG	3:C:29:PHE:HD2	2.16	0.57
1:A:1631:VAL:HG23	1:A:1632:TYR:CD2	2.39	0.57
2:B:201:ARG:HB2	2:B:205:TYR:CD2	2.40	0.57
2:B:743:VAL:CG2	2:B:999:TYR:HE2	2.16	0.57
2:B:854:VAL:CG1	9:L:34:ILE:HG21	2.33	0.57
1:A:84:PRO:HD3	1:A:335:VAL:HG22	1.85	0.57
1:A:1519:THR:HG23	1:A:1520:GLU:CD	2.29	0.57
2:B:524:PHE:CE2	2:B:616:PRO:HG3	2.39	0.57
4:E:122:ALA:HB1	4:E:123:PRO:HD2	1.85	0.57
1:A:93:PHE:CZ	1:A:223:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:HIS:O	1:A:656:LEU:HB2	2.04	0.57
1:A:749:LEU:HD23	1:A:754:TYR:CE2	2.39	0.57
1:A:1349:LEU:HA	1:A:1352:GLU:CD	2.30	0.57
1:A:1533:LEU:H	1:A:1535:LYS:HZ2	1.51	0.57
3:C:138:LEU:HD21	3:C:190:ILE:HD13	1.86	0.57
1:A:739:ILE:HD13	1:A:761:LEU:HD13	1.87	0.57
2:B:781:LEU:HD23	2:B:792:LEU:HD22	1.85	0.57
3:C:267:VAL:CG1	3:C:272:VAL:HG12	2.24	0.57
10:N:49:ALA:HA	12:M:86:ARG:HG3	1.87	0.57
2:B:696:MET:HG3	2:B:712:TYR:HB3	1.87	0.57
12:M:33:LEU:CD1	12:M:39:MET:CE	2.83	0.57
12:M:111:PRO:HD2	13:I:18:ASP:OD2	2.04	0.57
2:B:742:ILE:CD1	2:B:996:VAL:HG22	2.34	0.56
10:N:45:ILE:HB	12:M:88:PHE:HB2	1.87	0.56
1:A:1003:TYR:CE2	5:F:108:ARG:HB3	2.39	0.56
1:A:1326:TYR:HB3	13:I:60:VAL:O	2.04	0.56
10:N:146:ARG:NH1	10:N:148:ARG:HH22	1.96	0.56
1:A:309:TYR:CE1	2:B:1114:TYR:CE1	2.88	0.56
1:A:431:HIS:HA	2:B:1024:GLN:HE22	1.69	0.56
1:A:1531:LEU:HB3	1:A:1535:LYS:CD	2.36	0.56
1:A:1715:LEU:HD22	5:F:104:ILE:CG2	2.35	0.56
2:B:103:CYS:SG	2:B:171:ILE:HG21	2.46	0.56
2:B:141:VAL:HG12	2:B:142:LYS:HG2	1.87	0.56
2:B:186:ARG:HG3	2:B:187:ARG:H	1.69	0.56
2:B:260:SER:HB2	12:M:30:ASN:CG	2.25	0.56
2:B:527:THR:OG1	2:B:530:ILE:HD12	2.05	0.56
2:B:530:ILE:HB	2:B:531:PRO:HD3	1.87	0.56
3:C:98:THR:O	3:C:206:GLN:HG2	2.05	0.56
4:E:80:PRO:O	4:E:108:GLN:HB2	2.05	0.56
4:E:165:LEU:HD23	4:E:169:GLN:HE21	1.68	0.56
6:H:36:LYS:HA	6:H:36:LYS:HE3	1.87	0.56
12:M:66:ARG:CD	13:I:37:THR:HB	2.31	0.56
1:A:502:GLY:O	1:A:503:SER:OG	2.18	0.56
2:B:909:MET:HE3	7:J:44:CYS:HB3	1.87	0.56
12:M:33:LEU:CD1	12:M:39:MET:HE1	2.34	0.56
1:A:123:GLN:O	1:A:127:LEU:HD23	2.06	0.56
1:A:619:LEU:HD22	1:A:624:GLY:O	2.06	0.56
1:A:969:MET:HG2	2:B:489:LEU:HB3	1.88	0.56
1:A:1497:ALA:O	1:A:1498:MET:C	2.47	0.56
1:A:1512:ILE:HD12	1:A:1527:VAL:HG21	1.86	0.56
12:M:11:TRP:CZ2	12:M:101:VAL:HG21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:CD2	1:A:518:VAL:HG11	2.35	0.56
1:A:1083:LEU:HD12	1:A:1083:LEU:O	2.06	0.56
1:A:1318:ARG:CD	1:A:1524:TRP:HE3	2.19	0.56
1:A:1605:ILE:HG21	1:A:1621:ILE:CG1	2.36	0.56
7:J:63:ALA:HB1	9:L:23:HIS:NE2	2.20	0.56
1:A:14:GLY:HA2	1:A:1691:ASP:O	2.06	0.56
1:A:827:VAL:HG22	1:A:861:ILE:CG2	2.35	0.56
1:A:1239:MET:HG3	1:A:1239:MET:O	2.05	0.56
2:B:333:CYS:HB3	2:B:342:LYS:HG3	1.88	0.56
2:B:745:VAL:HG12	2:B:917:PRO:HB3	1.86	0.56
3:C:75:ALA:HA	8:K:50:THR:HG23	1.86	0.56
10:N:70:LYS:HE2	10:N:79:ARG:CZ	2.34	0.56
1:A:8:PRO:O	1:A:9:TRP:HB3	2.05	0.56
1:A:603:LEU:HG	5:F:67:GLY:HA3	1.88	0.56
1:A:914:CYS:O	1:A:915:LEU:HB2	2.05	0.56
2:B:600:MET:HB3	2:B:608:PRO:CB	2.32	0.56
2:B:785:ILE:HD12	2:B:791:SER:HB2	1.88	0.56
12:M:111:PRO:CB	13:I:18:ASP:HB2	2.36	0.56
1:A:711:ILE:N	1:A:750:ASP:OD2	2.35	0.56
1:A:907:VAL:HB	13:I:111:VAL:HG21	1.86	0.56
1:A:1003:TYR:CD2	5:F:108:ARG:HB3	2.41	0.56
2:B:547:HIS:CE1	10:N:83:LEU:CD1	2.84	0.56
6:H:103:GLU:OE1	6:H:103:GLU:N	2.28	0.56
1:A:465:LYS:HZ2	2:B:1014:THR:HG22	1.70	0.56
1:A:674:SER:HB3	1:A:686:GLN:OE1	2.05	0.56
1:A:881:MET:HE1	1:A:895:GLN:NE2	2.20	0.56
1:A:968:CYS:HB3	2:B:686:MET:HE2	1.88	0.56
1:A:1618:LEU:HD11	1:A:1649:CYS:HB2	1.87	0.56
2:B:651:VAL:HG21	10:N:130:LEU:CD2	2.36	0.56
3:C:28:ASP:O	3:C:29:PHE:HD1	1.89	0.56
15:T:8:DA:H2''	15:T:9:DT:C5	2.41	0.56
1:A:225:ILE:HG23	1:A:256:LEU:HD11	1.88	0.55
1:A:429:ARG:NH2	15:T:1:DG:OP1	2.38	0.55
1:A:1213:LEU:O	1:A:1217:GLN:HG3	2.07	0.55
1:A:1637:ASP:OD2	1:A:1639:ARG:HD3	2.06	0.55
12:M:66:ARG:CD	13:I:37:THR:CG2	2.73	0.55
1:A:19:MET:HG2	1:A:296:VAL:CG1	2.37	0.55
1:A:505:THR:HG23	1:A:505:THR:O	2.06	0.55
2:B:399:ALA:O	2:B:418:ARG:NH1	2.40	0.55
8:K:89:THR:HG23	8:K:90:LEU:N	2.21	0.55
1:A:310:ARG:HB3	1:A:322:ASN:HD22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:PRO:HB2	1:A:572:GLU:O	2.06	0.55
1:A:606:ALA:O	1:A:610:VAL:HG23	2.06	0.55
1:A:678:PRO:HG2	6:H:90:TYR:HD1	1.71	0.55
1:A:1502:VAL:O	1:A:1505:VAL:HG12	2.06	0.55
1:A:1583:ILE:HD12	1:A:1604:ASP:HB2	1.88	0.55
2:B:86:THR:HG23	2:B:96:ALA:O	2.05	0.55
3:C:74:ASN:O	3:C:78:ARG:HG3	2.06	0.55
3:C:183:ASP:O	3:C:184:LEU:HB3	2.06	0.55
7:J:1:MET:CE	7:J:56:ILE:HD13	2.24	0.55
9:L:19:CYS:HB3	9:L:23:HIS:H	1.71	0.55
12:M:68:SER:HB2	12:M:112:LEU:CB	2.36	0.55
15:T:-6:DA:H5'	15:T:-6:DA:C8	2.42	0.55
1:A:661:LEU:HG	1:A:691:LEU:HD12	1.89	0.55
1:A:1693:LEU:HD13	1:A:1702:VAL:HG21	1.88	0.55
1:A:929:MET:CB	2:B:492:GLU:OE2	2.54	0.55
1:A:1008:ARG:NH2	4:E:163:TYR:O	2.39	0.55
2:B:721:LEU:HD21	7:J:50:LEU:HD23	1.87	0.55
1:A:961:PRO:HD2	1:A:962:PRO:HD2	1.88	0.55
1:A:1128:ASP:HB3	1:A:1133:ARG:HD3	1.88	0.55
2:B:568:LYS:HG3	2:B:600:MET:CE	2.37	0.55
2:B:651:VAL:HG13	2:B:656:THR:CG2	2.36	0.55
2:B:702:THR:HG22	7:J:62:TYR:CE2	2.41	0.55
2:B:808:ASP:HB3	2:B:814:PHE:CE2	2.42	0.55
2:B:1067:ALA:HB2	2:B:1117:ARG:HD3	1.88	0.55
4:E:152:THR:HG23	4:E:154:GLU:HG2	1.89	0.55
6:H:110:THR:HG23	6:H:110:THR:O	2.06	0.55
1:A:921:LEU:HA	1:A:973:GLU:OE2	2.06	0.55
1:A:1516:GLN:CG	1:A:1526:GLN:HG3	2.36	0.55
2:B:61:ILE:HG22	2:B:61:ILE:O	2.05	0.55
2:B:903:PRO:HB2	2:B:979:LEU:HD23	1.89	0.55
3:C:288:PHE:CZ	3:C:299:LEU:HD21	2.42	0.55
1:A:220:ASN:O	1:A:221:SER:HB2	2.07	0.55
1:A:795:PHE:HE2	1:A:897:MET:HE2	1.72	0.55
10:N:83:LEU:HD12	10:N:116:ARG:NH1	2.22	0.55
12:M:111:PRO:CG	13:I:18:ASP:HB2	2.37	0.55
15:T:2:DT:H2'	15:T:3:DC:C6	2.42	0.55
1:A:121:LEU:O	1:A:125:ARG:HG3	2.07	0.54
5:F:61:GLU:O	5:F:65:VAL:HG23	2.07	0.54
6:H:104:THR:HB	6:H:109:ALA:CB	2.37	0.54
1:A:1108:GLU:N	1:A:1108:GLU:OE1	2.40	0.54
3:C:30:PRO:HA	3:C:38:ASP:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:122:ALA:HB1	4:E:123:PRO:CD	2.37	0.54
5:F:125:ILE:HG13	5:F:125:ILE:O	2.07	0.54
1:A:430:LYS:CA	2:B:1036:ARG:NH2	2.54	0.54
1:A:741:GLU:OE2	6:H:138:ASP:OD2	2.25	0.54
2:B:536:ASN:OD1	10:N:48:PRO:HB3	2.06	0.54
2:B:736:PRO:HG2	7:J:53:VAL:HG11	1.87	0.54
4:E:54:ARG:HD2	4:E:57:ASP:CB	2.36	0.54
1:A:402:PHE:CE2	2:B:1126:MET:HG2	2.42	0.54
1:A:522:LEU:O	1:A:523:LEU:HB2	2.08	0.54
1:A:799:VAL:O	1:A:803:LEU:HG	2.07	0.54
1:A:873:SER:HB3	1:A:915:LEU:CD2	2.38	0.54
1:A:1034:PRO:O	1:A:1035:LYS:HB3	2.06	0.54
2:B:399:ALA:HB2	2:B:422:MET:HE2	1.88	0.54
4:E:61:LEU:HD12	4:E:72:MET:O	2.07	0.54
1:A:422:GLU:O	1:A:423:LYS:HB2	2.08	0.54
1:A:1598:ARG:HA	4:E:142:HIS:HD2	1.73	0.54
8:K:86:THR:HG22	8:K:92:ALA:HB2	1.89	0.54
1:A:1293:VAL:HA	1:A:1322:LEU:HD12	1.88	0.54
2:B:66:PHE:HE1	2:B:75:PHE:CE2	2.24	0.54
2:B:194:ILE:HG12	2:B:208:TYR:CD1	2.42	0.54
2:B:965:MET:HE2	10:N:141:ILE:HD13	1.88	0.54
6:H:90:TYR:OH	6:H:92:MET:HE3	2.08	0.54
1:A:1529:VAL:HG12	1:A:1530:LYS:N	2.22	0.54
2:B:319:PRO:HB2	2:B:321:GLU:HG2	1.89	0.54
2:B:951:ILE:HD12	10:N:139:PRO:CG	2.38	0.54
3:C:53:VAL:HG13	3:C:61:LEU:HD11	1.89	0.54
6:H:37:MET:HE1	6:H:132:LEU:HD21	1.89	0.54
1:A:972:ARG:HH21	2:B:509:GLY:HA3	1.64	0.54
1:A:1605:ILE:HG12	1:A:1620:VAL:HG12	1.89	0.54
2:B:10:LEU:CD1	2:B:11:PRO:HD2	2.30	0.54
12:M:68:SER:HB2	12:M:112:LEU:HB3	1.90	0.54
1:A:968:CYS:HA	2:B:686:MET:CE	2.38	0.54
1:A:1170:TYR:CE2	1:A:1192:LEU:HD21	2.42	0.54
2:B:141:VAL:O	2:B:146:CYS:SG	2.66	0.54
2:B:703:TYR:O	2:B:704:GLN:HB3	2.08	0.54
2:B:940:LEU:HD23	2:B:969:ALA:CB	2.37	0.54
5:F:57:MET:HE1	5:F:120:VAL:HG13	1.90	0.54
8:K:55:LEU:HD23	8:K:82:LEU:HD11	1.90	0.54
1:A:180:HIS:HB3	1:A:1692:GLU:OE2	2.08	0.54
3:C:184:LEU:CD2	3:C:185:PHE:CE2	2.91	0.54
3:C:239:ILE:HD13	3:C:261:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:340:LEU:HD23	8:K:97:GLN:HB2	1.90	0.54
16:U:7:DT:H2''	16:U:8:DC:O4'	2.08	0.54
1:A:602:GLU:CD	5:F:89:PRO:HG2	2.34	0.53
1:A:739:ILE:CD1	1:A:761:LEU:HD13	2.37	0.53
1:A:931:SER:OG	2:B:640:ILE:HG21	2.03	0.53
1:A:1068:HIS:CE1	1:A:1144:ASP:O	2.61	0.53
1:A:1245:ILE:N	1:A:1246:PRO:HD2	2.24	0.53
1:A:1324:HIS:HA	1:A:1327:TYR:CE1	2.43	0.53
1:A:1640:HIS:O	1:A:1644:VAL:HG23	2.07	0.53
2:B:178:VAL:O	2:B:178:VAL:HG13	2.07	0.53
2:B:835:GLU:HG3	2:B:837:PHE:CZ	2.43	0.53
1:A:91:LEU:CD1	2:B:1128:ILE:HD11	2.38	0.53
2:B:548:ARG:C	10:N:88:GLN:HE22	2.10	0.53
3:C:13:ARG:HA	3:C:301:ARG:O	2.08	0.53
3:C:15:VAL:HG23	3:C:22:ARG:HB2	1.89	0.53
12:M:67:LEU:HD23	13:I:17:LEU:HD23	1.89	0.53
1:A:20:TYR:CE1	2:B:1129:LYS:HD3	2.43	0.53
1:A:308:ARG:HD3	2:B:1114:TYR:OH	2.08	0.53
1:A:914:CYS:H	1:A:954:ARG:CD	2.20	0.53
1:A:1133:ARG:C	1:A:1134:LYS:HE2	2.33	0.53
1:A:1221:GLU:HB3	1:A:1222:PRO:HD3	1.89	0.53
2:B:1013:ARG:HD2	2:B:1034:GLY:CA	2.38	0.53
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.44	0.53
1:A:438:ASP:CB	2:B:1014:THR:O	2.56	0.53
1:A:960:LYS:HB3	1:A:961:PRO:CD	2.39	0.53
1:A:972:ARG:HD2	2:B:502:THR:HG21	1.89	0.53
3:C:14:VAL:O	3:C:300:ALA:HB1	2.07	0.53
1:A:105:LEU:HD12	1:A:264:HIS:ND1	2.24	0.53
1:A:312:VAL:CG2	1:A:320:PHE:CB	2.85	0.53
3:C:12:SER:O	3:C:303:ARG:HB2	2.08	0.53
4:E:13:ILE:HD11	4:E:132:GLN:HG3	1.91	0.53
10:N:11:ARG:O	10:N:12:PHE:C	2.49	0.53
10:N:95:LEU:HD11	12:M:26:VAL:HG11	1.89	0.53
1:A:931:SER:OG	2:B:640:ILE:HG23	2.06	0.53
1:A:969:MET:CG	2:B:489:LEU:HD22	2.33	0.53
1:A:1044:TYR:HD1	1:A:1195:LEU:HD22	1.72	0.53
1:A:1566:GLU:H	1:A:1566:GLU:CD	2.16	0.53
2:B:270:LYS:HG3	2:B:550:TYR:CD2	2.44	0.53
2:B:1014:THR:HG23	2:B:1015:THR:H	1.73	0.53
1:A:120:LEU:O	1:A:124:LEU:HD23	2.08	0.53
1:A:1088:ALA:O	1:A:1091:SER:OG	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1618:LEU:O	1:A:1622:GLU:HG3	2.08	0.53
2:B:75:PHE:CG	2:B:397:LYS:HE3	2.43	0.53
12:M:66:ARG:CB	13:I:17:LEU:HD21	2.39	0.53
1:A:312:VAL:CG2	1:A:320:PHE:HA	2.39	0.53
1:A:682:TRP:N	1:A:682:TRP:CD1	2.76	0.53
1:A:1610:ASN:O	4:E:178:PRO:CG	2.57	0.53
2:B:514:LEU:HD22	2:B:518:CYS:SG	2.48	0.53
2:B:643:ASN:ND2	2:B:655:VAL:HG13	2.24	0.53
2:B:1056:ASP:O	2:B:1057:ARG:C	2.50	0.53
3:C:339:GLU:HG2	8:K:26:ALA:CB	2.39	0.53
1:A:30:VAL:HB	1:A:66:THR:HG21	1.90	0.53
1:A:182:LYS:O	1:A:183:ASN:HB2	2.09	0.53
2:B:110:TYR:CZ	2:B:146:CYS:SG	2.89	0.53
2:B:695:THR:CG2	2:B:1000:GLN:HB3	2.39	0.53
4:E:72:MET:HE1	4:E:103:LEU:HD12	1.91	0.53
4:E:205:THR:HG22	4:E:206:TYR:H	1.74	0.53
1:A:968:CYS:CB	2:B:686:MET:HE2	2.39	0.53
2:B:217:GLU:HB2	2:B:219:HIS:CE1	2.43	0.53
3:C:173:MET:HE3	3:C:212:MET:HE1	1.91	0.53
15:T:-8:DG:H2'	15:T:-7:DG:O4'	2.08	0.53
1:A:609:TYR:CD2	5:F:90:LEU:CD2	2.92	0.52
1:A:652:HIS:CE1	3:C:24:VAL:HG13	2.44	0.52
1:A:1518:ASP:OD2	1:A:1525:CYS:HB3	2.10	0.52
1:A:1518:ASP:HB3	1:A:1523:LEU:H	1.73	0.52
2:B:48:TYR:CE1	2:B:52:GLU:HG2	2.45	0.52
2:B:396:ILE:HG13	2:B:397:LYS:N	2.23	0.52
2:B:656:THR:HG22	2:B:656:THR:O	2.09	0.52
2:B:716:THR:O	2:B:716:THR:HG23	2.09	0.52
2:B:757:MET:HE3	2:B:759:VAL:HG23	1.90	0.52
2:B:808:ASP:HB3	2:B:814:PHE:CZ	2.44	0.52
4:E:20:LEU:HD12	4:E:20:LEU:O	2.08	0.52
8:K:58:MET:HG3	8:K:103:LEU:HB2	1.90	0.52
1:A:404:SER:HB2	1:A:416:GLY:H	1.73	0.52
2:B:1013:ARG:NH2	2:B:1025:PRO:HA	2.25	0.52
3:C:18:GLU:OE1	3:C:18:GLU:HA	2.08	0.52
6:H:29:HIS:CE1	6:H:40:ILE:HD12	2.44	0.52
7:J:53:VAL:HG13	7:J:53:VAL:O	2.09	0.52
12:M:67:LEU:CD2	12:M:69:TYR:OH	2.45	0.52
2:B:113:LYS:HG3	2:B:133:PHE:CE1	2.42	0.52
4:E:173:ILE:CG2	4:E:209:VAL:HA	2.38	0.52
1:A:972:ARG:CZ	2:B:509:GLY:CA	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:ILE:HG23	1:A:1154:ILE:O	2.10	0.52
1:A:1349:LEU:HG	1:A:1547:LEU:HD21	1.91	0.52
1:A:85:LEU:CD2	1:A:391:TRP:HE1	2.23	0.52
1:A:457:GLY:HA2	1:A:567:ARG:O	2.09	0.52
1:A:613:CYS:O	1:A:617:GLN:HG2	2.09	0.52
2:B:595:VAL:HA	2:B:612:LEU:HD23	1.91	0.52
6:H:65:TYR:HB3	6:H:67:ASP:OD2	2.10	0.52
13:I:7:ALA:O	13:I:9:THR:N	2.28	0.52
1:A:1624:GLU:O	1:A:1628:VAL:HG23	2.09	0.52
2:B:69:LYS:HD3	2:B:407:THR:H	1.73	0.52
2:B:411:MET:HE2	2:B:411:MET:N	2.24	0.52
3:C:68:ILE:HD11	3:C:72:ILE:HG21	1.91	0.52
3:C:312:SER:HB3	3:C:321:LEU:CD1	2.39	0.52
15:T:-7:DG:H2"	15:T:-6:DA:C8	2.45	0.52
1:A:166:THR:O	1:A:170:GLN:HG2	2.09	0.52
1:A:1293:VAL:O	1:A:1293:VAL:HG13	2.09	0.52
1:A:1359:ASN:O	1:A:1360:LYS:HD2	2.10	0.52
3:C:66:VAL:HG22	3:C:305:HIS:CE1	2.44	0.52
6:H:137:VAL:O	6:H:138:ASP:HB2	2.09	0.52
1:A:521:GLN:CA	1:A:524:THR:HB	2.25	0.52
1:A:618:TYR:CE2	1:A:626:PRO:HB3	2.44	0.52
1:A:651:GLU:CD	3:C:29:PHE:HD2	2.17	0.52
1:A:712:THR:HG22	1:A:714:LYS:H	1.74	0.52
2:B:77:ILE:HG12	2:B:118:ILE:HG22	1.91	0.52
2:B:224:MET:HE1	2:B:346:LEU:HD21	1.91	0.52
2:B:260:SER:CB	12:M:30:ASN:ND2	2.72	0.52
2:B:295:SER:O	13:I:19:PHE:CZ	2.63	0.52
8:K:124:GLN:O	8:K:128:ARG:HG2	2.09	0.52
1:A:33:ILE:HD11	1:A:81:ILE:HG13	1.92	0.52
1:A:550:LEU:HD23	1:A:594:MET:SD	2.49	0.52
1:A:929:MET:HG3	2:B:491:PRO:HG2	1.91	0.52
3:C:15:VAL:HA	3:C:300:ALA:CB	2.40	0.52
4:E:190:VAL:HG22	4:E:208:LEU:CD1	2.38	0.52
13:I:24:GLY:HA2	13:I:30:PRO:HD3	1.91	0.52
1:A:215:VAL:HG22	1:A:225:ILE:HG22	1.92	0.52
1:A:305:PRO:HG3	2:B:1125:ALA:HB2	1.92	0.52
1:A:713:GLY:O	6:H:20:LYS:CE	2.58	0.52
1:A:1589:PHE:HA	1:A:1597:LEU:HD13	1.91	0.52
2:B:178:VAL:O	2:B:179:ILE:C	2.53	0.52
2:B:648:GLU:HG2	2:B:649:ASP:N	2.25	0.52
3:C:221:ASP:OD2	9:L:58:ARG:NH2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:121:ASP:OD1	5:F:122:GLU:N	2.43	0.52
1:A:1003:TYR:OH	5:F:61:GLU:OE2	2.10	0.51
1:A:1029:THR:O	1:A:1033:GLN:NE2	2.41	0.51
1:A:1651:GLU:C	4:E:172:ARG:HB2	2.35	0.51
2:B:169:TYR:CE1	2:B:176:GLU:HG2	2.44	0.51
1:A:1096:ILE:HA	1:A:1120:MET:CE	2.40	0.51
2:B:194:ILE:HG12	2:B:208:TYR:CE1	2.45	0.51
2:B:473:HIS:HD2	2:B:475:GLY:H	1.58	0.51
1:A:181:VAL:CG1	4:E:166:ARG:HH22	2.20	0.51
1:A:677:LYS:HE2	6:H:88:PHE:O	2.11	0.51
1:A:1318:ARG:HH21	1:A:1526:GLN:HG2	1.75	0.51
2:B:742:ILE:HD12	7:J:43:TYR:HE1	1.75	0.51
1:A:912:ILE:CG1	2:B:924:MET:CG	2.81	0.51
2:B:639:GLN:O	2:B:639:GLN:HG2	2.09	0.51
2:B:1113:PRO:HD2	2:B:1116:PHE:HB2	1.93	0.51
5:F:104:ILE:O	5:F:120:VAL:HG23	2.10	0.51
1:A:312:VAL:CG2	1:A:320:PHE:CA	2.88	0.51
1:A:1348:LYS:CE	1:A:1508:ILE:HB	2.40	0.51
1:A:1512:ILE:HD12	1:A:1527:VAL:CG2	2.39	0.51
13:I:7:ALA:N	13:I:15:SER:O	2.43	0.51
1:A:607:GLU:HB3	2:B:1050:THR:HG22	1.92	0.51
1:A:543:LYS:HG3	1:A:543:LYS:O	2.09	0.51
1:A:927:PRO:HG3	2:B:488:ARG:CZ	2.41	0.51
1:A:965:PHE:CE2	2:B:489:LEU:HD21	2.40	0.51
1:A:1610:ASN:O	4:E:178:PRO:HG3	2.11	0.51
2:B:791:SER:C	2:B:792:LEU:HD23	2.36	0.51
2:B:1124:ALA:C	2:B:1126:MET:H	2.18	0.51
1:A:1110:ARG:HD3	1:A:1110:ARG:C	2.35	0.51
1:A:1114:SER:OG	1:A:1115:PRO:HD2	2.11	0.51
1:A:1353:SER:OG	1:A:1543:LEU:HD11	2.11	0.51
2:B:102:GLU:O	2:B:103:CYS:SG	2.68	0.51
2:B:212:MET:SD	2:B:345:MET:HE3	2.51	0.51
2:B:262:TYR:C	2:B:262:TYR:HD1	2.19	0.51
2:B:785:ILE:HG12	2:B:786:LYS:O	2.11	0.51
3:C:29:PHE:HB3	3:C:30:PRO:CD	2.41	0.51
12:M:34:GLN:HA	13:I:8:ASN:HB2	1.93	0.51
1:A:123:GLN:O	1:A:126:VAL:HG22	2.10	0.51
1:A:166:THR:HA	1:A:169:VAL:CG2	2.41	0.51
1:A:802:ILE:HG22	1:A:894:LEU:HD22	1.92	0.51
1:A:1147:LEU:HD22	1:A:1152:PRO:HB3	1.93	0.51
1:A:1583:ILE:HD11	1:A:1607:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:ARG:HD2	2:B:615:THR:CB	2.40	0.51
2:B:691:MET:CE	2:B:884:ALA:HB1	2.41	0.51
3:C:335:ARG:NH2	8:K:25:THR:O	2.43	0.51
12:M:34:GLN:CG	13:I:8:ASN:CA	2.88	0.51
13:I:84:ASP:HA	13:I:96:ALA:HA	1.92	0.51
1:A:441:ALA:HB2	2:B:1012:VAL:HG13	1.93	0.51
1:A:499:ASN:HD22	1:A:536:LYS:HD2	1.76	0.51
1:A:841:GLU:O	1:A:845:LYS:HG2	2.11	0.51
1:A:1068:HIS:HE1	1:A:1144:ASP:O	1.93	0.51
1:A:1134:LYS:HE2	1:A:1134:LYS:HA	1.92	0.51
1:A:1279:LYS:O	1:A:1283:LYS:HD3	2.11	0.51
2:B:624:GLN:NE2	2:B:629:GLY:HA2	2.26	0.51
12:M:111:PRO:HG2	13:I:18:ASP:CA	2.39	0.51
1:A:428:PHE:O	1:A:432:MET:HB3	2.11	0.50
1:A:766:TYR:HD1	1:A:771:GLY:HA2	1.75	0.50
1:A:1625:ILE:HG21	1:A:1641:LEU:HD22	1.93	0.50
2:B:172:ILE:HG12	2:B:434:PHE:HB3	1.93	0.50
2:B:262:TYR:C	2:B:262:TYR:CD1	2.89	0.50
4:E:10:LEU:CD2	4:E:58:LEU:HD11	2.41	0.50
13:I:88:PRO:HG3	13:I:92:HIS:CD2	2.47	0.50
1:A:57:PRO:HD3	1:A:64:CYS:HB3	1.93	0.50
1:A:1125:TYR:HE1	4:E:68:PRO:HB3	1.76	0.50
2:B:396:ILE:CG2	2:B:422:MET:HB2	2.33	0.50
2:B:659:GLN:HG3	2:B:660:GLU:N	2.23	0.50
4:E:154:GLU:O	4:E:158:GLU:HG3	2.11	0.50
1:A:163:GLN:O	1:A:166:THR:HG22	2.11	0.50
1:A:465:LYS:O	1:A:467:THR:HG23	2.12	0.50
1:A:869:VAL:HG21	1:A:918:GLN:HE21	1.76	0.50
2:B:87:VAL:HB	2:B:92:ILE:HD12	1.93	0.50
2:B:948:THR:O	2:B:951:ILE:HG12	2.11	0.50
4:E:87:ILE:HG22	4:E:121:MET:HE1	1.93	0.50
12:M:34:GLN:H	13:I:7:ALA:CB	2.19	0.50
1:A:163:GLN:HG3	1:A:164:TYR:N	2.26	0.50
1:A:601:SER:O	1:A:602:GLU:HB3	2.10	0.50
2:B:419:ILE:HG13	2:B:420:PHE:N	2.27	0.50
2:B:570:LEU:HD21	10:N:81:ARG:NE	2.26	0.50
2:B:657:THR:HG22	2:B:658:HIS:ND1	2.27	0.50
2:B:743:VAL:CG2	2:B:997:VAL:HG22	2.41	0.50
2:B:920:PHE:N	2:B:921:PRO:HD2	2.26	0.50
1:A:19:MET:HG2	1:A:296:VAL:HG11	1.93	0.50
1:A:1300:GLN:HB2	1:A:1316:GLN:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:GLU:O	2:B:568:LYS:HB2	2.11	0.50
2:B:1080:LEU:O	2:B:1096:TYR:HA	2.11	0.50
2:B:262:TYR:HB3	12:M:30:ASN:CB	2.42	0.50
2:B:341:GLU:OE1	12:M:80:LYS:HE3	2.12	0.50
2:B:655:VAL:HG12	2:B:656:THR:H	1.76	0.50
3:C:15:VAL:HG12	3:C:298:ARG:HH21	1.77	0.50
8:K:42:PHE:HE1	8:K:84:ILE:HD12	1.73	0.50
8:K:86:THR:OG1	8:K:90:LEU:HD21	2.11	0.50
10:N:121:PRO:HD2	10:N:121:PRO:O	2.10	0.50
13:I:82:VAL:HG13	13:I:98:HIS:CE1	2.47	0.50
1:A:795:PHE:CE2	1:A:897:MET:HE2	2.47	0.50
1:A:865:PHE:C	1:A:867:GLU:N	2.70	0.50
1:A:1151:ARG:HG3	1:A:1153:ASP:OD1	2.11	0.50
2:B:615:THR:HB	2:B:616:PRO:HD2	1.94	0.50
2:B:695:THR:HG21	2:B:1000:GLN:HB3	1.94	0.50
5:F:107:ARG:HD2	5:F:115:TYR:CG	2.46	0.50
12:M:33:LEU:HD13	12:M:39:MET:CE	2.41	0.50
1:A:225:ILE:HG23	1:A:256:LEU:CG	2.40	0.50
1:A:636:VAL:HG11	1:A:795:PHE:CZ	2.47	0.50
1:A:815:ILE:HD13	1:A:875:GLU:HG3	1.93	0.50
1:A:929:MET:HE2	2:B:491:PRO:C	2.36	0.50
1:A:1147:LEU:CD2	1:A:1152:PRO:HB3	2.42	0.50
1:A:1326:TYR:C	13:I:60:VAL:HG11	2.33	0.50
1:A:1632:TYR:HB2	1:A:1634:ILE:HD12	1.94	0.50
2:B:6:ARG:O	2:B:6:ARG:HD3	2.12	0.50
2:B:91:THR:HG22	2:B:91:THR:O	2.12	0.50
2:B:417:MET:O	2:B:421:THR:OG1	2.30	0.50
1:A:425:GLU:CG	1:A:426:GLY:H	2.24	0.50
2:B:118:ILE:HD11	2:B:419:ILE:HG21	1.93	0.50
2:B:721:LEU:HD22	7:J:50:LEU:HD23	1.94	0.50
2:B:882:LYS:HD2	2:B:1002:LEU:CD2	2.41	0.50
16:U:4:DC:H2'	16:U:5:DT:C6	2.47	0.50
1:A:897:MET:HG3	2:B:918:HIS:CE1	2.47	0.49
1:A:1086:ARG:CZ	1:A:1086:ARG:HB2	2.42	0.49
2:B:29:GLU:H	2:B:29:GLU:CD	2.20	0.49
2:B:743:VAL:HG21	2:B:999:TYR:CE2	2.42	0.49
12:M:74:PHE:N	12:M:78:ALA:HB2	2.27	0.49
1:A:425:GLU:HG3	1:A:426:GLY:N	2.24	0.49
1:A:1222:PRO:O	1:A:1226:MET:N	2.44	0.49
2:B:262:TYR:HD1	2:B:262:TYR:O	1.95	0.49
2:B:547:HIS:CE1	10:N:116:ARG:HH12	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:802:ARG:HB3	2:B:838:VAL:HG21	1.94	0.49
3:C:163:TYR:CD1	3:C:166:HIS:HB3	2.39	0.49
13:I:28:PRO:O	13:I:41:CYS:HA	2.12	0.49
1:A:20:TYR:CD2	2:B:1129:LYS:HB2	2.47	0.49
1:A:257:THR:HB	1:A:391:TRP:HZ3	1.77	0.49
2:B:187:ARG:NH1	2:B:616:PRO:HD2	2.27	0.49
2:B:387:GLU:OE1	2:B:445:LEU:HD11	2.13	0.49
3:C:114:PRO:HG3	7:J:13:ILE:CD1	2.42	0.49
16:U:13:DG:H1'	16:U:14:DG:H5'	1.94	0.49
1:A:423:LYS:HG3	1:A:424:LYS:N	2.27	0.49
1:A:908:ASN:HD21	13:I:126:SER:HG	1.55	0.49
1:A:912:ILE:HG13	2:B:924:MET:HG2	1.88	0.49
1:A:961:PRO:CD	1:A:962:PRO:HD2	2.41	0.49
1:A:1255:ALA:HB3	1:A:1656:PRO:HB3	1.94	0.49
1:A:1662:ILE:HD13	1:A:1674:PHE:HD2	1.78	0.49
2:B:319:PRO:HG2	2:B:322:GLN:HB2	1.93	0.49
2:B:684:ARG:NH2	13:I:107:GLU:N	2.59	0.49
2:B:781:LEU:O	2:B:792:LEU:HD22	2.13	0.49
3:C:29:PHE:HB3	3:C:30:PRO:HD2	1.94	0.49
3:C:56:MET:HE2	8:K:121:TYR:CD2	2.47	0.49
3:C:93:LEU:HB3	9:L:52:LEU:HD11	1.94	0.49
13:I:14:GLN:HG2	13:I:17:LEU:HD12	1.95	0.49
1:A:322:ASN:HB3	1:A:325:THR:HG23	1.94	0.49
1:A:465:LYS:HZ2	2:B:1014:THR:CG2	2.25	0.49
1:A:968:CYS:SG	2:B:686:MET:HE2	2.51	0.49
2:B:315:PRO:O	2:B:318:TYR:HB2	2.12	0.49
2:B:1126:MET:O	2:B:1127:ASN:HB2	2.12	0.49
6:H:39:LEU:HD11	6:H:123:MET:SD	2.52	0.49
1:A:25:LEU:O	1:A:28:LEU:HB2	2.13	0.49
1:A:428:PHE:CE1	1:A:432:MET:HE3	2.48	0.49
1:A:656:LEU:HD13	1:A:792:TYR:HE2	1.77	0.49
1:A:931:SER:OG	2:B:640:ILE:HG22	2.08	0.49
1:A:1504:ALA:O	1:A:1507:GLU:HB3	2.12	0.49
2:B:426:LEU:HD23	2:B:426:LEU:O	2.13	0.49
2:B:626:LEU:O	2:B:627:ALA:HB3	2.12	0.49
2:B:785:ILE:CG2	2:B:792:LEU:CD2	2.81	0.49
3:C:340:LEU:O	3:C:343:VAL:HG22	2.12	0.49
10:N:30:PHE:HZ	12:M:102:TYR:CG	2.31	0.49
13:I:119:LYS:NZ	13:I:121:GLN:OE1	2.44	0.49
1:A:480:LEU:O	1:A:484:VAL:HG12	2.11	0.49
1:A:588:ASP:OD1	2:B:754:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LYS:CB	6:H:91:VAL:H	2.25	0.49
2:B:497:LEU:HD23	2:B:512:ASN:CB	2.43	0.49
2:B:648:GLU:HG2	2:B:649:ASP:H	1.77	0.49
4:E:123:PRO:HA	4:E:126:ILE:CG2	2.42	0.49
8:K:31:GLN:OE1	8:K:37:ARG:HA	2.12	0.49
1:A:47:ALA:O	1:A:48:ASN:HB2	2.12	0.49
1:A:222:LYS:C	1:A:223:LEU:HD12	2.38	0.49
2:B:987:GLU:CD	3:C:301:ARG:HE	2.20	0.49
7:J:3:ILE:HD11	7:J:49:LEU:HD23	1.95	0.49
2:B:408:SER:HA	2:B:411:MET:CB	2.38	0.49
2:B:571:ALA:HB3	2:B:572:PRO:HD3	1.94	0.49
2:B:752:ASP:HB3	2:B:758:ILE:HG12	1.95	0.49
2:B:854:VAL:O	9:L:43:ILE:HA	2.13	0.49
3:C:14:VAL:C	3:C:300:ALA:HB1	2.38	0.49
3:C:33:TYR:HB3	3:C:36:TYR:CB	2.39	0.49
4:E:92:GLN:HA	4:E:95:GLN:CD	2.37	0.49
10:N:41:GLU:OE1	12:M:94:LYS:HD3	2.12	0.49
1:A:71:PHE:O	1:A:72:SER:OG	2.21	0.49
1:A:137:GLU:OE1	1:A:137:GLU:HA	2.12	0.49
1:A:915:LEU:HD12	1:A:952:THR:HA	1.95	0.49
1:A:930:ALA:O	2:B:362:MET:HE1	2.13	0.49
1:A:1016:GLN:NE2	1:A:1646:ASP:OD2	2.46	0.49
1:A:1281:LEU:HD21	1:A:1595:LEU:HD11	1.94	0.49
2:B:796:ILE:HD12	2:B:809:ASP:H	1.77	0.49
1:A:968:CYS:CA	2:B:686:MET:CE	2.91	0.48
1:A:1085:ARG:NH2	4:E:19:GLN:HG2	2.29	0.48
1:A:1223:SER:HB2	1:A:1245:ILE:HD11	1.94	0.48
1:A:1326:TYR:C	13:I:60:VAL:CG1	2.86	0.48
1:A:1505:VAL:HG11	1:A:1515:TYR:CZ	2.48	0.48
2:B:92:ILE:CD1	2:B:859:THR:HA	2.40	0.48
2:B:583:VAL:CG1	2:B:630:LYS:HB3	2.43	0.48
2:B:926:ILE:O	2:B:930:ILE:HG13	2.13	0.48
2:B:262:TYR:HE2	13:I:9:THR:CB	2.24	0.48
3:C:110:LEU:HD13	3:C:212:MET:SD	2.53	0.48
1:A:402:PHE:CD2	2:B:1126:MET:HG2	2.48	0.48
1:A:1281:LEU:HD11	1:A:1591:TYR:CE2	2.48	0.48
2:B:58:VAL:O	2:B:61:ILE:HB	2.13	0.48
4:E:189:GLN:O	4:E:209:VAL:HG23	2.13	0.48
4:E:205:THR:HG22	4:E:206:TYR:N	2.27	0.48
1:A:89:ASN:HD21	1:A:92:LEU:HD12	1.78	0.48
1:A:127:LEU:HD11	1:A:187:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TYR:O	1:A:168:ILE:HG12	2.14	0.48
1:A:497:VAL:O	1:A:505:THR:HG22	2.13	0.48
1:A:990:ARG:O	1:A:994:LYS:HG2	2.13	0.48
2:B:539:VAL:HG22	2:B:566:VAL:HB	1.95	0.48
2:B:1070:CYS:O	2:B:1074:GLY:N	2.45	0.48
3:C:30:PRO:HG2	8:K:61:LYS:HA	1.95	0.48
3:C:90:GLU:HB2	3:C:215:VAL:HG22	1.94	0.48
3:C:140:PHE:HE2	3:C:214:CYS:HG	1.61	0.48
4:E:17:ILE:HD11	4:E:105:VAL:HG21	1.95	0.48
4:E:80:PRO:HA	4:E:107:GLN:HG3	1.95	0.48
8:K:55:LEU:HD21	8:K:96:PHE:HE1	1.76	0.48
2:B:251:PHE:CE1	2:B:290:MET:HE3	2.48	0.48
2:B:785:ILE:HD12	2:B:791:SER:CB	2.43	0.48
2:B:1114:TYR:O	2:B:1118:TYR:N	2.45	0.48
6:H:106:THR:O	6:H:106:THR:HG22	2.13	0.48
9:L:19:CYS:SG	9:L:20:GLY:N	2.86	0.48
1:A:163:GLN:HG3	1:A:164:TYR:H	1.79	0.48
1:A:397:HIS:NE2	1:A:410:MET:HE1	2.28	0.48
1:A:812:ARG:HH11	1:A:914:CYS:C	2.21	0.48
1:A:1024:LEU:HD23	1:A:1029:THR:HG22	1.95	0.48
1:A:1590:LYS:CE	4:E:133:GLN:NE2	2.76	0.48
2:B:166:MET:O	2:B:166:MET:HG2	2.14	0.48
2:B:745:VAL:CG1	2:B:917:PRO:HB3	2.43	0.48
12:M:81:CYS:SG	12:M:85:CYS:SG	3.05	0.48
1:A:654:MET:C	1:A:656:LEU:H	2.22	0.48
1:A:874:ASN:N	13:I:83:VAL:HG23	2.28	0.48
1:A:960:LYS:HB3	1:A:961:PRO:HD2	1.96	0.48
1:A:968:CYS:HB3	2:B:686:MET:CE	2.42	0.48
2:B:981:SER:HB2	2:B:988:LEU:HD21	1.96	0.48
6:H:13:LYS:HE2	6:H:13:LYS:HA	1.95	0.48
1:A:34:THR:HA	1:A:332:MET:HE1	1.95	0.48
1:A:968:CYS:SG	2:B:686:MET:CE	3.01	0.48
1:A:1597:LEU:CD1	4:E:137:ILE:HG21	2.38	0.48
2:B:905:THR:CG2	2:B:909:MET:HB2	2.43	0.48
2:B:1017:ALA:HB3	2:B:1026:ILE:CG2	2.44	0.48
3:C:171:ARG:HG3	3:C:195:ASP:HB2	1.94	0.48
3:C:222:HIS:CD2	9:L:58:ARG:HD3	2.49	0.48
4:E:67:ASP:CG	4:E:70:ASP:HB2	2.39	0.48
4:E:87:ILE:CG2	4:E:121:MET:HE1	2.43	0.48
1:A:961:PRO:HB3	2:B:666:LEU:CD2	2.43	0.48
1:A:1605:ILE:HG21	1:A:1621:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ARG:O	2:B:9:ASN:ND2	2.47	0.48
2:B:648:GLU:OE1	10:N:134:PRO:HB2	2.13	0.48
2:B:951:ILE:HD12	10:N:139:PRO:HG2	1.95	0.48
12:M:34:GLN:CG	13:I:7:ALA:C	2.75	0.48
12:M:34:GLN:N	13:I:7:ALA:HB3	2.19	0.48
1:A:9:TRP:CG	1:A:9:TRP:O	2.66	0.48
1:A:221:SER:HB3	1:A:395:GLN:HB3	1.95	0.48
1:A:1122:ARG:O	1:A:1127:LEU:HD13	2.14	0.48
1:A:1558:GLY:O	1:A:1582:GLY:HA3	2.14	0.48
2:B:178:VAL:O	2:B:178:VAL:HG22	2.14	0.48
3:C:250:ALA:HB1	3:C:273:ALA:HB2	1.96	0.48
6:H:105:SER:O	6:H:106:THR:HB	2.14	0.48
10:N:29:ARG:C	10:N:31:SER:H	2.22	0.48
1:A:677:LYS:HB3	1:A:678:PRO:HD3	1.94	0.47
1:A:683:THR:HG22	1:A:683:THR:O	2.12	0.47
1:A:1670:GLN:C	1:A:1672:MET:H	2.22	0.47
1:A:1702:VAL:CG2	1:A:1704:LYS:HG3	2.43	0.47
2:B:527:THR:HG23	2:B:527:THR:O	2.14	0.47
2:B:1081:LEU:HD22	2:B:1094:ARG:HB3	1.95	0.47
8:K:47:GLU:OE1	8:K:47:GLU:HA	2.14	0.47
12:M:33:LEU:HD21	12:M:39:MET:CE	2.08	0.47
1:A:603:LEU:HD22	2:B:1052:PHE:CB	2.44	0.47
1:A:609:TYR:CD2	5:F:90:LEU:HD22	2.49	0.47
1:A:1037:PHE:H	1:A:1038:PRO:HD2	1.78	0.47
1:A:1580:THR:HG22	1:A:1581:GLU:N	2.29	0.47
2:B:746:ILE:HG22	2:B:914:LEU:HD22	1.95	0.47
2:B:973:PHE:N	3:C:286:GLU:OE2	2.43	0.47
1:A:162:GLU:HA	1:A:165:THR:OG1	2.13	0.47
1:A:1253:MET:O	1:A:1658:ASN:HB3	2.14	0.47
1:A:1615:GLU:HG3	4:E:193:ILE:CD1	2.26	0.47
2:B:162:GLU:C	2:B:164:GLU:N	2.72	0.47
2:B:286:LEU:O	2:B:290:MET:HB2	2.13	0.47
2:B:576:ASP:OD1	2:B:576:ASP:C	2.57	0.47
3:C:147:THR:N	3:C:164:VAL:HG22	2.26	0.47
3:C:182:ALA:O	3:C:185:PHE:O	2.32	0.47
1:A:119:LEU:HB2	1:A:142:LEU:HD22	1.96	0.47
1:A:441:ALA:CB	2:B:1012:VAL:HG13	2.45	0.47
1:A:479:GLU:CD	5:F:87:THR:HG21	2.39	0.47
1:A:958:GLY:CA	2:B:678:ASP:O	2.62	0.47
1:A:1106:GLU:N	1:A:1106:GLU:OE2	2.48	0.47
1:A:1287:ARG:HG2	1:A:1555:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ILE:HG12	2:B:454:CYS:HB2	1.96	0.47
2:B:504:ASP:OD2	13:I:105:ALA:CB	2.62	0.47
3:C:86:THR:HG21	3:C:227:PRO:HB3	1.96	0.47
4:E:139:ILE:HG13	4:E:140:THR:N	2.28	0.47
12:M:26:VAL:HG12	12:M:60:LEU:CD2	2.44	0.47
13:I:28:PRO:HD2	13:I:30:PRO:HA	1.96	0.47
1:A:308:ARG:CZ	2:B:1114:TYR:OH	2.63	0.47
1:A:732:MET:HE2	6:H:27:ARG:NH1	2.29	0.47
1:A:1716:LYS:CB	5:F:105:ILE:HB	2.42	0.47
2:B:122:VAL:O	2:B:123:ASN:HB2	2.14	0.47
2:B:392:TRP:CE3	2:B:393:LEU:HD23	2.49	0.47
2:B:498:CYS:CB	2:B:668:SER:HB2	2.43	0.47
2:B:743:VAL:HG21	2:B:997:VAL:HG22	1.97	0.47
2:B:1071:VAL:HG22	2:B:1134:VAL:HG11	1.96	0.47
3:C:162:LEU:HG	3:C:204:PRO:HD3	1.95	0.47
1:A:464:THR:HG22	1:A:464:THR:O	2.14	0.47
1:A:872:TYR:O	1:A:876:ILE:HG13	2.14	0.47
2:B:570:LEU:CD2	10:N:81:ARG:HD3	2.44	0.47
2:B:742:ILE:HD12	7:J:43:TYR:CE1	2.49	0.47
3:C:53:VAL:HG21	8:K:118:ILE:CD1	2.37	0.47
1:A:89:ASN:OD1	1:A:92:LEU:HB2	2.14	0.47
1:A:173:LEU:O	1:A:174:LEU:CB	2.63	0.47
1:A:257:THR:HB	1:A:391:TRP:CZ3	2.50	0.47
1:A:433:MET:HB3	2:B:1039:GLU:HG2	1.95	0.47
1:A:753:HIS:O	1:A:754:TYR:HB2	2.14	0.47
1:A:791:LEU:CD2	2:B:984:SER:HB3	2.44	0.47
1:A:845:LYS:HA	1:A:845:LYS:HE2	1.97	0.47
1:A:1518:ASP:CB	1:A:1522:SER:HA	2.45	0.47
1:A:1527:VAL:HG22	1:A:1528:THR:N	2.30	0.47
1:A:1655:LYS:HB3	1:A:1655:LYS:HE3	1.69	0.47
1:A:1711:GLY:HA2	5:F:64:ARG:NH1	2.29	0.47
2:B:140:MET:HE3	2:B:168:GLY:C	2.40	0.47
2:B:181:MET:SD	2:B:520:VAL:HG21	2.55	0.47
2:B:278:LEU:HD11	2:B:354:PHE:HB3	1.95	0.47
2:B:625:ASN:O	2:B:629:GLY:N	2.48	0.47
3:C:240:THR:CG2	3:C:298:ARG:HB3	2.44	0.47
3:C:245:VAL:HG21	3:C:253:LEU:HD23	1.97	0.47
4:E:72:MET:CE	4:E:103:LEU:HD12	2.45	0.47
5:F:66:LEU:HD21	5:F:97:LEU:HD22	1.96	0.47
12:M:67:LEU:CG	12:M:69:TYR:CE1	2.98	0.47
13:I:27:LEU:HB3	13:I:28:PRO:CD	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1565:ASN:HD22	1:A:1579:ASN:HD22	1.63	0.47
4:E:159:LEU:HD11	4:E:206:TYR:CD2	2.50	0.47
1:A:1106:GLU:O	1:A:1107:SER:OG	2.29	0.47
1:A:1326:TYR:CD2	13:I:60:VAL:HG13	2.34	0.47
1:A:1498:MET:HA	1:A:1501:ARG:NH1	2.29	0.47
1:A:1575:GLU:O	1:A:1576:LEU:HD22	2.15	0.47
1:A:1669:LEU:O	1:A:1673:THR:HG23	2.15	0.47
2:B:60:ALA:O	2:B:61:ILE:C	2.58	0.47
2:B:259:PHE:CA	12:M:110:GLN:NE2	2.55	0.47
2:B:332:ILE:HG13	2:B:332:ILE:O	2.14	0.47
2:B:853:LYS:HG2	9:L:45:TYR:CE2	2.49	0.47
3:C:31:GLY:HA2	3:C:37:ASP:OD1	2.15	0.47
3:C:337:LEU:HD21	8:K:100:LEU:HB2	1.97	0.47
4:E:53:PRO:HB2	4:E:54:ARG:CZ	2.45	0.47
10:N:105:LEU:HB2	12:M:41:PHE:HB2	1.95	0.47
13:I:97:TYR:HA	13:I:112:PHE:O	2.14	0.47
1:A:677:LYS:HG2	6:H:89:GLU:C	2.40	0.47
2:B:141:VAL:O	2:B:146:CYS:CB	2.63	0.47
1:A:469:PRO:HD3	1:A:600:GLN:NE2	2.30	0.46
1:A:497:VAL:HG13	1:A:505:THR:CG2	2.45	0.46
1:A:652:HIS:ND1	3:C:24:VAL:HG13	2.31	0.46
2:B:626:LEU:HD13	2:B:659:GLN:HB3	1.97	0.46
2:B:926:ILE:O	2:B:926:ILE:HG22	2.15	0.46
3:C:299:LEU:HD23	3:C:299:LEU:H	1.79	0.46
3:C:339:GLU:HG2	8:K:26:ALA:HB3	1.97	0.46
6:H:35:PHE:HB3	6:H:37:MET:HG3	1.96	0.46
8:K:83:ARG:HH11	8:K:85:GLN:NE2	2.11	0.46
1:A:1084:LEU:HG	1:A:1084:LEU:O	2.14	0.46
2:B:263:GLN:CA	12:M:29:SER:O	2.63	0.46
2:B:333:CYS:SG	2:B:345:MET:SD	3.13	0.46
2:B:410:SER:HB3	2:B:411:MET:HE2	1.97	0.46
5:F:71:LEU:HD12	5:F:71:LEU:O	2.15	0.46
5:F:81:VAL:O	5:F:81:VAL:HG22	2.14	0.46
12:M:66:ARG:CZ	13:I:37:THR:CB	2.92	0.46
15:T:9:DT:H2"	15:T:10:DA:N7	2.30	0.46
1:A:969:MET:HG3	2:B:489:LEU:HB3	1.97	0.46
1:A:1332:CYS:O	1:A:1332:CYS:SG	2.73	0.46
1:A:1715:LEU:HD13	5:F:104:ILE:HD13	1.98	0.46
2:B:269:ILE:HD11	2:B:282:VAL:HG21	1.97	0.46
2:B:269:ILE:HD13	2:B:278:LEU:HD23	1.98	0.46
3:C:15:VAL:HG12	3:C:298:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:THR:O	3:C:27:THR:HG22	2.14	0.46
3:C:161:GLU:H	3:C:161:GLU:HG3	1.67	0.46
3:C:173:MET:SD	3:C:212:MET:HE1	2.56	0.46
8:K:62:ASN:O	8:K:65:VAL:HG22	2.15	0.46
12:M:32:LYS:HB3	13:I:8:ASN:HB3	1.98	0.46
1:A:127:LEU:HD21	1:A:135:VAL:HG21	1.98	0.46
1:A:512:MET:HG3	1:A:512:MET:O	2.15	0.46
1:A:804:VAL:HG13	1:A:884:GLY:O	2.14	0.46
1:A:1000:VAL:HG12	1:A:1210:ALA:HA	1.96	0.46
1:A:1354:ILE:HD12	1:A:1540:MET:CE	2.45	0.46
2:B:66:PHE:CE1	2:B:75:PHE:CE2	3.02	0.46
2:B:175:ILE:O	2:B:175:ILE:CG2	2.64	0.46
2:B:262:TYR:CE2	12:M:30:ASN:O	2.65	0.46
2:B:673:PHE:CZ	2:B:732:MET:HE3	2.50	0.46
2:B:790:SER:C	2:B:792:LEU:H	2.22	0.46
3:C:61:LEU:HG	3:C:63:PHE:HD1	1.80	0.46
1:A:100:LEU:HD21	1:A:265:LEU:HD22	1.96	0.46
1:A:434:GLY:O	2:B:1036:ARG:HG3	2.16	0.46
1:A:811:LYS:O	1:A:814:ARG:HG2	2.15	0.46
1:A:889:PHE:O	1:A:890:PRO:C	2.56	0.46
1:A:897:MET:SD	2:B:921:PRO:HG3	2.56	0.46
1:A:1180:LYS:HD3	1:A:1180:LYS:HA	1.83	0.46
2:B:39:THR:HG21	2:B:166:MET:HG2	1.98	0.46
2:B:403:LYS:HB3	2:B:418:ARG:NH2	2.26	0.46
2:B:821:TYR:HB2	2:B:844:LYS:HZ2	1.80	0.46
1:A:89:ASN:HB3	1:A:299:LEU:HG	1.97	0.46
1:A:258:PRO:HD2	1:A:391:TRP:CE3	2.50	0.46
1:A:498:ILE:O	1:A:536:LYS:HA	2.16	0.46
1:A:551:ASN:O	1:A:594:MET:HG3	2.15	0.46
1:A:812:ARG:HD2	1:A:914:CYS:CA	2.46	0.46
1:A:1014:VAL:HG23	4:E:165:LEU:CD2	2.42	0.46
1:A:1269:LEU:HD22	1:A:1269:LEU:HA	1.81	0.46
2:B:262:TYR:HE2	13:I:9:THR:CG2	2.28	0.46
2:B:386:LYS:O	2:B:390:GLU:HG3	2.16	0.46
2:B:570:LEU:HD23	10:N:81:ARG:CZ	2.24	0.46
2:B:632:GLU:HG2	2:B:633:LEU:N	2.31	0.46
2:B:722:VAL:HG21	2:B:934:ALA:CB	2.44	0.46
2:B:864:PHE:H	9:L:34:ILE:HG13	1.80	0.46
13:I:7:ALA:HB2	13:I:16:ASP:HA	1.98	0.46
1:A:558:ARG:HB3	1:A:559:PRO:HD3	1.96	0.46
1:A:1288:VAL:HB	1:A:1331:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:CYS:SG	2:B:511:MET:HG2	2.56	0.46
2:B:700:LEU:HD11	2:B:706:ARG:CG	2.39	0.46
2:B:906:GLU:CD	3:C:301:ARG:HH22	2.24	0.46
10:N:24:ALA:HB3	10:N:27:SER:HB3	1.98	0.46
1:A:33:ILE:HD13	1:A:304:VAL:HG11	1.98	0.46
1:A:606:ALA:HA	5:F:90:LEU:HD21	1.98	0.46
1:A:1106:GLU:O	1:A:1106:GLU:HG2	2.14	0.46
1:A:1207:PRO:HD2	5:F:58:THR:CG2	2.46	0.46
1:A:1518:ASP:CG	1:A:1524:TRP:H	2.23	0.46
2:B:141:VAL:HB	2:B:167:GLY:HA3	1.97	0.46
2:B:393:LEU:O	2:B:396:ILE:HG12	2.16	0.46
3:C:138:LEU:HD21	3:C:190:ILE:HG21	1.98	0.46
1:A:138:LEU:HD11	1:A:165:THR:CG2	2.42	0.46
1:A:214:VAL:HG21	1:A:216:ARG:NH2	2.31	0.46
1:A:1343:GLU:HG3	1:A:1505:VAL:CG2	2.46	0.46
1:A:1511:PHE:HB3	1:A:1529:VAL:HG13	1.97	0.46
2:B:69:LYS:HE2	2:B:69:LYS:HB3	1.57	0.46
2:B:183:ILE:HG13	2:B:472:VAL:HG12	1.98	0.46
2:B:707:SER:HB2	2:B:868:CYS:SG	2.56	0.46
6:H:86:ASP:C	6:H:88:PHE:H	2.23	0.46
1:A:872:TYR:O	1:A:876:ILE:N	2.49	0.46
1:A:1045:GLU:H	1:A:1045:GLU:HG2	1.43	0.46
1:A:1247:ARG:HG2	1:A:1628:VAL:HG22	1.97	0.46
2:B:140:MET:HE2	2:B:168:GLY:HA2	1.98	0.46
2:B:847:CYS:SG	2:B:871:MET:HG2	2.56	0.46
3:C:53:VAL:HA	3:C:63:PHE:HA	1.97	0.46
3:C:290:ASN:HD22	3:C:293:LEU:HB2	1.81	0.46
4:E:125:TYR:O	4:E:127:LEU:HD12	2.16	0.46
12:M:16:ALA:HB3	12:M:19:GLY:HA2	1.98	0.46
12:M:66:ARG:HB2	13:I:17:LEU:HD21	1.98	0.46
13:I:49:ASP:HB3	13:I:51:GLU:OE1	2.16	0.46
1:A:865:PHE:HA	1:A:868:GLU:OE2	2.16	0.45
1:A:881:MET:HB3	1:A:881:MET:HE3	1.63	0.45
1:A:881:MET:HB2	13:I:85:ARG:NH2	2.31	0.45
2:B:167:GLY:O	2:B:169:TYR:CD2	2.68	0.45
2:B:184:MET:HB3	2:B:185:PRO:HD2	1.98	0.45
3:C:245:VAL:HG21	3:C:253:LEU:HD22	1.98	0.45
1:A:140:ARG:NH1	1:A:144:ARG:HH12	2.09	0.45
1:A:314:ARG:HD2	1:A:319:MET:HE3	1.98	0.45
2:B:39:THR:CG2	2:B:166:MET:HG2	2.45	0.45
2:B:64:PHE:HE2	2:B:397:LYS:CB	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:PHE:CD2	2:B:75:PHE:N	2.82	0.45
2:B:206:THR:OG1	2:B:228:TYR:O	2.34	0.45
2:B:642:MET:HE3	2:B:658:HIS:ND1	2.31	0.45
2:B:722:VAL:HG21	2:B:934:ALA:HB3	1.98	0.45
1:A:716:TRP:HZ2	1:A:748:VAL:HG11	1.80	0.45
1:A:926:PRO:HB3	1:A:969:MET:HE1	1.98	0.45
1:A:1128:ASP:CB	1:A:1133:ARG:HD3	2.46	0.45
1:A:1162:THR:HG21	4:E:199:THR:O	2.17	0.45
2:B:336:LEU:CD2	2:B:561:VAL:HG22	2.46	0.45
2:B:538:GLY:O	10:N:116:ARG:NH2	2.49	0.45
2:B:674:ILE:HG12	2:B:688:GLN:HG3	1.98	0.45
2:B:800:ASP:HB3	2:B:803:VAL:HG22	1.99	0.45
2:B:905:THR:HG21	2:B:909:MET:HB2	1.99	0.45
2:B:1084:PRO:HD3	2:B:1094:ARG:NH1	2.31	0.45
3:C:236:LEU:HD22	3:C:305:HIS:CD2	2.51	0.45
8:K:90:LEU:HD12	8:K:95:PRO:HD3	1.98	0.45
1:A:387:LEU:HD12	1:A:390:ILE:HD11	1.97	0.45
1:A:1605:ILE:HG21	1:A:1621:ILE:HG13	1.98	0.45
2:B:797:LYS:HE2	2:B:797:LYS:HB3	1.81	0.45
2:B:951:ILE:HD12	10:N:139:PRO:HG3	1.98	0.45
2:B:972:ASN:HA	3:C:286:GLU:OE2	2.17	0.45
5:F:53:THR:OG1	5:F:108:ARG:NH1	2.48	0.45
5:F:55:PRO:O	5:F:123:LEU:HD12	2.16	0.45
1:A:105:LEU:HD12	1:A:264:HIS:CE1	2.52	0.45
1:A:430:LYS:O	1:A:431:HIS:HB2	2.16	0.45
1:A:518:VAL:HG22	1:A:518:VAL:O	2.17	0.45
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.45
1:A:1533:LEU:H	1:A:1535:LYS:NZ	2.14	0.45
2:B:238:PHE:CE1	2:B:327:LEU:HD11	2.52	0.45
2:B:336:LEU:HD22	2:B:561:VAL:HG22	1.99	0.45
2:B:730:TYR:O	2:B:731:ASP:C	2.57	0.45
2:B:818:LYS:HG2	2:B:848:VAL:HG12	1.99	0.45
3:C:236:LEU:HB2	3:C:305:HIS:HD2	1.82	0.45
3:C:261:VAL:HG21	3:C:281:ASP:HB2	1.97	0.45
5:F:122:GLU:O	5:F:122:GLU:HG3	2.15	0.45
13:I:85:ARG:HG3	13:I:86:ARG:N	2.32	0.45
1:A:1348:LYS:NZ	1:A:1509:HIS:HB3	2.32	0.45
2:B:269:ILE:HG22	2:B:273:GLU:HA	1.98	0.45
2:B:482:ARG:CB	16:U:1:DG:O5'	2.60	0.45
2:B:698:PHE:HE2	2:B:701:LEU:HD23	1.80	0.45
2:B:705:ASP:HA	2:B:853:LYS:HZ3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:63:THR:HG22	6:H:71:ASP:OD1	2.17	0.45
14:R:-5:C:H2'	14:R:-4:U:O4'	2.17	0.45
15:T:-1:DG:H22	16:U:2:DT:H3	1.65	0.45
2:B:106:ARG:HG3	9:L:43:ILE:HD11	1.99	0.45
2:B:543:ASP:CB	12:M:81:CYS:CB	2.77	0.45
2:B:781:LEU:HD22	2:B:792:LEU:CB	2.37	0.45
10:N:81:ARG:HB3	10:N:118:LEU:HG	1.98	0.45
12:M:67:LEU:HD11	12:M:69:TYR:CE1	2.52	0.45
15:T:-7:DG:C2	15:T:-6:DA:C6	3.05	0.45
1:A:8:PRO:HB3	2:B:1109:THR:C	2.42	0.45
1:A:1275:LEU:O	1:A:1278:VAL:HG12	2.15	0.45
2:B:143:SER:O	2:B:144:LYS:HB2	2.17	0.45
2:B:400:PHE:HA	2:B:418:ARG:NH1	2.30	0.45
2:B:808:ASP:O	2:B:809:ASP:HB2	2.15	0.45
3:C:193:VAL:HG11	3:C:314:GLY:HA3	1.99	0.45
8:K:22:GLU:HG2	8:K:25:THR:CB	2.46	0.45
9:L:37:ARG:O	9:L:38:GLU:HB3	2.15	0.45
12:M:39:MET:HG2	12:M:64:THR:HG22	1.99	0.45
13:I:7:ALA:HA	13:I:15:SER:C	2.42	0.45
1:A:619:LEU:HD23	1:A:626:PRO:HA	1.99	0.45
2:B:149:ARG:O	2:B:150:ASN:HB2	2.17	0.45
2:B:262:TYR:CG	12:M:30:ASN:C	2.95	0.45
2:B:496:PHE:C	2:B:497:LEU:HD12	2.41	0.45
2:B:655:VAL:HG12	2:B:656:THR:N	2.32	0.45
2:B:760:ASN:OD1	2:B:761:LYS:N	2.50	0.45
6:H:14:ASP:HB3	6:H:17:PRO:HG3	1.99	0.45
13:I:14:GLN:O	13:I:17:LEU:N	2.50	0.45
16:U:9:DC:H3'	16:U:9:DC:OP2	2.17	0.45
1:A:91:LEU:HD13	2:B:1128:ILE:HD11	2.00	0.45
1:A:472:VAL:CG2	1:A:477:VAL:HG23	2.47	0.45
1:A:716:TRP:CZ2	1:A:748:VAL:HG11	2.53	0.45
1:A:929:MET:HE2	2:B:492:GLU:CG	2.46	0.45
4:E:87:ILE:HD11	4:E:110:MET:HE2	1.99	0.45
7:J:24:LEU:O	7:J:29:TYR:HB2	2.17	0.45
1:A:174:LEU:HG	1:A:174:LEU:O	2.17	0.44
1:A:429:ARG:HG2	2:B:1039:GLU:OE2	2.17	0.44
1:A:544:ASN:HA	1:A:566:ALA:O	2.17	0.44
1:A:1531:LEU:CB	1:A:1535:LYS:HD3	2.47	0.44
2:B:5:SER:O	2:B:6:ARG:HB3	2.17	0.44
2:B:98:VAL:O	2:B:110:TYR:HE1	2.00	0.44
2:B:205:TYR:CD1	2:B:229:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:651:VAL:HG22	2:B:656:THR:HG21	1.99	0.44
3:C:241:LEU:HD23	3:C:297:VAL:CG2	2.47	0.44
4:E:13:ILE:CD1	4:E:132:GLN:HG3	2.47	0.44
10:N:38:PRO:O	12:M:94:LYS:NZ	2.47	0.44
1:A:95:LYS:HD3	1:A:95:LYS:HA	1.74	0.44
1:A:822:CYS:SG	1:A:868:GLU:HB2	2.57	0.44
6:H:92:MET:HE2	6:H:121:LEU:HD12	1.99	0.44
1:A:715:ALA:HB2	1:A:899:GLN:NE2	2.33	0.44
1:A:1512:ILE:HG22	1:A:1513:ASP:N	2.31	0.44
1:A:1589:PHE:HA	1:A:1597:LEU:CD1	2.47	0.44
1:A:1598:ARG:O	1:A:1599:ARG:HB2	2.17	0.44
2:B:92:ILE:CG2	2:B:93:CYS:H	2.24	0.44
2:B:186:ARG:O	2:B:213:HIS:HB3	2.18	0.44
2:B:239:ILE:HB	2:B:244:LEU:HD23	1.99	0.44
2:B:337:LYS:HB2	2:B:337:LYS:HE2	1.66	0.44
3:C:53:VAL:C	10:N:157:PRO:HD3	2.43	0.44
3:C:241:LEU:HD21	3:C:253:LEU:HD21	1.99	0.44
4:E:11:TRP:HB2	4:E:40:PHE:CD2	2.52	0.44
4:E:87:ILE:HD11	4:E:110:MET:CE	2.48	0.44
13:I:122:GLU:HG2	13:I:124:GLU:OE2	2.18	0.44
1:A:29:SER:HB3	1:A:80:HIS:HD2	1.82	0.44
1:A:121:LEU:HD23	1:A:121:LEU:C	2.43	0.44
1:A:132:LEU:HG	4:E:210:GLN:HE22	1.82	0.44
1:A:422:GLU:HG2	1:A:1677:SER:HB3	1.99	0.44
1:A:464:THR:O	1:A:464:THR:CG2	2.66	0.44
1:A:908:ASN:HB3	2:B:921:PRO:O	2.17	0.44
2:B:197:LYS:HG2	2:B:197:LYS:O	2.18	0.44
2:B:247:LEU:HD12	2:B:248:PRO:HD2	1.98	0.44
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.47	0.44
1:A:854:ASP:O	1:A:855:GLN:HB2	2.17	0.44
1:A:1531:LEU:HB3	1:A:1535:LYS:HD3	1.98	0.44
1:A:1628:VAL:O	1:A:1631:VAL:HG22	2.17	0.44
2:B:647:PHE:CE1	2:B:663:PRO:HB3	2.53	0.44
3:C:149:ASN:OD1	3:C:161:GLU:HA	2.17	0.44
4:E:168:ASN:HA	4:E:172:ARG:HH12	1.82	0.44
6:H:40:ILE:O	6:H:123:MET:HA	2.17	0.44
12:M:69:TYR:HA	12:M:110:GLN:O	2.18	0.44
15:T:-9:DA:H61	16:U:10:DT:H1'	1.83	0.44
1:A:268:LEU:HD23	1:A:268:LEU:O	2.17	0.44
3:C:75:ALA:O	3:C:79:ILE:HG12	2.18	0.44
3:C:142:LEU:HD21	3:C:168:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:168:ASN:HA	4:E:172:ARG:HH22	1.83	0.44
1:A:26:LYS:O	1:A:27:LYS:HB2	2.18	0.44
1:A:1009:ASP:OD1	1:A:1010:SER:N	2.47	0.44
2:B:525:VAL:HG21	2:B:590:PRO:HG3	2.00	0.44
8:K:89:THR:HG23	8:K:90:LEU:H	1.81	0.44
1:A:186:GLU:HB2	1:A:1664:SER:HB2	2.00	0.44
1:A:766:TYR:CD1	1:A:771:GLY:HA2	2.52	0.44
2:B:55:GLY:O	2:B:59:GLN:HG2	2.18	0.44
2:B:156:LEU:HG	2:B:161:GLU:HB2	2.00	0.44
2:B:570:LEU:HD22	10:N:81:ARG:HD3	2.00	0.44
2:B:782:SER:HA	2:B:792:LEU:HD13	2.00	0.44
2:B:804:LEU:HG	2:B:805:GLN:OE1	2.18	0.44
2:B:855:CYS:HA	9:L:42:ARG:O	2.17	0.44
10:N:146:ARG:NH1	10:N:148:ARG:NH2	2.63	0.44
1:A:976:VAL:O	1:A:980:VAL:HG13	2.18	0.44
1:A:1090:LEU:CD1	4:E:22:HIS:NE2	2.80	0.44
1:A:1530:LYS:C	1:A:1531:LEU:HD12	2.43	0.44
1:A:1583:ILE:CD1	1:A:1604:ASP:HB2	2.48	0.44
2:B:109:THR:HA	2:B:171:ILE:O	2.18	0.44
2:B:526:TYR:O	2:B:527:THR:HG22	2.17	0.44
2:B:674:ILE:HG12	2:B:688:GLN:CG	2.48	0.44
2:B:792:LEU:CD1	2:B:865:LYS:HD2	2.41	0.44
2:B:811:GLY:O	2:B:812:LEU:HD23	2.18	0.44
3:C:30:PRO:HG3	8:K:61:LYS:HA	1.99	0.44
6:H:56:PHE:HE1	6:H:58:LEU:HD12	1.83	0.44
10:N:30:PHE:O	10:N:96:ALA:HB1	2.18	0.44
10:N:84:SER:OG	10:N:115:LEU:CD2	2.66	0.44
12:M:11:TRP:CZ2	12:M:101:VAL:HG11	2.53	0.44
13:I:89:ARG:HG2	13:I:120:PHE:CE2	2.53	0.44
13:I:115:CYS:SG	13:I:116:THR:N	2.91	0.44
1:A:132:LEU:HD23	4:E:172:ARG:HH21	1.83	0.43
1:A:811:LYS:O	1:A:815:ILE:HG13	2.18	0.43
1:A:1113:ARG:O	1:A:1114:SER:HB2	2.17	0.43
2:B:115:THR:HG22	2:B:133:PHE:HA	1.99	0.43
2:B:538:GLY:CA	10:N:118:LEU:CB	2.89	0.43
3:C:26:THR:OG1	3:C:303:ARG:NE	2.45	0.43
4:E:122:ALA:O	4:E:124:LYS:N	2.50	0.43
5:F:57:MET:HE2	5:F:106:ILE:HD11	2.00	0.43
6:H:118:TYR:OH	6:H:143:LEU:HB2	2.18	0.43
9:L:15:MET:HA	9:L:15:MET:HE3	2.00	0.43
12:M:34:GLN:CG	13:I:8:ASN:HA	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:CG1	1:A:66:THR:HG21	2.48	0.43
1:A:93:PHE:O	1:A:96:LEU:HB3	2.18	0.43
1:A:472:VAL:O	1:A:535:THR:HG21	2.19	0.43
1:A:606:ALA:HB2	5:F:90:LEU:CD1	2.41	0.43
1:A:955:PHE:CD2	2:B:924:MET:HB3	2.53	0.43
1:A:56:GLY:HA2	1:A:64:CYS:HB3	2.00	0.43
1:A:833:LEU:HD13	1:A:834:PRO:HD2	2.00	0.43
1:A:865:PHE:CZ	1:A:945:PRO:HA	2.53	0.43
1:A:968:CYS:O	2:B:686:MET:HE1	2.18	0.43
1:A:1348:LYS:O	1:A:1352:GLU:HG3	2.18	0.43
2:B:240:TYR:HB2	2:B:331:CYS:SG	2.58	0.43
2:B:248:PRO:HB2	2:B:251:PHE:HD2	1.82	0.43
2:B:262:TYR:HE2	13:I:9:THR:HG1	0.62	0.43
2:B:667:LEU:HD12	2:B:667:LEU:HA	1.86	0.43
2:B:689:CYS:O	2:B:693:LYS:HD3	2.18	0.43
2:B:743:VAL:HG21	2:B:997:VAL:CG2	2.47	0.43
2:B:1132:LEU:HD12	2:B:1132:LEU:O	2.18	0.43
10:N:39:ASP:HA	12:M:94:LYS:HE3	1.99	0.43
1:A:64:CYS:SG	1:A:67:CYS:O	2.75	0.43
1:A:598:PHE:O	1:A:600:GLN:HG2	2.18	0.43
1:A:846:TRP:NE1	1:A:858:PHE:HE1	2.13	0.43
1:A:1095:LYS:O	1:A:1098:GLU:HB3	2.19	0.43
1:A:1134:LYS:HE2	1:A:1134:LYS:CA	2.49	0.43
1:A:1207:PRO:HD2	5:F:58:THR:HG22	2.00	0.43
1:A:1318:ARG:HB2	1:A:1526:GLN:HB3	1.99	0.43
2:B:18:HIS:HE1	2:B:723:ARG:HH22	1.66	0.43
2:B:116:ALA:H	2:B:134:LEU:HD23	1.83	0.43
2:B:403:LYS:CB	2:B:418:ARG:HH12	2.20	0.43
2:B:767:GLY:HA2	2:B:770:HIS:CE1	2.53	0.43
4:E:143:GLU:HG3	4:E:144:LEU:HG	2.00	0.43
9:L:37:ARG:C	9:L:39:CYS:H	2.25	0.43
1:A:100:LEU:HD21	1:A:265:LEU:CD2	2.48	0.43
1:A:131:ALA:HB2	1:A:172:ASN:HD22	1.83	0.43
1:A:221:SER:CB	1:A:395:GLN:HB3	2.49	0.43
1:A:459:PRO:HB2	1:A:572:GLU:C	2.43	0.43
1:A:743:GLU:OE2	6:H:140:ARG:NH2	2.51	0.43
1:A:801:ASP:HB3	1:A:887:ARG:HD2	2.00	0.43
1:A:1008:ARG:CZ	5:F:111:PRO:HG3	2.48	0.43
1:A:1062:PRO:HB3	1:A:1156:PHE:HD2	1.83	0.43
1:A:1206:GLU:OE1	5:F:58:THR:HA	2.19	0.43
1:A:1209:GLU:OE1	5:F:60:TYR:OH	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1631:VAL:HG23	1:A:1632:TYR:CE2	2.54	0.43
1:A:1715:LEU:HD12	5:F:68:THR:HG21	2.01	0.43
2:B:704:GLN:HG3	2:B:704:GLN:O	2.18	0.43
4:E:82:VAL:HG13	4:E:86:THR:HB	1.99	0.43
15:T:9:DT:H2''	15:T:10:DA:C8	2.53	0.43
1:A:217:LYS:HD2	1:A:218:GLU:O	2.19	0.43
1:A:1114:SER:HB3	1:A:1117:THR:H	1.84	0.43
1:A:1515:TYR:O	1:A:1526:GLN:NE2	2.52	0.43
1:A:1590:LYS:HE3	4:E:133:GLN:NE2	2.33	0.43
2:B:35:LEU:HD13	2:B:35:LEU:HA	1.87	0.43
2:B:758:ILE:HD12	2:B:895:ARG:HB2	1.95	0.43
2:B:796:ILE:HD11	2:B:807:LEU:CB	2.41	0.43
2:B:828:TYR:CD1	2:B:828:TYR:N	2.86	0.43
4:E:73:PHE:HB2	4:E:99:ILE:HD13	2.00	0.43
12:M:66:ARG:HB3	13:I:17:LEU:HD21	2.01	0.43
1:A:404:SER:CB	1:A:415:PRO:HA	2.42	0.43
2:B:18:HIS:O	2:B:21:ASP:HB2	2.19	0.43
2:B:172:ILE:O	2:B:173:ASN:HB2	2.17	0.43
2:B:863:LYS:O	2:B:865:LYS:HG2	2.19	0.43
2:B:1003:ARG:O	2:B:1003:ARG:CD	2.64	0.43
3:C:246:GLU:HG2	3:C:272:VAL:HA	2.01	0.43
4:E:85:LYS:HE2	4:E:85:LYS:HB3	1.87	0.43
1:A:40:ASP:HB2	1:A:44:ASN:O	2.18	0.43
1:A:472:VAL:HG12	1:A:536:LYS:O	2.19	0.43
1:A:1085:ARG:HD3	4:E:22:HIS:ND1	2.34	0.43
2:B:73:ILE:HG22	2:B:75:PHE:CZ	2.51	0.43
2:B:175:ILE:O	2:B:175:ILE:HG22	2.19	0.43
2:B:290:MET:HA	2:B:290:MET:HE2	2.00	0.43
9:L:15:MET:HE3	9:L:15:MET:CA	2.48	0.43
15:T:-6:DA:H1'	15:T:-5:DC:O4'	2.19	0.43
1:A:186:GLU:HG2	1:A:190:LYS:HE3	2.01	0.43
1:A:280:PHE:O	1:A:281:SER:OG	2.17	0.43
1:A:754:TYR:CE1	1:A:781:LEU:HD22	2.54	0.43
1:A:968:CYS:CA	2:B:686:MET:HE1	2.49	0.43
2:B:32:LYS:O	2:B:33:ALA:HB3	2.19	0.43
2:B:258:SER:HB3	2:B:297:GLN:OE1	2.19	0.43
8:K:65:VAL:HA	8:K:86:THR:HA	2.00	0.43
12:M:113:PHE:HE1	13:I:35:THR:HG23	1.84	0.43
1:A:332:MET:HB3	1:A:332:MET:HE2	1.69	0.43
1:A:806:PRO:C	1:A:808:ALA:H	2.26	0.43
1:A:1243:LEU:O	1:A:1246:PRO:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1652:GLY:HA2	4:E:172:ARG:O	2.19	0.43
2:B:388:LYS:HE3	2:B:429:PRO:HB3	2.01	0.43
3:C:30:PRO:HB3	3:C:38:ASP:O	2.19	0.43
3:C:100:ILE:HG13	7:J:60:LEU:HD23	2.00	0.43
6:H:32:SER:HB3	6:H:37:MET:H	1.83	0.43
1:A:121:LEU:HD23	1:A:125:ARG:HG3	2.01	0.42
1:A:205:CYS:HB3	1:A:208:CYS:O	2.18	0.42
1:A:427:LEU:HG	1:A:427:LEU:O	2.19	0.42
1:A:440:ALA:CB	2:B:1035:ILE:HD11	2.47	0.42
1:A:927:PRO:CG	2:B:488:ARG:HH22	2.32	0.42
1:A:1590:LYS:HZ1	4:E:133:GLN:NE2	2.08	0.42
2:B:282:VAL:HA	2:B:285:MET:HE3	2.00	0.42
2:B:519:GLU:HG3	2:B:620:VAL:HG23	2.01	0.42
2:B:718:GLN:HB3	7:J:51:ALA:O	2.19	0.42
2:B:804:LEU:N	2:B:804:LEU:HD23	2.34	0.42
3:C:102:GLN:O	3:C:106:LEU:HB2	2.19	0.42
4:E:43:GLN:O	4:E:44:SER:HB3	2.18	0.42
6:H:37:MET:HE3	6:H:127:GLY:CA	2.45	0.42
1:A:218:GLU:HG2	1:A:219:HIS:H	1.82	0.42
1:A:1008:ARG:NH1	5:F:111:PRO:CG	2.79	0.42
1:A:1129:GLU:OE1	1:A:1132:ARG:CB	2.67	0.42
1:A:1523:LEU:HD12	1:A:1524:TRP:HB2	2.01	0.42
1:A:1531:LEU:O	1:A:1535:LYS:HD3	2.19	0.42
1:A:1559:ILE:HG23	1:A:1580:THR:HG23	2.01	0.42
1:A:1566:GLU:O	1:A:1576:LEU:HD22	2.19	0.42
1:A:1713:PHE:CZ	5:F:61:GLU:HG2	2.54	0.42
2:B:430:PHE:O	2:B:434:PHE:HD1	2.02	0.42
2:B:918:HIS:C	2:B:921:PRO:HD2	2.43	0.42
4:E:169:GLN:O	4:E:169:GLN:CG	2.67	0.42
13:I:13:PHE:HD1	13:I:20:CYS:CB	2.32	0.42
1:A:459:PRO:O	1:A:461:VAL:N	2.52	0.42
1:A:727:PHE:HE1	6:H:40:ILE:HG13	1.84	0.42
1:A:936:PRO:CD	2:B:494:TRP:CB	2.96	0.42
1:A:961:PRO:N	1:A:962:PRO:HD2	2.33	0.42
1:A:1268:VAL:HG23	1:A:1576:LEU:O	2.19	0.42
2:B:263:GLN:N	12:M:29:SER:O	2.51	0.42
2:B:269:ILE:HG22	2:B:269:ILE:O	2.19	0.42
2:B:908:GLY:HA2	3:C:232:SER:OG	2.19	0.42
4:E:56:THR:O	4:E:56:THR:HG22	2.18	0.42
12:M:30:ASN:ND2	13:I:18:ASP:O	2.53	0.42
12:M:83:THR:O	12:M:84:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HE3	1:A:61:LYS:HB2	1.86	0.42
1:A:225:ILE:CG2	1:A:256:LEU:HD11	2.49	0.42
1:A:330:ALA:HB1	1:A:397:HIS:CE1	2.54	0.42
1:A:406:MET:HE2	1:A:406:MET:HB2	1.81	0.42
1:A:463:ALA:CB	1:A:568:ILE:HD12	2.49	0.42
1:A:705:LEU:CD1	1:A:761:LEU:HA	2.50	0.42
1:A:860:MET:HE2	1:A:864:LYS:CE	2.38	0.42
1:A:1006:THR:CG2	1:A:1008:ARG:HE	2.29	0.42
1:A:1078:LYS:HB2	1:A:1078:LYS:HE3	1.82	0.42
1:A:1357:LYS:HZ1	1:A:1538:PHE:HE1	1.67	0.42
1:A:1535:LYS:HD2	1:A:1535:LYS:N	2.34	0.42
2:B:63:PRO:HB3	2:B:76:THR:HG22	2.00	0.42
2:B:116:ALA:N	2:B:134:LEU:HD23	2.34	0.42
2:B:194:ILE:HD12	2:B:363:GLU:HB2	2.01	0.42
2:B:214:CYS:O	2:B:221:ALA:HA	2.19	0.42
2:B:681:GLN:O	2:B:684:ARG:HB2	2.19	0.42
2:B:720:PRO:O	2:B:723:ARG:HD3	2.19	0.42
4:E:159:LEU:CD2	4:E:160:LEU:HD23	2.45	0.42
5:F:53:THR:HG23	5:F:116:GLU:CD	2.45	0.42
6:H:107:GLU:HG3	6:H:108:ALA:N	2.34	0.42
10:N:61:VAL:HG21	12:M:11:TRP:HE3	1.84	0.42
1:A:85:LEU:HD22	1:A:391:TRP:NE1	2.33	0.42
1:A:543:LYS:O	1:A:543:LYS:CG	2.68	0.42
1:A:636:VAL:HG11	1:A:795:PHE:CE1	2.54	0.42
1:A:927:PRO:HG3	2:B:488:ARG:HH22	1.80	0.42
1:A:1016:GLN:OE1	1:A:1643:LEU:HD13	2.19	0.42
1:A:1335:PRO:C	1:A:1338:ILE:HG22	2.45	0.42
2:B:920:PHE:N	2:B:921:PRO:CD	2.82	0.42
2:B:997:VAL:CG2	2:B:999:TYR:CE2	3.02	0.42
1:A:459:PRO:C	1:A:461:VAL:H	2.26	0.42
1:A:602:GLU:O	1:A:602:GLU:HG3	2.19	0.42
1:A:703:LEU:HD23	1:A:703:LEU:H	1.84	0.42
1:A:727:PHE:O	1:A:729:PRO:HD3	2.18	0.42
1:A:912:ILE:HG13	2:B:924:MET:SD	2.59	0.42
1:A:1247:ARG:HG2	1:A:1628:VAL:CG2	2.50	0.42
1:A:1672:MET:O	1:A:1677:SER:HB2	2.19	0.42
2:B:75:PHE:CD1	2:B:120:TRP:CB	3.03	0.42
2:B:746:ILE:CG2	2:B:914:LEU:HD22	2.50	0.42
2:B:854:VAL:HG12	9:L:34:ILE:CG2	2.41	0.42
3:C:86:THR:HA	3:C:119:PRO:CG	2.49	0.42
3:C:312:SER:HB3	3:C:321:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:6:GLU:O	4:E:10:LEU:HD13	2.19	0.42
1:A:454:ASN:HA	1:A:614:THR:HG21	2.00	0.42
1:A:1713:PHE:CE1	5:F:61:GLU:HG2	2.55	0.42
2:B:370:VAL:HG13	2:B:637:MET:HA	2.01	0.42
4:E:103:LEU:HD21	4:E:130:PHE:CD2	2.55	0.42
1:A:312:VAL:HG23	1:A:320:PHE:C	2.44	0.42
1:A:1086:ARG:HB2	1:A:1086:ARG:NH1	2.35	0.42
1:A:1639:ARG:HE	4:E:199:THR:HG21	1.85	0.42
1:A:1715:LEU:HD23	1:A:1715:LEU:HA	1.85	0.42
2:B:489:LEU:HD23	2:B:489:LEU:O	2.19	0.42
2:B:541:PRO:HD2	10:N:46:GLN:HE22	1.82	0.42
3:C:236:LEU:HB2	3:C:305:HIS:CD2	2.55	0.42
3:C:337:LEU:HD21	8:K:100:LEU:CB	2.49	0.42
4:E:110:MET:SD	4:E:118:LEU:CD1	3.06	0.42
10:N:56:PHE:HZ	10:N:80:TYR:HB2	1.83	0.42
13:I:85:ARG:HG3	13:I:86:ARG:H	1.85	0.42
1:A:860:MET:HE2	1:A:864:LYS:HG3	2.01	0.42
1:A:992:ILE:HD11	1:A:1252:LEU:HD13	2.01	0.42
1:A:1266:VAL:HG12	1:A:1596:ASP:O	2.19	0.42
1:A:1268:VAL:O	1:A:1268:VAL:HG12	2.19	0.42
1:A:1268:VAL:HG13	1:A:1595:LEU:HD23	2.01	0.42
1:A:1280:SER:O	1:A:1284:GLN:HB2	2.19	0.42
1:A:1711:GLY:HA2	5:F:64:ARG:HH11	1.84	0.42
2:B:167:GLY:O	2:B:169:TYR:HD2	2.02	0.42
2:B:668:SER:O	2:B:672:ASN:ND2	2.53	0.42
2:B:804:LEU:HD23	2:B:804:LEU:H	1.85	0.42
3:C:40:TRP:HZ2	8:K:106:VAL:CG2	2.33	0.42
3:C:240:THR:O	3:C:240:THR:HG23	2.20	0.42
4:E:73:PHE:HD2	4:E:75:PHE:CZ	2.38	0.42
1:A:402:PHE:CZ	2:B:1126:MET:HA	2.54	0.42
1:A:642:THR:HB	1:A:748:VAL:O	2.19	0.42
1:A:659:ARG:HD3	1:A:787:ALA:HB1	2.02	0.42
1:A:711:ILE:HG13	1:A:750:ASP:OD2	2.19	0.42
1:A:896:MET:O	1:A:896:MET:HG3	2.19	0.42
1:A:1020:GLY:O	1:A:1021:GLU:HB2	2.20	0.42
1:A:1034:PRO:C	1:A:1036:GLN:H	2.28	0.42
1:A:1150:TRP:O	1:A:1151:ARG:C	2.62	0.42
1:A:1324:HIS:HD2	1:A:1328:GLN:HG3	1.84	0.42
1:A:1334:ARG:HG3	1:A:1335:PRO:CD	2.40	0.42
1:A:1648:MET:HE2	1:A:1654:TYR:CE1	2.55	0.42
2:B:210:VAL:HG21	2:B:349:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:GLN:O	2:B:288:ILE:HB	2.19	0.42
3:C:50:ARG:HG3	3:C:66:VAL:HB	2.02	0.42
6:H:26:SER:HB3	6:H:45:ILE:HG21	2.02	0.42
7:J:17:LYS:HE3	7:J:38:LEU:O	2.20	0.42
12:M:30:ASN:ND2	13:I:18:ASP:HA	2.35	0.42
1:A:78:LEU:HD12	1:A:306:PRO:HD3	2.01	0.41
1:A:513:THR:HG23	1:A:514:GLN:N	2.34	0.41
1:A:1092:TYR:CZ	1:A:1095:LYS:HD2	2.55	0.41
1:A:1133:ARG:O	1:A:1133:ARG:CG	2.66	0.41
1:A:1570:ASN:OD1	1:A:1571:LYS:N	2.53	0.41
2:B:171:ILE:CG2	2:B:174:GLY:HA2	2.47	0.41
2:B:521:VAL:O	2:B:616:PRO:O	2.38	0.41
3:C:263:GLU:CB	3:C:276:ALA:HB2	2.50	0.41
13:I:83:VAL:H	13:I:83:VAL:HG12	1.59	0.41
13:I:103:ARG:NH2	13:I:107:GLU:HG3	2.35	0.41
15:T:-8:DG:H8	15:T:-8:DG:O5'	2.03	0.41
1:A:408:LYS:H	1:A:408:LYS:HD3	1.84	0.41
1:A:679:PHE:CE1	6:H:47:ILE:HG12	2.55	0.41
1:A:754:TYR:HE1	1:A:781:LEU:HD22	1.85	0.41
1:A:896:MET:O	1:A:896:MET:CG	2.67	0.41
2:B:162:GLU:HB2	2:B:165:GLU:HB3	2.01	0.41
3:C:135:ILE:H	3:C:135:ILE:HG12	1.48	0.41
4:E:122:ALA:C	4:E:124:LYS:N	2.77	0.41
13:I:87:CYS:HA	13:I:88:PRO:HD3	1.92	0.41
1:A:326:VAL:HG11	1:A:414:TYR:CE1	2.55	0.41
1:A:613:CYS:SG	1:A:614:THR:N	2.93	0.41
1:A:1037:PHE:N	1:A:1038:PRO:CD	2.82	0.41
1:A:1200:TRP:CD1	1:A:1200:TRP:C	2.98	0.41
1:A:1580:THR:CG2	1:A:1581:GLU:N	2.84	0.41
2:B:179:ILE:HD11	2:B:434:PHE:CE2	2.55	0.41
2:B:210:VAL:HG23	2:B:349:MET:HE2	2.02	0.41
3:C:336:PHE:CZ	8:K:44:LEU:HB3	2.55	0.41
4:E:179:VAL:O	4:E:179:VAL:HG12	2.18	0.41
6:H:105:SER:C	6:H:107:GLU:H	2.28	0.41
15:T:-4:DA:H1'	15:T:-3:DG:H5'	2.03	0.41
1:A:496:MET:HB2	1:A:496:MET:HE3	1.73	0.41
1:A:661:LEU:HG	1:A:691:LEU:CD1	2.51	0.41
2:B:346:LEU:HD23	2:B:346:LEU:HA	1.93	0.41
2:B:549:SER:C	2:B:551:SER:H	2.28	0.41
2:B:566:VAL:HG23	2:B:574:ILE:HD12	2.02	0.41
3:C:267:VAL:HG11	3:C:272:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:67:ASP:O	4:E:70:ASP:N	2.53	0.41
6:H:39:LEU:HD12	6:H:125:LEU:HD13	2.00	0.41
8:K:45:HIS:O	8:K:46:GLU:HB2	2.19	0.41
13:I:17:LEU:HD13	13:I:35:THR:O	2.20	0.41
1:A:927:PRO:CG	2:B:488:ARG:NH2	2.79	0.41
1:A:1618:LEU:HD11	1:A:1649:CYS:CB	2.49	0.41
2:B:35:LEU:HD13	2:B:730:TYR:HD2	1.85	0.41
2:B:804:LEU:HG	2:B:805:GLN:N	2.36	0.41
1:A:569:LEU:HA	1:A:570:PRO:HD3	1.95	0.41
1:A:796:THR:OG1	2:B:745:VAL:O	2.35	0.41
1:A:968:CYS:HA	2:B:686:MET:HE3	2.03	0.41
1:A:1162:THR:O	1:A:1166:LYS:HG3	2.20	0.41
1:A:1324:HIS:CD2	1:A:1328:GLN:HG3	2.56	0.41
1:A:1704:LYS:HE2	1:A:1704:LYS:HB3	1.74	0.41
2:B:66:PHE:CZ	2:B:400:PHE:CD2	3.06	0.41
2:B:86:THR:HG22	2:B:87:VAL:N	2.35	0.41
2:B:104:ARG:NH2	2:B:169:TYR:OH	2.52	0.41
3:C:29:PHE:CE1	8:K:57:TYR:HE1	2.39	0.41
3:C:40:TRP:HB2	8:K:61:LYS:HB3	2.02	0.41
5:F:110:LEU:HB3	5:F:111:PRO:HD2	2.01	0.41
8:K:60:MET:SD	8:K:68:CYS:HB3	2.60	0.41
16:U:7:DT:H6	16:U:7:DT:H2'	1.58	0.41
1:A:33:ILE:HD11	1:A:81:ILE:CG1	2.51	0.41
1:A:593:GLU:OE2	2:B:1009:LYS:O	2.39	0.41
1:A:897:MET:HG3	2:B:918:HIS:HE1	1.85	0.41
1:A:939:GLU:HG2	1:A:940:PRO:N	2.34	0.41
1:A:1504:ALA:O	1:A:1508:ILE:HG13	2.21	0.41
2:B:215:VAL:HA	2:B:220:SER:O	2.20	0.41
2:B:247:LEU:HD11	2:B:304:LEU:HD21	2.03	0.41
2:B:1042:ARG:HG2	2:B:1054:LEU:HD21	2.03	0.41
12:M:68:SER:HB2	12:M:112:LEU:HB2	2.02	0.41
1:A:874:ASN:HB2	13:I:83:VAL:O	2.20	0.41
1:A:975:LEU:HD22	13:I:104:SER:CA	2.33	0.41
1:A:1104:LYS:HD2	1:A:1104:LYS:O	2.20	0.41
2:B:185:PRO:O	2:B:186:ARG:HB2	2.21	0.41
2:B:267:GLU:HA	2:B:270:LYS:HD3	2.02	0.41
2:B:396:ILE:HA	2:B:422:MET:CB	2.51	0.41
2:B:416:LEU:HD12	2:B:419:ILE:HD11	2.02	0.41
2:B:786:LYS:O	2:B:788:GLY:N	2.52	0.41
3:C:84:VAL:HA	3:C:85:PRO:HD3	1.94	0.41
3:C:312:SER:HB3	3:C:321:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:LEU:HD21	4:E:58:LEU:HD11	2.02	0.41
12:M:67:LEU:HD12	12:M:68:SER:N	2.36	0.41
1:A:20:TYR:CD1	2:B:1129:LYS:HD3	2.55	0.41
1:A:26:LYS:HE3	1:A:301:PHE:CE2	2.55	0.41
1:A:468:TYR:HB2	1:A:598:PHE:CE2	2.56	0.41
1:A:585:TYR:O	1:A:586:ASN:HB3	2.21	0.41
1:A:678:PRO:HB2	6:H:47:ILE:HG21	1.96	0.41
1:A:705:LEU:HD23	1:A:706:SER:N	2.36	0.41
1:A:734:GLU:HG3	6:H:22:PHE:CZ	2.55	0.41
1:A:753:HIS:C	1:A:755:GLY:H	2.29	0.41
1:A:792:TYR:HB3	3:C:24:VAL:HG11	2.03	0.41
1:A:850:HIS:HD2	1:A:941:TYR:OH	2.04	0.41
1:A:910:MET:C	1:A:912:ILE:H	2.28	0.41
1:A:1034:PRO:O	1:A:1035:LYS:CB	2.69	0.41
1:A:1184:LYS:HE3	1:A:1184:LYS:HB3	1.84	0.41
1:A:1341:PHE:CE1	1:A:1345:ARG:HD2	2.56	0.41
1:A:1348:LYS:HE3	1:A:1508:ILE:HB	2.02	0.41
1:A:1543:LEU:HD23	1:A:1543:LEU:C	2.46	0.41
1:A:1568:THR:HG21	1:A:1577:VAL:HG11	2.01	0.41
2:B:92:ILE:CG2	2:B:93:CYS:N	2.82	0.41
2:B:180:ARG:NH1	14:R:-5:C:OP1	2.44	0.41
2:B:399:ALA:HB2	2:B:422:MET:SD	2.61	0.41
3:C:203:ARG:O	3:C:204:PRO:C	2.64	0.41
4:E:17:ILE:HG21	4:E:74:VAL:HG11	2.03	0.41
8:K:92:ALA:C	8:K:95:PRO:HD2	2.46	0.41
8:K:93:VAL:O	8:K:93:VAL:HG12	2.21	0.41
10:N:61:VAL:N	12:M:9:ALA:O	2.54	0.41
1:A:127:LEU:HD21	1:A:135:VAL:HG22	2.01	0.41
1:A:445:ILE:HD11	1:A:587:ALA:HB1	2.03	0.41
1:A:811:LYS:HA	1:A:814:ARG:HG2	2.03	0.41
1:A:934:SER:C	2:B:491:PRO:HB2	2.44	0.41
1:A:967:HIS:CD2	2:B:682:SER:OG	2.74	0.41
1:A:1300:GLN:O	1:A:1315:TYR:HA	2.20	0.41
1:A:1557:LYS:O	1:A:1584:ASN:ND2	2.53	0.41
1:A:1583:ILE:HG23	1:A:1583:ILE:O	2.21	0.41
1:A:1598:ARG:HA	4:E:142:HIS:CD2	2.55	0.41
2:B:46:PHE:CE1	2:B:50:VAL:HG11	2.56	0.41
2:B:364:ASP:OD1	2:B:606:LEU:HD22	2.21	0.41
2:B:681:GLN:HG3	2:B:683:PRO:HD2	2.03	0.41
2:B:700:LEU:HA	2:B:735:TYR:HE1	1.85	0.41
2:B:987:GLU:OE1	3:C:301:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:VAL:HG22	3:C:214:CYS:SG	2.61	0.41
3:C:245:VAL:O	3:C:246:GLU:HG3	2.21	0.41
3:C:337:LEU:HD12	8:K:104:MET:HE3	2.02	0.41
6:H:80:ASP:O	6:H:82:PRO:HD3	2.21	0.41
12:M:28:PHE:HB2	12:M:31:GLY:O	2.21	0.41
1:A:215:VAL:HG22	1:A:225:ILE:CG2	2.50	0.40
1:A:439:TYR:H	2:B:1014:THR:HA	1.86	0.40
1:A:737:VAL:HA	1:A:746:CYS:O	2.20	0.40
1:A:847:GLN:NE2	2:B:603:LYS:HD2	2.35	0.40
1:A:1602:SER:HB3	1:A:1608:ILE:HD11	2.02	0.40
2:B:82:ILE:HD13	2:B:137:VAL:HG21	2.02	0.40
2:B:262:TYR:CG	12:M:30:ASN:HA	2.54	0.40
2:B:333:CYS:SG	2:B:333:CYS:O	2.79	0.40
2:B:648:GLU:C	2:B:650:GLU:H	2.28	0.40
2:B:808:ASP:OD2	9:L:46:LYS:NZ	2.54	0.40
2:B:1056:ASP:O	2:B:1057:ARG:O	2.39	0.40
3:C:45:PHE:CZ	8:K:106:VAL:HG13	2.56	0.40
3:C:180:ASN:HD22	3:C:180:ASN:HA	1.77	0.40
7:J:63:ALA:HB1	7:J:64:PRO:HD2	2.03	0.40
10:N:70:LYS:HE2	10:N:79:ARG:NH1	2.36	0.40
10:N:94:LEU:HD13	12:M:89:VAL:HG21	2.03	0.40
10:N:131:GLN:HB2	10:N:134:PRO:HB3	2.02	0.40
13:I:28:PRO:HA	13:I:41:CYS:HA	2.02	0.40
13:I:88:PRO:HB3	13:I:92:HIS:CD2	2.56	0.40
1:A:681:LEU:CD1	6:H:47:ILE:HD11	2.52	0.40
1:A:956:LEU:O	2:B:679:HIS:HD2	2.04	0.40
1:A:976:VAL:HG13	2:B:484:THR:HG21	2.03	0.40
1:A:1104:LYS:HD3	1:A:1116:GLY:CA	2.52	0.40
1:A:1590:LYS:CE	4:E:133:GLN:HE21	2.35	0.40
2:B:179:ILE:HG23	2:B:453:LEU:O	2.21	0.40
2:B:284:GLN:HG3	2:B:288:ILE:HG13	2.04	0.40
2:B:365:ASN:OD1	2:B:365:ASN:N	2.52	0.40
2:B:1035:ILE:O	2:B:1036:ARG:C	2.64	0.40
6:H:88:PHE:HA	6:H:146:LYS:HB2	2.04	0.40
8:K:24:LYS:C	8:K:26:ALA:N	2.76	0.40
10:N:49:ALA:HB2	12:M:84:LEU:O	2.21	0.40
1:A:327:ASN:HB3	1:A:401:VAL:HG22	2.02	0.40
1:A:448:ASP:O	1:A:449:MET:CB	2.69	0.40
1:A:1267:PRO:HG2	1:A:1596:ASP:HB3	2.03	0.40
1:A:1281:LEU:CD2	1:A:1595:LEU:HD11	2.51	0.40
1:A:1289:CYS:SG	1:A:1549:HIS:O	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1610:ASN:O	4:E:178:PRO:HG2	2.20	0.40
2:B:15:SER:O	2:B:723:ARG:NH2	2.55	0.40
2:B:42:HIS:C	2:B:140:MET:HE1	2.47	0.40
2:B:263:GLN:HB2	12:M:29:SER:CA	2.52	0.40
2:B:410:SER:C	2:B:411:MET:HE2	2.46	0.40
2:B:759:VAL:O	2:B:896:LEU:HA	2.21	0.40
2:B:820:GLN:O	2:B:823:ASP:HB2	2.21	0.40
2:B:909:MET:HE2	2:B:909:MET:HB3	1.72	0.40
2:B:1069:VAL:CG2	2:B:1134:VAL:HG21	2.50	0.40
4:E:81:LYS:HB2	4:E:81:LYS:HE3	1.84	0.40
8:K:90:LEU:HA	8:K:91:PRO:HD3	1.91	0.40
1:A:975:LEU:CD2	13:I:105:ALA:N	2.84	0.40
1:A:1318:ARG:HD2	1:A:1524:TRP:CE3	2.50	0.40
2:B:791:SER:HB3	2:B:792:LEU:CD2	2.48	0.40
2:B:937:SER:OG	2:B:965:MET:HB3	2.22	0.40
4:E:169:GLN:O	4:E:169:GLN:HG2	2.21	0.40
1:A:32:SER:HB2	1:A:80:HIS:CE1	2.57	0.40
1:A:293:ASN:O	1:A:296:VAL:HG23	2.22	0.40
1:A:603:LEU:HD22	2:B:1052:PHE:HB3	2.04	0.40
1:A:642:THR:CG2	1:A:744:LEU:HD21	2.52	0.40
1:A:740:ARG:O	1:A:741:GLU:HB2	2.22	0.40
1:A:866:LYS:HD3	1:A:925:ARG:HG3	2.03	0.40
1:A:955:PHE:CE1	2:B:681:GLN:HA	2.56	0.40
2:B:31:GLN:HG3	2:B:153:PRO:HG3	2.02	0.40
2:B:95:GLU:HA	2:B:95:GLU:OE1	2.21	0.40
2:B:1017:ALA:HB3	2:B:1026:ILE:HG21	2.04	0.40
3:C:157:SER:O	3:C:161:GLU:HG3	2.21	0.40
13:I:96:ALA:O	13:I:114:THR:N	2.52	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	A	1459/1719 (85%)	1310 (90%)	141 (10%)	8 (0%)	24	59
2	B	1119/1135 (99%)	1017 (91%)	99 (9%)	3 (0%)	36	68
3	C	335/346 (97%)	312 (93%)	23 (7%)	0	100	100
4	E	195/210 (93%)	185 (95%)	10 (5%)	0	100	100
5	F	74/127 (58%)	70 (95%)	4 (5%)	0	100	100
6	H	144/150 (96%)	130 (90%)	14 (10%)	0	100	100
7	J	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
8	K	106/133 (80%)	96 (91%)	9 (8%)	1 (1%)	14	46
9	L	43/58 (74%)	37 (86%)	6 (14%)	0	100	100
10	N	149/510 (29%)	134 (90%)	13 (9%)	2 (1%)	9	36
11	G	153/338 (45%)	138 (90%)	14 (9%)	1 (1%)	18	51
12	M	108/419 (26%)	107 (99%)	1 (1%)	0	100	100
13	I	103/126 (82%)	68 (66%)	32 (31%)	3 (3%)	3	18
All	All	4050/5338 (76%)	3663 (90%)	369 (9%)	18 (0%)	31	63

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	1605	ILE
2	B	1125	ALA
10	N	156	PRO
13	I	28	PRO
2	B	1033	GLY
11	G	102	LEU
1	A	677	LYS
10	N	132	PRO
13	I	8	ASN
13	I	27	LEU
1	A	719	GLU
1	A	866	LYS
1	A	22	ALA
1	A	206	PRO
8	K	24	LYS
2	B	1031	VAL
1	A	311	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1298/1503 (86%)	1218 (94%)	80 (6%)	16	47
2	B	982/992 (99%)	896 (91%)	86 (9%)	9	33
3	C	296/302 (98%)	274 (93%)	22 (7%)	13	40
4	E	183/192 (95%)	180 (98%)	3 (2%)	55	78
5	F	66/111 (60%)	66 (100%)	0	100	100
6	H	129/131 (98%)	125 (97%)	4 (3%)	35	67
7	J	53/56 (95%)	50 (94%)	3 (6%)	18	50
8	K	96/119 (81%)	94 (98%)	2 (2%)	47	74
9	L	42/55 (76%)	41 (98%)	1 (2%)	43	72
10	N	119/427 (28%)	113 (95%)	6 (5%)	22	54
11	G	135/288 (47%)	130 (96%)	5 (4%)	30	63
12	M	94/366 (26%)	90 (96%)	4 (4%)	26	59
13	I	94/111 (85%)	91 (97%)	3 (3%)	34	66
All	All	3587/4653 (77%)	3368 (94%)	219 (6%)	19	47

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	16	SER
1	A	19	MET
1	A	65	SER
1	A	82	GLU
1	A	83	LEU
1	A	85	LEU
1	A	86	THR
1	A	200	MET
1	A	204	ARG
1	A	206	PRO
1	A	209	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	292	PHE
1	A	295	SER
1	A	296	VAL
1	A	303	VAL
1	A	304	VAL
1	A	312	VAL
1	A	315	LEU
1	A	318	GLN
1	A	319	MET
1	A	341	LEU
1	A	348	GLU
1	A	381	GLN
1	A	383	LEU
1	A	408	LYS
1	A	409	LEU
1	A	410	MET
1	A	412	ASP
1	A	453	THR
1	A	454	ASN
1	A	484	VAL
1	A	535	THR
1	A	550	LEU
1	A	553	GLN
1	A	555	THR
1	A	557	HIS
1	A	561	ILE
1	A	635	MET
1	A	664	LYS
1	A	676	LEU
1	A	680	PRO
1	A	701	ILE
1	A	718	LYS
1	A	833	LEU
1	A	868	GLU
1	A	869	VAL
1	A	870	ASN
1	A	878	LYS
1	A	885	LEU
1	A	888	GLN
1	A	891	GLU
1	A	906	THR
1	A	1045	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1046	VAL
1	A	1051	GLN
1	A	1055	GLU
1	A	1057	LEU
1	A	1145	PRO
1	A	1184	LYS
1	A	1186	GLU
1	A	1260	LYS
1	A	1263	MET
1	A	1266	VAL
1	A	1268	VAL
1	A	1269	LEU
1	A	1272	LYS
1	A	1288	VAL
1	A	1313	GLN
1	A	1316	GLN
1	A	1317	LEU
1	A	1340	ARG
1	A	1505	VAL
1	A	1507	GLU
1	A	1508	ILE
1	A	1509	HIS
1	A	1556	THR
1	A	1603	ASN
1	A	1606	HIS
1	A	1677	SER
2	B	26	ILE
2	B	29	GLU
2	B	31	GLN
2	B	32	LYS
2	B	35	LEU
2	B	71	GLU
2	B	73	ILE
2	B	74	SER
2	B	76	THR
2	B	111	ARG
2	B	144	LYS
2	B	222	VAL
2	B	224	MET
2	B	226	LEU
2	B	229	LEU
2	B	231	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	235	MET
2	B	249	LEU
2	B	260	SER
2	B	267	GLU
2	B	273	GLU
2	B	274	ASP
2	B	276	SER
2	B	278	LEU
2	B	289	VAL
2	B	290	MET
2	B	292	GLU
2	B	307	CYS
2	B	314	VAL
2	B	318	TYR
2	B	321	GLU
2	B	325	GLU
2	B	327	LEU
2	B	330	GLN
2	B	332	ILE
2	B	334	ILE
2	B	337	LYS
2	B	338	SER
2	B	345	MET
2	B	348	LEU
2	B	353	LEU
2	B	361	CYS
2	B	365	ASN
2	B	429	PRO
2	B	430	PHE
2	B	454	CYS
2	B	461	ASN
2	B	463	ILE
2	B	466	LEU
2	B	506	GLU
2	B	537	LEU
2	B	542	ILE
2	B	547	HIS
2	B	582	LYS
2	B	601	THR
2	B	659	GLN
2	B	666	LEU
2	B	667	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	678	ASP
2	B	680	ASN
2	B	728	ASP
2	B	755	ASP
2	B	792	LEU
2	B	793	VAL
2	B	797	LYS
2	B	828	TYR
2	B	859	THR
2	B	864	PHE
2	B	866	CYS
2	B	1011	GLN
2	B	1012	VAL
2	B	1015	THR
2	B	1018	ARG
2	B	1025	PRO
2	B	1031	VAL
2	B	1046	LEU
2	B	1056	ASP
2	B	1059	PHE
2	B	1063	ASP
2	B	1064	ARG
2	B	1069	VAL
2	B	1077	LEU
2	B	1105	ASP
2	B	1109	THR
2	B	1111	SER
2	B	1119	PHE
3	C	21	VAL
3	C	55	HIS
3	C	58	GLU
3	C	94	VAL
3	C	96	ASN
3	C	114	PRO
3	C	121	LEU
3	C	133	THR
3	C	134	GLU
3	C	135	ILE
3	C	136	ASP
3	C	137	THR
3	C	138	LEU
3	C	144	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	151	HIS
3	C	161	GLU
3	C	166	HIS
3	C	196	ASP
3	C	266	GLU
3	C	267	VAL
3	C	274	ARG
3	C	275	VAL
4	E	31	ASP
4	E	107	GLN
4	E	185	ILE
6	H	15	ILE
6	H	80	ASP
6	H	83	SER
6	H	89	GLU
7	J	5	VAL
7	J	9	THR
7	J	28	GLU
8	K	27	LEU
8	K	30	VAL
9	L	52	LEU
10	N	25	SER
10	N	60	HIS
10	N	116	ARG
10	N	118	LEU
10	N	130	LEU
10	N	133	ILE
11	G	95	ASN
11	G	97	LYS
11	G	98	VAL
11	G	102	LEU
11	G	169	MET
12	M	67	LEU
12	M	81	CYS
12	M	110	GLN
12	M	112	LEU
13	I	37	THR
13	I	82	VAL
13	I	83	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	89	ASN
1	A	108	HIS
1	A	163	GLN
1	A	170	GLN
1	A	324	GLN
1	A	347	GLN
1	A	397	HIS
1	A	478	GLN
1	A	482	GLN
1	A	486	ASN
1	A	499	ASN
1	A	564	HIS
1	A	578	HIS
1	A	597	HIS
1	A	600	GLN
1	A	616	GLN
1	A	632	GLN
1	A	652	HIS
1	A	728	ASN
1	A	753	HIS
1	A	790	GLN
1	A	832	ASN
1	A	847	GLN
1	A	850	HIS
1	A	877	ASN
1	A	908	ASN
1	A	918	GLN
1	A	967	HIS
1	A	989	GLN
1	A	1051	GLN
1	A	1068	HIS
1	A	1076	GLN
1	A	1094	GLN
1	A	1109	ASN
1	A	1111	ASN
1	A	1118	GLN
1	A	1136	GLN
1	A	1177	GLN
1	A	1258	ASN
1	A	1313	GLN
1	A	1565	ASN
1	A	1579	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1603	ASN
1	A	1683	GLN
1	A	1690	HIS
2	B	9	ASN
2	B	18	HIS
2	B	30	GLN
2	B	31	GLN
2	B	36	GLN
2	B	97	ASN
2	B	147	ASN
2	B	150	ASN
2	B	219	HIS
2	B	223	ASN
2	B	237	ASN
2	B	313	ASN
2	B	371	ASN
2	B	473	HIS
2	B	501	HIS
2	B	523	GLN
2	B	639	GLN
2	B	672	ASN
2	B	679	HIS
2	B	715	GLN
2	B	846	ASN
2	B	887	HIS
2	B	1004	HIS
2	B	1024	GLN
2	B	1032	GLN
2	B	1097	ASN
3	C	48	ASN
3	C	59	ASN
3	C	102	GLN
3	C	116	HIS
3	C	127	GLN
3	C	166	HIS
3	C	180	ASN
3	C	181	GLN
3	C	222	HIS
3	C	277	ASN
3	C	290	ASN
3	C	305	HIS
4	E	132	GLN

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Mol	Chain	Res	Type
4	E	133	GLN
4	E	169	GLN
6	H	126	GLN
7	J	61	ASN
8	K	85	GLN
10	N	46	GLN
12	M	98	GLN
12	M	110	GLN
13	I	92	HIS
13	I	117	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	5/6 (83%)	2 (40%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	-6	G
14	R	-5	C

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

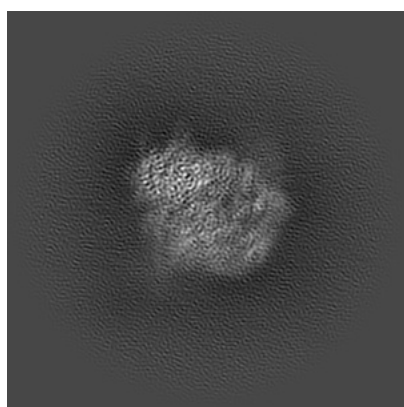
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31878. These allow visual inspection of the internal detail of the map and identification of artifacts.

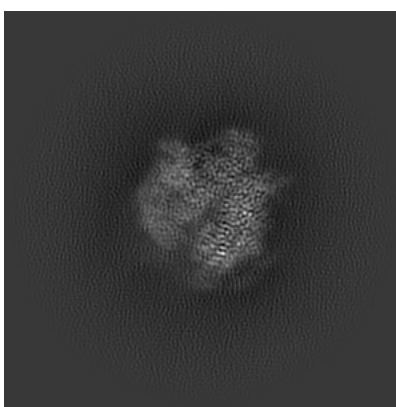
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

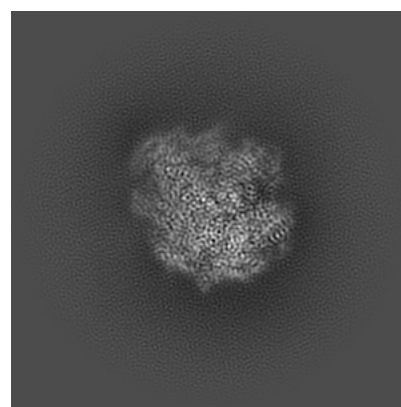
#### 6.1.1 Primary map



X



Y

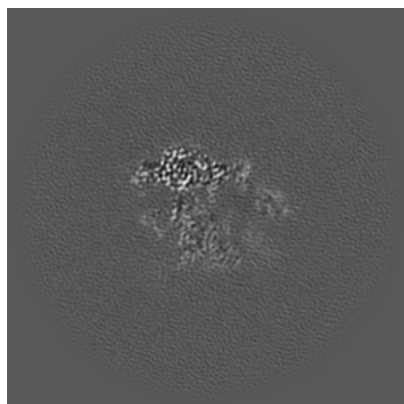


Z

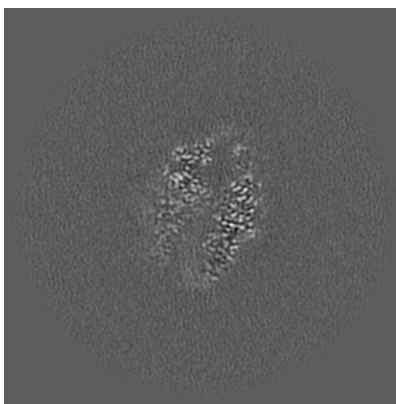
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

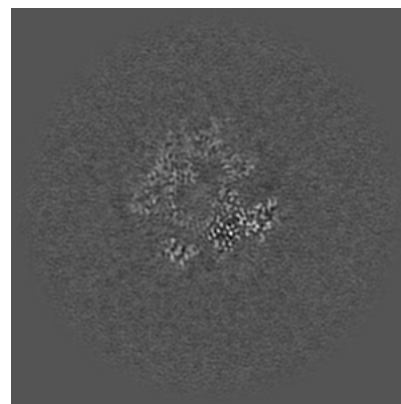
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

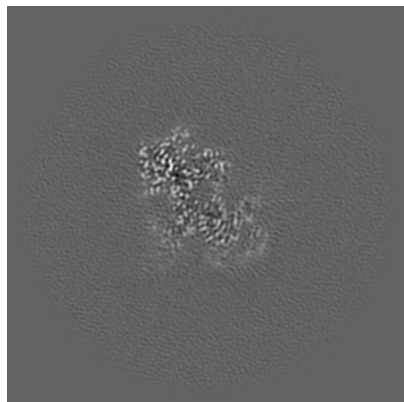


Z Index: 160

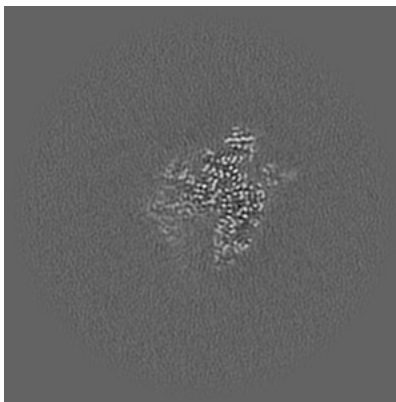
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

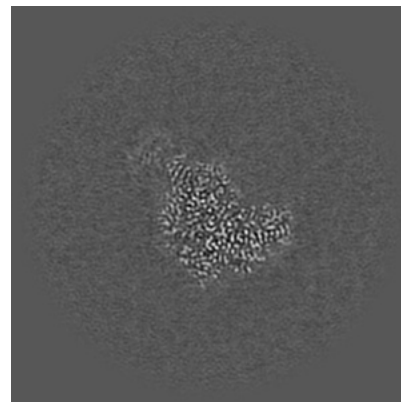
### 6.3.1 Primary map



X Index: 179



Y Index: 139

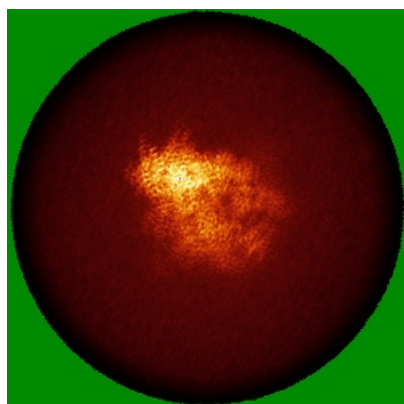


Z Index: 185

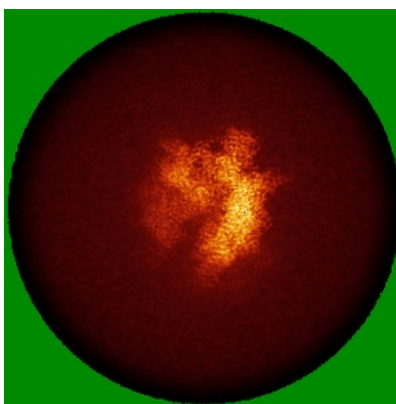
The images above show the largest variance slices of the map in three orthogonal directions.

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

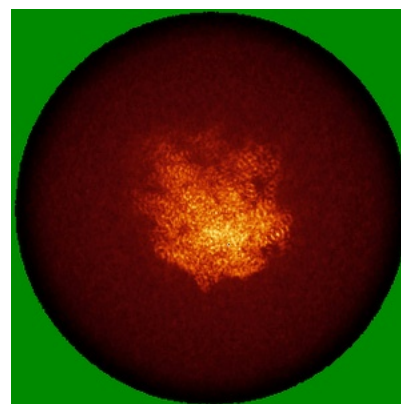
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

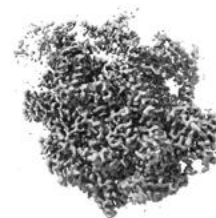
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.575. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

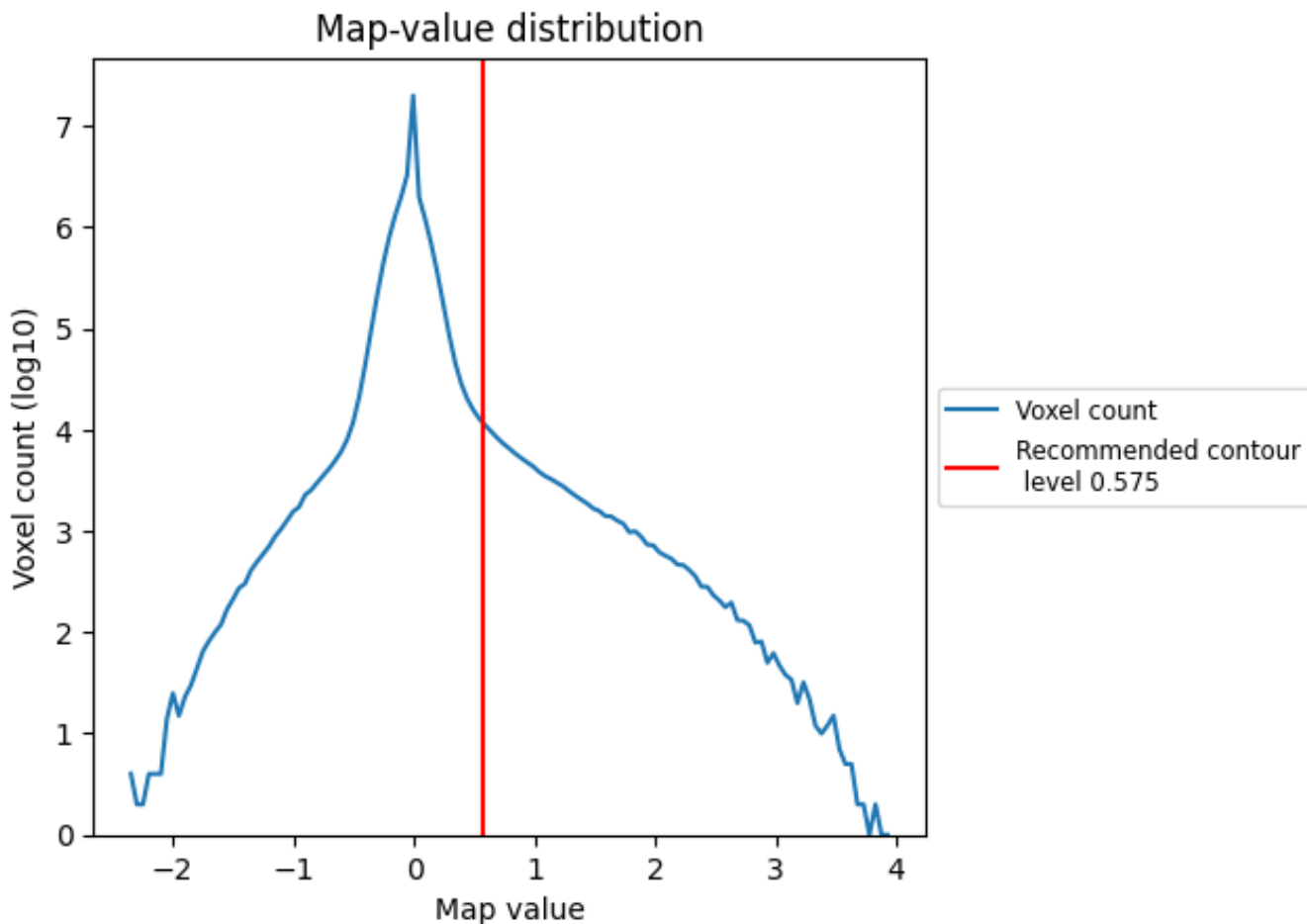
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

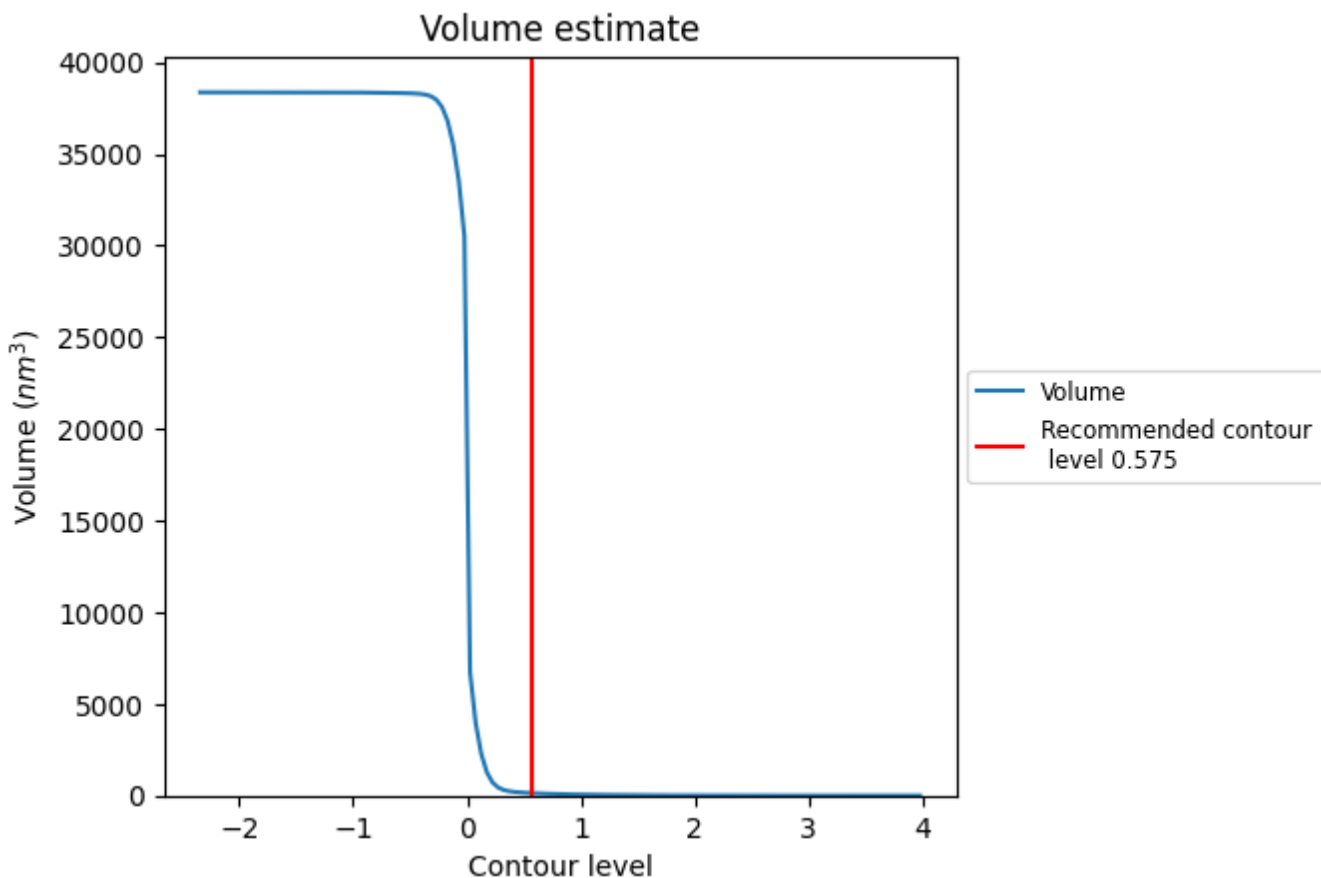
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

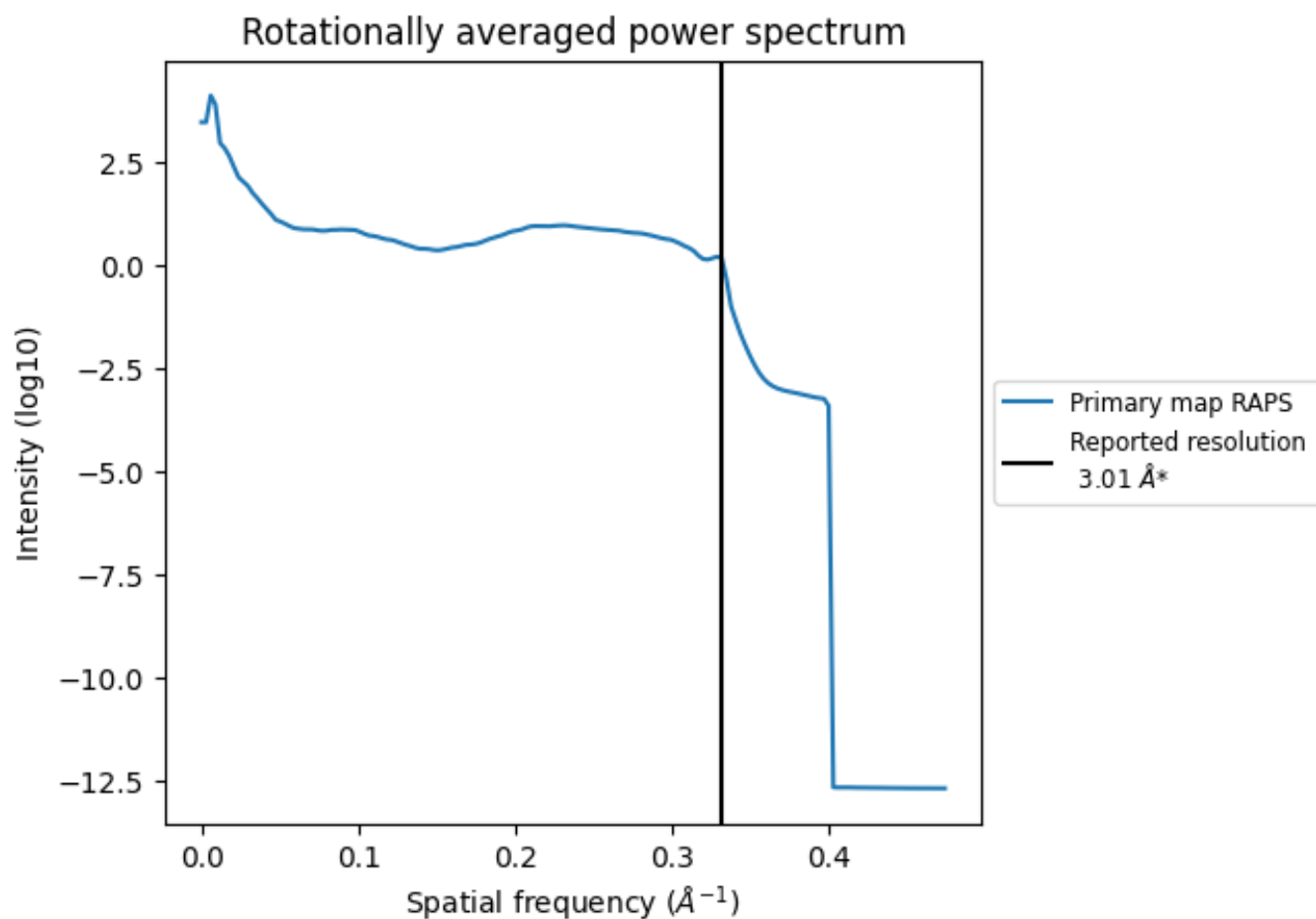
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm<sup>3</sup>; this corresponds to an approximate mass of 117 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.332 \text{\AA}^{-1}$

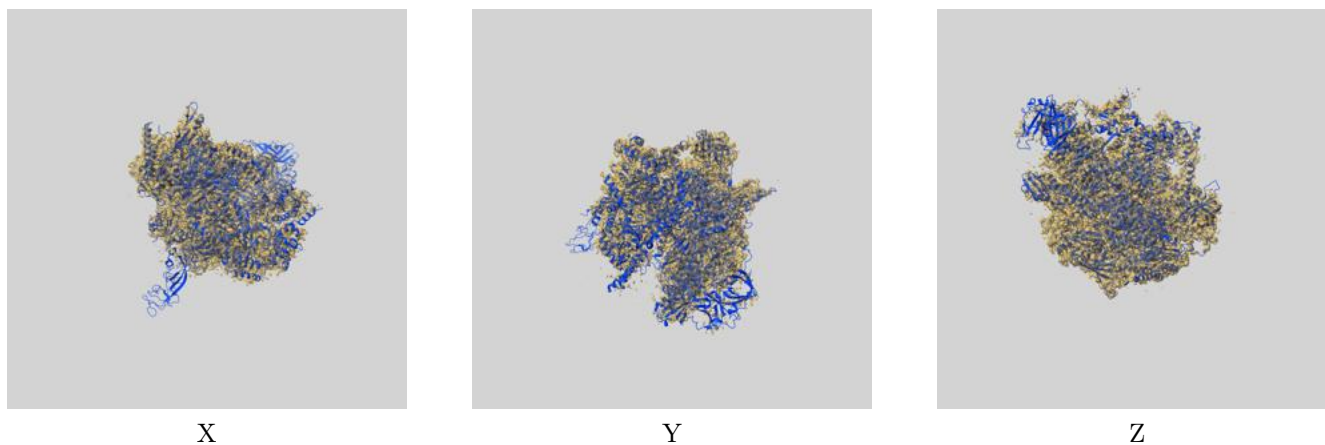
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

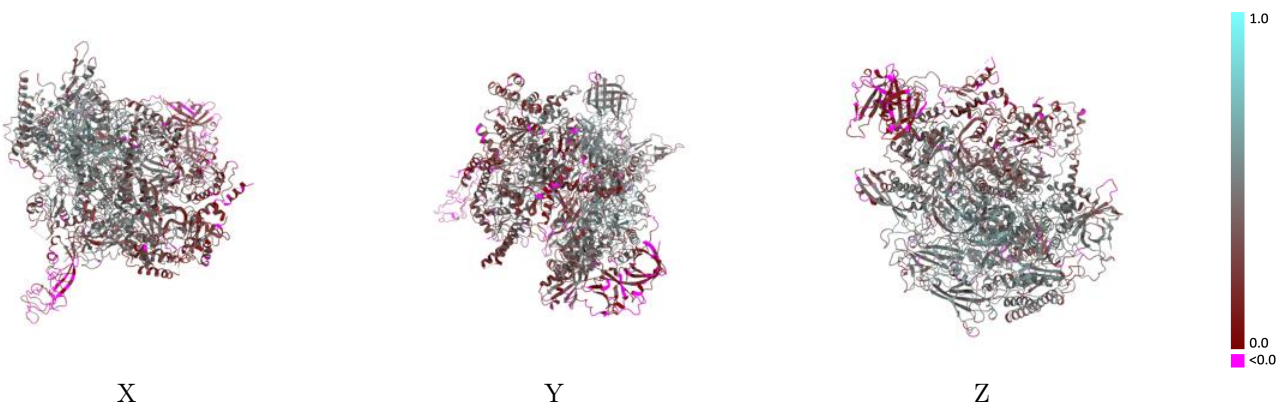
This section contains information regarding the fit between EMDB map EMD-31878 and PDB model 7VBC. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



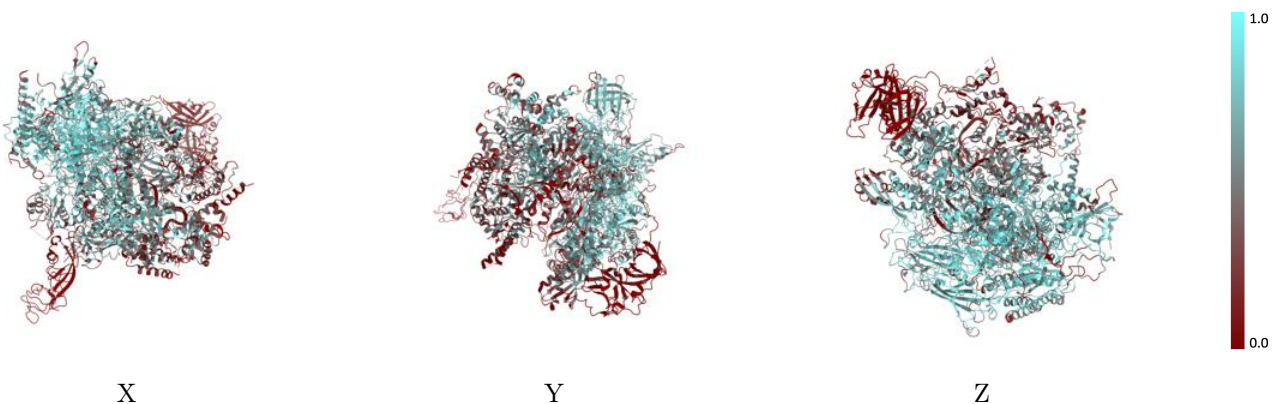
The images above show the 3D surface view of the map at the recommended contour level 0.575 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



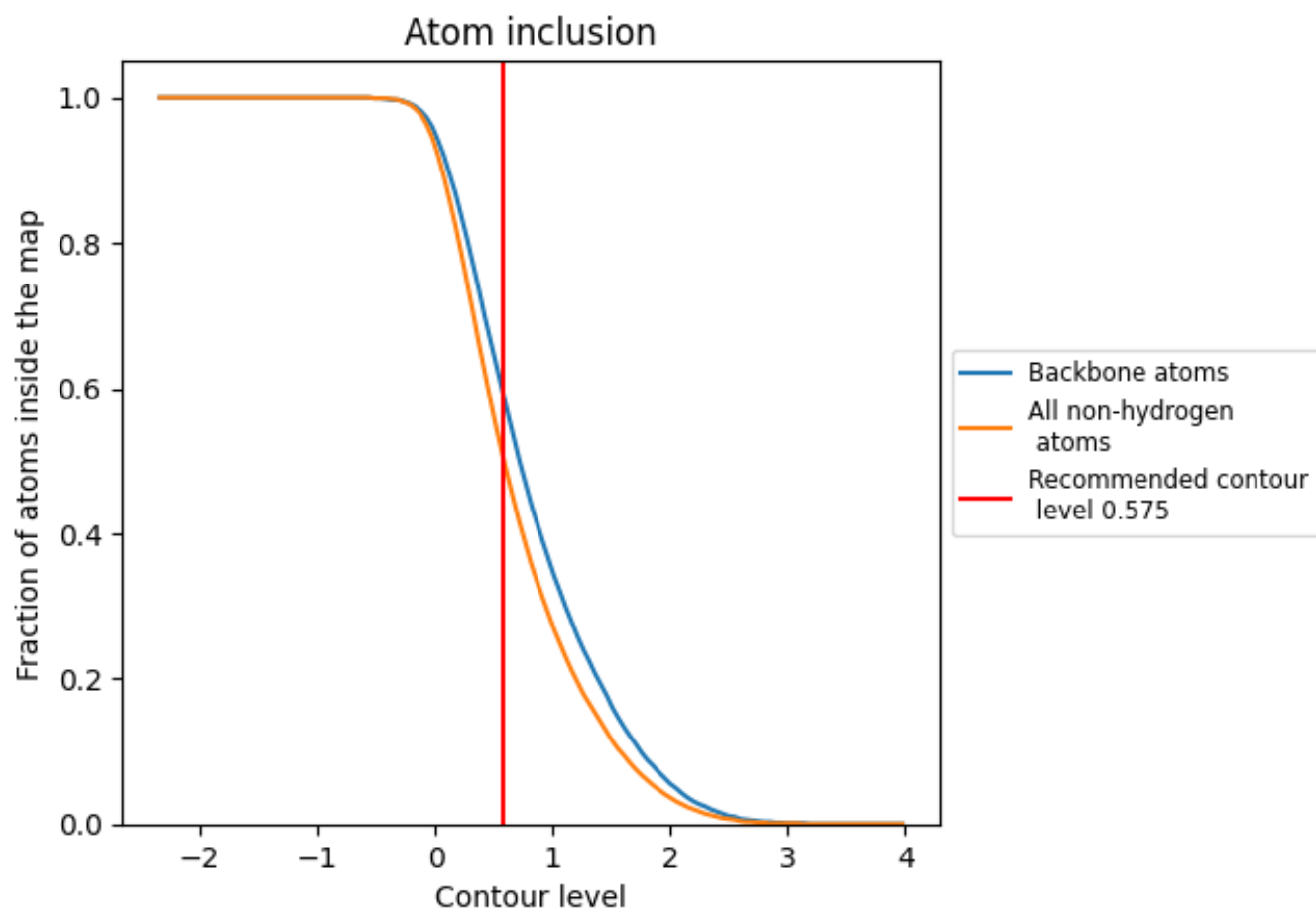
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.575).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 51% 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 (0.575) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5060	 0.3730
A	 0.5020	 0.3710
B	 0.6550	 0.4570
C	 0.6220	 0.4270
E	 0.4240	 0.2760
F	 0.4380	 0.3070
G	 0.0260	 0.0550
H	 0.6330	 0.4230
I	 0.2490	 0.3950
J	 0.8360	 0.5340
K	 0.6630	 0.4370
L	 0.6970	 0.4290
M	 0.0490	 0.1320
N	 0.0330	 0.0980
R	 0.4220	 0.5210
T	 0.2820	 0.3820
U	 0.1170	 0.3040

