



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:48 AM UTC

PDB ID : 7VBB / pdb_00007vbb
EMDB ID : EMD-31877
Title : Structure of the post state human RNA Polymerase I Elongation Complex
Authors : Zhao, D.; Liu, W.; Chen, K.; Yang, H.; Xu, Y.
Deposited on : 2021-08-31
Resolution : 2.81 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

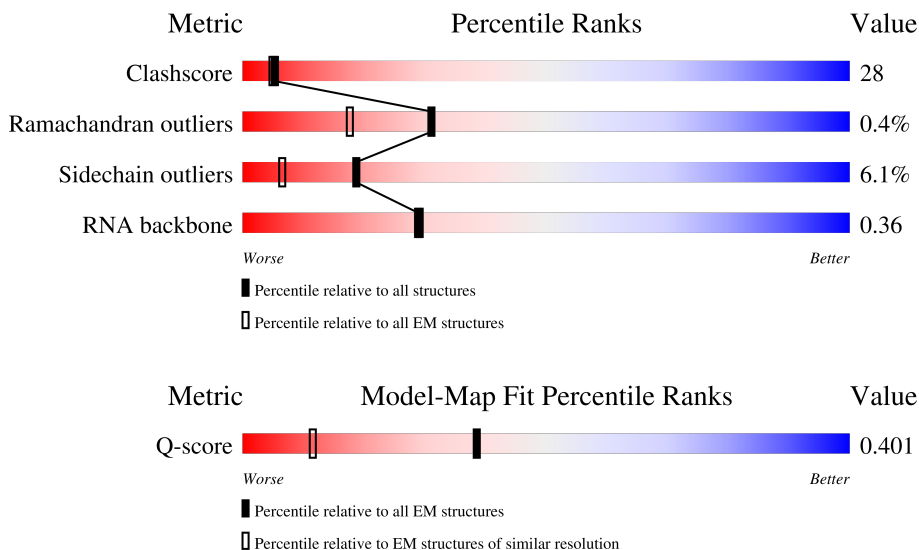
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.81 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	11740 (2.31 - 3.31)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	I	126	
8	J	67	
9	K	133	
10	L	58	
11	N	510	
12	G	338	
13	M	419	
14	R	8	
15	T	25	
16	U	14	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 33151 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	1473	11749	7474	2063	2134	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 polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	60	447	277	76	89	5	0	0

- Molecule 8 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		
8	J	64	507	328	86	87	6	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 10 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		
10	L	45	379	236	73	64	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA34.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA43.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
14	R	8	Total	C	N	O	P	0	0
			168	75	27	58	8		

- Molecule 15 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms				AltConf	Trace	
15	T	25	Total	C	N	O	P	0	0
			514	243	105	142	24		

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
16	U	14	Total	C	N	O	P	0	0
			281	135	48	85	13		

- 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	

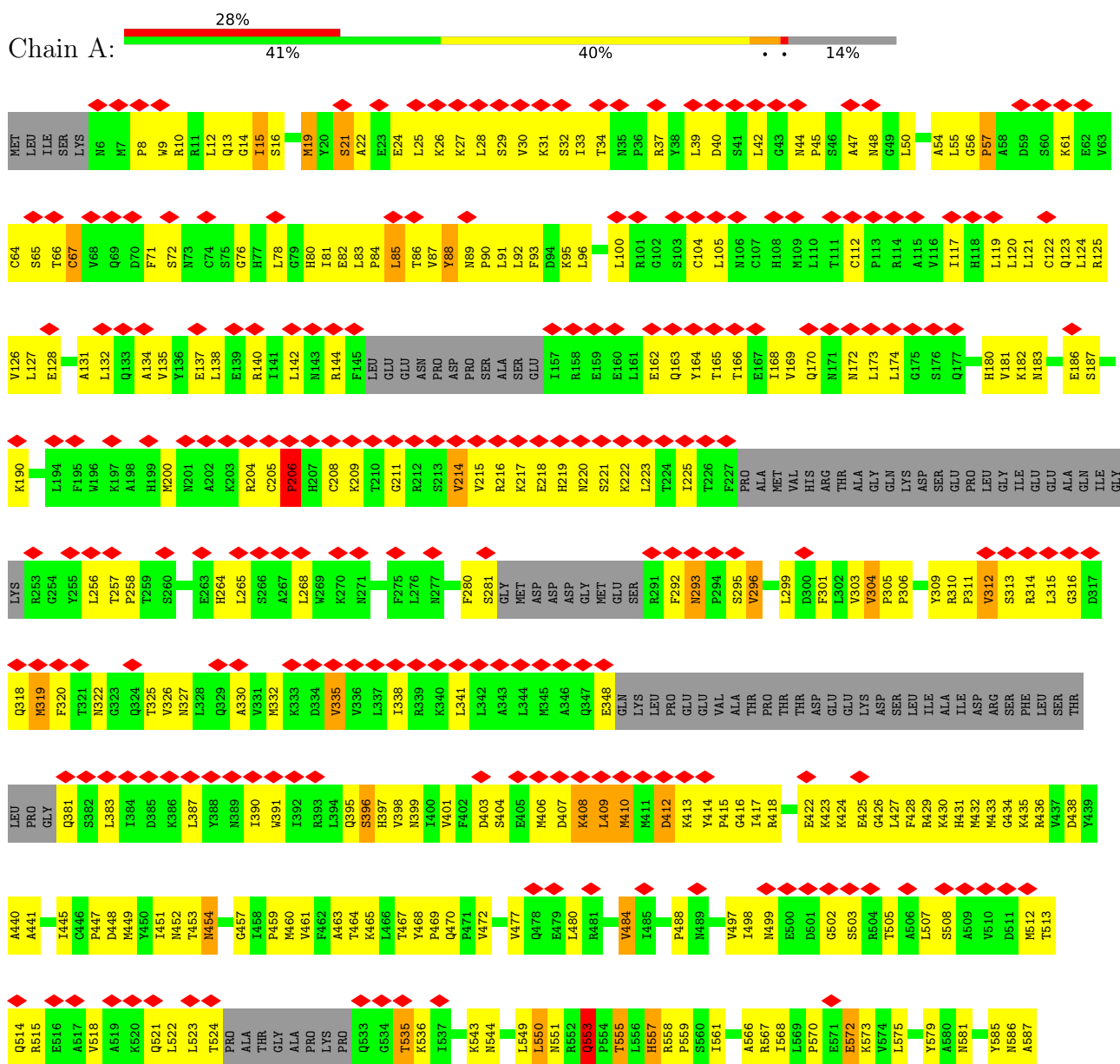
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

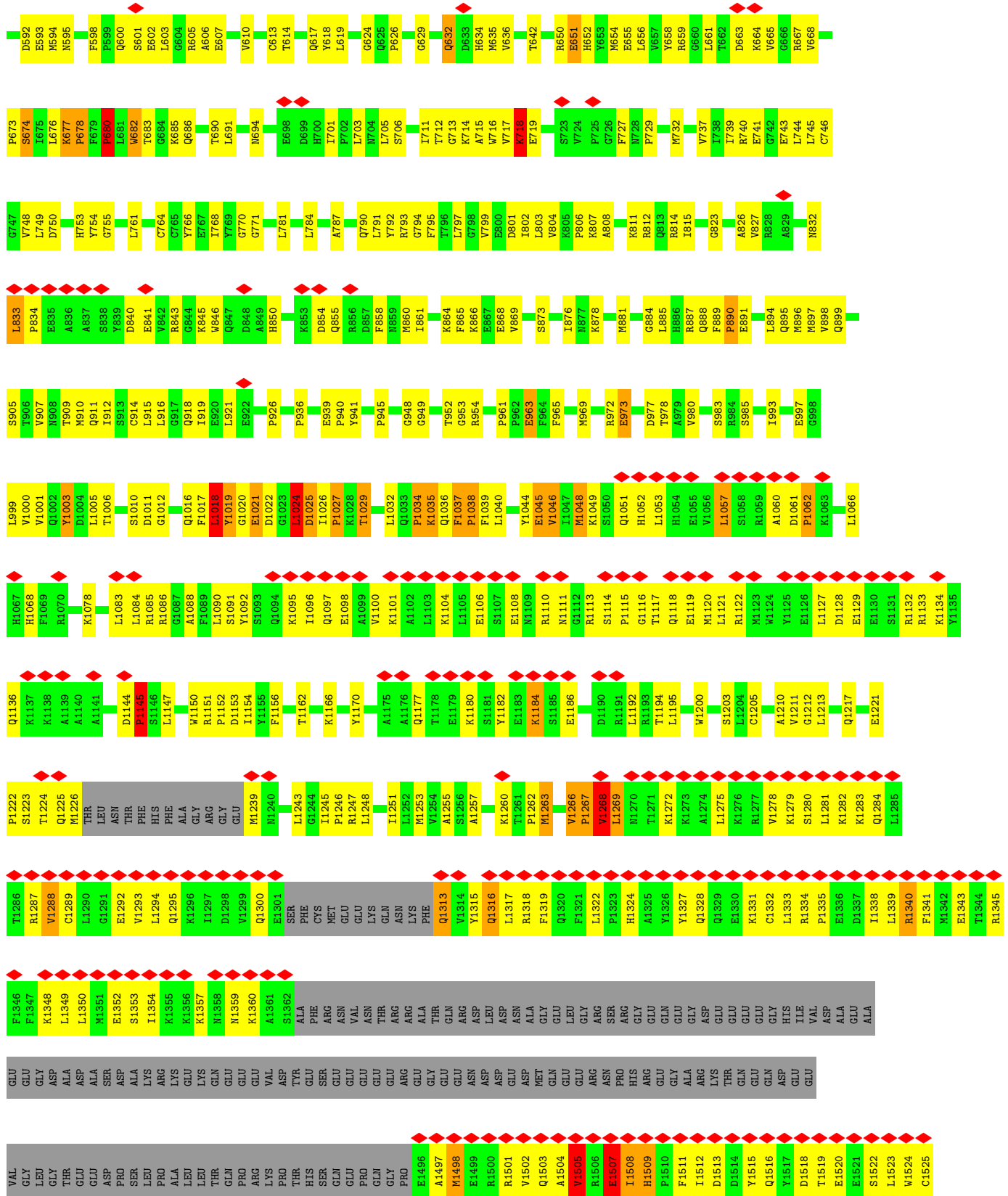
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

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

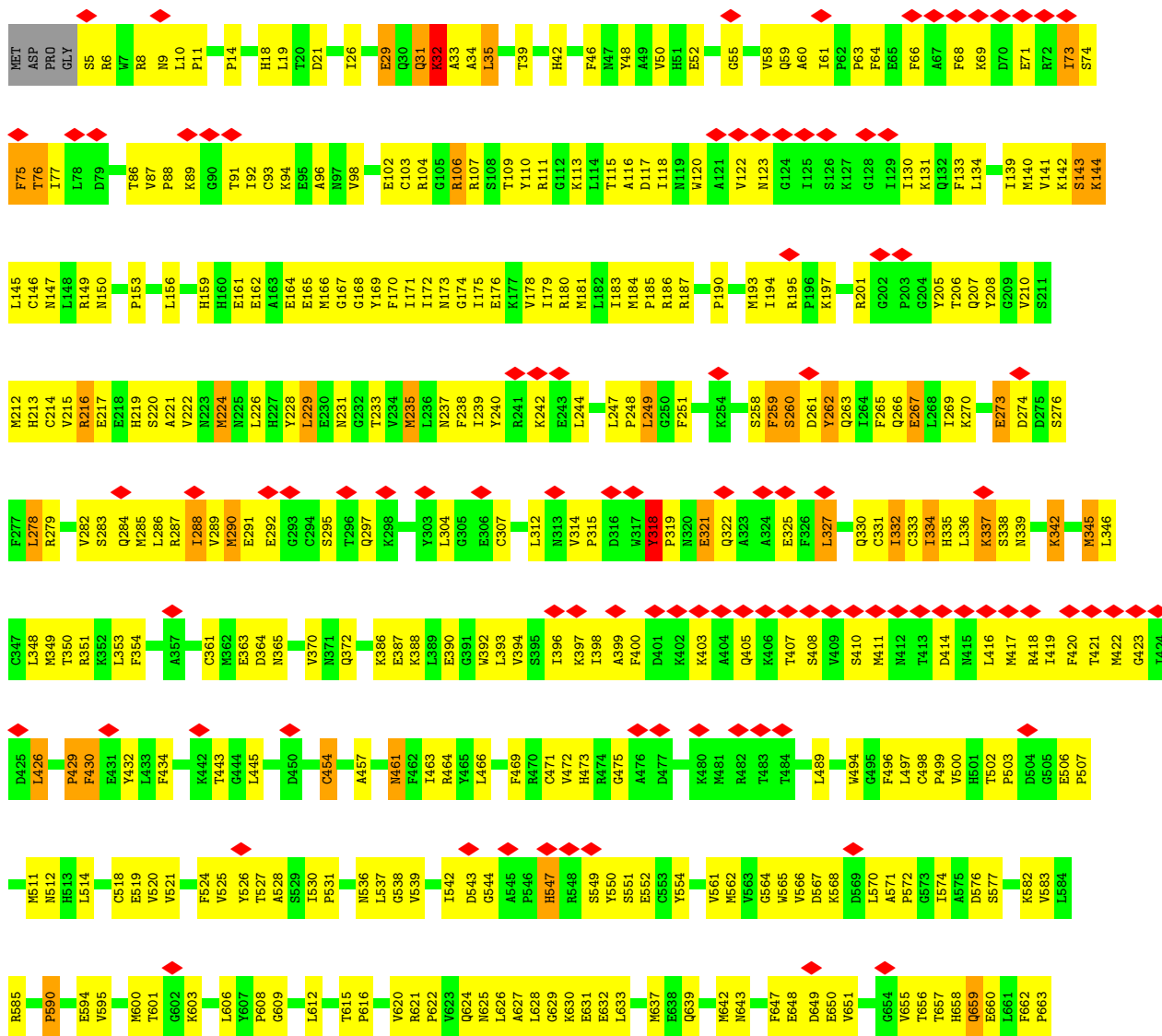
- Molecule 1: DNA-directed RNA polymerase I subunit RPA1

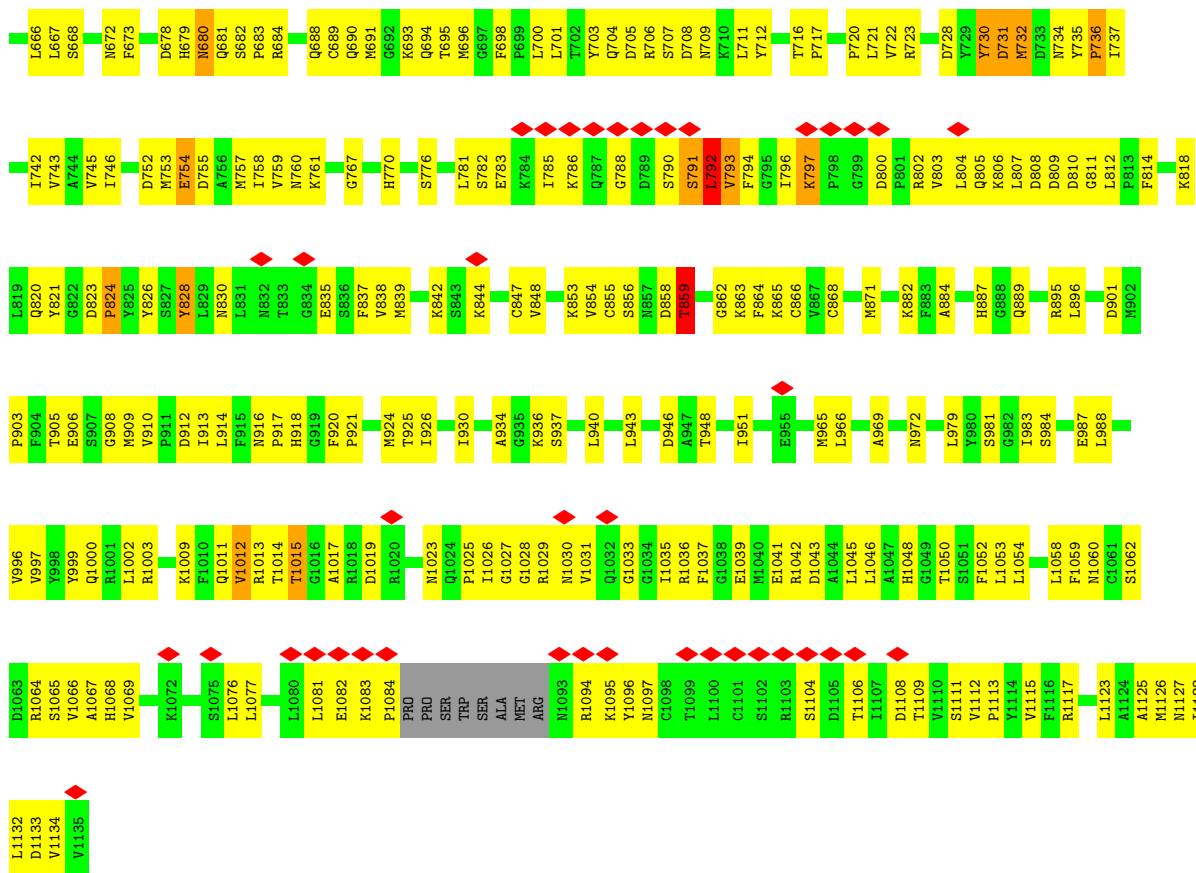




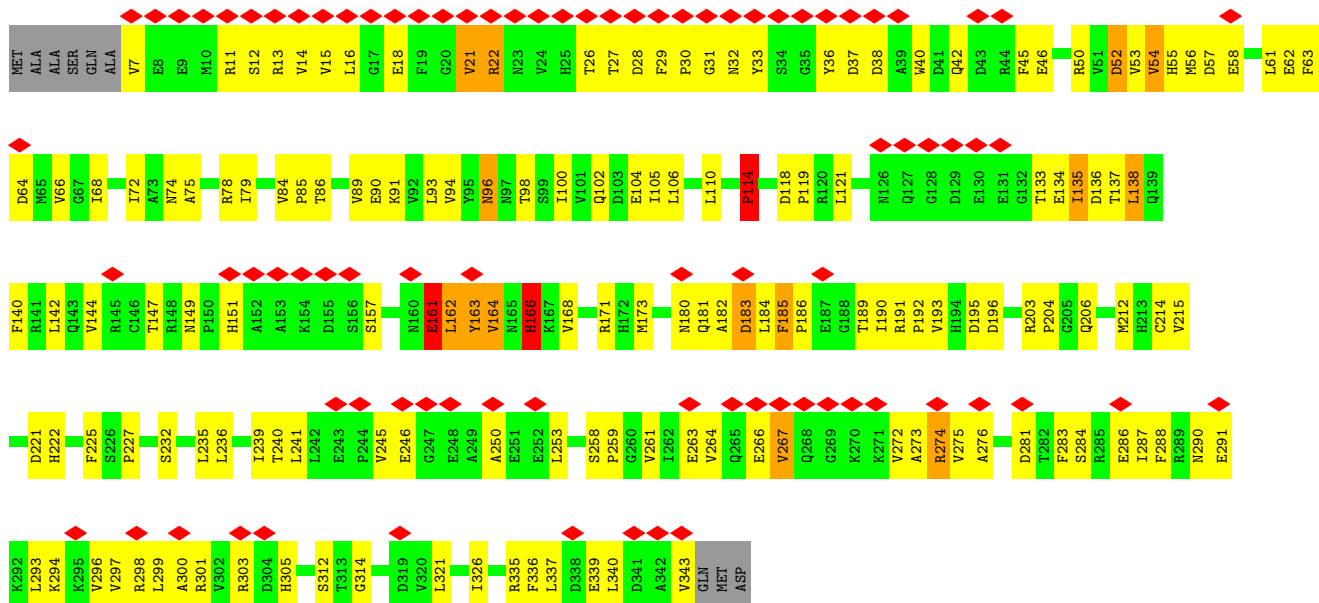


• Molecule 2: DNA-directed RNA polymerase I subunit RPA2





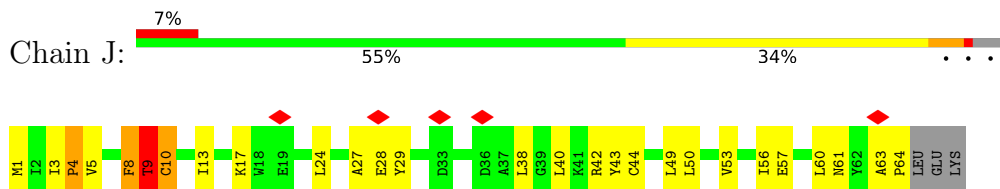
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



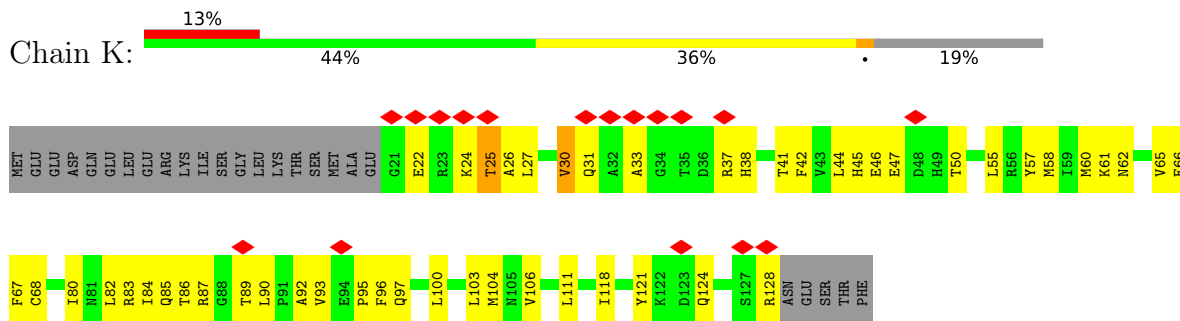
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

GLN
GLU
LYS
GLU
ASP
SER

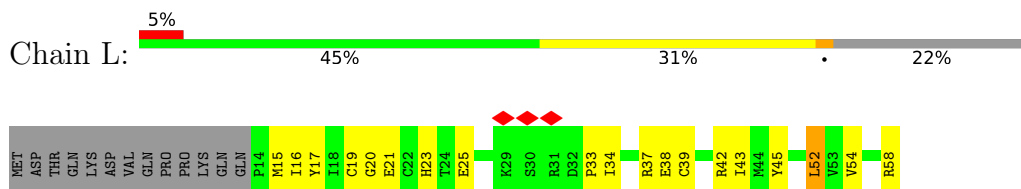
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



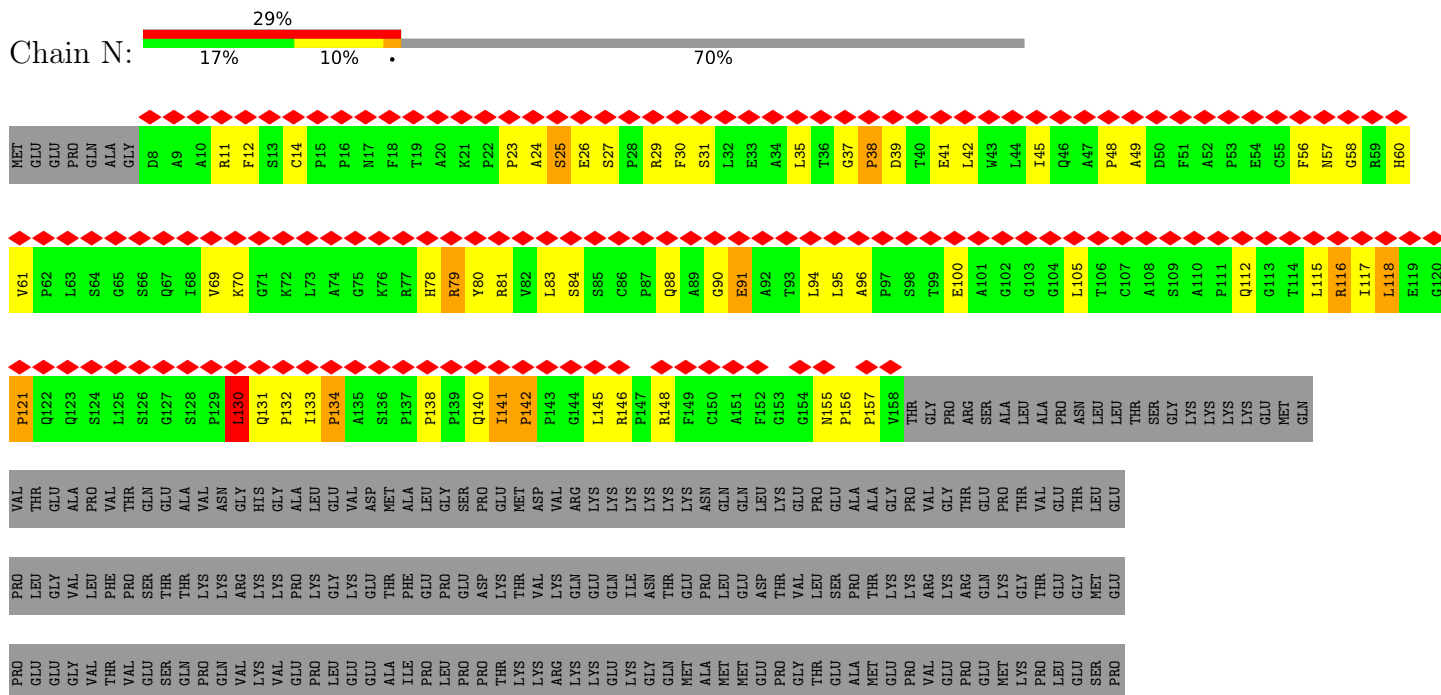
- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: DNA-directed RNA polymerase I subunit RPA34



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183087	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	5.000	Depositor
Minimum map value	-3.528	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.687	Depositor
Map size (\AA)	334.08002, 334.08002, 334.08002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.044, 1.044, 1.044	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	0.70	10/11988 (0.1%)	1.06	73/16184 (0.5%)
2	B	0.71	6/9127 (0.1%)	1.10	67/12350 (0.5%)
3	C	0.75	2/2751 (0.1%)	1.19	30/3729 (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	4/1614 (0.2%)
7	I	1.34	1/454 (0.2%)	1.65	9/615 (1.5%)
8	J	0.66	0/516	1.14	5/696 (0.7%)
9	K	0.39	0/878	0.82	1/1182 (0.1%)
10	L	0.35	0/385	0.66	0/511
11	N	1.10	9/1140 (0.8%)	1.43	21/1560 (1.3%)
12	G	0.38	0/1252	0.64	1/1691 (0.1%)
13	M	1.06	7/884 (0.8%)	1.29	13/1192 (1.1%)
14	R	0.19	0/186	0.35	0/287
15	T	0.25	0/579	0.39	0/892
16	U	0.19	0/313	0.38	0/481
All	All	0.69	35/33939 (0.1%)	1.04	225/46077 (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
8	J	0	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	20	CYS	C-N	25.44	1.69	1.33
13	M	66	ARG	C-N	-9.02	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	590	PRO	C-O	-8.21	1.18	1.25
13	M	61	ALA	C-N	-7.70	1.23	1.33
11	N	155	ASN	C-N	7.54	1.42	1.33
11	N	100	GLU	C-N	-7.51	1.24	1.33
1	A	1498	MET	C-O	7.19	1.32	1.24
11	N	57	ASN	C-N	7.00	1.44	1.33
1	A	1503	GLN	C-O	-6.45	1.16	1.24
2	B	682	SER	CA-CB	-6.40	1.44	1.53
2	B	143	SER	CA-CB	-6.37	1.44	1.53
11	N	58	GLY	C-N	-6.29	1.24	1.33
13	M	57	GLN	C-N	-6.06	1.25	1.33
13	M	32	LYS	C-N	-6.05	1.25	1.33
11	N	69	VAL	C-N	-5.93	1.25	1.33
13	M	39	MET	C-N	-5.93	1.25	1.33
1	A	629	GLY	C-O	-5.89	1.17	1.24
1	A	632	GLN	C-O	-5.88	1.19	1.24
11	N	38	PRO	N-CD	5.82	1.55	1.47
2	B	507	PRO	C-O	-5.71	1.18	1.23
11	N	14	CYS	C-N	-5.50	1.28	1.33
2	B	283	SER	CA-CB	-5.46	1.44	1.53
2	B	683	PRO	C-O	-5.44	1.17	1.24
1	A	674	SER	CA-CB	-5.41	1.44	1.53
13	M	33	LEU	C-N	-5.39	1.26	1.34
1	A	581	ASN	C-O	-5.32	1.16	1.24
11	N	91	GLU	C-N	-5.31	1.26	1.33
1	A	447	PRO	C-O	-5.31	1.18	1.23
1	A	961	PRO	C-O	-5.26	1.18	1.24
1	A	673	PRO	C-O	-5.25	1.17	1.23
1	A	57	PRO	C-O	-5.17	1.18	1.23
11	N	90	GLY	C-N	-5.14	1.26	1.33
3	C	114	PRO	C-O	-5.11	1.18	1.23
3	C	284	SER	CA-CB	-5.02	1.46	1.54
13	M	88	PHE	C-N	-5.01	1.27	1.33

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	13	PHE	O-C-N	16.15	143.31	122.96
7	I	20	CYS	O-C-N	-16.14	104.82	123.22
3	C	164	VAL	N-CA-C	-16.07	98.62	112.12
8	J	10	CYS	CB-CA-C	-14.05	86.78	110.24
7	I	13	PHE	CA-C-N	-13.90	97.51	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	13	PHE	C-N-CA	-13.90	97.51	120.72
1	A	1507	GLU	N-CA-C	-11.00	99.30	111.07
9	K	25	THR	N-CA-C	-10.17	100.88	113.18
2	B	19	LEU	N-CA-C	-9.83	97.56	110.53
2	B	159	HIS	N-CA-C	-9.44	95.31	110.32
1	A	1598	ARG	N-CA-C	-9.21	95.34	110.17
11	N	121	PRO	CA-N-CD	-8.96	99.45	112.00
11	N	155	ASN	CA-C-N	8.86	129.50	120.38
11	N	155	ASN	C-N-CA	8.86	129.50	120.38
2	B	1009	LYS	CB-CA-C	-8.82	98.88	111.85
7	I	20	CYS	CA-C-N	8.69	138.13	121.54
7	I	20	CYS	C-N-CA	8.69	138.13	121.54
3	C	163	TYR	CB-CA-C	-8.57	100.19	111.42
1	A	1606	HIS	N-CA-C	-8.53	103.39	113.88
2	B	734	ASN	N-CA-C	-8.35	102.14	111.82
1	A	1505	VAL	CA-C-O	-8.15	112.48	120.95
3	C	166	HIS	CA-CB-CG	8.04	121.84	113.80
1	A	398	VAL	CA-C-N	-8.02	110.06	120.65
1	A	398	VAL	C-N-CA	-8.02	110.06	120.65
2	B	791	SER	N-CA-C	-7.93	103.67	112.72
1	A	634	HIS	N-CA-C	-7.89	103.68	113.38
3	C	191	ARG	CB-CA-C	-7.81	99.91	110.22
1	A	1062	PRO	N-CA-C	7.72	124.56	114.68
1	A	1032	LEU	N-CA-C	-7.61	104.04	112.72
8	J	27	ALA	N-CA-C	-7.60	99.78	110.50
1	A	57	PRO	CB-CA-C	-7.59	104.49	111.40
2	B	291	GLU	N-CA-C	-7.58	104.01	113.18
3	C	191	ARG	N-CA-CB	-7.57	103.16	111.10
13	M	111	PRO	N-CA-C	7.56	123.23	111.21
1	A	313	SER	CA-C-O	-7.48	115.50	119.77
2	B	662	PHE	CA-CB-CG	7.38	121.18	113.80
1	A	1021	GLU	CB-CA-C	7.35	121.13	110.04
11	N	155	ASN	CA-C-O	-7.34	110.10	120.16
2	B	288	ILE	CA-C-N	-7.34	111.75	122.69
2	B	288	ILE	C-N-CA	-7.34	111.75	122.69
1	A	1268	VAL	N-CA-C	7.28	119.13	112.29
1	A	313	SER	O-C-N	7.24	126.19	120.83
2	B	736	PRO	CB-CA-C	7.16	122.03	111.22
2	B	730	TYR	CB-CA-C	-7.13	99.33	111.31
2	B	544	GLY	N-CA-C	7.12	120.81	110.63
2	B	791	SER	CA-C-N	-7.06	112.83	122.86
2	B	791	SER	C-N-CA	-7.06	112.83	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	4	PRO	CB-CA-C	7.04	120.54	111.46
2	B	34	ALA	N-CA-C	-6.99	104.38	113.12
1	A	412	ASP	N-CA-C	-6.99	104.70	113.23
3	C	163	TYR	CA-C-N	-6.97	115.45	122.77
3	C	163	TYR	C-N-CA	-6.97	115.45	122.77
13	M	14	CYS	N-CA-C	-6.96	103.62	111.07
2	B	839	MET	CA-C-O	-6.93	113.44	122.45
3	C	284	SER	N-CA-C	-6.92	105.78	114.56
1	A	680	PRO	N-CA-CB	-6.89	97.07	103.27
11	N	138	PRO	N-CA-C	6.86	119.07	110.70
3	C	183	ASP	N-CA-C	-6.81	101.74	110.53
1	A	1676	THR	CB-CA-C	6.80	121.55	111.89
2	B	732	MET	N-CA-C	-6.80	104.10	112.88
11	N	25	SER	N-CA-C	-6.79	104.99	113.28
13	M	19	GLY	N-CA-C	-6.73	106.52	115.40
11	N	134	PRO	N-CA-C	6.71	121.77	111.57
3	C	114	PRO	N-CA-CB	-6.68	97.82	103.36
1	A	1034	PRO	CA-C-O	-6.64	114.13	121.23
1	A	470	GLN	CB-CA-C	-6.62	99.21	109.08
13	M	110	GLN	CA-C-N	6.55	126.53	119.78
13	M	110	GLN	C-N-CA	6.55	126.53	119.78
2	B	75	PHE	CA-CB-CG	-6.54	107.26	113.80
6	H	77	PRO	N-CA-C	-6.54	106.18	114.35
3	C	22	ARG	N-CA-C	6.49	118.44	111.36
1	A	553	GLN	N-CA-C	6.49	122.53	113.57
1	A	678	PRO	N-CA-C	-6.47	103.30	113.78
2	B	339	ASN	N-CA-C	-6.46	105.55	113.50
3	C	258	SER	N-CA-C	-6.42	101.49	109.64
6	H	87	GLN	N-CA-C	-6.41	105.57	113.19
2	B	443	THR	CB-CA-C	-6.40	98.64	109.72
4	E	180	ALA	N-CA-C	-6.37	105.64	113.41
2	B	547	HIS	CB-CA-C	6.36	119.65	110.04
2	B	730	TYR	CA-C-O	-6.35	113.98	120.84
3	C	225	PHE	CA-CB-CG	6.35	120.15	113.80
2	B	259	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	1267	PRO	CB-CA-C	6.29	119.23	111.12
2	B	145	LEU	N-CA-C	-6.28	103.01	111.87
2	B	590	PRO	N-CA-CB	-6.28	99.67	103.19
1	A	447	PRO	CB-CA-C	-6.28	102.86	111.21
2	B	32	LYS	N-CA-C	6.27	118.11	111.28
2	B	106	ARG	N-CA-C	-6.26	102.45	110.53
11	N	78	HIS	CA-C-N	-6.24	114.19	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	78	HIS	C-N-CA	-6.24	114.19	122.99
1	A	55	LEU	N-CA-C	-6.21	105.56	113.02
2	B	279	ARG	N-CA-C	-6.21	104.51	111.28
3	C	166	HIS	CB-CA-C	6.21	121.41	110.85
1	A	1177	GLN	N-CA-C	-6.19	106.36	114.04
2	B	351	ARG	N-CA-C	-6.14	104.65	111.71
2	B	794	PHE	CB-CA-C	6.14	120.14	109.65
2	B	216	ARG	CB-CA-C	-6.13	100.14	110.19
3	C	259	PRO	N-CA-C	6.10	122.84	113.75
1	A	1062	PRO	N-CA-CB	-6.08	96.72	101.83
2	B	265	PHE	CA-CB-CG	6.08	119.88	113.80
2	B	585	ARG	CB-CA-C	6.07	120.35	111.73
1	A	1319	PHE	CB-CA-C	6.06	121.15	110.85
2	B	500	VAL	N-CA-C	6.01	116.79	110.72
2	B	603	LYS	CB-CA-C	6.00	120.30	109.45
1	A	1182	TYR	CB-CA-C	5.99	120.68	110.56
12	G	168	THR	N-CA-C	5.97	117.46	111.07
1	A	1034	PRO	N-CA-C	-5.97	101.84	111.03
1	A	1503	GLN	CA-C-O	-5.95	114.58	120.82
7	I	17	LEU	CA-C-N	-5.95	110.18	121.54
7	I	17	LEU	C-N-CA	-5.95	110.18	121.54
13	M	77	GLY	CA-C-N	-5.90	112.69	120.95
13	M	77	GLY	C-N-CA	-5.90	112.69	120.95
13	M	110	GLN	CB-CA-C	-5.87	100.33	109.55
8	J	8	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	1061	ASP	CB-CA-C	-5.87	101.50	109.42
2	B	824	PRO	N-CA-CB	-5.86	98.09	103.31
1	A	88	TYR	CA-C-O	-5.84	114.61	121.16
11	N	141	ILE	N-CA-C	5.83	114.67	108.95
3	C	96	ASN	CA-C-N	-5.83	112.74	121.72
3	C	96	ASN	C-N-CA	-5.83	112.74	121.72
6	H	15	ILE	CA-C-O	-5.82	114.48	120.71
3	C	180	ASN	N-CA-C	-5.79	106.08	113.02
1	A	1049	LYS	CB-CA-C	-5.76	101.80	110.90
2	B	464	ARG	N-CA-C	-5.72	103.80	112.04
2	B	266	GLN	CB-CA-C	5.71	121.20	110.63
2	B	731	ASP	CB-CA-C	5.71	118.00	110.06
2	B	826	TYR	CB-CA-C	5.70	122.34	111.17
2	B	318	TYR	CB-CA-C	-5.68	100.62	109.08
3	C	183	ASP	CA-C-O	-5.68	115.41	121.94
2	B	32	LYS	CA-C-O	-5.66	114.55	120.55
2	B	147	ASN	CB-CA-C	5.66	120.86	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	164	VAL	CB-CA-C	5.65	116.45	110.91
1	A	890	PRO	N-CA-C	-5.65	105.67	113.53
2	B	859	THR	CB-CA-C	5.65	120.36	110.64
3	C	161	GLU	CA-C-O	-5.64	115.02	121.68
1	A	1263	MET	CA-C-O	-5.64	115.42	121.45
1	A	678	PRO	CB-CA-C	5.63	122.71	113.20
1	A	90	PRO	N-CA-C	5.63	121.16	113.84
2	B	609	GLY	CA-C-O	-5.63	116.23	122.14
1	A	832	ASN	CB-CA-C	5.63	120.01	111.80
2	B	287	ARG	CB-CA-C	-5.62	100.85	110.24
11	N	26	GLU	N-CA-C	-5.60	106.22	113.16
1	A	293	ASN	N-CA-C	-5.59	103.13	110.39
1	A	1022	ASP	CB-CA-C	-5.58	99.33	110.42
2	B	461	ASN	N-CA-C	-5.56	100.68	108.96
2	B	594	GLU	CB-CA-C	-5.54	102.00	111.31
1	A	1018	LEU	N-CA-C	-5.54	100.29	108.99
3	C	118	ASP	CA-CB-CG	5.52	118.12	112.60
11	N	130	LEU	N-CA-CB	-5.51	102.02	110.01
3	C	162	LEU	N-CA-C	-5.50	105.20	112.24
1	A	718	LYS	CA-C-O	-5.48	114.45	120.43
2	B	19	LEU	CA-C-O	-5.47	115.52	121.87
13	M	69	TYR	CA-C-N	-5.46	115.41	122.99
13	M	69	TYR	C-N-CA	-5.46	115.41	122.99
2	B	754	GLU	CA-C-O	-5.44	115.28	121.65
3	C	185	PHE	CB-CA-C	5.43	116.39	110.15
3	C	192	PRO	CB-CA-C	5.42	118.09	110.98
13	M	111	PRO	CB-CA-C	-5.42	104.29	111.23
1	A	1027	PRO	CB-CA-C	-5.42	103.68	112.62
2	B	279	ARG	CB-CA-C	5.42	119.79	110.79
1	A	1257	ALA	N-CA-C	-5.42	106.51	113.23
1	A	54	ALA	N-CA-C	-5.41	107.05	113.97
1	A	1145	PRO	N-CA-CB	-5.41	98.78	103.32
1	A	1019	TYR	N-CA-C	5.39	116.83	111.07
2	B	262	TYR	CB-CA-C	-5.37	101.73	110.85
3	C	164	VAL	N-CA-CB	5.37	119.25	111.90
1	A	1012	GLY	N-CA-C	-5.35	107.73	115.27
2	B	351	ARG	CB-CA-C	5.34	120.52	110.63
2	B	342	LYS	CB-CA-C	5.34	119.66	110.79
1	A	452	ASN	CA-CB-CG	5.32	117.92	112.60
11	N	79	ARG	CB-CA-C	5.32	119.44	109.71
2	B	792	LEU	N-CA-CB	-5.32	102.76	110.84
1	A	961	PRO	N-CA-C	5.30	117.17	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ASN	CB-CA-C	5.29	119.27	109.54
2	B	106	ARG	CA-C-N	-5.28	114.94	123.23
2	B	106	ARG	C-N-CA	-5.28	114.94	123.23
1	A	1003	TYR	CB-CA-C	5.27	120.38	110.63
1	A	579	TYR	CB-CA-C	-5.25	99.51	109.95
1	A	575	LEU	CA-C-O	-5.24	115.09	120.54
1	A	309	TYR	N-CA-C	-5.23	106.29	113.30
11	N	23	PRO	CB-CA-C	-5.23	103.33	111.22
1	A	770	GLY	CA-C-O	-5.23	117.18	122.56
11	N	37	GLY	CA-C-N	5.22	124.89	119.56
11	N	37	GLY	C-N-CA	5.22	124.89	119.56
1	A	1029	THR	CB-CA-C	-5.22	101.74	110.56
7	I	29	LEU	N-CA-C	-5.22	103.15	109.57
2	B	679	HIS	CA-CB-CG	5.21	119.01	113.80
2	B	793	VAL	N-CA-C	-5.19	98.55	109.34
2	B	107	ARG	CB-CA-C	5.19	120.23	111.41
13	M	82	ASN	CB-CA-C	5.18	120.61	110.67
8	J	9	THR	CB-CA-C	5.15	118.97	110.88
3	C	283	PHE	CB-CA-C	5.15	119.36	110.77
3	C	57	ASP	CB-CA-C	-5.14	101.70	113.33
1	A	682	TRP	CA-C-O	-5.13	114.64	121.46
1	A	1037	PHE	CB-CA-C	5.13	120.28	110.17
1	A	840	ASP	CA-C-N	-5.12	112.52	120.31
1	A	840	ASP	C-N-CA	-5.12	112.52	120.31
11	N	142	PRO	N-CA-C	-5.12	104.45	110.70
1	A	67	CYS	CA-C-N	-5.12	113.50	121.18
1	A	67	CYS	C-N-CA	-5.12	113.50	121.18
2	B	335	HIS	CA-CB-CG	5.11	118.91	113.80
11	N	23	PRO	CA-C-N	-5.11	115.97	122.77
11	N	23	PRO	C-N-CA	-5.11	115.97	122.77
1	A	557	HIS	CA-CB-CG	5.11	118.91	113.80
1	A	651	GLU	N-CA-CB	-5.10	102.44	110.30
1	A	451	ILE	N-CA-C	-5.10	100.55	108.86
1	A	1598	ARG	CA-C-O	-5.10	115.26	121.28
1	A	572	GLU	CA-C-O	-5.10	115.98	121.38
2	B	249	LEU	N-CA-C	-5.10	103.80	110.53
3	C	52	ASP	CA-C-O	-5.09	114.84	120.24
1	A	206	PRO	CB-CA-C	-5.08	103.17	111.56
11	N	140	GLN	N-CA-C	5.08	116.53	108.96
3	C	52	ASP	CB-CA-C	-5.08	102.02	110.14
1	A	335	VAL	N-CA-C	-5.06	105.45	110.62
1	A	21	SER	CA-C-O	-5.06	115.19	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	130	LEU	N-CA-C	5.05	116.47	111.07
1	A	573	LYS	N-CA-C	-5.05	104.92	112.54
2	B	426	LEU	O-C-N	-5.03	115.73	122.43
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
2	B	499	PRO	CA-C-N	5.02	127.54	120.42
2	B	499	PRO	C-N-CA	5.02	127.54	120.42
1	A	1340	ARG	N-CA-C	-5.01	105.94	111.71
13	M	81	CYS	CB-CA-C	-5.01	101.36	110.63
6	H	22	PHE	CB-CA-C	5.00	121.61	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	8	PHE	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	11749	0	11888	753	0
2	B	8912	0	8896	580	0
3	C	2697	0	2676	157	0
4	E	1641	0	1671	110	0
5	F	610	0	642	21	0
6	H	1176	0	1137	59	0
7	I	447	0	429	73	0
8	J	507	0	523	27	0
9	K	863	0	850	69	0
10	L	379	0	387	26	0
11	N	1105	0	1098	50	0
12	G	1229	0	1212	0	0
13	M	867	0	844	69	0
14	R	168	0	85	6	0
15	T	514	0	279	40	0
16	U	281	0	160	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	33151	0	32777	1790	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 28.

All (1790) 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)
13:M:33:LEU:CD2	13:M:39:MET:HE1	1.31	1.58
7:I:20:CYS:C	7:I:21:SER:N	1.69	1.50
2:B:260:SER:HB3	7:I:18:ASP:CB	1.44	1.45
13:M:33:LEU:HD22	13:M:39:MET:CE	1.47	1.43
2:B:260:SER:CB	7:I:18:ASP:HB2	1.45	1.42
11:N:142:PRO:CG	11:N:145:LEU:HD21	1.50	1.42
11:N:142:PRO:HG2	11:N:145:LEU:CD2	1.54	1.34
1:A:408:LYS:NZ	1:A:409:LEU:HD22	1.46	1.30
13:M:28:PHE:CZ	13:M:33:LEU:HD11	1.73	1.22
13:M:33:LEU:CD2	13:M:39:MET:CE	2.10	1.21
1:A:408:LYS:NZ	1:A:409:LEU:CD2	2.06	1.18
1:A:407:ASP:OD2	1:A:410:MET:HG3	1.40	1.17
1:A:408:LYS:HZ3	1:A:409:LEU:CD2	1.57	1.15
2:B:792:LEU:HB2	2:B:865:LYS:HD3	1.24	1.13
13:M:67:LEU:HD21	13:M:69:TYR:CZ	1.83	1.11
2:B:180:ARG:NH2	14:R:-4:G:OP1	1.84	1.10
2:B:785:ILE:HG21	2:B:792:LEU:HD21	1.27	1.10
7:I:13:PHE:CE1	7:I:20:CYS:HB3	1.88	1.09
13:M:33:LEU:HD21	13:M:39:MET:HE1	1.16	1.08
13:M:33:LEU:HD13	13:M:39:MET:SD	1.94	1.07
1:A:521:GLN:HA	1:A:524:THR:HB	1.36	1.07
13:M:33:LEU:HD22	13:M:39:MET:HE3	1.27	1.06
3:C:267:VAL:HG12	3:C:272:VAL:CG1	1.86	1.06
2:B:73:ILE:HB	2:B:75:PHE:CZ	1.91	1.05
1:A:312:VAL:HG21	1:A:320:PHE:HB3	1.34	1.05
2:B:14:PRO:HD3	2:B:946:ASP:HB3	1.36	1.04
8:J:1:MET:HE3	8:J:56:ILE:HD13	1.37	1.03
1:A:881:MET:HG3	1:A:910:MET:HG2	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:ASP:HB2	7:I:19:PHE:HA	1.39	1.02
3:C:267:VAL:HG12	3:C:272:VAL:HG12	1.36	1.01
3:C:291:GLU:HA	3:C:294:LYS:HE3	1.36	1.01
1:A:754:TYR:CE1	1:A:781:LEU:HD13	1.95	1.01
13:M:67:LEU:HD21	13:M:69:TYR:OH	1.59	1.00
2:B:110:TYR:CE2	2:B:146:CYS:SG	2.56	0.99
13:M:28:PHE:CZ	13:M:33:LEU:CD1	2.45	0.99
2:B:110:TYR:HE2	2:B:146:CYS:SG	1.85	0.98
2:B:568:LYS:HE2	2:B:600:MET:HE3	1.47	0.97
2:B:785:ILE:CG2	2:B:792:LEU:HD21	1.95	0.96
1:A:418:ARG:NH2	15:T:13:DA:OP1	1.98	0.96
1:A:132:LEU:HG	4:E:210:GLN:HE22	1.27	0.96
2:B:10:LEU:HD12	2:B:11:PRO:HD2	1.48	0.95
4:E:110:MET:HE1	4:E:118:LEU:HD11	1.49	0.95
4:E:72:MET:HE2	4:E:103:LEU:HB2	1.49	0.94
2:B:260:SER:HB3	7:I:18:ASP:HB3	1.46	0.94
2:B:396:ILE:HG22	2:B:422:MET:HB2	1.48	0.94
1:A:1512:ILE:HG21	1:A:1515:TYR:HE1	1.28	0.93
13:M:12:GLN:OE1	13:M:98:GLN:NE2	2.01	0.93
11:N:35:LEU:HD22	11:N:42:LEU:HD21	1.50	0.93
1:A:1282:LYS:HE3	1:A:1564:LEU:HD13	1.49	0.93
3:C:53:VAL:HA	3:C:63:PHE:HA	1.51	0.92
1:A:1090:LEU:HD22	4:E:30:GLN:HG2	1.51	0.92
1:A:1145:PRO:HD2	4:E:204:ILE:HD11	1.52	0.92
1:A:754:TYR:HE1	1:A:781:LEU:HD13	1.32	0.91
1:A:939:GLU:HG2	1:A:940:PRO:HD2	1.48	0.91
2:B:88:PRO:HD2	2:B:92:ILE:HD12	1.51	0.91
1:A:969:MET:HG2	2:B:489:LEU:HD22	1.53	0.91
1:A:408:LYS:HZ2	1:A:409:LEU:HD22	1.32	0.90
6:H:104:THR:HG22	6:H:107:GLU:HB3	1.54	0.90
11:N:146:ARG:HH12	11:N:148:ARG:HH22	1.17	0.90
13:M:67:LEU:HD21	13:M:69:TYR:CE1	2.05	0.90
2:B:260:SER:HB3	7:I:18:ASP:HB2	0.90	0.89
1:A:1313:GLN:HE22	1:A:1535:LYS:HB2	1.37	0.89
1:A:408:LYS:HZ3	1:A:409:LEU:HD22	1.11	0.89
1:A:122:CYS:HB3	1:A:165:THR:HG21	1.53	0.88
2:B:73:ILE:HB	2:B:75:PHE:HZ	1.38	0.88
5:F:79:VAL:HG12	5:F:81:VAL:HG12	1.53	0.88
2:B:600:MET:HB3	2:B:608:PRO:HB3	1.54	0.88
1:A:869:VAL:HG21	1:A:918:GLN:HE21	1.39	0.88
2:B:792:LEU:HB2	2:B:865:LYS:CD	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:OD2	1:A:410:MET:CG	2.22	0.88
1:A:1580:THR:HG22	1:A:1582:GLY:H	1.35	0.88
2:B:216:ARG:HB2	2:B:334:ILE:HG22	1.54	0.88
2:B:403:LYS:HB2	2:B:418:ARG:HH12	1.40	0.87
1:A:316:GLY:HA2	15:T:25:DA:H2'	1.55	0.87
2:B:392:TRP:HE1	2:B:423:GLY:HA2	1.39	0.87
7:I:40:ARG:HD2	7:I:43:PHE:HA	1.55	0.86
2:B:408:SER:HA	2:B:411:MET:HB2	1.56	0.86
2:B:117:ASP:HB3	2:B:131:LYS:HE2	1.56	0.86
13:M:33:LEU:CD1	13:M:39:MET:SD	2.64	0.85
2:B:432:TYR:HE1	15:T:25:DA:H5''	1.40	0.85
3:C:53:VAL:O	11:N:157:PRO:HD3	1.76	0.85
2:B:648:GLU:HG3	11:N:130:LEU:HD22	1.59	0.85
2:B:68:PHE:HA	2:B:405:GLN:HE22	1.42	0.84
4:E:94:MET:HG2	4:E:99:ILE:HD11	1.59	0.84
1:A:713:GLY:O	6:H:20:LYS:HE3	1.78	0.84
4:E:85:LYS:O	4:E:89:VAL:HG13	1.78	0.83
2:B:1068:HIS:HB3	2:B:1109:THR:HA	1.60	0.83
2:B:260:SER:HB2	7:I:18:ASP:HB2	1.57	0.83
2:B:781:LEU:HD22	2:B:792:LEU:HB3	1.60	0.83
2:B:178:VAL:HB	2:B:457:ALA:HB2	1.60	0.83
1:A:860:MET:HE2	1:A:864:LYS:HE3	1.60	0.83
1:A:1334:ARG:HG3	1:A:1335:PRO:HD2	1.58	0.83
2:B:260:SER:HA	7:I:18:ASP:OD2	1.79	0.83
1:A:555:THR:HG21	2:B:1041:GLU:HG3	1.61	0.82
1:A:1619:ARG:HH22	4:E:196:PRO:HD2	1.45	0.82
1:A:912:ILE:HD11	2:B:924:MET:HG2	1.61	0.82
2:B:400:PHE:HA	2:B:418:ARG:CZ	2.10	0.82
2:B:758:ILE:HB	2:B:914:LEU:HB2	1.62	0.82
2:B:792:LEU:HD12	2:B:865:LYS:HD2	1.61	0.82
1:A:312:VAL:CG2	1:A:320:PHE:HB3	2.10	0.82
2:B:796:ILE:HD11	2:B:807:LEU:HB2	1.61	0.82
3:C:91:LYS:HE2	10:L:54:VAL:HG11	1.62	0.81
3:C:104:GLU:HG2	3:C:105:ILE:HD12	1.61	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
2:B:700:LEU:HD11	2:B:706:ARG:HG3	1.63	0.80
2:B:567:ASP:OD1	2:B:568:LYS:N	2.15	0.80
2:B:940:LEU:HD12	8:J:43:TYR:HB3	1.63	0.80
7:I:13:PHE:HE1	7:I:20:CYS:HB3	1.38	0.80
2:B:396:ILE:HA	2:B:422:MET:HG3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:22:GLU:HG3	9:K:25:THR:H	1.44	0.80
2:B:708:ASP:O	2:B:776:SER:HB3	1.80	0.80
2:B:783:GLU:OE1	2:B:783:GLU:N	2.15	0.80
1:A:417:ILE:HB	2:B:1126:MET:HE3	1.62	0.80
1:A:1512:ILE:HG21	1:A:1515:TYR:CE1	2.15	0.80
2:B:631:GLU:HG3	2:B:631:GLU:O	1.80	0.80
2:B:73:ILE:CB	2:B:75:PHE:CZ	2.65	0.80
8:J:40:LEU:HD11	8:J:49:LEU:HD12	1.64	0.79
1:A:658:TYR:HB2	9:K:67:PHE:HZ	1.47	0.79
2:B:14:PRO:CD	2:B:946:ASP:HB3	2.10	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:1354:ILE:O	1:A:1357:LYS:HG2	1.81	0.79
1:A:1531:LEU:HB3	1:A:1535:LYS:HE2	1.64	0.79
1:A:404:SER:HB2	1:A:415:PRO:HA	1.65	0.78
1:A:8:PRO:HG3	2:B:1066:VAL:HG13	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
2:B:92:ILE:HD11	2:B:859:THR:HA	1.66	0.78
1:A:465:LYS:HZ2	2:B:1014:THR:HG22	1.46	0.78
2:B:536:ASN:HA	11:N:48:PRO:HG3	1.63	0.78
1:A:310:ARG:HE	1:A:325:THR:HG22	1.48	0.78
3:C:53:VAL:HG22	3:C:63:PHE:HB3	1.66	0.78
3:C:267:VAL:CG1	3:C:272:VAL:CG1	2.62	0.78
2:B:856:SER:HB3	10:L:42:ARG:HB3	1.64	0.77
1:A:914:CYS:H	1:A:954:ARG:HD3	1.48	0.77
1:A:1350:LEU:O	1:A:1354:ILE:HG12	1.83	0.77
1:A:403:ASP:HB3	1:A:406:MET:HE2	1.66	0.77
1:A:1029:THR:HG21	1:A:1639:ARG:HH12	1.49	0.77
2:B:758:ILE:CD1	2:B:895:ARG:HB2	2.13	0.77
1:A:1531:LEU:HB3	1:A:1535:LYS:CE	2.15	0.77
1:A:408:LYS:HZ3	1:A:409:LEU:HD21	1.47	0.77
9:K:90:LEU:HD23	9:K:90:LEU:H	1.50	0.77
1:A:425:GLU:HG3	1:A:426:GLY:H	1.48	0.77
4:E:86:THR:O	4:E:89:VAL:HG22	1.84	0.77
5:F:81:VAL:HB	5:F:96:GLU:HG2	1.66	0.77
1:A:430:LYS:HE3	1:A:431:HIS:HE1	1.51	0.76
1:A:122:CYS:CB	1:A:165:THR:HG21	2.16	0.76
13:M:28:PHE:CE1	13:M:33:LEU:HD12	2.19	0.76
1:A:668:VAL:H	9:K:85:GLN:HE22	1.32	0.76
1:A:1515:TYR:O	1:A:1516:GLN:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1675:GLU:HG2	15:T:14:DG:H5''	1.67	0.76
1:A:1288:VAL:HG21	1:A:1333:LEU:HD22	1.67	0.76
2:B:75:PHE:CD2	2:B:397:LYS:HE3	2.21	0.76
2:B:916:ASN:OD1	2:B:917:PRO:HD2	1.86	0.76
4:E:168:ASN:O	4:E:169:GLN:HB3	1.84	0.76
3:C:147:THR:H	3:C:164:VAL:HG22	1.50	0.76
2:B:73:ILE:CB	2:B:75:PHE:HZ	1.99	0.76
2:B:68:PHE:HA	2:B:405:GLN:NE2	2.00	0.76
4:E:110:MET:CE	4:E:118:LEU:HD11	2.16	0.76
13:M:67:LEU:HD12	13:M:68:SER:O	1.86	0.76
2:B:709:ASN:ND2	15:T:22:DG:H5''	2.01	0.75
7:I:9:THR:CG2	7:I:15:SER:HA	2.16	0.75
1:A:667:ARG:NH1	9:K:66:GLU:OE2	2.20	0.75
1:A:939:GLU:HG2	1:A:940:PRO:CD	2.17	0.75
1:A:793:ARG:HG3	1:A:794:GLY:N	2.02	0.75
2:B:432:TYR:CE1	15:T:25:DA:H5''	2.22	0.75
3:C:186:PRO:HG2	3:C:189:THR:OG1	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
11:N:88:GLN:O	11:N:91:GLU:HG3	1.86	0.74
2:B:1003:ARG:HD2	2:B:1003:ARG:O	1.87	0.74
3:C:267:VAL:HG12	3:C:272:VAL:HG11	1.68	0.74
1:A:423:LYS:NZ	15:T:14:DG:OP2	2.20	0.74
1:A:1545:VAL:HG21	7:I:53:LYS:HE3	1.69	0.74
6:H:37:MET:HE3	6:H:127:GLY:HA3	1.70	0.74
2:B:88:PRO:HD2	2:B:92:ILE:CD1	2.17	0.74
1:A:312:VAL:HG23	1:A:320:PHE:HA	1.70	0.73
2:B:403:LYS:HB3	2:B:418:ARG:HH22	1.52	0.73
13:M:28:PHE:CE1	13:M:33:LEU:CD1	2.71	0.73
2:B:170:PHE:O	2:B:176:GLU:HA	1.87	0.73
2:B:1060:ASN:OD1	2:B:1064:ARG:NH1	2.20	0.73
1:A:125:ARG:O	1:A:128:GLU:HG2	1.88	0.73
1:A:1225:GLN:O	1:A:1226:MET:HB2	1.86	0.73
1:A:1295:GLN:O	7:I:59:VAL:HG12	1.89	0.73
1:A:134:ALA:O	1:A:138:LEU:HD23	1.89	0.73
3:C:27:THR:HA	3:C:32:ASN:ND2	2.03	0.73
1:A:1289:CYS:HA	1:A:1552:VAL:HA	1.71	0.73
2:B:64:PHE:HE2	2:B:397:LYS:HB2	1.54	0.73
2:B:743:VAL:HG21	2:B:999:TYR:HE2	1.53	0.73
1:A:1615:GLU:HG3	4:E:193:ILE:HD13	1.71	0.73
7:I:13:PHE:CE1	7:I:20:CYS:CB	2.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:HIS:CE1	1:A:410:MET:HE1	2.24	0.72
8:J:57:GLU:O	8:J:61:ASN:ND2	2.21	0.72
1:A:1328:GLN:NE2	1:A:1333:LEU:O	2.22	0.72
15:T:8:DA:H2'	15:T:9:DG:C8	2.24	0.72
1:A:911:GLN:HA	1:A:915:LEU:O	1.89	0.72
2:B:181:MET:HE1	2:B:514:LEU:HD11	1.72	0.72
1:A:1334:ARG:CG	1:A:1335:PRO:HD2	2.19	0.72
1:A:1349:LEU:HD21	1:A:1547:LEU:HD11	1.72	0.72
2:B:536:ASN:HA	11:N:48:PRO:CG	2.19	0.72
9:K:30:VAL:HG23	9:K:41:THR:HB	1.70	0.72
1:A:749:LEU:HB3	1:A:754:TYR:HE2	1.53	0.72
2:B:92:ILE:HG22	2:B:93:CYS:H	1.53	0.72
4:E:61:LEU:HD13	4:E:73:PHE:HD1	1.55	0.72
1:A:1335:PRO:O	1:A:1338:ILE:HG22	1.90	0.72
1:A:1026:ILE:H	1:A:1026:ILE:HD12	1.55	0.72
3:C:287:ILE:HD11	3:C:299:LEU:HD22	1.71	0.72
1:A:713:GLY:O	6:H:20:LYS:CE	2.37	0.71
2:B:73:ILE:HB	2:B:75:PHE:CE2	2.24	0.71
2:B:396:ILE:HA	2:B:422:MET:CG	2.19	0.71
1:A:749:LEU:HD23	1:A:754:TYR:OH	1.90	0.71
2:B:260:SER:CA	7:I:18:ASP:HB2	2.20	0.71
2:B:193:MET:SD	2:B:195:ARG:NH2	2.63	0.71
1:A:19:MET:HE1	1:A:91:LEU:HD11	1.72	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
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:430:LYS:HE3	1:A:431:HIS:CE1	2.25	0.70
6:H:104:THR:CG2	6:H:107:GLU:HB3	2.21	0.70
13:M:28:PHE:CE2	13:M:33:LEU:HD11	2.24	0.70
1:A:650:ARG:HG2	1:A:654:MET:HE2	1.72	0.70
1:A:850:HIS:O	1:A:855:GLN:NE2	2.24	0.70
2:B:622:PRO:HB3	2:B:631:GLU:OE2	1.91	0.70
1:A:997:GLU:HA	1:A:1213:LEU:HD13	1.73	0.70
1:A:1619:ARG:NH2	4:E:196:PRO:HD2	2.06	0.70
7:I:13:PHE:CD1	7:I:20:CYS:HA	2.25	0.70
1:A:512:MET:SD	1:A:515:ARG:NH2	2.65	0.70
1:A:1145:PRO:HD2	4:E:204:ILE:CD1	2.21	0.70
1:A:1686:MET:HG3	1:A:1687:LEU:HD12	1.74	0.70
2:B:58:VAL:HA	2:B:61:ILE:HG13	1.71	0.70
1:A:686:GLN:O	1:A:690:THR:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:33:LEU:CG	13:M:39:MET:HE1	2.21	0.70
2:B:140:MET:CE	2:B:168:GLY:HA2	2.21	0.70
2:B:576:ASP:OD1	2:B:577:SER:N	2.25	0.70
2:B:781:LEU:HD23	2:B:781:LEU:O	1.92	0.70
4:E:13:ILE:O	4:E:17:ILE:HG13	1.91	0.70
2:B:46:PHE:O	2:B:50:VAL:HG22	1.92	0.70
4:E:159:LEU:HD23	4:E:160:LEU:HD23	1.74	0.70
3:C:184:LEU:HD23	3:C:185:PHE:CE2	2.27	0.70
6:H:104:THR:HB	6:H:109:ALA:HB2	1.74	0.70
7:I:14:GLN:NE2	7:I:32:ALA:HB3	2.06	0.70
2:B:691:MET:HE3	2:B:884:ALA:HB1	1.73	0.70
1:A:312:VAL:HG23	1:A:320:PHE:CA	2.22	0.69
2:B:717:PRO:HB2	2:B:736:PRO:HB2	1.74	0.69
3:C:54:VAL:HG12	3:C:62:GLU:HB2	1.71	0.69
4:E:92:GLN:O	4:E:95:GLN:HG2	1.92	0.69
2:B:394:VAL:O	2:B:398:ILE:HG12	1.91	0.69
4:E:93:ARG:NH1	4:E:97:GLU:OE2	2.26	0.69
7:I:7:ALA:HB3	13:M:32:LYS:O	1.93	0.69
1:A:793:ARG:HG3	1:A:794:GLY:H	1.57	0.69
3:C:267:VAL:CG1	3:C:272:VAL:HG11	2.22	0.69
4:E:54:ARG:HD2	4:E:57:ASP:HB3	1.72	0.69
4:E:190:VAL:HG22	4:E:208:LEU:HD12	1.73	0.69
1:A:1097:GLN:HA	1:A:1100:VAL:HG22	1.75	0.69
1:A:258:PRO:HD2	1:A:391:TRP:CZ3	2.27	0.69
2:B:392:TRP:O	2:B:396:ILE:HG23	1.93	0.69
1:A:691:LEU:HD22	1:A:784:LEU:HD22	1.74	0.69
6:H:101:GLY:HA2	6:H:112:LEU:HD23	1.74	0.69
1:A:654:MET:HE1	9:K:60:MET:HE1	1.73	0.69
1:A:1545:VAL:HG21	7:I:53:LYS:CE	2.22	0.69
6:H:96:VAL:HG22	6:H:116:VAL:HG22	1.73	0.69
2:B:568:LYS:HG3	2:B:600:MET:HE2	1.75	0.69
1:A:754:TYR:HE1	1:A:781:LEU:CD1	2.05	0.69
3:C:138:LEU:HD12	3:C:181:GLN:HE22	1.58	0.68
1:A:1516:GLN:HG3	1:A:1526:GLN:HG3	1.76	0.68
1:A:1702:VAL:HG23	1:A:1704:LYS:HG3	1.76	0.68
2:B:400:PHE:CD1	2:B:418:ARG:HG2	2.29	0.68
1:A:745:LEU:HD22	6:H:117:SER:OG	1.93	0.68
1:A:1262:PRO:HA	1:A:1603:ASN:HD21	1.58	0.68
2:B:392:TRP:NE1	2:B:423:GLY:HA2	2.09	0.68
3:C:291:GLU:CA	3:C:294:LYS:HE3	2.21	0.68
1:A:1534:MET:C	1:A:1535:LYS:HD2	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:651:VAL:HG13	2:B:656:THR:HG21	1.75	0.68
1:A:860:MET:CE	1:A:864:LYS:HE3	2.24	0.67
1:A:13:GLN:O	2:B:1133:ASP:HB2	1.94	0.67
1:A:910:MET:O	1:A:911:GLN:HB3	1.93	0.67
8:J:3:ILE:HD12	8:J:4:PRO:HD2	1.75	0.67
1:A:44:ASN:HB2	1:A:45:PRO:HD2	1.75	0.67
11:N:48:PRO:HD3	11:N:117:ILE:O	1.95	0.67
15:T:5:DC:H42	16:U:10:DG:H22	1.42	0.67
1:A:843:ARG:NH1	1:A:939:GLU:OE2	2.27	0.67
1:A:1515:TYR:CD1	1:A:1527:VAL:HG23	2.30	0.67
1:A:338:ILE:HG12	1:A:390:ILE:HD12	1.77	0.67
1:A:690:THR:O	1:A:694:ASN:ND2	2.27	0.67
2:B:187:ARG:HD2	2:B:615:THR:HB	1.77	0.67
7:I:9:THR:HG22	7:I:15:SER:HA	1.76	0.67
2:B:110:TYR:OH	2:B:146:CYS:SG	2.48	0.67
3:C:16:LEU:HD12	3:C:21:VAL:HG23	1.77	0.67
1:A:806:PRO:O	1:A:807:LYS:HB3	1.93	0.67
1:A:1512:ILE:HD13	1:A:1529:VAL:HG22	1.77	0.67
11:N:70:LYS:HG2	11:N:79:ARG:HG2	1.74	0.67
1:A:140:ARG:HH11	1:A:144:ARG:HH12	1.42	0.67
1:A:465:LYS:NZ	2:B:1014:THR:HG22	2.11	0.67
2:B:75:PHE:CE1	2:B:120:TRP:HB2	2.29	0.67
1:A:434:GLY:HA3	2:B:1036:ARG:NH2	2.10	0.66
1:A:1566:GLU:HA	1:A:1576:LEU:HD13	1.75	0.66
1:A:166:THR:HA	1:A:169:VAL:HG22	1.77	0.66
3:C:53:VAL:HG21	9:K:118:ILE:HD13	1.76	0.66
1:A:654:MET:CE	9:K:60:MET:HE1	2.24	0.66
4:E:84:ILE:O	4:E:88:LYS:HG2	1.95	0.66
1:A:916:LEU:HB2	1:A:953:GLY:O	1.96	0.66
3:C:235:LEU:HB2	3:C:301:ARG:HD3	1.76	0.66
1:A:430:LYS:HG2	1:A:431:HIS:ND1	2.11	0.66
4:E:127:LEU:O	4:E:128:GLU:HG3	1.95	0.66
2:B:233:THR:HG23	2:B:285:MET:HG2	1.78	0.66
2:B:690:GLN:OE1	2:B:694:GLN:NE2	2.27	0.66
4:E:77:PRO:HD2	4:E:105:VAL:O	1.96	0.66
7:I:33:GLN:HG3	7:I:34:ASP:OD1	1.96	0.66
1:A:603:LEU:O	1:A:603:LEU:HD23	1.96	0.66
2:B:566:VAL:HG21	2:B:574:ILE:HD12	1.78	0.66
3:C:245:VAL:CG2	3:C:273:ALA:HB3	2.26	0.66
9:K:42:PHE:CE1	9:K:84:ILE:HD12	2.31	0.66
2:B:194:ILE:HG23	2:B:207:GLN:OE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1066:VAL:O	2:B:1066:VAL:HG12	1.96	0.65
5:F:79:VAL:CG1	5:F:81:VAL:HG12	2.25	0.65
1:A:1104:LYS:CB	1:A:1116:GLY:HA2	2.27	0.65
6:H:102:ASP:OD2	6:H:111:ARG:HB2	1.96	0.65
11:N:112:GLN:OE1	11:N:112:GLN:N	2.30	0.65
1:A:173:LEU:O	1:A:174:LEU:HB3	1.96	0.65
4:E:94:MET:SD	4:E:102:ALA:HB2	2.37	0.65
1:A:1566:GLU:HA	1:A:1576:LEU:CD1	2.26	0.65
2:B:403:LYS:HE2	2:B:418:ARG:NH2	2.11	0.65
1:A:642:THR:O	1:A:685:LYS:HE2	1.96	0.65
2:B:757:MET:HE3	2:B:759:VAL:CG2	2.26	0.65
6:H:48:TYR:OH	6:H:147:LYS:HG3	1.96	0.65
1:A:12:LEU:HD21	2:B:1132:LEU:HD13	1.78	0.65
2:B:709:ASN:HD21	15:T:22:DG:H5"	1.60	0.65
8:J:1:MET:HE3	8:J:56:ILE:CD1	2.22	0.65
1:A:1133:ARG:HG2	1:A:1133:ARG:O	1.97	0.65
2:B:1042:ARG:NH1	2:B:1043:ASP:OD1	2.30	0.65
2:B:806:LYS:HG2	2:B:824:PRO:HD2	1.78	0.65
1:A:137:GLU:HG2	1:A:164:TYR:OH	1.97	0.65
1:A:1096:ILE:O	1:A:1100:VAL:HG13	1.97	0.65
1:A:1349:LEU:CD2	1:A:1547:LEU:HD11	2.26	0.65
1:A:1516:GLN:HG3	1:A:1526:GLN:H	1.62	0.65
1:A:807:LYS:HG3	1:A:807:LYS:O	1.97	0.64
1:A:1334:ARG:CD	1:A:1335:PRO:HD2	2.27	0.64
1:A:1016:GLN:OE1	1:A:1643:LEU:HD13	1.98	0.64
2:B:73:ILE:CG2	2:B:75:PHE:HZ	2.09	0.64
2:B:842:LYS:O	2:B:844:LYS:HE2	1.97	0.64
10:L:21:GLU:OE1	10:L:21:GLU:N	2.31	0.64
1:A:1104:LYS:HB2	1:A:1116:GLY:HA2	1.78	0.64
2:B:909:MET:HG2	8:J:42:ARG:HD3	1.80	0.64
1:A:812:ARG:HD2	1:A:914:CYS:HA	1.78	0.64
2:B:936:LYS:HG2	2:B:966:LEU:HD21	1.79	0.64
3:C:11:ARG:O	3:C:303:ARG:HD3	1.97	0.64
4:E:20:LEU:HD11	4:E:24:ARG:HE	1.61	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
2:B:346:LEU:O	2:B:350:THR:HG23	1.97	0.64
4:E:110:MET:SD	4:E:118:LEU:HD11	2.37	0.64
1:A:85:LEU:HD22	1:A:391:TRP:HE1	1.63	0.64
1:A:658:TYR:HB2	9:K:67:PHE:CZ	2.31	0.64
2:B:566:VAL:CG2	2:B:574:ILE:HD12	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1028:GLY:O	2:B:1033:GLY:HA3	1.97	0.64
7:I:16:ASP:C	13:M:67:LEU:HD22	2.22	0.64
1:A:749:LEU:HD23	1:A:754:TYR:CZ	2.32	0.64
4:E:90:TYR:OH	4:E:104:ILE:HD13	1.97	0.64
4:E:185:ILE:HD12	4:E:191:VAL:HG11	1.80	0.64
11:N:146:ARG:HH12	11:N:148:ARG:NH2	1.92	0.64
1:A:430:LYS:HG2	1:A:431:HIS:CE1	2.34	0.63
1:A:1057:LEU:HD13	1:A:1194:THR:HG21	1.79	0.63
2:B:146:CYS:O	2:B:149:ARG:HG2	1.97	0.63
2:B:570:LEU:HD11	11:N:83:LEU:HD11	1.80	0.63
3:C:274:ARG:HB3	3:C:274:ARG:HH11	1.61	0.63
2:B:75:PHE:CD1	2:B:120:TRP:HB2	2.34	0.63
2:B:216:ARG:HB2	2:B:334:ILE:CG2	2.26	0.63
6:H:39:LEU:HD13	6:H:125:LEU:HD13	1.80	0.63
1:A:21:SER:HB3	1:A:24:GLU:HG2	1.81	0.63
1:A:460:MET:HG3	1:A:570:PRO:HA	1.81	0.63
1:A:1293:VAL:O	1:A:1294:LEU:HG	1.99	0.63
2:B:229:LEU:HD11	2:B:235:MET:HE3	1.79	0.63
3:C:7:VAL:N	6:H:49:PRO:HD2	2.13	0.63
4:E:9:ARG:HD2	4:E:132:GLN:HE21	1.64	0.63
2:B:400:PHE:HD1	2:B:418:ARG:HG2	1.61	0.63
10:L:34:ILE:O	10:L:34:ILE:HG22	1.98	0.63
1:A:414:TYR:HB3	1:A:415:PRO:HD2	1.81	0.63
2:B:538:GLY:O	11:N:116:ARG:NH2	2.31	0.63
2:B:936:LYS:HE3	2:B:966:LEU:CD2	2.29	0.63
1:A:1338:ILE:HG23	1:A:1339:LEU:HD12	1.81	0.63
2:B:171:ILE:HG23	2:B:174:GLY:HA2	1.81	0.63
1:A:823:GLY:HA2	1:A:865:PHE:HE1	1.64	0.63
2:B:791:SER:HB3	2:B:792:LEU:HD23	1.81	0.63
2:B:1067:ALA:HB1	2:B:1076:LEU:HD11	1.80	0.63
2:B:936:LYS:HE3	2:B:966:LEU:HD22	1.80	0.62
2:B:1013:ARG:NH2	2:B:1017:ALA:O	2.31	0.62
3:C:15:VAL:HA	3:C:300:ALA:HB2	1.81	0.62
1:A:1282:LYS:CE	1:A:1564:LEU:HD13	2.27	0.62
2:B:791:SER:HA	2:B:830:ASN:HA	1.81	0.62
4:E:59:THR:HG23	4:E:74:VAL:O	1.99	0.62
2:B:743:VAL:HG22	2:B:913:ILE:HB	1.81	0.62
1:A:122:CYS:SG	1:A:165:THR:HG21	2.40	0.62
6:H:39:LEU:CD1	6:H:125:LEU:HD13	2.28	0.62
9:K:55:LEU:HD21	9:K:96:PHE:CE1	2.34	0.62
1:A:225:ILE:HG23	1:A:256:LEU:CD1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LYS:HG3	1:A:424:LYS:H	1.64	0.62
1:A:1289:CYS:N	1:A:1292:GLU:OE2	2.31	0.62
1:A:1322:LEU:HD13	7:I:60:VAL:HB	1.81	0.62
2:B:190:PRO:HB3	2:B:349:MET:HG2	1.79	0.62
1:A:846:TRP:HE1	1:A:858:PHE:HE1	1.48	0.62
1:A:1119:GLU:OE1	1:A:1122:ARG:NH1	2.22	0.62
2:B:647:PHE:O	2:B:650:GLU:HB2	1.99	0.62
3:C:326:ILE:HG21	9:K:111:LEU:HB2	1.82	0.62
1:A:790:GLN:NE2	2:B:983:ILE:HD13	2.15	0.62
1:A:939:GLU:CG	1:A:940:PRO:HD2	2.26	0.62
1:A:1569:ASN:O	1:A:1573:GLU:HA	2.00	0.62
2:B:312:LEU:HD21	2:B:327:LEU:HD12	1.82	0.62
1:A:127:LEU:HD21	1:A:135:VAL:CG2	2.30	0.62
1:A:1034:PRO:O	1:A:1035:LYS:HB2	1.98	0.62
1:A:1223:SER:HB2	1:A:1245:ILE:CD1	2.29	0.62
2:B:392:TRP:HE1	2:B:423:GLY:CA	2.13	0.62
2:B:695:THR:HG21	2:B:737:ILE:HG12	1.81	0.62
2:B:791:SER:HA	2:B:830:ASN:OD1	2.00	0.62
4:E:173:ILE:HG23	4:E:209:VAL:HA	1.81	0.62
1:A:1583:ILE:HD11	1:A:1607:ALA:CB	2.30	0.61
2:B:583:VAL:HG13	2:B:630:LYS:HB3	1.81	0.61
1:A:1670:GLN:O	1:A:1671:GLN:HB3	2.00	0.61
2:B:965:MET:HE1	11:N:142:PRO:HD3	1.81	0.61
4:E:126:ILE:O	4:E:126:ILE:HG13	1.99	0.61
9:K:25:THR:HB	9:K:46:GLU:OE1	2.00	0.61
10:L:16:ILE:HG23	10:L:25:GLU:HB3	1.81	0.61
2:B:64:PHE:CE2	2:B:397:LYS:HB2	2.35	0.61
2:B:113:LYS:HG3	2:B:133:PHE:HE1	1.65	0.61
2:B:260:SER:CB	7:I:18:ASP:CB	2.29	0.61
2:B:680:ASN:HD21	2:B:887:HIS:HD2	1.46	0.61
2:B:742:ILE:HD13	2:B:996:VAL:HG22	1.81	0.61
1:A:677:LYS:O	1:A:678:PRO:C	2.42	0.61
1:A:1020:GLY:HA3	1:A:1639:ARG:HG3	1.81	0.61
1:A:1335:PRO:HA	1:A:1338:ILE:HG22	1.82	0.61
1:A:1681:LEU:HD21	2:B:1123:LEU:HD21	1.81	0.61
2:B:237:ASN:HD21	2:B:244:LEU:HD22	1.65	0.61
3:C:264:VAL:HG13	3:C:264:VAL:O	2.00	0.61
1:A:607:GLU:HB3	2:B:1050:THR:HG22	1.81	0.61
2:B:785:ILE:HG21	2:B:792:LEU:CD2	2.17	0.61
13:M:67:LEU:CD2	13:M:69:TYR:CE1	2.81	0.61
1:A:223:LEU:O	1:A:256:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HD11	2:B:1053:LEU:HD13	1.81	0.61
1:A:926:PRO:HD2	1:A:948:GLY:O	2.01	0.61
3:C:33:TYR:CB	3:C:36:TYR:HB3	2.29	0.61
3:C:241:LEU:HD23	3:C:297:VAL:HG22	1.80	0.61
1:A:502:GLY:O	1:A:503:SER:OG	2.18	0.61
1:A:895:GLN:O	1:A:896:MET:HB3	2.01	0.61
1:A:1498:MET:HA	1:A:1501:ARG:HH12	1.65	0.61
2:B:92:ILE:HG22	2:B:93:CYS:N	2.16	0.61
3:C:18:GLU:HB2	3:C:288:PHE:CD2	2.36	0.61
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
11:N:142:PRO:HG2	11:N:145:LEU:HD21	0.70	0.60
1:A:664:LYS:N	1:A:664:LYS:HD2	2.16	0.60
1:A:812:ARG:HG3	1:A:876:ILE:HG23	1.82	0.60
2:B:691:MET:HE3	2:B:884:ALA:CB	2.31	0.60
1:A:137:GLU:OE1	1:A:140:ARG:NH2	2.34	0.60
1:A:919:ILE:HG12	1:A:949:GLY:O	2.01	0.60
11:N:61:VAL:HG11	13:M:11:TRP:CE3	2.35	0.60
2:B:201:ARG:HB2	2:B:205:TYR:HD2	1.67	0.60
9:K:83:ARG:HH11	9:K:85:GLN:HE21	1.48	0.60
1:A:37:ARG:HH11	1:A:40:ASP:HA	1.66	0.60
2:B:526:TYR:CE2	2:B:528:ALA:HB3	2.37	0.60
2:B:752:ASP:O	2:B:916:ASN:HB2	2.00	0.60
2:B:1067:ALA:HB2	2:B:1117:ARG:NE	2.16	0.60
3:C:30:PRO:CG	9:K:61:LYS:HA	2.31	0.60
8:J:40:LEU:CD1	8:J:49:LEU:HD12	2.31	0.60
1:A:898:VAL:HG21	1:A:909:THR:HG21	1.83	0.60
2:B:185:PRO:O	2:B:372:GLN:HA	2.01	0.60
1:A:1541:SER:HA	1:A:1544:VAL:HG22	1.83	0.60
2:B:498:CYS:HB2	2:B:668:SER:HB2	1.84	0.60
1:A:468:TYR:CE2	1:A:605:ARG:HD2	2.37	0.60
1:A:1170:TYR:HE2	1:A:1192:LEU:HD21	1.67	0.60
1:A:1318:ARG:HD2	1:A:1524:TRP:HE3	1.67	0.60
2:B:703:TYR:HE1	2:B:711:LEU:HD22	1.67	0.60
4:E:37:LEU:O	4:E:41:LYS:HG2	2.01	0.60
9:K:22:GLU:HG2	9:K:25:THR:OG1	2.02	0.60
2:B:1030:ASN:OD1	2:B:1031:VAL:N	2.35	0.59
1:A:316:GLY:CA	15:T:25:DA:H2'	2.28	0.59
1:A:1005:LEU:HD11	1:A:1153:ASP:HB3	1.84	0.59
1:A:1523:LEU:HD12	1:A:1524:TRP:N	2.17	0.59
3:C:337:LEU:HD12	9:K:104:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:34:ASP:O	7:I:35:THR:OG1	2.18	0.59
14:R:-7:G:H2'	14:R:-6:C:C6	2.37	0.59
2:B:1068:HIS:CB	2:B:1109:THR:HA	2.31	0.59
3:C:337:LEU:HD12	9:K:104:MET:HE1	1.83	0.59
1:A:1048:MET:HG2	1:A:1195:LEU:HD13	1.83	0.59
1:A:1565:ASN:HD22	1:A:1579:ASN:ND2	2.01	0.59
3:C:245:VAL:HG21	3:C:253:LEU:CD2	2.32	0.59
1:A:768:ILE:CG2	1:A:1046:VAL:HB	2.32	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:1026:ILE:HG22	2:B:1033:GLY:HA2	1.84	0.59
11:N:142:PRO:HG2	11:N:145:LEU:CG	2.27	0.59
1:A:651:GLU:CD	3:C:29:PHE:HD2	2.09	0.59
2:B:139:ILE:HG22	2:B:140:MET:O	2.02	0.59
2:B:403:LYS:HB2	2:B:418:ARG:NH1	2.14	0.59
2:B:758:ILE:HD13	2:B:895:ARG:HB2	1.84	0.59
9:K:66:GLU:HB3	9:K:87:ARG:HE	1.67	0.59
1:A:1505:VAL:HG22	1:A:1509:HIS:CE1	2.38	0.59
2:B:549:SER:O	2:B:550:TYR:HB2	2.02	0.59
1:A:754:TYR:CD1	1:A:781:LEU:HD13	2.37	0.59
2:B:39:THR:HG22	2:B:469:PHE:CG	2.38	0.59
2:B:229:LEU:HD21	2:B:235:MET:HB2	1.85	0.59
2:B:414:ASP:CB	2:B:417:MET:HE3	2.33	0.59
6:H:24:ARG:HG2	6:H:46:GLN:OE1	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
1:A:603:LEU:HD22	2:B:1052:PHE:CD2	2.38	0.59
2:B:562:MET:HE2	2:B:564:GLY:HA2	1.83	0.59
2:B:753:MET:HA	2:B:916:ASN:HD22	1.68	0.59
4:E:35:GLN:HA	4:E:39:GLU:OE2	2.03	0.59
1:A:764:CYS:HB3	1:A:1039:PHE:CZ	2.38	0.58
2:B:162:GLU:C	2:B:164:GLU:H	2.11	0.58
2:B:536:ASN:OD1	11:N:48:PRO:HB3	2.03	0.58
4:E:60:VAL:HG22	4:E:74:VAL:HB	1.84	0.58
6:H:14:ASP:HB2	6:H:29:HIS:HB2	1.85	0.58
1:A:435:LYS:HD2	2:B:1058:LEU:O	2.03	0.58
1:A:1117:THR:O	1:A:1121:LEU:HD23	2.03	0.58
2:B:75:PHE:CE2	2:B:397:LYS:HE3	2.37	0.58
2:B:239:ILE:HD11	2:B:242:LYS:HA	1.85	0.58
2:B:821:TYR:HB2	2:B:844:LYS:HZ2	1.68	0.58
3:C:42:GLN:O	3:C:46:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:9:THR:HG21	7:I:15:SER:HA	1.85	0.58
1:A:112:CYS:HB2	1:A:117:ILE:HD11	1.85	0.58
1:A:718:LYS:HG3	6:H:21:LYS:HB2	1.85	0.58
1:A:1145:PRO:HG2	4:E:202:ARG:O	2.03	0.58
3:C:245:VAL:HG23	3:C:273:ALA:HB3	1.85	0.58
6:H:100:GLU:HG3	6:H:100:GLU:O	2.02	0.58
1:A:396:SER:HA	1:A:399:ASN:HB2	1.85	0.58
1:A:866:LYS:HA	1:A:869:VAL:HG22	1.84	0.58
2:B:68:PHE:HB3	2:B:73:ILE:HD11	1.83	0.58
3:C:30:PRO:HG2	9:K:60:MET:O	2.03	0.58
1:A:122:CYS:HB3	1:A:165:THR:CG2	2.31	0.58
1:A:438:ASP:HB3	2:B:1014:THR:O	2.04	0.58
1:A:1669:LEU:HB2	1:A:1691:ASP:OD2	2.03	0.58
2:B:882:LYS:HD2	2:B:1002:LEU:HD23	1.85	0.58
3:C:91:LYS:HE2	10:L:54:VAL:CG1	2.32	0.58
3:C:93:LEU:HD22	10:L:54:VAL:HG22	1.84	0.58
11:N:142:PRO:HG3	11:N:145:LEU:HD21	1.72	0.58
13:M:68:SER:O	13:M:111:PRO:HA	2.02	0.58
13:M:72:ASN:ND2	13:M:74:PHE:O	2.36	0.58
2:B:92:ILE:HD11	2:B:858:ASP:O	2.03	0.58
2:B:703:TYR:HE1	2:B:711:LEU:CD2	2.17	0.58
1:A:33:ILE:CD1	1:A:50:LEU:HD13	2.34	0.58
1:A:91:LEU:H	1:A:91:LEU:HD23	1.69	0.58
2:B:66:PHE:HZ	2:B:400:PHE:CD2	2.21	0.58
2:B:416:LEU:HA	2:B:419:ILE:HG12	1.85	0.58
2:B:821:TYR:HB2	2:B:844:LYS:NZ	2.18	0.58
4:E:73:PHE:HB2	4:E:99:ILE:CD1	2.34	0.58
9:K:44:LEU:HD12	9:K:80:ILE:HD11	1.84	0.58
3:C:290:ASN:ND2	3:C:293:LEU:HD12	2.18	0.58
1:A:488:PRO:HG3	1:A:508:SER:HA	1.86	0.58
1:A:873:SER:HB2	1:A:915:LEU:CD2	2.34	0.58
1:A:1110:ARG:HB3	1:A:1118:GLN:HE22	1.69	0.58
2:B:106:ARG:HG2	2:B:855:CYS:HB3	1.84	0.58
2:B:130:ILE:HG21	2:B:419:ILE:HD13	1.86	0.58
2:B:781:LEU:CD2	2:B:792:LEU:HB3	2.31	0.58
14:R:-8:U:H2'	14:R:-7:G:C8	2.39	0.58
1:A:225:ILE:HG23	1:A:256:LEU:HG	1.85	0.58
7:I:36:VAL:O	7:I:36:VAL:HG12	2.02	0.58
13:M:11:TRP:CE2	13:M:101:VAL:HG21	2.39	0.58
1:A:1117:THR:HG22	1:A:1121:LEU:HD23	1.86	0.57
1:A:76:GLY:HA3	1:A:306:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:554:TYR:O	2:B:565:TRP:HA	2.05	0.57
2:B:648:GLU:O	2:B:649:ASP:HB2	2.03	0.57
4:E:142:HIS:HB3	4:E:145:VAL:HG23	1.85	0.57
1:A:137:GLU:HG2	1:A:164:TYR:CZ	2.39	0.57
1:A:521:GLN:HA	1:A:524:THR:CB	2.24	0.57
1:A:797:LEU:HD12	1:A:897:MET:CE	2.34	0.57
1:A:1318:ARG:HA	1:A:1526:GLN:HA	1.85	0.57
3:C:86:THR:CG2	3:C:227:PRO:HB3	2.34	0.57
3:C:245:VAL:CG1	3:C:296:VAL:HG11	2.35	0.57
6:H:147:LYS:O	6:H:148:LEU:HD23	2.04	0.57
9:K:25:THR:HB	9:K:46:GLU:CD	2.29	0.57
15:T:21:DA:H2'	15:T:22:DG:C8	2.38	0.57
1:A:1519:THR:HG23	1:A:1520:GLU:CD	2.29	0.57
1:A:42:LEU:O	1:A:42:LEU:HD23	2.04	0.57
1:A:654:MET:O	1:A:655:GLU:HB3	2.05	0.57
1:A:1110:ARG:HB3	1:A:1118:GLN:NE2	2.18	0.57
1:A:1585:LEU:HB2	1:A:1586:PRO:HD3	1.87	0.57
2:B:201:ARG:HB2	2:B:205:TYR:CD2	2.40	0.57
1:A:93:PHE:CZ	1:A:223:LEU:HD11	2.39	0.57
1:A:316:GLY:HA2	15:T:25:DA:C2'	2.29	0.57
1:A:652:HIS:O	1:A:656:LEU:HB2	2.04	0.57
1:A:983:SER:HA	15:T:16:DG:H5'	1.86	0.57
13:M:33:LEU:CD1	13:M:39:MET:CE	2.83	0.57
1:A:651:GLU:HG3	9:K:60:MET:HE2	1.85	0.57
1:A:739:ILE:HD13	1:A:761:LEU:HD13	1.87	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:1585:LEU:HD12	1:A:1600:LEU:HD21	1.87	0.57
2:B:524:PHE:CE2	2:B:616:PRO:HG3	2.39	0.57
2:B:568:LYS:HE2	2:B:600:MET:CE	2.29	0.57
2:B:854:VAL:HG12	10:L:34:ILE:HG21	1.87	0.57
1:A:1533:LEU:H	1:A:1535:LYS:HZ2	1.51	0.57
7:I:44:ASN:OD1	7:I:45:ILE:N	2.37	0.57
1:A:1036:GLN:O	1:A:1040:LEU:HG	2.05	0.57
1:A:1631:VAL:HG23	1:A:1632:TYR:CD2	2.39	0.57
2:B:700:LEU:HD21	2:B:711:LEU:HD11	1.86	0.57
3:C:267:VAL:CG1	3:C:272:VAL:HG12	2.24	0.57
2:B:104:ARG:O	2:B:707:SER:OG	2.22	0.57
2:B:742:ILE:CD1	2:B:996:VAL:HG22	2.34	0.57
2:B:743:VAL:CG2	2:B:999:TYR:HE2	2.16	0.57
8:J:1:MET:CE	8:J:56:ILE:HD13	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:45:ILE:HB	13:M:88:PHE:HB2	1.87	0.57
1:A:84:PRO:HD3	1:A:335:VAL:HG22	1.85	0.56
1:A:132:LEU:CG	4:E:210:GLN:HE22	2.08	0.56
2:B:745:VAL:HG12	2:B:917:PRO:HB3	1.86	0.56
3:C:138:LEU:HD21	3:C:190:ILE:HD13	1.86	0.56
11:N:49:ALA:HA	13:M:86:ARG:HG3	1.87	0.56
11:N:70:LYS:HE2	11:N:79:ARG:CZ	2.34	0.56
13:M:33:LEU:CD1	13:M:39:MET:HE1	2.34	0.56
4:E:165:LEU:HD23	4:E:169:GLN:HE21	1.68	0.56
1:A:881:MET:HE1	1:A:895:GLN:NE2	2.20	0.56
1:A:921:LEU:HD21	1:A:969:MET:HE2	1.87	0.56
1:A:1213:LEU:HD22	2:B:1046:LEU:CD1	2.35	0.56
1:A:1685:THR:HG21	2:B:1128:ILE:HG12	1.86	0.56
2:B:889:GLN:NE2	2:B:925:THR:OG1	2.36	0.56
2:B:1059:PHE:CE2	2:B:1064:ARG:HD3	2.40	0.56
3:C:98:THR:O	3:C:206:GLN:HG2	2.05	0.56
6:H:36:LYS:HA	6:H:36:LYS:HE3	1.87	0.56
8:J:63:ALA:HB1	10:L:23:HIS:NE2	2.20	0.56
1:A:1083:LEU:HD12	1:A:1083:LEU:O	2.06	0.56
1:A:1300:GLN:HE21	7:I:48:ARG:HH11	1.52	0.56
2:B:103:CYS:SG	2:B:171:ILE:HG21	2.46	0.56
3:C:75:ALA:HA	9:K:50:THR:HG23	1.86	0.56
4:E:122:ALA:HB1	4:E:123:PRO:HD2	1.86	0.56
6:H:103:GLU:OE1	6:H:103:GLU:N	2.29	0.56
1:A:316:GLY:CA	15:T:25:DA:C2'	2.83	0.56
1:A:1512:ILE:HD12	1:A:1527:VAL:HG21	1.86	0.56
2:B:333:CYS:HB3	2:B:342:LYS:HG3	1.88	0.56
2:B:781:LEU:HD23	2:B:792:LEU:HD22	1.85	0.56
1:A:827:VAL:HG22	1:A:861:ILE:CG2	2.35	0.56
1:A:1062:PRO:HB2	1:A:1066:LEU:HG	1.88	0.56
1:A:1318:ARG:CD	1:A:1524:TRP:HE3	2.19	0.56
1:A:1497:ALA:O	1:A:1498:MET:C	2.47	0.56
1:A:1618:LEU:HD11	1:A:1649:CYS:HB2	1.87	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:527:THR:OG1	2:B:530:ILE:HD12	2.05	0.56
2:B:696:MET:HG3	2:B:712:TYR:HB3	1.87	0.56
1:A:430:LYS:HA	2:B:1036:ARG:HH21	1.70	0.56
1:A:914:CYS:O	1:A:915:LEU:HB2	2.05	0.56
1:A:1531:LEU:HB3	1:A:1535:LYS:CD	2.36	0.56
2:B:1028:GLY:H	2:B:1033:GLY:HA3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:20:CYS:O	7:I:21:SER:N	2.33	0.56
9:K:89:THR:HG23	9:K:90:LEU:N	2.21	0.56
11:N:146:ARG:NH1	11:N:148:ARG:HH22	1.96	0.56
1:A:14:GLY:HA2	1:A:1691:ASP:O	2.06	0.56
1:A:123:GLN:O	1:A:127:LEU:HD23	2.06	0.56
1:A:438:ASP:OD1	2:B:1025:PRO:HG3	2.06	0.56
1:A:507:LEU:CD2	1:A:518:VAL:HG11	2.35	0.56
2:B:261:ASP:HB2	7:I:19:PHE:CA	2.27	0.56
4:E:80:PRO:O	4:E:108:GLN:HB2	2.05	0.56
1:A:619:LEU:HD22	1:A:624:GLY:O	2.06	0.56
1:A:1605:ILE:HG21	1:A:1621:ILE:CG1	2.36	0.56
13:M:11:TRP:CZ2	13:M:101:VAL:HG21	2.40	0.56
1:A:1025:ASP:O	1:A:1029:THR:HG23	2.06	0.56
2:B:86:THR:HG23	2:B:96:ALA:O	2.05	0.56
2:B:965:MET:HE1	11:N:142:PRO:CD	2.36	0.56
3:C:74:ASN:O	3:C:78:ARG:HG3	2.06	0.56
1:A:674:SER:HB3	1:A:686:GLN:OE1	2.05	0.55
2:B:61:ILE:HG22	2:B:61:ILE:O	2.06	0.55
2:B:530:ILE:HB	2:B:531:PRO:HD3	1.87	0.55
1:A:8:PRO:O	1:A:9:TRP:HB3	2.05	0.55
1:A:19:MET:HG2	1:A:296:VAL:CG1	2.37	0.55
1:A:1502:VAL:O	1:A:1505:VAL:HG12	2.06	0.55
2:B:399:ALA:O	2:B:418:ARG:NH1	2.40	0.55
2:B:736:PRO:HG2	8:J:53:VAL:HG11	1.87	0.55
3:C:28:ASP:O	3:C:29:PHE:HD1	1.89	0.55
3:C:52:ASP:HB2	3:C:64:ASP:HB2	1.88	0.55
1:A:225:ILE:HG23	1:A:256:LEU:HD11	1.88	0.55
1:A:310:ARG:HB3	1:A:322:ASN:HD22	1.72	0.55
1:A:1090:LEU:HD11	4:E:33:LEU:CD1	2.36	0.55
1:A:1213:LEU:O	1:A:1217:GLN:HG3	2.07	0.55
1:A:1239:MET:HG3	1:A:1239:MET:O	2.05	0.55
10:L:19:CYS:HB3	10:L:23:HIS:H	1.71	0.55
13:M:68:SER:HB2	13:M:112:LEU:CB	2.36	0.55
1:A:1583:ILE:HD12	1:A:1604:ASP:HB2	1.88	0.55
2:B:651:VAL:HG13	2:B:656:THR:CG2	2.36	0.55
2:B:785:ILE:HD12	2:B:791:SER:HB2	1.88	0.55
2:B:1036:ARG:NH1	15:T:18:DG:OP1	2.39	0.55
1:A:10:ARG:HD2	2:B:1108:ASP:HB3	1.87	0.55
1:A:397:HIS:O	1:A:401:VAL:HG23	2.07	0.55
1:A:459:PRO:HB2	1:A:572:GLU:O	2.06	0.55
1:A:1637:ASP:OD2	1:A:1639:ARG:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:TYR:HE1	15:T:25:DA:C5'	2.14	0.55
1:A:505:THR:HG23	1:A:505:THR:O	2.06	0.55
1:A:606:ALA:O	1:A:610:VAL:HG23	2.06	0.55
1:A:661:LEU:HG	1:A:691:LEU:HD12	1.89	0.55
1:A:711:ILE:N	1:A:750:ASP:OD2	2.35	0.55
1:A:795:PHE:HE2	1:A:897:MET:HE2	1.72	0.55
1:A:1024:LEU:HA	1:A:1203:SER:O	2.06	0.55
1:A:1128:ASP:HB3	1:A:1133:ARG:HD3	1.88	0.55
2:B:600:MET:HB3	2:B:608:PRO:CB	2.33	0.55
4:E:152:THR:HG23	4:E:154:GLU:HG2	1.89	0.55
11:N:83:LEU:HD12	11:N:116:ARG:NH1	2.22	0.55
15:T:9:DG:H2''	15:T:10:DG:H8	1.72	0.55
1:A:1001:VAL:HG21	1:A:1205:CYS:SG	2.47	0.55
2:B:568:LYS:HG3	2:B:600:MET:CE	2.37	0.55
5:F:61:GLU:O	5:F:65:VAL:HG23	2.07	0.55
7:I:13:PHE:CD1	7:I:20:CYS:CA	2.89	0.55
1:A:912:ILE:CD1	2:B:924:MET:HG2	2.35	0.55
1:A:1516:GLN:CG	1:A:1526:GLN:HG3	2.36	0.55
2:B:66:PHE:HE1	2:B:75:PHE:CE2	2.24	0.55
2:B:110:TYR:CZ	2:B:146:CYS:SG	2.89	0.55
1:A:1693:LEU:HD13	1:A:1702:VAL:HG21	1.88	0.55
2:B:1026:ILE:HG21	2:B:1031:VAL:CG1	2.37	0.55
4:E:61:LEU:HD12	4:E:72:MET:O	2.07	0.55
6:H:110:THR:HG23	6:H:110:THR:O	2.06	0.55
1:A:220:ASN:O	1:A:221:SER:HB2	2.07	0.55
1:A:799:VAL:O	1:A:803:LEU:HG	2.07	0.55
2:B:194:ILE:HG12	2:B:208:TYR:CD1	2.42	0.55
2:B:987:GLU:CD	3:C:301:ARG:HE	2.15	0.55
3:C:30:PRO:HA	3:C:38:ASP:H	1.72	0.55
1:A:1044:TYR:HD1	1:A:1195:LEU:HD22	1.71	0.54
2:B:263:GLN:CD	13:M:29:SER:HB2	2.32	0.54
2:B:1112:VAL:HG22	2:B:1113:PRO:HD2	1.88	0.54
3:C:183:ASP:O	3:C:184:LEU:HB3	2.06	0.54
4:E:54:ARG:HD2	4:E:57:ASP:CB	2.36	0.54
7:I:55:VAL:HA	7:I:59:VAL:HG11	1.89	0.54
2:B:113:LYS:HG3	2:B:133:PHE:CE1	2.42	0.54
2:B:903:PRO:HB2	2:B:979:LEU:HD23	1.89	0.54
1:A:121:LEU:O	1:A:125:ARG:HG3	2.07	0.54
1:A:522:LEU:O	1:A:523:LEU:HB2	2.08	0.54
1:A:1714:GLU:HG2	5:F:109:TYR:HE2	1.72	0.54
2:B:808:ASP:HB3	2:B:814:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:940:LEU:HD23	2:B:969:ALA:CB	2.37	0.54
3:C:288:PHE:CZ	3:C:299:LEU:HD21	2.41	0.54
5:F:125:ILE:HG13	5:F:125:ILE:O	2.07	0.54
1:A:1293:VAL:HA	1:A:1322:LEU:HD12	1.87	0.54
1:A:1357:LYS:HZ1	1:A:1538:PHE:HE1	1.55	0.54
2:B:399:ALA:HB2	2:B:422:MET:HE2	1.88	0.54
6:H:104:THR:HB	6:H:109:ALA:CB	2.37	0.54
7:I:7:ALA:HB1	13:M:34:GLN:H	1.70	0.54
1:A:422:GLU:O	1:A:423:LYS:HB2	2.08	0.54
1:A:1108:GLU:N	1:A:1108:GLU:OE1	2.40	0.54
1:A:1605:ILE:HG12	1:A:1620:VAL:HG12	1.89	0.54
2:B:1069:VAL:HG21	2:B:1134:VAL:HG21	1.89	0.54
4:E:122:ALA:HB1	4:E:123:PRO:CD	2.37	0.54
6:H:37:MET:HE1	6:H:132:LEU:HD21	1.89	0.54
9:K:86:THR:HG22	9:K:92:ALA:HB2	1.89	0.54
1:A:312:VAL:CG2	1:A:320:PHE:CB	2.85	0.54
1:A:330:ALA:HB1	1:A:397:HIS:CE1	2.43	0.54
11:N:11:ARG:O	11:N:12:PHE:C	2.49	0.54
1:A:1529:VAL:HG12	1:A:1530:LYS:N	2.23	0.54
2:B:178:VAL:O	2:B:178:VAL:HG13	2.07	0.54
5:F:57:MET:HE1	5:F:120:VAL:HG13	1.90	0.54
13:M:67:LEU:CD2	13:M:69:TYR:OH	2.45	0.54
1:A:1000:VAL:HA	1:A:1210:ALA:HA	1.89	0.54
1:A:1068:HIS:CE1	1:A:1144:ASP:O	2.61	0.54
2:B:141:VAL:O	2:B:146:CYS:SG	2.66	0.54
2:B:319:PRO:HB2	2:B:321:GLU:HG2	1.89	0.54
2:B:703:TYR:O	2:B:704:GLN:HB3	2.08	0.54
7:I:54:VAL:HG12	7:I:55:VAL:H	1.73	0.54
13:M:68:SER:HB2	13:M:112:LEU:HB3	1.90	0.54
1:A:1324:HIS:HA	1:A:1327:TYR:CE1	2.43	0.54
3:C:13:ARG:HA	3:C:301:ARG:O	2.08	0.54
6:H:90:TYR:OH	6:H:92:MET:HE3	2.08	0.54
7:I:48:ARG:HD3	7:I:50:PHE:CZ	2.43	0.54
1:A:739:ILE:CD1	1:A:761:LEU:HD13	2.37	0.53
1:A:1034:PRO:HD3	1:A:1166:LYS:HD3	1.90	0.53
1:A:1170:TYR:CE2	1:A:1192:LEU:HD21	2.42	0.53
1:A:1221:GLU:HB3	1:A:1222:PRO:HD3	1.89	0.53
1:A:1640:HIS:O	1:A:1644:VAL:HG23	2.07	0.53
1:A:1714:GLU:HB2	5:F:107:ARG:HB3	1.89	0.53
2:B:514:LEU:HD22	2:B:518:CYS:SG	2.48	0.53
2:B:757:MET:HE3	2:B:759:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:VAL:HG23	3:C:22:ARG:HB2	1.89	0.53
3:C:239:ILE:HD13	3:C:261:VAL:HG11	1.90	0.53
9:K:55:LEU:HD23	9:K:82:LEU:HD11	1.90	0.53
1:A:120:LEU:O	1:A:124:LEU:HD23	2.08	0.53
1:A:727:PHE:O	1:A:729:PRO:HD3	2.08	0.53
2:B:835:GLU:HG3	2:B:837:PHE:CZ	2.43	0.53
1:A:1245:ILE:N	1:A:1246:PRO:HD2	2.24	0.53
1:A:1618:LEU:O	1:A:1622:GLU:HG3	2.08	0.53
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.44	0.53
11:N:95:LEU:HD11	13:M:26:VAL:HG11	1.89	0.53
15:T:12:DC:H2"	15:T:13:DA:C8	2.43	0.53
1:A:316:GLY:HA3	15:T:25:DA:H2"	1.90	0.53
1:A:1133:ARG:C	1:A:1134:LYS:HE2	2.33	0.53
3:C:340:LEU:HD23	9:K:97:GLN:HB2	1.90	0.53
4:E:13:ILE:HD11	4:E:132:GLN:HG3	1.91	0.53
1:A:105:LEU:HD12	1:A:264:HIS:ND1	2.24	0.53
1:A:180:HIS:HB3	1:A:1692:GLU:OE2	2.08	0.53
1:A:182:LYS:O	1:A:183:ASN:HB2	2.09	0.53
1:A:682:TRP:N	1:A:682:TRP:CD1	2.76	0.53
1:A:905:SER:OG	1:A:907:VAL:HG12	2.08	0.53
1:A:1052:HIS:O	1:A:1053:LEU:HB2	2.08	0.53
2:B:69:LYS:HD3	2:B:407:THR:H	1.73	0.53
2:B:270:LYS:HG3	2:B:550:TYR:CD2	2.44	0.53
2:B:910:VAL:O	8:J:9:THR:HG22	2.09	0.53
3:C:184:LEU:CD2	3:C:185:PHE:CE2	2.91	0.53
1:A:632:GLN:HE22	2:B:754:GLU:H	1.57	0.53
1:A:667:ARG:HH21	9:K:38:HIS:HB2	1.74	0.53
1:A:1518:ASP:HB3	1:A:1523:LEU:H	1.73	0.53
2:B:695:THR:CG2	2:B:1000:GLN:HB3	2.39	0.53
2:B:906:GLU:CD	3:C:301:ARG:HH22	2.17	0.53
3:C:12:SER:O	3:C:303:ARG:HB2	2.08	0.53
3:C:173:MET:HE3	3:C:212:MET:HE1	1.91	0.53
4:E:205:THR:HG22	4:E:206:TYR:H	1.74	0.53
1:A:312:VAL:CG2	1:A:320:PHE:HA	2.39	0.53
1:A:404:SER:HB2	1:A:416:GLY:H	1.73	0.53
1:A:914:CYS:H	1:A:954:ARG:CD	2.20	0.53
1:A:1300:GLN:NE2	7:I:48:ARG:HH11	2.06	0.53
1:A:1718:PRO:HD2	5:F:103:PRO:O	2.08	0.53
2:B:217:GLU:HB2	2:B:219:HIS:CE1	2.43	0.53
2:B:808:ASP:HB3	2:B:814:PHE:CZ	2.44	0.53
2:B:862:GLY:O	10:L:33:PRO:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:943:LEU:HD11	11:N:142:PRO:HG3	1.91	0.53
1:A:1566:GLU:H	1:A:1566:GLU:CD	2.16	0.53
2:B:396:ILE:HG13	2:B:397:LYS:N	2.23	0.53
3:C:14:VAL:O	3:C:300:ALA:HB1	2.07	0.53
3:C:18:GLU:OE1	3:C:18:GLU:HA	2.09	0.53
4:E:72:MET:HE1	4:E:103:LEU:HD12	1.91	0.53
7:I:40:ARG:CD	7:I:43:PHE:HA	2.36	0.53
1:A:8:PRO:HG2	2:B:1111:SER:HB3	1.89	0.53
1:A:457:GLY:HA2	1:A:567:ARG:O	2.09	0.53
2:B:48:TYR:CE1	2:B:52:GLU:HG2	2.44	0.53
2:B:75:PHE:CG	2:B:397:LYS:HE3	2.43	0.53
15:T:13:DA:H2''	15:T:14:DG:C8	2.44	0.53
1:A:521:GLN:CA	1:A:524:THR:HB	2.25	0.52
1:A:1518:ASP:OD2	1:A:1525:CYS:HB3	2.09	0.52
2:B:10:LEU:CD1	2:B:11:PRO:HD2	2.31	0.52
2:B:259:PHE:HA	13:M:110:GLN:HE22	1.74	0.52
2:B:643:ASN:ND2	2:B:655:VAL:HG13	2.24	0.52
2:B:1014:THR:HG23	2:B:1015:THR:H	1.73	0.52
3:C:339:GLU:HG2	9:K:26:ALA:CB	2.39	0.52
8:J:53:VAL:HG13	8:J:53:VAL:O	2.09	0.52
16:U:8:DC:H2'	16:U:9:DT:H71	1.90	0.52
1:A:30:VAL:HB	1:A:66:THR:HG21	1.90	0.52
1:A:465:LYS:HD3	2:B:1012:VAL:HB	1.92	0.52
1:A:618:TYR:CE2	1:A:626:PRO:HB3	2.44	0.52
1:A:668:VAL:H	9:K:85:GLN:NE2	2.04	0.52
1:A:1624:GLU:O	1:A:1628:VAL:HG23	2.09	0.52
2:B:656:THR:HG22	2:B:656:THR:O	2.09	0.52
4:E:20:LEU:HD12	4:E:20:LEU:O	2.08	0.52
7:I:54:VAL:HG12	7:I:55:VAL:N	2.23	0.52
9:K:58:MET:HG3	9:K:103:LEU:HB2	1.90	0.52
1:A:1293:VAL:O	1:A:1293:VAL:HG13	2.09	0.52
2:B:1067:ALA:HB2	2:B:1117:ARG:CZ	2.40	0.52
1:A:1349:LEU:HG	1:A:1547:LEU:HD21	1.91	0.52
4:E:173:ILE:CG2	4:E:209:VAL:HA	2.38	0.52
1:A:85:LEU:CD2	1:A:391:TRP:HE1	2.23	0.52
1:A:1619:ARG:HH12	4:E:196:PRO:HG2	1.74	0.52
2:B:224:MET:HE1	2:B:346:LEU:HD21	1.91	0.52
2:B:595:VAL:HA	2:B:612:LEU:HD23	1.91	0.52
2:B:972:ASN:HA	3:C:286:GLU:OE2	2.10	0.52
1:A:613:CYS:O	1:A:617:GLN:HG2	2.09	0.52
2:B:1082:GLU:HG3	2:B:1095:LYS:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:312:SER:HB3	3:C:321:LEU:CD1	2.39	0.52
6:H:29:HIS:CE1	6:H:40:ILE:HD12	2.45	0.52
9:K:124:GLN:O	9:K:128:ARG:HG2	2.09	0.52
1:A:15:ILE:HD13	2:B:1132:LEU:HB3	1.92	0.52
1:A:553:GLN:HG2	15:T:18:DG:H4'	1.92	0.52
1:A:712:THR:HG22	1:A:714:LYS:H	1.73	0.52
1:A:1154:ILE:HG23	1:A:1154:ILE:O	2.10	0.52
1:A:1589:PHE:HA	1:A:1597:LEU:HD13	1.91	0.52
2:B:411:MET:HE2	2:B:411:MET:N	2.24	0.52
2:B:473:HIS:HD2	2:B:475:GLY:H	1.58	0.52
2:B:716:THR:O	2:B:716:THR:HG23	2.09	0.52
3:C:68:ILE:HD11	3:C:72:ILE:HG21	1.91	0.52
6:H:137:VAL:O	6:H:138:ASP:HB2	2.09	0.52
1:A:33:ILE:HD11	1:A:81:ILE:HG13	1.92	0.52
1:A:1359:ASN:O	1:A:1360:LYS:HD2	2.10	0.52
2:B:77:ILE:HG12	2:B:118:ILE:HG22	1.91	0.52
2:B:262:TYR:HD2	13:M:30:ASN:HA	1.74	0.52
2:B:639:GLN:O	2:B:639:GLN:HG2	2.09	0.52
7:I:16:ASP:O	13:M:67:LEU:HD22	2.09	0.52
2:B:648:GLU:HG2	2:B:649:ASP:N	2.25	0.52
2:B:1068:HIS:HB3	2:B:1109:THR:HG22	1.91	0.52
3:C:66:VAL:HG22	3:C:305:HIS:CE1	2.44	0.52
6:H:65:TYR:HB3	6:H:67:ASP:OD2	2.10	0.52
1:A:1096:ILE:HA	1:A:1120:MET:CE	2.40	0.52
2:B:721:LEU:CD2	8:J:50:LEU:HD23	2.40	0.52
2:B:965:MET:HE2	11:N:141:ILE:HD13	1.92	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
7:I:43:PHE:CE1	7:I:46:ASN:HA	2.45	0.52
1:A:166:THR:O	1:A:170:GLN:HG2	2.09	0.51
1:A:550:LEU:HD23	1:A:594:MET:SD	2.49	0.51
1:A:603:LEU:HD22	2:B:1052:PHE:CG	2.45	0.51
1:A:873:SER:HB2	1:A:915:LEU:HD21	1.91	0.51
1:A:1090:LEU:CD2	4:E:30:GLN:HG2	2.34	0.51
2:B:659:GLN:HG3	2:B:660:GLU:N	2.23	0.51
1:A:429:ARG:NH2	15:T:17:DA:OP1	2.44	0.51
1:A:1088:ALA:O	1:A:1091:SER:OG	2.20	0.51
2:B:212:MET:SD	2:B:345:MET:HE3	2.51	0.51
2:B:742:ILE:HD12	8:J:43:TYR:HE1	1.75	0.51
5:F:121:ASP:OD1	5:F:122:GLU:N	2.43	0.51
1:A:132:LEU:HG	4:E:210:GLN:NE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ASN:HD21	2:B:1041:GLU:HG2	1.74	0.51
2:B:178:VAL:O	2:B:179:ILE:C	2.53	0.51
5:F:104:ILE:O	5:F:120:VAL:HG23	2.10	0.51
1:A:215:VAL:HG22	1:A:225:ILE:HG22	1.93	0.51
1:A:1020:GLY:O	1:A:1021:GLU:HB2	2.11	0.51
1:A:1348:LYS:CE	1:A:1508:ILE:HB	2.40	0.51
1:A:802:ILE:HG22	1:A:894:LEU:HD22	1.92	0.51
1:A:1318:ARG:HH21	1:A:1526:GLN:HG2	1.75	0.51
1:A:1512:ILE:HD12	1:A:1527:VAL:CG2	2.39	0.51
2:B:169:TYR:CE1	2:B:176:GLU:HG2	2.44	0.51
2:B:187:ARG:HD2	2:B:615:THR:CB	2.40	0.51
2:B:194:ILE:HG12	2:B:208:TYR:CE1	2.45	0.51
1:A:732:MET:HE2	6:H:27:ARG:HH12	1.76	0.51
1:A:985:SER:CB	1:A:1224:THR:HA	2.40	0.51
3:C:29:PHE:HB3	3:C:30:PRO:CD	2.41	0.51
3:C:53:VAL:HG21	9:K:118:ILE:CD1	2.41	0.51
9:K:42:PHE:HE1	9:K:84:ILE:HD12	1.73	0.51
1:A:1353:SER:OG	1:A:1543:LEU:HD11	2.11	0.51
2:B:882:LYS:HD2	2:B:1002:LEU:CD2	2.40	0.51
4:E:154:GLU:O	4:E:158:GLU:HG3	2.11	0.51
1:A:543:LYS:HG3	1:A:543:LYS:O	2.10	0.51
2:B:94:LYS:HG2	10:L:39:CYS:HA	1.91	0.51
2:B:102:GLU:O	2:B:103:CYS:SG	2.68	0.51
2:B:785:ILE:HG12	2:B:786:LYS:O	2.11	0.51
2:B:791:SER:C	2:B:792:LEU:HD23	2.36	0.51
3:C:221:ASP:OD2	10:L:58:ARG:NH2	2.40	0.51
3:C:335:ARG:NH2	9:K:25:THR:O	2.43	0.51
1:A:163:GLN:HG3	1:A:164:TYR:N	2.26	0.51
1:A:428:PHE:O	1:A:432:MET:HB3	2.11	0.51
1:A:440:ALA:HB1	2:B:1035:ILE:HD11	1.92	0.51
1:A:1147:LEU:HD22	1:A:1152:PRO:HB3	1.93	0.51
2:B:948:THR:O	2:B:951:ILE:HG12	2.11	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:312:VAL:CG2	1:A:320:PHE:CA	2.88	0.51
1:A:1134:LYS:HE2	1:A:1134:LYS:HA	1.92	0.51
1:A:1583:ILE:HD11	1:A:1607:ALA:HB3	1.93	0.51
2:B:172:ILE:HG12	2:B:434:PHE:HB3	1.93	0.51
1:A:57:PRO:HD3	1:A:64:CYS:HB3	1.93	0.50
1:A:936:PRO:HG2	2:B:494:TRP:CD1	2.45	0.50
1:A:1114:SER:OG	1:A:1115:PRO:HD2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:ILE:CG2	2:B:792:LEU:CD2	2.81	0.50
1:A:163:GLN:O	1:A:166:THR:HG22	2.11	0.50
1:A:499:ASN:HD22	1:A:536:LYS:HD2	1.76	0.50
1:A:766:TYR:HD1	1:A:771:GLY:HA2	1.75	0.50
1:A:841:GLU:O	1:A:845:LYS:HG2	2.11	0.50
1:A:1625:ILE:HG21	1:A:1641:LEU:HD22	1.93	0.50
1:A:465:LYS:O	1:A:467:THR:HG23	2.12	0.50
1:A:601:SER:O	1:A:602:GLU:HB3	2.10	0.50
1:A:1068:HIS:HE1	1:A:1144:ASP:O	1.93	0.50
1:A:1110:ARG:HD3	1:A:1110:ARG:C	2.35	0.50
2:B:91:THR:HG22	2:B:91:THR:O	2.12	0.50
2:B:92:ILE:CD1	2:B:859:THR:HA	2.40	0.50
2:B:624:GLN:NE2	2:B:629:GLY:HA2	2.26	0.50
2:B:743:VAL:HG21	2:B:999:TYR:CE2	2.42	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
3:C:15:VAL:HG12	3:C:298:ARG:HH21	1.77	0.50
4:E:10:LEU:CD2	4:E:58:LEU:HD11	2.41	0.50
1:A:1279:LYS:O	1:A:1283:LYS:HD3	2.11	0.50
1:A:1300:GLN:HB2	1:A:1316:GLN:HG2	1.94	0.50
11:N:121:PRO:HD2	11:N:121:PRO:O	2.10	0.50
1:A:19:MET:HG2	1:A:296:VAL:HG11	1.93	0.50
1:A:225:ILE:HG23	1:A:256:LEU:CG	2.40	0.50
2:B:6:ARG:O	2:B:6:ARG:HD3	2.12	0.50
2:B:691:MET:CE	2:B:884:ALA:HB1	2.41	0.50
15:T:1:DT:H2''	15:T:2:DC:C5	2.47	0.50
2:B:118:ILE:HD11	2:B:419:ILE:HG21	1.93	0.50
2:B:319:PRO:HG2	2:B:322:GLN:HB2	1.93	0.50
2:B:417:MET:O	2:B:421:THR:OG1	2.30	0.50
2:B:615:THR:HB	2:B:616:PRO:HD2	1.94	0.50
2:B:657:THR:HG22	2:B:658:HIS:ND1	2.27	0.50
2:B:1029:ARG:HD2	15:T:20:DC:H5''	1.93	0.50
1:A:1147:LEU:CD2	1:A:1152:PRO:HB3	2.42	0.50
1:A:1222:PRO:O	1:A:1226:MET:N	2.44	0.50
1:A:1632:TYR:HB2	1:A:1634:ILE:HD12	1.94	0.50
2:B:552:GLU:O	2:B:568:LYS:HB2	2.11	0.50
4:E:87:ILE:HG22	4:E:121:MET:HE1	1.93	0.50
7:I:7:ALA:HB3	13:M:33:LEU:HA	1.92	0.50
9:K:55:LEU:HD21	9:K:96:PHE:HE1	1.76	0.50
9:K:86:THR:OG1	9:K:90:LEU:HD21	2.11	0.50
1:A:480:LEU:O	1:A:484:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:PHE:HE1	6:H:40:ILE:HG21	1.77	0.50
1:A:1086:ARG:CZ	1:A:1086:ARG:HB2	2.42	0.50
1:A:280:PHE:O	1:A:281:SER:OG	2.17	0.50
2:B:695:THR:HG21	2:B:1000:GLN:HB3	1.94	0.50
1:A:425:GLU:CG	1:A:426:GLY:H	2.24	0.49
1:A:795:PHE:CE2	1:A:897:MET:HE2	2.47	0.49
1:A:1062:PRO:HB3	1:A:1156:PHE:HD2	1.76	0.49
1:A:1619:ARG:HH22	4:E:196:PRO:CD	2.20	0.49
5:F:107:ARG:HD2	5:F:115:TYR:CG	2.46	0.49
1:A:423:LYS:HG3	1:A:424:LYS:N	2.27	0.49
1:A:1151:ARG:HG3	1:A:1153:ASP:OD1	2.11	0.49
1:A:1545:VAL:HG21	7:I:53:LYS:NZ	2.28	0.49
2:B:419:ILE:HG13	2:B:420:PHE:N	2.26	0.49
2:B:655:VAL:HG12	2:B:656:THR:H	1.76	0.49
3:C:140:PHE:HE2	3:C:214:CYS:HG	1.60	0.49
7:I:17:LEU:HD13	7:I:35:THR:OG1	2.12	0.49
1:A:322:ASN:HB3	1:A:325:THR:HG23	1.94	0.49
1:A:418:ARG:HH22	15:T:13:DA:P	2.32	0.49
1:A:551:ASN:ND2	2:B:1041:GLU:HG2	2.26	0.49
1:A:1251:ILE:O	1:A:1654:TYR:OH	2.30	0.49
2:B:792:LEU:HD12	2:B:865:LYS:CD	2.40	0.49
3:C:29:PHE:HB3	3:C:30:PRO:HD2	1.94	0.49
3:C:56:MET:HE2	9:K:121:TYR:CD2	2.47	0.49
3:C:93:LEU:HB3	10:L:52:LEU:HD11	1.94	0.49
1:A:257:THR:HB	1:A:391:TRP:HZ3	1.77	0.49
1:A:668:VAL:N	9:K:85:GLN:HE22	2.05	0.49
1:A:1662:ILE:HD13	1:A:1674:PHE:HD2	1.78	0.49
2:B:29:GLU:H	2:B:29:GLU:CD	2.20	0.49
2:B:87:VAL:HB	2:B:92:ILE:HD12	1.93	0.49
2:B:426:LEU:HD23	2:B:426:LEU:O	2.13	0.49
2:B:1126:MET:O	2:B:1127:ASN:HB2	2.12	0.49
1:A:636:VAL:HG11	1:A:795:PHE:CZ	2.47	0.49
2:B:387:GLU:OE1	2:B:445:LEU:HD11	2.13	0.49
2:B:781:LEU:O	2:B:792:LEU:HD22	2.13	0.49
3:C:52:ASP:O	3:C:64:ASP:N	2.45	0.49
3:C:114:PRO:HG3	8:J:13:ILE:CD1	2.42	0.49
4:E:123:PRO:HA	4:E:126:ILE:CG2	2.42	0.49
1:A:25:LEU:O	1:A:28:LEU:HB2	2.13	0.49
1:A:764:CYS:HB3	1:A:1039:PHE:CE1	2.48	0.49
1:A:1255:ALA:HB3	1:A:1656:PRO:HB3	1.94	0.49
1:A:1504:ALA:O	1:A:1507:GLU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:PRO:O	2:B:318:TYR:HB2	2.12	0.49
2:B:396:ILE:CG2	2:B:422:MET:HB2	2.33	0.49
2:B:648:GLU:HG2	2:B:649:ASP:H	1.77	0.49
11:N:41:GLU:OE1	13: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: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:663:ASP:OD1	1:A:664:LYS:N	2.45	0.49
1:A:972:ARG:NH1	2:B:489:LEU:HD12	2.28	0.49
6:H:39:LEU:HD11	6:H:123:MET:SD	2.52	0.49
7:I:31:GLY:HA3	7:I:36:VAL:HG13	1.95	0.49
11:N:30:PHE:HZ	13:M:102:TYR:CG	2.31	0.49
13:M:74:PHE:N	13:M:78:ALA:HB2	2.27	0.49
1:A:222:LYS:C	1:A:223:LEU:HD12	2.38	0.49
1:A:717:VAL:HG22	6:H:20:LYS:HG2	1.95	0.49
1:A:1281:LEU:HD21	1:A:1595:LEU:HD11	1.94	0.49
1:A:1505:VAL:HG11	1:A:1515:TYR:CZ	2.48	0.49
4:E:189:GLN:O	4:E:209:VAL:HG23	2.12	0.49
4:E:205:THR:HG22	4:E:206:TYR:N	2.27	0.49
16:U:11:DG:H2''	16:U:12:DC:C5	2.47	0.49
1:A:497:VAL:O	1:A:505:THR:HG22	2.13	0.49
1:A:791:LEU:HD22	2:B:984:SER:HB3	1.94	0.49
1:A:915:LEU:HD12	1:A:952:THR:HA	1.95	0.49
2:B:802:ARG:HB3	2:B:838:VAL:HG21	1.94	0.49
3:C:90:GLU:HB2	3:C:215:VAL:HG22	1.94	0.49
2:B:187:ARG:NH1	2:B:616:PRO:HD2	2.27	0.49
15:T:24:DA:H2''	15:T:25:DA:C8	2.48	0.49
2:B:626:LEU:O	2:B:627:ALA:HB3	2.12	0.48
4:E:80:PRO:HA	4:E:107:GLN:HG3	1.95	0.48
7:I:60:VAL:O	7:I:60:VAL:HG12	2.10	0.48
1:A:1223:SER:HB2	1:A:1245:ILE:HD11	1.94	0.48
2:B:497:LEU:HD23	2:B:512:ASN:CB	2.43	0.48
2:B:583:VAL:CG1	2:B:630:LYS:HB3	2.43	0.48
2:B:752:ASP:HB3	2:B:758:ILE:HG12	1.95	0.48
2:B:796:ILE:HD12	2:B:809:ASP:H	1.77	0.48
3:C:14:VAL:C	3:C:300:ALA:HB1	2.38	0.48
3:C:33:TYR:HB3	3:C:36:TYR:CB	2.39	0.48
9:K:31:GLN:OE1	9:K:37:ARG:HA	2.12	0.48
1:A:408:LYS:NZ	1:A:409:LEU:HD21	2.12	0.48
1:A:1281:LEU:HD11	1:A:1591:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1069:VAL:CG2	2:B:1134:VAL:HG21	2.44	0.48
3:C:52:ASP:HB2	3:C:64:ASP:OD2	2.13	0.48
3:C:163:TYR:CD1	3:C:166:HIS:HB3	2.39	0.48
3:C:340:LEU:O	3:C:343:VAL:HG22	2.12	0.48
4:E:92:GLN:HA	4:E:95:GLN:CD	2.37	0.48
1:A:47:ALA:O	1:A:48:ASN:HB2	2.12	0.48
1:A:127:LEU:HD11	1:A:187:SER:OG	2.13	0.48
1:A:1558:GLY:O	1:A:1582:GLY:HA3	2.13	0.48
2:B:251:PHE:CE1	2:B:290:MET:HE3	2.48	0.48
2:B:539:VAL:HG22	2:B:566:VAL:HB	1.95	0.48
2:B:785:ILE:HD12	2:B:791:SER:CB	2.43	0.48
2:B:905:THR:CG2	2:B:909:MET:HB2	2.43	0.48
3:C:110:LEU:HD13	3:C:212:MET:SD	2.53	0.48
6:H:106:THR:O	6:H:106:THR:HG22	2.13	0.48
7:I:9:THR:CG2	7:I:15:SER:CA	2.90	0.48
7:I:30:PRO:O	7:I:31:GLY:C	2.57	0.48
7:I:35:THR:HG21	13:M:113:PHE:CE1	2.49	0.48
8:J:3:ILE:HD11	8:J:49:LEU:HD23	1.95	0.48
1:A:164:TYR:O	1:A:168:ILE:HG12	2.14	0.48
2:B:571:ALA:HB3	2:B:572:PRO:HD3	1.94	0.48
3:C:147:THR:N	3:C:164:VAL:HG22	2.26	0.48
1:A:144:ARG:CD	4:E:122:ALA:HB2	2.43	0.48
1:A:812:ARG:HH11	1:A:914:CYS:C	2.21	0.48
1:A:1060:ALA:HB1	1:A:1156:PHE:CD1	2.49	0.48
1:A:1702:VAL:CG2	1:A:1704:LYS:HG3	2.43	0.48
2:B:166:MET:O	2:B:166:MET:HG2	2.14	0.48
4:E:67:ASP:CG	4:E:70:ASP:HB2	2.39	0.48
7:I:13:PHE:HD1	7:I:20:CYS:HA	1.78	0.48
2:B:178:VAL:O	2:B:178:VAL:HG22	2.14	0.48
2:B:527:THR:HG23	2:B:527:THR:O	2.14	0.48
2:B:909:MET:HE3	8:J:44:CYS:HB3	1.94	0.48
3:C:222:HIS:CD2	10:L:58:ARG:HD3	2.49	0.48
7:I:14:GLN:O	7:I:15:SER:HB2	2.13	0.48
1:A:162:GLU:HA	1:A:165:THR:OG1	2.13	0.48
1:A:163:GLN:HG3	1:A:164:TYR:H	1.79	0.48
2:B:926:ILE:O	2:B:930:ILE:HG13	2.13	0.48
7:I:14:GLN:HE21	7:I:32:ALA:HB3	1.76	0.48
10:L:19:CYS:SG	10:L:20:GLY:N	2.86	0.48
1:A:34:THR:HA	1:A:332:MET:HE1	1.95	0.48
1:A:89:ASN:HD21	1:A:92:LEU:HD12	1.78	0.48
1:A:654:MET:C	1:A:656:LEU:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LYS:HB3	1:A:678:PRO:HD3	1.94	0.48
2:B:8:ARG:O	2:B:9:ASN:ND2	2.47	0.48
2:B:745:VAL:CG1	2:B:917:PRO:HB3	2.43	0.48
2:B:746:ILE:HG22	2:B:914:LEU:HD22	1.95	0.48
2:B:912:ASP:HB3	8:J:9:THR:HG23	1.96	0.48
3:C:30:PRO:HG2	9:K:61:LYS:HA	1.95	0.48
4:E:139:ILE:HG13	4:E:140:THR:N	2.28	0.48
13:M:33:LEU:HD21	13:M:39:MET:CE	2.08	0.48
1:A:1122:ARG:O	1:A:1127:LEU:HD13	2.14	0.48
1:A:1605:ILE:HG21	1:A:1621:ILE:HG12	1.96	0.48
2:B:179:ILE:HG12	2:B:454:CYS:HB2	1.96	0.48
2:B:278:LEU:HD11	2:B:354:PHE:HB3	1.95	0.48
2:B:392:TRP:CE3	2:B:393:LEU:HD23	2.49	0.48
2:B:408:SER:HA	2:B:411:MET:CB	2.38	0.48
2:B:498:CYS:CB	2:B:668:SER:HB2	2.43	0.48
4:E:17:ILE:HD11	4:E:105:VAL:HG21	1.95	0.48
6:H:13:LYS:HE2	6:H:13:LYS:HA	1.95	0.48
1:A:9:TRP:O	1:A:9:TRP:CG	2.66	0.47
1:A:683:THR:HG22	1:A:683:THR:O	2.12	0.47
1:A:1213:LEU:HD22	2:B:1046:LEU:HD11	1.95	0.47
2:B:576:ASP:OD1	2:B:576:ASP:C	2.57	0.47
2:B:1026:ILE:HG21	2:B:1031:VAL:HG12	1.96	0.47
11:N:29:ARG:C	11:N:31:SER:H	2.22	0.47
13:M:26:VAL:HG12	13:M:60:LEU:CD2	2.44	0.47
1:A:768:ILE:HG21	1:A:1046:VAL:HB	1.96	0.47
2:B:286:LEU:O	2:B:290:MET:HB2	2.13	0.47
3:C:171:ARG:HG3	3:C:195:ASP:HB2	1.94	0.47
3:C:250:ALA:HB1	3:C:273:ALA:HB2	1.96	0.47
7:I:47:VAL:HG23	7:I:47:VAL:O	2.14	0.47
1:A:1253:MET:O	1:A:1658:ASN:HB3	2.14	0.47
1:A:1287:ARG:HG2	1:A:1555:ALA:HB1	1.96	0.47
1:A:1681:LEU:HD21	2:B:1123:LEU:CD2	2.45	0.47
2:B:743:VAL:HG21	2:B:997:VAL:HG22	1.97	0.47
4:E:87:ILE:CG2	4:E:121:MET:HE1	2.43	0.47
1:A:464:THR:HG22	1:A:464:THR:O	2.14	0.47
1:A:1106:GLU:N	1:A:1106:GLU:OE2	2.48	0.47
1:A:1580:THR:HG22	1:A:1581:GLU:N	2.29	0.47
2:B:58:VAL:O	2:B:61:ILE:HB	2.13	0.47
2:B:122:VAL:O	2:B:123:ASN:HB2	2.14	0.47
2:B:403:LYS:HB3	2:B:418:ARG:NH2	2.26	0.47
2:B:730:TYR:O	2:B:731:ASP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:981:SER:HB2	2:B:988:LEU:HD21	1.96	0.47
3:C:240:THR:CG2	3:C:298:ARG:HB3	2.44	0.47
6:H:105:SER:O	6:H:106:THR:HB	2.14	0.47
13:M:33:LEU:HD13	13:M:39:MET:CE	2.41	0.47
15:T:1:DT:H2''	15:T:2:DC:C4	2.50	0.47
1:A:181:VAL:HG11	4:E:166:ARG:HH21	1.79	0.47
1:A:595:ASN:HD22	2:B:1035:ILE:HD12	1.79	0.47
1:A:1498:MET:HA	1:A:1501:ARG:NH1	2.29	0.47
1:A:1518:ASP:CB	1:A:1522:SER:HA	2.45	0.47
1:A:1670:GLN:C	1:A:1672:MET:H	2.22	0.47
3:C:86:THR:HG21	3:C:227:PRO:HB3	1.96	0.47
3:C:182:ALA:O	3:C:185:PHE:O	2.32	0.47
5:F:66:LEU:HD21	5:F:97:LEU:HD22	1.96	0.47
9:K:47:GLU:OE1	9:K:47:GLU:HA	2.14	0.47
11:N:105:LEU:HB2	13:M:41:PHE:HB2	1.96	0.47
1:A:678:PRO:HB2	6:H:47:ILE:HG23	1.95	0.47
1:A:845:LYS:HA	1:A:845:LYS:HE2	1.97	0.47
2:B:625:ASN:O	2:B:629:GLY:N	2.48	0.47
3:C:162:LEU:HG	3:C:204:PRO:HD3	1.95	0.47
1:A:89:ASN:OD1	1:A:92:LEU:HB2	2.14	0.47
1:A:119:LEU:HB2	1:A:142:LEU:HD22	1.97	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:753:HIS:O	1:A:754:TYR:HB2	2.14	0.47
1:A:1527:VAL:HG22	1:A:1528:THR:N	2.30	0.47
2:B:140:MET:HE3	2:B:168:GLY:C	2.40	0.47
3:C:245:VAL:HG21	3:C:253:LEU:HD23	1.97	0.47
4:E:159:LEU:HD11	4:E:206:TYR:CD2	2.50	0.47
8:J:10:CYS:SG	8:J:42:ARG:HD2	2.54	0.47
16:U:3:DG:H2'	16:U:4:DT:C6	2.49	0.47
1:A:404:SER:CB	1:A:415:PRO:HA	2.42	0.47
1:A:889:PHE:O	1:A:890:PRO:C	2.56	0.47
1:A:1575:GLU:O	1:A:1576:LEU:HD22	2.15	0.47
2:B:162:GLU:C	2:B:164:GLU:N	2.72	0.47
3:C:337:LEU:HD21	9:K:100:LEU:HB2	1.97	0.47
4:E:72:MET:CE	4:E:103:LEU:HD12	2.45	0.47
7:I:55:VAL:HA	7:I:59:VAL:CG1	2.45	0.47
1:A:66:THR:O	2:B:1083:LYS:HE3	2.14	0.47
1:A:181:VAL:HG11	4:E:166:ARG:NH2	2.30	0.47
1:A:1085:ARG:NH2	4:E:19:GLN:HG2	2.30	0.47
1:A:1162:THR:HG21	4:E:199:THR:O	2.14	0.47

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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	0.47
6:H:35:PHE:HB3	6:H:37:MET:HG3	1.96	0.47
13:M:67:LEU:CG	13:M:69:TYR:CE1	2.98	0.47
1:A:553:GLN:HG2	15:T:18:DG:C4'	2.45	0.47
1:A:1084:LEU:HG	1:A:1084:LEU:O	2.14	0.47
1:A:1669:LEU:O	1:A:1673:THR:HG23	2.15	0.47
2:B:66:PHE:CE1	2:B:75:PHE:CE2	3.02	0.47
2:B:742:ILE:HD12	8:J:43:TYR:CE1	2.50	0.47
2:B:901:ASP:OD1	3:C:78:ARG:NH1	2.38	0.47
2:B:926:ILE:O	2:B:926:ILE:HG22	2.15	0.47
4:E:53:PRO:HB2	4:E:54:ARG:CZ	2.45	0.47
5:F:81:VAL:O	5:F:81:VAL:HG22	2.14	0.47
1:A:1332:CYS:O	1:A:1332:CYS:SG	2.73	0.46
2:B:333:CYS:SG	2:B:345:MET:SD	3.13	0.46
9:K:62:ASN:O	9:K:65:VAL:HG22	2.15	0.46
1:A:89:ASN:HB3	1:A:299:LEU:HG	1.97	0.46
1:A:100:LEU:HD21	1:A:265:LEU:HD22	1.96	0.46
1:A:258:PRO:HD2	1:A:391:TRP:CE3	2.50	0.46
1:A:713:GLY:O	6:H:20:LYS:HE2	2.15	0.46
1:A:1565:ASN:HD22	1:A:1579:ASN:HD22	1.63	0.46
2:B:60:ALA:O	2:B:61:ILE:C	2.58	0.46
2:B:181:MET:SD	2:B:520:VAL:HG21	2.55	0.46
3:C:15:VAL:HG12	3:C:298:ARG:NH2	2.30	0.46
3:C:339:GLU:HG2	9:K:26:ALA:HB3	1.97	0.46
1:A:497:VAL:HG13	1:A:505:THR:CG2	2.45	0.46
1:A:551:ASN:O	1:A:594:MET:HG3	2.15	0.46
2:B:386:LYS:O	2:B:390:GLU:HG3	2.16	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
3:C:299:LEU:HD23	3:C:299:LEU:H	1.79	0.46
13:M:81:CYS:SG	13:M:85:CYS:SG	3.05	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:811:LYS:O	1:A:814:ARG:HG2	2.15	0.46
2:B:141:VAL:O	2:B:146:CYS:CB	2.63	0.46
2:B:1037:PHE:CD2	2:B:1058:LEU:HD21	2.51	0.46
3:C:173:MET:SD	3:C:212:MET:HE1	2.56	0.46
7:I:7:ALA:HB1	13:M:34:GLN:HG3	1.96	0.46
9:K:83:ARG:HH11	9:K:85:GLN:NE2	2.11	0.46
15:T:12:DC:H2''	15:T:13:DA:H8	1.80	0.46
1:A:469:PRO:HD3	1:A:600:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:HD11	2:B:282:VAL:HG21	1.97	0.46
2:B:393:LEU:O	2:B:396:ILE:HG12	2.16	0.46
2:B:410:SER:HB3	2:B:411:MET:HE2	1.97	0.46
2:B:626:LEU:HD13	2:B:659:GLN:HB3	1.97	0.46
2:B:940:LEU:HD12	8:J:43:TYR:CB	2.41	0.46
2:B:1069:VAL:HG12	2:B:1076:LEU:HD13	1.98	0.46
3:C:31:GLY:HA2	3:C:37:ASP:OD1	2.15	0.46
5:F:71:LEU:HD12	5:F:71:LEU:O	2.15	0.46
7:I:29:LEU:N	7:I:41:CYS:HA	2.30	0.46
9:K:90:LEU:H	9:K:90:LEU:CD2	2.26	0.46
1:A:558:ARG:HB3	1:A:559:PRO:HD3	1.96	0.46
1:A:936:PRO:HG2	2:B:494:TRP:CG	2.50	0.46
1:A:1106:GLU:O	1:A:1106:GLU:HG2	2.14	0.46
1:A:1247:ARG:HG2	1:A:1628:VAL:HG22	1.97	0.46
1:A:1518:ASP:CG	1:A:1524:TRP:H	2.23	0.46
2:B:167:GLY:O	2:B:169:TYR:CD2	2.68	0.46
2:B:183:ILE:HG13	2:B:472:VAL:HG12	1.98	0.46
2:B:269:ILE:HD13	2:B:278:LEU:HD23	1.98	0.46
2:B:673:PHE:CZ	2:B:732:MET:HE3	2.50	0.46
3:C:27:THR:O	3:C:27:THR:HG22	2.14	0.46
6:H:86:ASP:C	6:H:88:PHE:H	2.23	0.46
1:A:498:ILE:O	1:A:536:LYS:HA	2.16	0.46
1:A:812:ARG:HD2	1:A:914:CYS:CA	2.46	0.46
1:A:1354:ILE:HD12	1:A:1540:MET:CE	2.45	0.46
2:B:39:THR:HG21	2:B:166:MET:HG2	1.98	0.46
2:B:642:MET:HE3	2:B:658:HIS:ND1	2.31	0.46
2:B:707:SER:HB2	2:B:868:CYS:SG	2.56	0.46
2:B:721:LEU:HD21	8:J:50:LEU:HD23	1.97	0.46
3:C:138:LEU:HD21	3:C:190:ILE:HG21	1.98	0.46
1:A:127:LEU:HD21	1:A:135:VAL: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:1180:LYS:HD3	1:A:1180:LYS:HA	1.83	0.46
2:B:705:ASP:HA	2:B:853:LYS:HZ3	1.80	0.46
2:B:847:CYS:SG	2:B:871:MET:HG2	2.56	0.46
3:C:61:LEU:HG	3:C:63:PHE:HD1	1.80	0.46
11:N:24:ALA:HB3	11:N:27:SER:HB3	1.98	0.46
1:A:897:MET:SD	2:B:921:PRO:HG3	2.56	0.46
2:B:39:THR:CG2	2:B:166:MET:HG2	2.45	0.46
2:B:175:ILE:CG2	2:B:175:ILE:O	2.64	0.46
2:B:471:CYS:SG	2:B:511:MET:HG2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HD13	1:A:304:VAL:HG11	1.98	0.46
2:B:332:ILE:HG13	2:B:332:ILE:O	2.14	0.46
2:B:336:LEU:CD2	2:B:561:VAL:HG22	2.46	0.46
2:B:810:ASP:OD2	10:L:17:TYR:OH	2.30	0.46
3:C:236:LEU:HD22	3:C:305:HIS:CD2	2.51	0.46
3:C:290:ASN:HD22	3:C:293:LEU:HB2	1.81	0.46
5:F:53:THR:OG1	5:F:108:ARG:NH1	2.48	0.46
9:K:90:LEU:HD12	9:K:95:PRO:HD3	1.98	0.46
1:A:1090:LEU:HD21	4:E:33:LEU:HD12	1.99	0.45
1:A:1288:VAL:HB	1:A:1331:LYS:HE3	1.98	0.45
1:A:1511:PHE:HB3	1:A:1529:VAL:HG13	1.97	0.45
4:E:125:TYR:O	4:E:127:LEU:HD12	2.16	0.45
7:I:13:PHE:CD1	7:I:20:CYS:CB	2.99	0.45
13:M:16:ALA:HB3	13:M:19:GLY:HA2	1.98	0.45
1:A:833:LEU:HD22	1:A:833:LEU:HA	1.85	0.45
1:A:1533:LEU:H	1:A:1535:LYS:NZ	2.14	0.45
1:A:1545:VAL:CG2	7:I:53:LYS:HE3	2.41	0.45
2:B:92:ILE:CG2	2:B:93:CYS:H	2.24	0.45
2:B:141:VAL:HB	2:B:167:GLY:HA3	1.97	0.45
2:B:700:LEU:HD11	2:B:706:ARG:CG	2.39	0.45
2:B:722:VAL:HG21	2:B:934:ALA:HB3	1.98	0.45
2:B:792:LEU:CD1	2:B:865:LYS:HD2	2.41	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	1.98	0.45
5:F:122:GLU:O	5:F:122:GLU:HG3	2.15	0.45
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.45
1:A:665:VAL:CG1	9:K:33:ALA:HB2	2.45	0.45
3:C:245:VAL:HG21	3:C:253:LEU:HD22	1.98	0.45
3:C:261:VAL:HG21	3:C:281:ASP:HB2	1.97	0.45
1:A:314:ARG:HD2	1:A:319:MET:HE3	1.98	0.45
1:A:430:LYS:O	1:A:431:HIS:HB2	2.16	0.45
1:A:716:TRP:HZ2	1:A:748:VAL:HG11	1.80	0.45
1:A:936:PRO:HG2	2:B:494:TRP:HB3	1.97	0.45
1:A:1343:GLU:HG3	1:A:1505:VAL:CG2	2.46	0.45
2:B:64:PHE:HE2	2:B:397:LYS:CB	2.25	0.45
2:B:760:ASN:OD1	2:B:761:LYS:N	2.50	0.45
2:B:790:SER:C	2:B:792:LEU:H	2.22	0.45
1:A:422:GLU:OE2	15:T:14:DG:OP1	2.34	0.45
1:A:619:LEU:HD23	1:A:626:PRO:HA	1.99	0.45
1:A:869:VAL:HG21	1:A:918:GLN:NE2	2.20	0.45
1:A:1348:LYS:NZ	1:A:1509:HIS:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LEU:HD22	2:B:561:VAL:HG22	1.99	0.45
2:B:496:PHE:C	2:B:497:LEU:HD12	2.41	0.45
2:B:808:ASP:O	2:B:809:ASP:HB2	2.15	0.45
5:F:55:PRO:O	5:F:123:LEU:HD12	2.16	0.45
15:T:21:DA:H2'	15:T:22:DG:H8	1.81	0.45
1:A:1269:LEU:HD22	1:A:1269:LEU:HA	1.81	0.45
1:A:1275:LEU:O	1:A:1278:VAL:HG12	2.15	0.45
2:B:140:MET:HE2	2:B:168:GLY:HA2	1.98	0.45
2:B:143:SER:O	2:B:144:LYS:HB2	2.17	0.45
2:B:184:MET:HB3	2:B:185:PRO:HD2	1.98	0.45
2:B:269:ILE:HG22	2:B:273:GLU:HA	1.98	0.45
3:C:236:LEU:HB2	3:C:305:HIS:HD2	1.82	0.45
7:I:65:GLY:O	7:I:66:THR:C	2.59	0.45
10:L:37:ARG:O	10:L:38:GLU:HB3	2.15	0.45
11:N:38:PRO:O	13:M:94:LYS:NZ	2.47	0.45
1:A:105:LEU:HD12	1:A:264:HIS:CE1	2.52	0.45
1:A:140:ARG:NH1	1:A:144:ARG:HH12	2.09	0.45
1:A:518:VAL:HG22	1:A:518:VAL:O	2.17	0.45
1:A:678:PRO:HB2	6:H:47:ILE:CG2	2.47	0.45
1:A:1531:LEU:CB	1:A:1535:LYS:HD3	2.47	0.45
2:B:238:PHE:CE1	2:B:327:LEU:HD11	2.51	0.45
2:B:698:PHE:HE2	2:B:701:LEU:HD23	1.80	0.45
3:C:193:VAL:HG11	3:C:314:GLY:HA3	1.99	0.45
13:M:39:MET:HG2	13:M:64:THR:HG22	1.99	0.45
6:H:63:THR:HG22	6:H:71:ASP:OD1	2.17	0.45
9:K:22:GLU:HG2	9:K:25:THR:CB	2.46	0.45
1:A:387:LEU:HD12	1:A:390:ILE:HD11	1.97	0.45
1:A:1512:ILE:HG22	1:A:1513:ASP:N	2.31	0.45
2:B:689:CYS:O	2:B:693:LYS:HD3	2.17	0.45
2:B:781:LEU:HD22	2:B:792:LEU:CB	2.37	0.45
7:I:40:ARG:HG3	7:I:40:ARG:O	2.16	0.45
13:M:67:LEU:HD11	13:M:69:TYR:CE1	2.52	0.45
16:U:9:DT:H2''	16:U:10:DG:N7	2.31	0.45
1:A:174:LEU:HG	1:A:174:LEU:O	2.17	0.45
1:A:472:VAL:CG2	1:A:477:VAL:HG23	2.47	0.45
1:A:727:PHE:CD2	1:A:729:PRO:HA	2.52	0.45
2:B:239:ILE:HB	2:B:244:LEU:HD23	1.99	0.45
2:B:818:LYS:HG2	2:B:848:VAL:HG12	1.99	0.45
3:C:241:LEU:HD23	3:C:297:VAL:CG2	2.47	0.45
4:E:13:ILE:CD1	4:E:132:GLN:HG3	2.47	0.45
8:J:24:LEU:O	8:J:29:TYR:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:81:ARG:HB3	11:N:118:LEU:HG	1.98	0.45
1:A:95:LYS:HD3	1:A:95:LYS:HA	1.74	0.44
1:A:1128:ASP:CB	1:A:1133:ARG:HD3	2.46	0.44
2:B:149:ARG:O	2:B:150:ASN:HB2	2.17	0.44
2:B:400:PHE:HA	2:B:418:ARG:NH1	2.30	0.44
3:C:186:PRO:CG	3:C:189:THR:OG1	2.63	0.44
1:A:87:VAL:HB	1:A:395:GLN:OE1	2.18	0.44
1:A:433:MET:HB3	2:B:1039:GLU:HG2	1.98	0.44
1:A:544:ASN:HA	1:A:566:ALA:O	2.17	0.44
1:A:716:TRP:CZ2	1:A:748:VAL:HG11	2.53	0.44
1:A:881:MET:HE3	1:A:881:MET:HB3	1.63	0.44
1:A:1589:PHE:HA	1:A:1597:LEU:CD1	2.47	0.44
2:B:205:TYR:CD1	2:B:229:LEU:HD22	2.52	0.44
6:H:14:ASP:HB3	6:H:17:PRO:HG3	1.99	0.44
6:H:40:ILE:O	6:H:123:MET:HA	2.17	0.44
6:H:92:MET:HE2	6:H:121:LEU:HD12	1.98	0.44
1:A:715:ALA:HB2	1:A:899:GLN:NE2	2.33	0.44
1:A:1037:PHE:N	1:A:1038:PRO:CD	2.81	0.44
2:B:98:VAL:O	2:B:110:TYR:HE1	2.00	0.44
2:B:186:ARG:O	2:B:213:HIS:HB3	2.18	0.44
2:B:526:TYR:O	2:B:527:THR:HG22	2.17	0.44
2:B:853:LYS:HE2	10:L:45:TYR:HE2	1.82	0.44
3:C:142:LEU:HD21	3:C:168:VAL:HG11	1.99	0.44
3:C:149:ASN:OD1	3:C:161:GLU:HA	2.17	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:HE2	1.99	0.44
13:M:69:TYR:HA	13:M:110:GLN:O	2.18	0.44
1:A:464:THR:O	1:A:464:THR:CG2	2.66	0.44
2:B:5:SER:O	2:B:6:ARG:HB3	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
2:B:655:VAL:HG12	2:B:656:THR:N	2.32	0.44
2:B:743:VAL:HG21	2:B:997:VAL:CG2	2.47	0.44
4:E:168:ASN:HA	4:E:172:ARG:HH12	1.82	0.44
1:A:121:LEU:HD23	1:A:121:LEU:C	2.43	0.44
1:A:268:LEU:HD23	1:A:268:LEU:O	2.16	0.44
1:A:422:GLU:HG2	1:A:1677:SER:HB3	1.99	0.44
1:A:1628:VAL:O	1:A:1631:VAL:HG22	2.17	0.44
2:B:116:ALA:H	2:B:134:LEU:HD23	1.82	0.44
2:B:432:TYR:CE1	15:T:25:DA:C5'	2.95	0.44
2:B:651:VAL:HG22	2:B:656:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:9:THR:HG22	7:I:15:SER:OG	2.17	0.44
1:A:29:SER:HB3	1:A:80:HIS:HD2	1.81	0.44
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.47	0.44
1:A:1598:ARG:O	1:A:1599:ARG:HB2	2.17	0.44
2:B:106:ARG:HG3	10:L:43:ILE:HD11	1.98	0.44
2:B:811:GLY:O	2:B:812:LEU:HD23	2.18	0.44
3:C:75:ALA:O	3:C:79:ILE:HG12	2.18	0.44
4:E:87:ILE:HD11	4:E:110:MET:CE	2.48	0.44
15:T:21:DA:H2''	15:T:22:DG:H5'	1.99	0.44
1:A:766:TYR:CD1	1:A:771:GLY:HA2	2.52	0.44
1:A:854:ASP:O	1:A:855:GLN:HB2	2.17	0.44
1:A:921:LEU:HA	1:A:973:GLU:OE1	2.17	0.44
1:A:1003:TYR:CE2	1:A:1712:LEU:HD23	2.52	0.44
1:A:1530:LYS:C	1:A:1531:LEU:HD12	2.43	0.44
2:B:206:THR:OG1	2:B:228:TYR:O	2.34	0.44
2:B:647:PHE:CE1	2:B:663:PRO:HB3	2.53	0.44
2:B:782:SER:HA	2:B:792:LEU:HD13	2.00	0.44
3:C:30:PRO:HG3	9:K:61:LYS:HA	1.99	0.44
3:C:241:LEU:HD21	3:C:253:LEU:HD21	1.99	0.44
4:E:82:VAL:HG13	4:E:86:THR:HB	1.99	0.44
1:A:26:LYS:O	1:A:27:LYS:HB2	2.18	0.44
1:A:186:GLU:HB2	1:A:1664:SER:HB2	2.00	0.44
1:A:555:THR:HG23	2:B:1041:GLU:OE2	2.17	0.44
1:A:745:LEU:HD21	6:H:95:LYS:HD3	1.99	0.44
1:A:1006:THR:HG22	1:A:1017:PHE:HA	2.00	0.44
2:B:92:ILE:HG21	10:L:42:ARG:NH1	2.32	0.44
2:B:337:LYS:HB2	2:B:337:LYS:HE2	1.66	0.44
2:B:1132:LEU:HD12	2:B:1132:LEU:O	2.18	0.44
4:E:168:ASN:HA	4:E:172:ARG:HH22	1.83	0.44
13:M:11:TRP:CZ2	13:M:101:VAL:HG11	2.53	0.44
1:A:865:PHE:CZ	1:A:945:PRO:HA	2.53	0.44
1:A:1113:ARG:O	1:A:1114:SER:HB2	2.17	0.44
1:A:1318:ARG:HB2	1:A:1526:GLN:HB3	1.99	0.44
1:A:1583:ILE:CD1	1:A:1604:ASP:HB2	2.48	0.44
2:B:525:VAL:HG21	2:B:590:PRO:HG3	2.00	0.44
2:B:767:GLY:HA2	2:B:770:HIS:CE1	2.53	0.44
2:B:796:ILE:HD11	2:B:807:LEU:CB	2.41	0.44
2:B:804:LEU:HG	2:B:805:GLN:OE1	2.18	0.44
6:H:118:TYR:OH	6:H:143:LEU:HB2	2.18	0.44
9:K:89:THR:HG23	9:K:90:LEU:H	1.81	0.44
16:U:9:DT:H2''	16:U:10:DG:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:O	1:A:96:LEU:HB3	2.18	0.43
1:A:100:LEU:HD21	1:A:265:LEU:CD2	2.48	0.43
1:A:472:VAL:O	1:A:535:THR:HG21	2.18	0.43
2:B:688:GLN:OE1	2:B:688:GLN:HA	2.18	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
7:I:13:PHE:CD1	7:I:20:CYS:HB3	2.46	0.43
11:N:30:PHE:O	11:N:96:ALA:HB1	2.18	0.43
11:N:84:SER:OG	11:N:115:LEU:CD2	2.66	0.43
1:A:56:GLY:HA2	1:A:64:CYS:HB3	2.00	0.43
1:A:1639:ARG:HE	4:E:199:THR:HG21	1.83	0.43
4:E:143:GLU:HG3	4:E:144:LEU:HG	2.00	0.43
1:A:316:GLY:HA3	15:T:25:DA:C2'	2.48	0.43
1:A:425:GLU:HG3	1:A:426:GLY:N	2.24	0.43
1:A:459:PRO:HB2	1:A:572:GLU:C	2.43	0.43
1:A:598:PHE:O	1:A:600:GLN:HG2	2.18	0.43
1:A:801:ASP:HB3	1:A:887:ARG:HD2	2.00	0.43
1:A:846:TRP:NE1	1:A:858:PHE:HE1	2.13	0.43
1:A:1018:LEU:HD12	1:A:1018:LEU:HA	1.80	0.43
1:A:1631:VAL:HG23	1:A:1632:TYR:CE2	2.53	0.43
2:B:18:HIS:HE1	2:B:723:ARG:HH22	1.66	0.43
2:B:55:GLY:O	2:B:59:GLN:HG2	2.18	0.43
2:B:109:THR:HA	2:B:171:ILE:O	2.18	0.43
2:B:172:ILE:O	2:B:173:ASN:HB2	2.17	0.43
2:B:1027:GLY:H	2:B:1033:GLY:HA2	1.83	0.43
6:H:56:PHE:HE1	6:H:58:LEU:HD12	1.83	0.43
10:L:15:MET:HA	10:L:15:MET:HE3	2.00	0.43
1:A:131:ALA:HB2	1:A:172:ASN:HD22	1.83	0.43
1:A:431:HIS:O	2:B:1115:VAL:HG11	2.19	0.43
1:A:595:ASN:HB3	2:B:1035:ILE:HD12	2.00	0.43
1:A:811:LYS:O	1:A:815:ILE:HG13	2.18	0.43
1:A:866:LYS:O	1:A:869:VAL:HG22	2.19	0.43
1:A:1045:GLU:H	1:A:1045:GLU:HG2	1.37	0.43
1:A:1348:LYS:O	1:A:1352:GLU:HG3	2.18	0.43
1:A:1605:ILE:HG21	1:A:1621:ILE:HG13	1.98	0.43
2:B:240:TYR:HB2	2:B:331:CYS:SG	2.57	0.43
2:B:797:LYS:HB3	2:B:797:LYS:HE2	1.81	0.43
2:B:987:GLU:OE1	3:C:301:ARG:NH2	2.52	0.43
7:I:14:GLN:O	7:I:15:SER:CB	2.65	0.43
1:A:64:CYS:SG	1:A:67:CYS:O	2.75	0.43
1:A:833:LEU:HD13	1:A:834:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:LEU:HB3	1:A:1535:LYS:HD3	1.99	0.43
2:B:156:LEU:HG	2:B:161:GLU:HB2	2.00	0.43
11:N:39:ASP:HA	13:M:94:LYS:HE3	1.99	0.43
1:A:30:VAL:CG1	1:A:66:THR:HG21	2.48	0.43
1:A:332:MET:HB3	1:A:332:MET:HE2	1.68	0.43
1:A:460:MET:HE3	1:A:460:MET:HB3	1.91	0.43
1:A:754:TYR:CE1	1:A:781:LEU:HD22	2.54	0.43
1:A:1053:LEU:HA	1:A:1053:LEU:HD23	1.87	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:1300:GLN:NE2	7:I:48:ARG:HD3	2.34	0.43
1:A:1655:LYS:HB3	1:A:1655:LYS:HE3	1.69	0.43
7:I:18:ASP:HB3	13:M:30:ASN:HD21	1.84	0.43
1:A:205:CYS:HB3	1:A:208:CYS:O	2.18	0.43
1:A:472:VAL:HG12	1:A:536:LYS:O	2.19	0.43
1:A:860:MET:HE2	1:A:864:LYS:CE	2.38	0.43
2:B:248:PRO:HB2	2:B:251:PHE:HD2	1.82	0.43
2:B:704:GLN:HG3	2:B:704:GLN:O	2.18	0.43
3:C:30:PRO:HB3	3:C:38:ASP:O	2.19	0.43
3:C:100:ILE:HG13	8:J:60:LEU:HD23	2.00	0.43
4:E:43:GLN:O	4:E:44:SER:HB3	2.18	0.43
1:A:40:ASP:HB2	1:A:44:ASN:O	2.19	0.43
1:A:217:LYS:HD2	1:A:218:GLU:O	2.19	0.43
1:A:1300:GLN:HE22	7:I:48:ARG:HD3	1.83	0.43
2:B:32:LYS:O	2:B:33:ALA:HB3	2.19	0.43
2:B:753:MET:HA	2:B:916:ASN:ND2	2.34	0.43
2:B:828:TYR:CD1	2:B:828:TYR:N	2.86	0.43
3:C:26:THR:OG1	3:C:303:ARG:NE	2.45	0.43
3:C:246:GLU:HG2	3:C:272:VAL:HA	2.01	0.43
11:N:146:ARG:NH1	11:N:148:ARG:NH2	2.63	0.43
1:A:218:GLU:HG2	1:A:219:HIS:H	1.82	0.43
1:A:963:GLU:H	1:A:963:GLU:HG2	1.39	0.43
1:A:1114:SER:HB3	1:A:1117:THR:H	1.84	0.43
2:B:295:SER:HB3	7:I:34:ASP:OD2	2.19	0.43
2:B:1084:PRO:HD3	2:B:1094:ARG:NH2	2.33	0.43
7:I:7:ALA:CB	13:M:34:GLN:H	2.30	0.43
10:L:37:ARG:C	10:L:39:CYS:H	2.25	0.43
1:A:459:PRO:O	1:A:461:VAL:N	2.52	0.43
1:A:743:GLU:CD	6:H:140:ARG:HH22	2.27	0.43
1:A:1129:GLU:OE1	1:A:1132:ARG:CB	2.67	0.43
1:A:1268:VAL:HG23	1:A:1576:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:TYR:O	1:A:1526:GLN:NE2	2.52	0.43
1:A:1523:LEU:HD12	1:A:1524:TRP:HB2	2.01	0.43
1:A:1531:LEU:O	1:A:1535:LYS:HD3	2.19	0.43
2:B:18:HIS:O	2:B:21:ASP:HB2	2.19	0.43
2:B:171:ILE:CG2	2:B:174:GLY:HA2	2.47	0.43
2:B:290:MET:HA	2:B:290:MET:HE2	2.00	0.43
2:B:430:PHE:O	2:B:434:PHE:HD1	2.02	0.43
2:B:804:LEU:N	2:B:804:LEU:HD23	2.34	0.43
2:B:863:LYS:O	2:B:865:LYS:HG2	2.19	0.43
4:E:56:THR:O	4:E:56:THR:HG22	2.18	0.43
2:B:167:GLY:O	2:B:169:TYR:HD2	2.02	0.42
2:B:214:CYS:O	2:B:221:ALA:HA	2.19	0.42
2:B:519:GLU:HG3	2:B:620:VAL:HG23	2.01	0.42
2:B:918:HIS:C	2:B:921:PRO:HD2	2.43	0.42
4:E:73:PHE:HB2	4:E:99:ILE:HD13	2.00	0.42
4:E:169:GLN:O	4:E:169:GLN:CG	2.67	0.42
6:H:107:GLU:HG3	6:H:108:ALA:N	2.34	0.42
15:T:9:DG:H2''	15:T:10:DG:C8	2.53	0.42
1:A:121:LEU:HD23	1:A:125:ARG:HG3	2.01	0.42
1:A:186:GLU:HG2	1:A:190:LYS:HE3	2.01	0.42
1:A:427:LEU:HG	1:A:427:LEU:O	2.19	0.42
1:A:1559:ILE:HG23	1:A:1580:THR:HG23	2.01	0.42
2:B:175:ILE:O	2:B:175:ILE:HG22	2.18	0.42
3:C:102:GLN:O	3:C:106:LEU:HB2	2.19	0.42
10:L:15:MET:HE3	10:L:15:MET:CA	2.49	0.42
11:N:61:VAL:HG21	13:M:11:TRP:HE3	1.84	0.42
1:A:225:ILE:CG2	1:A:256:LEU:HD11	2.49	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	2.49	0.42
1:A:1335:PRO:C	1:A:1338:ILE:HG22	2.45	0.42
2:B:69:LYS:HB3	2:B:69:LYS:HE2	1.57	0.42
2:B:115:THR:HG22	2:B:133:PHE:HA	1.99	0.42
2:B:269:ILE:HG22	2:B:269:ILE:O	2.19	0.42
2:B:388:LYS:HE3	2:B:429:PRO:HB3	2.01	0.42
2:B:920:PHE:N	2:B:921:PRO:CD	2.83	0.42
6:H:32:SER:HB3	6:H:37:MET:H	1.83	0.42
9:K:65:VAL:HA	9:K:86:THR:HA	2.00	0.42
1:A:316:GLY:CA	15:T:25:DA:H2''	2.49	0.42
1:A:703:LEU:HD23	1:A:703:LEU:H	1.84	0.42
1:A:806:PRO:C	1:A:808:ALA:H	2.26	0.42
1:A:1133:ARG:O	1:A:1133:ARG:CG	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:LEU:O	1:A:1246:PRO:HG2	2.19	0.42
1:A:1535:LYS:HD2	1:A:1535:LYS:N	2.33	0.42
1:A:1566:GLU:O	1:A:1576:LEU:HD22	2.19	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:210:VAL:HG21	2:B:349:MET:HB3	2.01	0.42
2:B:370:VAL:HG13	2:B:637:MET:HA	2.01	0.42
3:C:86:THR:HA	3:C:119:PRO:CG	2.49	0.42
5:F:53:THR:HG23	5:F:116:GLU:CD	2.45	0.42
6:H:37:MET:HE3	6:H:127:GLY:CA	2.45	0.42
1:A:406:MET:HE2	1:A:406:MET:HB2	1.81	0.42
1:A:454:ASN:HA	1:A:614:THR:HG21	2.00	0.42
1:A:659:ARG:HD3	1:A:787:ALA:HB1	2.01	0.42
1:A:1150:TRP:O	1:A:1151:ARG:C	2.62	0.42
1:A:1247:ARG:HG2	1:A:1628:VAL:CG2	2.49	0.42
1:A:1334:ARG:HG3	1:A:1335:PRO:CD	2.40	0.42
2:B:162:GLU:HB2	2:B:165:GLU:HB3	2.01	0.42
2:B:258:SER:HB3	2:B:297:GLN:OE1	2.19	0.42
4:E:159:LEU:CD2	4:E:160:LEU:HD23	2.45	0.42
1:A:61:LYS:HE3	1:A:61:LYS:HB2	1.86	0.42
1:A:543:LYS:O	1:A:543:LYS:CG	2.68	0.42
1:A:1715:LEU:HD23	1:A:1715:LEU:HA	1.84	0.42
2:B:282:VAL:HA	2:B:285:MET:HE3	2.00	0.42
2:B:284:GLN:O	2:B:288:ILE:HB	2.19	0.42
2:B:681:GLN:O	2:B:684:ARG:HB2	2.19	0.42
2:B:758:ILE:HD12	2:B:895:ARG:HB2	1.95	0.42
2:B:908:GLY:HA2	3:C:232:SER:OG	2.19	0.42
4:E:179:VAL:O	4:E:179:VAL:HG12	2.18	0.42
1:A:636:VAL:HG11	1:A:795:PHE:CE1	2.54	0.42
1:A:642:THR:HB	1:A:748:VAL:O	2.19	0.42
1:A:977:ASP:O	1:A:980:VAL:HG22	2.19	0.42
1:A:1078:LYS:HB2	1:A:1078:LYS:HE3	1.82	0.42
1:A:1324:HIS:HD2	1:A:1328:GLN:HG3	1.84	0.42
1:A:1672:MET:O	1:A:1677:SER:HB2	2.19	0.42
2:B:549:SER:C	2:B:551:SER:H	2.28	0.42
2:B:746:ILE:CG2	2:B:914:LEU:HD22	2.49	0.42
2:B:997:VAL:CG2	2:B:999:TYR:CE2	3.02	0.42
3:C:40:TRP:HZ2	9:K:106:VAL:CG2	2.33	0.42
4:E:6:GLU:O	4:E:10:LEU:HD13	2.19	0.42
4:E:103:LEU:HD21	4:E:130:PHE:CD2	2.55	0.42
4:E:122:ALA:C	4:E:124:LYS:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:83:THR:O	13:M:84:LEU:C	2.62	0.42
1:A:459:PRO:C	1:A:461:VAL:H	2.26	0.42
1:A:1111:ASN:ND2	4:E:61:LEU:HD23	2.34	0.42
1:A:1268:VAL:HG13	1:A:1595:LEU:HD23	2.01	0.42
1:A:1618:LEU:HD11	1:A:1649:CYS:CB	2.49	0.42
2:B:295:SER:O	7:I:19:PHE:CE1	2.72	0.42
2:B:489:LEU:O	2:B:489:LEU:HD23	2.20	0.42
3:C:236:LEU:HB2	3:C:305:HIS:CD2	2.55	0.42
3:C:263:GLU:CB	3:C:276:ALA:HB2	2.50	0.42
4:E:110:MET:SD	4:E:118:LEU:CD1	3.06	0.42
1:A:312:VAL:HG23	1:A:320:PHE:C	2.44	0.42
1:A:674:SER:HB2	6:H:118:TYR:O	2.20	0.42
1:A:965:PHE:O	1:A:969:MET:HG3	2.20	0.42
1:A:1268:VAL:O	1:A:1268:VAL:HG12	2.20	0.42
2:B:194:ILE:HD12	2:B:363:GLU:HB2	2.01	0.42
2:B:1097:ASN:OD1	2:B:1104:SER:HB2	2.20	0.42
3:C:50:ARG:HG3	3:C:66:VAL:HB	2.02	0.42
3:C:312:SER:HB3	3:C:321:LEU:HD11	2.01	0.42
6:H:105:SER:C	6:H:107:GLU:H	2.28	0.42
1:A:408:LYS:HD3	1:A:408:LYS:H	1.84	0.42
1:A:513:THR:HG23	1:A:514:GLN:N	2.34	0.42
1:A:896:MET:O	1:A:896:MET:CG	2.67	0.42
1:A:1086:ARG:HB2	1:A:1086:ARG:NH1	2.35	0.42
1:A:1092:TYR:CZ	1:A:1095:LYS:HD2	2.55	0.42
1:A:1615:GLU:OE2	4:E:207:ARG:NE	2.46	0.42
1:A:1648:MET:HE2	1:A:1654:TYR:CE1	2.55	0.42
2:B:104:ARG:NH2	2:B:169:TYR:OH	2.52	0.42
2:B:210:VAL:HG23	2:B:349:MET:HE2	2.02	0.42
2:B:720:PRO:O	2:B:723:ARG:HD3	2.19	0.42
4:E:85:LYS:HE2	4:E:85:LYS:HB3	1.87	0.42
9:K:45:HIS:O	9:K:46:GLU:HB2	2.19	0.42
11:N:56:PHE:HZ	11:N:80:TYR:HB2	1.83	0.42
1:A:602:GLU:O	1:A:602:GLU:HG3	2.19	0.41
1:A:711:ILE:HG13	1:A:750:ASP:OD2	2.19	0.41
1:A:860:MET:HE2	1:A:864:LYS:HG3	2.01	0.41
1:A:1266:VAL:HG12	1:A:1596:ASP:O	2.19	0.41
2:B:75:PHE:CD1	2:B:120:TRP:CB	3.03	0.41
2:B:403:LYS:CB	2:B:418:ARG:HH12	2.20	0.41
13:M:68:SER:HB2	13:M:112:LEU:HB2	2.02	0.41
14:R:-6:C:H2'	14:R:-5:U:H6	1.85	0.41
2:B:626:LEU:C	2:B:628:LEU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1003:ARG:O	2:B:1003:ARG:CD	2.64	0.41
3:C:336:PHE:CZ	9:K:44:LEU:HB3	2.55	0.41
1:A:88:TYR:H	1:A:395:GLN:NE2	2.18	0.41
1:A:433:MET:CB	2:B:1039:GLU:HG2	2.51	0.41
1:A:654:MET:HE3	9:K:60:MET:HE1	2.00	0.41
1:A:866:LYS:HA	1:A:869:VAL:CG2	2.49	0.41
1:A:999:LEU:HB2	1:A:1212:GLY:HA3	2.02	0.41
1:A:1280:SER:O	1:A:1284:GLN:HB2	2.19	0.41
1:A:1678:PHE:CE1	2:B:1126:MET:HE1	2.56	0.41
2:B:267:GLU:HA	2:B:270:LYS:HD3	2.02	0.41
2:B:668:SER:O	2:B:672:ASN:ND2	2.53	0.41
2:B:804:LEU:HD23	2:B:804:LEU:H	1.85	0.41
2:B:856:SER:CB	10:L:42:ARG:HB3	2.43	0.41
3:C:240:THR:O	3:C:240:THR:HG23	2.20	0.41
3:C:337:LEU:HD21	9:K:100:LEU:CB	2.49	0.41
4:E:10:LEU:HD21	4:E:58:LEU:HD11	2.02	0.41
5:F:110:LEU:HB3	5:F:111:PRO:HD2	2.01	0.41
1:A:78:LEU:HD12	1:A:306:PRO:HD3	2.01	0.41
1:A:408:LYS:HZ1	1:A:409:LEU:CD2	2.22	0.41
1:A:441:ALA:HB2	2:B:1012:VAL:HG13	2.03	0.41
1:A:1184:LYS:HE3	1:A:1184:LYS:HB3	1.83	0.41
1:A:1504:ALA:O	1:A:1508:ILE:HG13	2.21	0.41
1:A:1580:THR:CG2	1:A:1581:GLU:N	2.84	0.41
2:B:66:PHE:CZ	2:B:400:PHE:CD2	3.06	0.41
2:B:73:ILE:HG22	2:B:75:PHE:CZ	2.51	0.41
2:B:179:ILE:HD11	2:B:434:PHE:CE2	2.55	0.41
2:B:215:VAL:HA	2:B:220:SER:O	2.20	0.41
2:B:416:LEU:HD12	2:B:419:ILE:HD11	2.02	0.41
4:E:81:LYS:HB2	4:E:81:LYS:HE3	1.84	0.41
6:H:26:SER:HB3	6:H:45:ILE:HG21	2.02	0.41
6:H:39:LEU:HD12	6:H:125:LEU:HD13	2.00	0.41
7:I:28:PRO:O	7:I:29:LEU:C	2.63	0.41
8:J:17:LYS:HE3	8:J:38:LEU:O	2.20	0.41
1:A:326:VAL:HG11	1:A:414:TYR:CE1	2.55	0.41
1:A:910:MET:C	1:A:912:ILE:H	2.28	0.41
1:A:1104:LYS:HD2	1:A:1104:LYS:O	2.20	0.41
1:A:1200:TRP:CD1	1:A:1200:TRP:C	2.98	0.41
1:A:1570:ASN:OD1	1:A:1571:LYS:N	2.53	0.41
2:B:35:LEU:HD13	2:B:730:TYR:HD2	1.86	0.41
2:B:185:PRO:O	2:B:186:ARG:HB2	2.21	0.41
2:B:791:SER:HB3	2:B:792:LEU:CD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:TRP:HB2	9:K:61:LYS:HB3	2.02	0.41
3:C:312:SER:HB3	3:C:321:LEU:HD12	2.02	0.41
4:E:73:PHE:HD2	4:E:75:PHE:CZ	2.38	0.41
1:A:661:LEU:HG	1:A:691:LEU:CD1	2.51	0.41
1:A:754:TYR:HE1	1:A:781:LEU:HD22	1.85	0.41
1:A:826:ALA:HB2	1:A:868:GLU:HG3	2.02	0.41
1:A:896:MET:O	1:A:896:MET:HG3	2.19	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
2:B:521:VAL:O	2:B:616:PRO:O	2.38	0.41
2:B:621:ARG:HA	2:B:622:PRO:HD3	1.93	0.41
2:B:804:LEU:HG	2:B:805:GLN:N	2.36	0.41
2:B:1026:ILE:HG21	2:B:1031:VAL:HG11	2.02	0.41
3:C:267:VAL:HG11	3:C:272:VAL:HG11	2.01	0.41
9:K:60:MET:SD	9:K:68:CYS:HB3	2.60	0.41
15:T:14:DG:H2'	15:T:15:DC:C6	2.56	0.41
1:A:585:TYR:O	1:A:586:ASN:HB3	2.21	0.41
1:A:939:GLU:HG2	1:A:940:PRO:N	2.34	0.41
1:A:972:ARG:HD2	2:B:502:THR:HG21	2.02	0.41
1:A:1025:ASP:OD1	1:A:1025:ASP:N	2.51	0.41
2:B:1065:SER:HB2	2:B:1117:ARG:NH2	2.36	0.41
3:C:89:VAL:HG22	3:C:214:CYS:SG	2.61	0.41
3:C:203:ARG:O	3:C:204:PRO:C	2.64	0.41
3:C:337:LEU:HD12	9:K:104:MET:HE3	2.02	0.41
9:K:92:ALA:C	9:K:95:PRO:HD2	2.46	0.41
14:R:-6:C:H2'	14:R:-5:U:C6	2.56	0.41
1:A:33:ILE:HD11	1:A:81:ILE:CG1	2.51	0.41
1:A:468:TYR:HB2	1:A:598:PHE:CE2	2.56	0.41
1:A:613:CYS:SG	1:A:614:THR:N	2.93	0.41
1:A:811:LYS:HA	1:A:814:ARG:HG2	2.03	0.41
1:A:1090:LEU:HD12	4:E:22:HIS:NE2	2.36	0.41
1:A:1348:LYS:HE3	1:A:1508:ILE:HB	2.02	0.41
2:B:86:THR:HG22	2:B:87:VAL:N	2.35	0.41
2:B:410:SER:C	2:B:411:MET:HE2	2.46	0.41
2:B:566:VAL:HG23	2:B:574:ILE:HD12	2.02	0.41
3:C:29:PHE:CE1	9:K:57:TYR:HE1	2.39	0.41
3:C:84:VAL:HA	3:C:85:PRO:HD3	1.94	0.41
4:E:67:ASP:O	4:E:70:ASP:N	2.53	0.41
1:A:436:ARG:O	2:B:1062:SER:HB3	2.21	0.41
1:A:558:ARG:HG2	2:B:1048:HIS:NE2	2.36	0.41
1:A:705:LEU:HD23	1:A:706:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:HIS:C	1:A:755:GLY:H	2.29	0.41
1:A:912:ILE:CG1	2:B:924:MET:HG2	2.50	0.41
1:A:1341:PHE:CE1	1:A:1345:ARG:HD2	2.56	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:131:LYS:HE3	2:B:131:LYS:HB2	1.78	0.41
2:B:247:LEU:HD11	2:B:304:LEU:HD21	2.02	0.41
2:B:820:GLN:O	2:B:823:ASP:HB2	2.21	0.41
2:B:1019:ASP:O	2:B:1023:ASN:N	2.50	0.41
7:I:53:LYS:HD3	7:I:53:LYS:HA	1.87	0.41
11:N:131:GLN:HB2	11:N:134:PRO:HB3	2.02	0.41
15:T:3:DG:H2''	15:T:4:DC:C6	2.56	0.41
1:A:417:ILE:HD12	2:B:1126:MET:HG3	2.02	0.41
1:A:850:HIS:HD2	1:A:941:TYR:OH	2.04	0.41
1:A:1318:ARG:HD2	1:A:1524:TRP:CE3	2.50	0.41
1:A:1639:ARG:HE	4:E:199:THR:CG2	2.34	0.41
2:B:700:LEU:HA	2:B:735:TYR:HE1	1.85	0.41
2:B:1069:VAL:HG21	2:B:1134:VAL:CG2	2.50	0.41
6:H:80:ASP:O	6:H:82:PRO:HD3	2.21	0.41
6:H:88:PHE:HA	6:H:146:LYS:HB2	2.03	0.41
8:J:63:ALA:HB1	8:J:64:PRO:HD2	2.03	0.41
11:N:61:VAL:N	13:M:9:ALA:O	2.54	0.41
13:M:67:LEU:HD12	13:M:68:SER:N	2.36	0.41
1:A:445:ILE:HD11	1:A:587:ALA:HB1	2.03	0.40
1:A:1000:VAL:HG12	1:A:1210:ALA:HA	2.03	0.40
1:A:1267:PRO:HG2	1:A:1596:ASP:HB3	2.03	0.40
2:B:333:CYS:SG	2:B:333:CYS:O	2.79	0.40
2:B:396:ILE:HA	2:B:422:MET:CB	2.51	0.40
2:B:786:LYS:O	2:B:788:GLY:N	2.52	0.40
2:B:1026:ILE:HD12	2:B:1026:ILE:HA	1.97	0.40
4:E:17:ILE:HG21	4:E:74:VAL:HG11	2.03	0.40
7:I:43:PHE:HE1	7:I:46:ASN:HA	1.84	0.40
9:K:93:VAL:O	9:K:93:VAL:HG12	2.21	0.40
11:N:49:ALA:HB2	13:M:84:LEU:O	2.21	0.40
14:R:-7:G:H2'	14:R:-6:C:H6	1.86	0.40
1:A:88:TYR:H	1:A:395:GLN:HE22	1.68	0.40
1:A:327:ASN:HB3	1:A:401:VAL:HG22	2.02	0.40
1:A:718:LYS:HE2	1:A:718:LYS:HB3	1.82	0.40
1:A:740:ARG:O	1:A:741:GLU:HB2	2.22	0.40
1:A:1104:LYS:HD3	1:A:1116:GLY:CA	2.52	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:1300:GLN:O	1:A:1315:TYR:HA	2.20	0.40
2:B:31:GLN:HG3	2:B:153:PRO:HG3	2.02	0.40
2:B:543:ASP:HB2	13:M:81:CYS:HB2	2.03	0.40
2:B:648:GLU:C	2:B:650:GLU:H	2.28	0.40
2:B:759:VAL:O	2:B:896:LEU:HA	2.21	0.40
2:B:1045:LEU:HD23	2:B:1054:LEU:HD13	2.03	0.40
3:C:135:ILE:H	3:C:135:ILE:HG12	1.48	0.40
3:C:245:VAL:O	3:C:246:GLU:HG3	2.21	0.40
11:N:70:LYS:HE2	11:N:79:ARG:NH1	2.36	0.40
1:A:293:ASN:O	1:A:296:VAL:HG23	2.22	0.40
1:A:436:ARG:NH1	15:T:19:DT:OP1	2.54	0.40
1:A:654:MET:SD	9:K:67:PHE:HA	2.61	0.40
1:A:680:PRO:HG2	3:C:31:GLY:O	2.22	0.40
1:A:915:LEU:CD1	1:A:952:THR:HA	2.51	0.40
1:A:1019:TYR:CE1	1:A:1211:VAL:HB	2.57	0.40
1:A:1136:GLN:HE21	1:A:1136:GLN:HB3	1.63	0.40
1:A:1557:LYS:O	1:A:1584:ASN:ND2	2.53	0.40
1:A:1583:ILE:HG23	1:A:1583:ILE:O	2.21	0.40
3:C:157:SER:O	3:C:161:GLU:HG3	2.21	0.40
9:K:22:GLU:CG	9:K:25:THR:H	2.25	0.40
1:A:26:LYS:HE3	1:A:301:PHE:CE2	2.56	0.40
1:A:32:SER:HB2	1:A:80:HIS:CE1	2.57	0.40
1:A:498:ILE:O	1:A:536:LYS:HG3	2.21	0.40
1:A:642:THR:CG2	1:A:744:LEU:HD21	2.52	0.40
1:A:1248:LEU:HD23	1:A:1248:LEU:HA	1.91	0.40
1:A:1357:LYS:NZ	1:A:1538:PHE:HE1	2.19	0.40
2:B:42:HIS:C	2:B:140:MET:HE1	2.46	0.40
2:B:89:LYS:O	2:B:89:LYS:HG3	2.22	0.40
2:B:364:ASP:OD1	2:B:606:LEU:HD22	2.21	0.40
2:B:853:LYS:HG2	10:L:45:TYR:CE2	2.56	0.40
2:B:937:SER:OG	2:B:965:MET:HB3	2.22	0.40
2:B:1068:HIS:CE1	2:B:1096:TYR:CE2	3.09	0.40
3:C:45:PHE:CZ	9:K:106:VAL:HG13	2.56	0.40
1:A:305:PRO:HG3	2:B:1125:ALA:HB2	2.02	0.40
1:A:448:ASP:O	1:A:449:MET:CB	2.69	0.40
1:A:737:VAL:HA	1:A:746:CYS:O	2.20	0.40
2:B:284:GLN:HG3	2:B:288:ILE:HG13	2.04	0.40
3:C:53:VAL:HA	3:C:63:PHE:CA	2.38	0.40
11:N:94:LEU:HD13	13:M:89:VAL:HG21	2.03	0.40
13:M:28:PHE:HB2	13:M:31:GLY:O	2.20	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	1455/1719 (85%)	1309 (90%)	137 (9%)	9 (1%)	21	48
2	B	1119/1135 (99%)	1019 (91%)	100 (9%)	0	100	100
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%)	71 (96%)	3 (4%)	0	100	100
6	H	144/150 (96%)	130 (90%)	14 (10%)	0	100	100
7	I	58/126 (46%)	41 (71%)	14 (24%)	3 (5%)	1	4
8	J	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
9	K	106/133 (80%)	96 (91%)	9 (8%)	1 (1%)	14	38
10	L	43/58 (74%)	37 (86%)	6 (14%)	0	100	100
11	N	149/510 (29%)	134 (90%)	13 (9%)	2 (1%)	9	29
12	G	153/338 (45%)	138 (90%)	14 (9%)	1 (1%)	18	45
13	M	108/419 (26%)	107 (99%)	1 (1%)	0	100	100
All	All	4001/5338 (75%)	3639 (91%)	346 (9%)	16 (0%)	31	58

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	1035	LYS
1	A	1605	ILE
7	I	21	SER
11	N	156	PRO
12	G	102	LEU
1	A	1024	LEU
7	I	19	PHE
11	N	132	PRO
1	A	677	LYS

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Mol	Chain	Res	Type
1	A	719	GLU
7	I	17	LEU
1	A	22	ALA
1	A	206	PRO
9	K	24	LYS
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	1295/1503 (86%)	1208 (93%)	87 (7%)	15 40
2	B	982/992 (99%)	907 (92%)	75 (8%)	12 35
3	C	296/302 (98%)	273 (92%)	23 (8%)	11 34
4	E	183/192 (95%)	180 (98%)	3 (2%)	55 82
5	F	66/111 (60%)	66 (100%)	0	100 100
6	H	129/131 (98%)	125 (97%)	4 (3%)	35 69
7	I	53/111 (48%)	49 (92%)	4 (8%)	12 35
8	J	53/56 (95%)	50 (94%)	3 (6%)	18 47
9	K	96/119 (81%)	94 (98%)	2 (2%)	47 78
10	L	42/55 (76%)	41 (98%)	1 (2%)	43 75
11	N	119/427 (28%)	113 (95%)	6 (5%)	22 53
12	G	135/288 (47%)	130 (96%)	5 (4%)	30 63
13	M	94/366 (26%)	90 (96%)	4 (4%)	26 58
All	All	3543/4653 (76%)	3326 (94%)	217 (6%)	19 44

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	16	SER

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Mol	Chain	Res	Type
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
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	396	SER
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	676	LEU
1	A	680	PRO
1	A	701	ILE
1	A	718	LYS

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Mol	Chain	Res	Type
1	A	833	LEU
1	A	878	LYS
1	A	885	LEU
1	A	888	GLN
1	A	891	GLU
1	A	963	GLU
1	A	973	GLU
1	A	978	THR
1	A	993	ILE
1	A	1010	SER
1	A	1011	ASP
1	A	1018	LEU
1	A	1024	LEU
1	A	1025	ASP
1	A	1027	PRO
1	A	1038	PRO
1	A	1045	GLU
1	A	1046	VAL
1	A	1048	MET
1	A	1051	GLN
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	1077	LEU
2	B	1081	LEU
2	B	1106	THR
3	C	21	VAL
3	C	54	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

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Mol	Chain	Res	Type
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
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	I	15	SER
7	I	17	LEU
7	I	27	LEU
7	I	29	LEU
8	J	5	VAL
8	J	9	THR
8	J	28	GLU
9	K	27	LEU
9	K	30	VAL
10	L	52	LEU
11	N	25	SER
11	N	60	HIS
11	N	116	ARG
11	N	118	LEU
11	N	130	LEU
11	N	133	ILE
12	G	95	ASN
12	G	97	LYS
12	G	98	VAL
12	G	102	LEU

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Mol	Chain	Res	Type
12	G	169	MET
13	M	67	LEU
13	M	81	CYS
13	M	110	GLN
13	M	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	89	ASN
1	A	106	ASN
1	A	108	HIS
1	A	133	GLN
1	A	163	GLN
1	A	170	GLN
1	A	324	GLN
1	A	347	GLN
1	A	395	GLN
1	A	397	HIS
1	A	431	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	595	ASN
1	A	597	HIS
1	A	600	GLN
1	A	616	GLN
1	A	617	GLN
1	A	632	GLN
1	A	652	HIS
1	A	753	HIS
1	A	790	GLN
1	A	832	ASN
1	A	847	GLN
1	A	850	HIS
1	A	859	ASN
1	A	918	GLN
1	A	1051	GLN

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Mol	Chain	Res	Type
1	A	1054	HIS
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	1295	GLN
1	A	1300	GLN
1	A	1313	GLN
1	A	1565	ASN
1	A	1579	ASN
1	A	1603	ASN
1	A	1683	GLN
1	A	1690	HIS
1	A	1717	GLN
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	547	HIS
2	B	639	GLN
2	B	672	ASN
2	B	690	GLN
2	B	694	GLN
2	B	709	ASN
2	B	846	ASN
2	B	887	HIS

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Mol	Chain	Res	Type
2	B	889	GLN
2	B	1011	GLN
2	B	1068	HIS
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	277	ASN
3	C	290	ASN
3	C	305	HIS
4	E	132	GLN
4	E	133	GLN
4	E	169	GLN
6	H	126	GLN
7	I	33	GLN
8	J	61	ASN
9	K	85	GLN
11	N	88	GLN
13	M	98	GLN
13	M	110	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	7/8 (87%)	3 (42%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	-6	C
14	R	-5	U
14	R	-4	G

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	20:CYS	C	21:SER	N	1.69

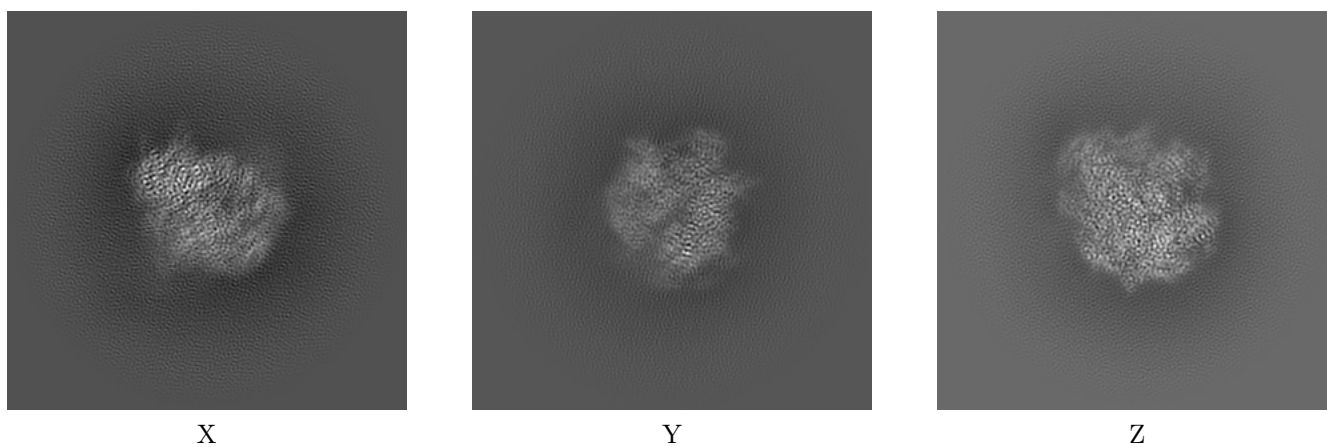
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31877. 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](#)

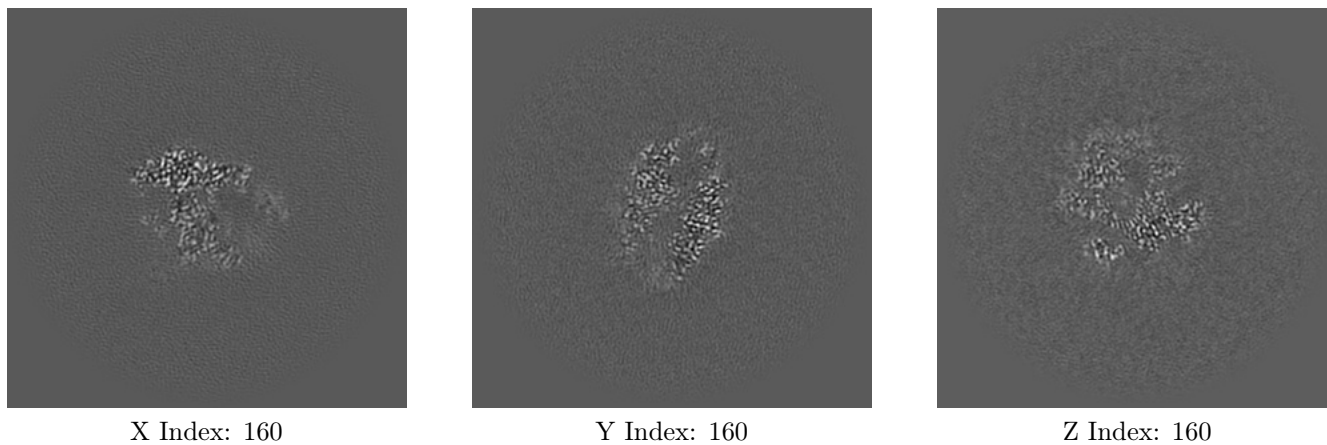
6.1.1 Primary map



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

6.2 Central slices [i](#)

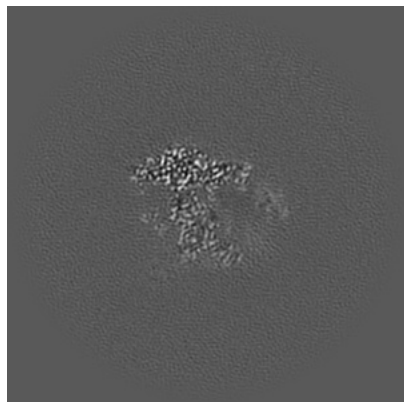
6.2.1 Primary map



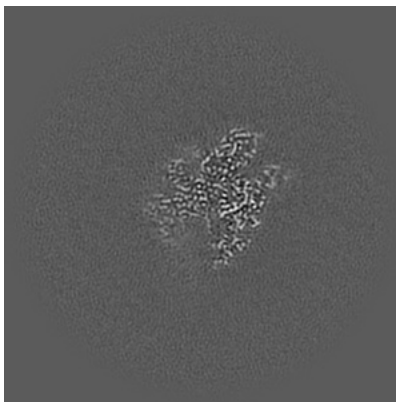
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

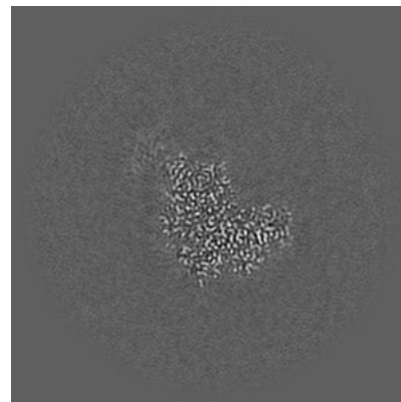
6.3.1 Primary map



X Index: 160



Y Index: 141

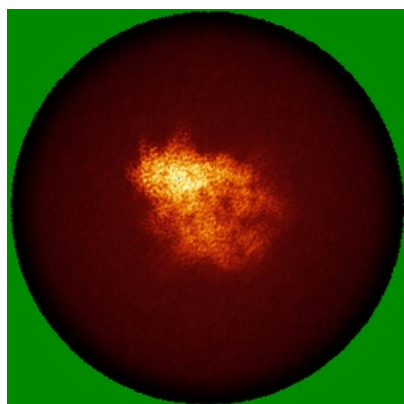


Z Index: 184

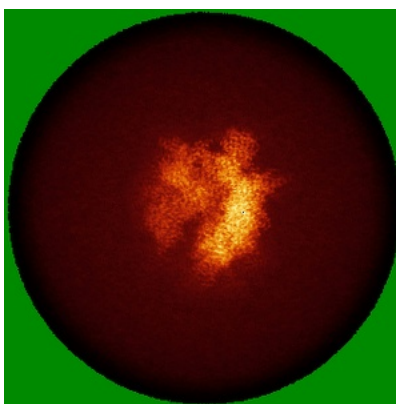
The images above show the largest variance slices of the map in three orthogonal directions.

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

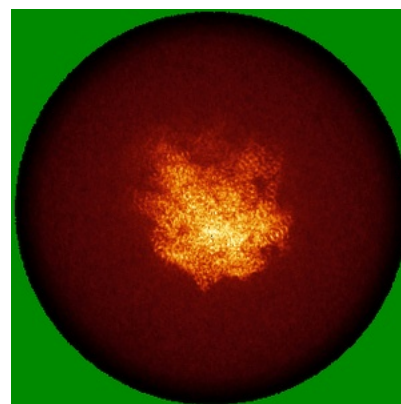
6.4.1 Primary map



X



Y

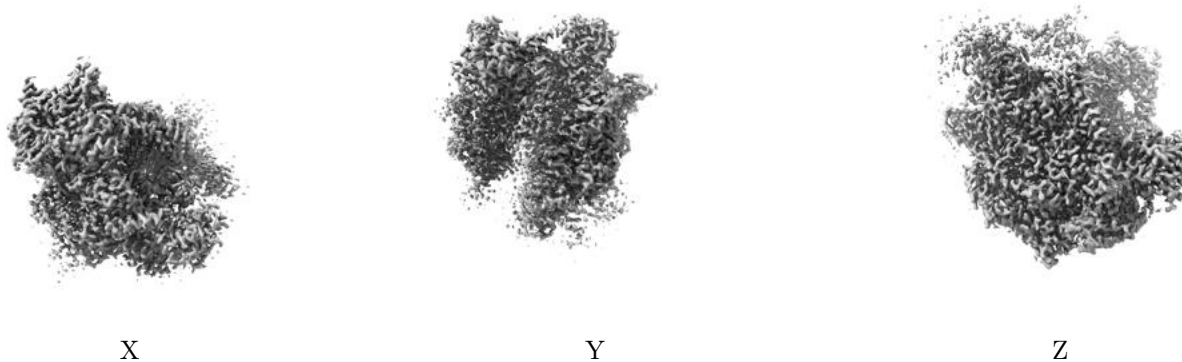


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.687. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

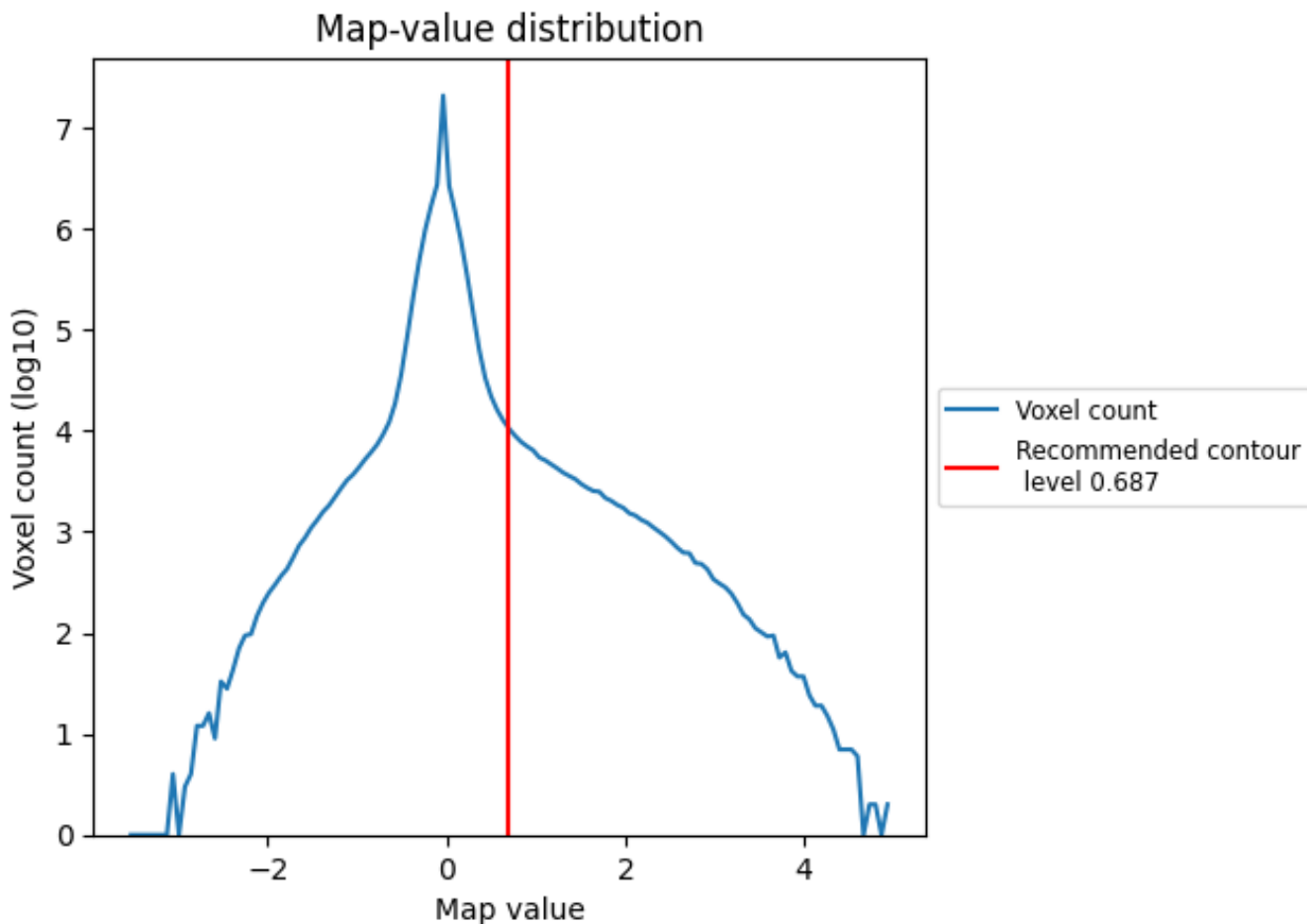
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

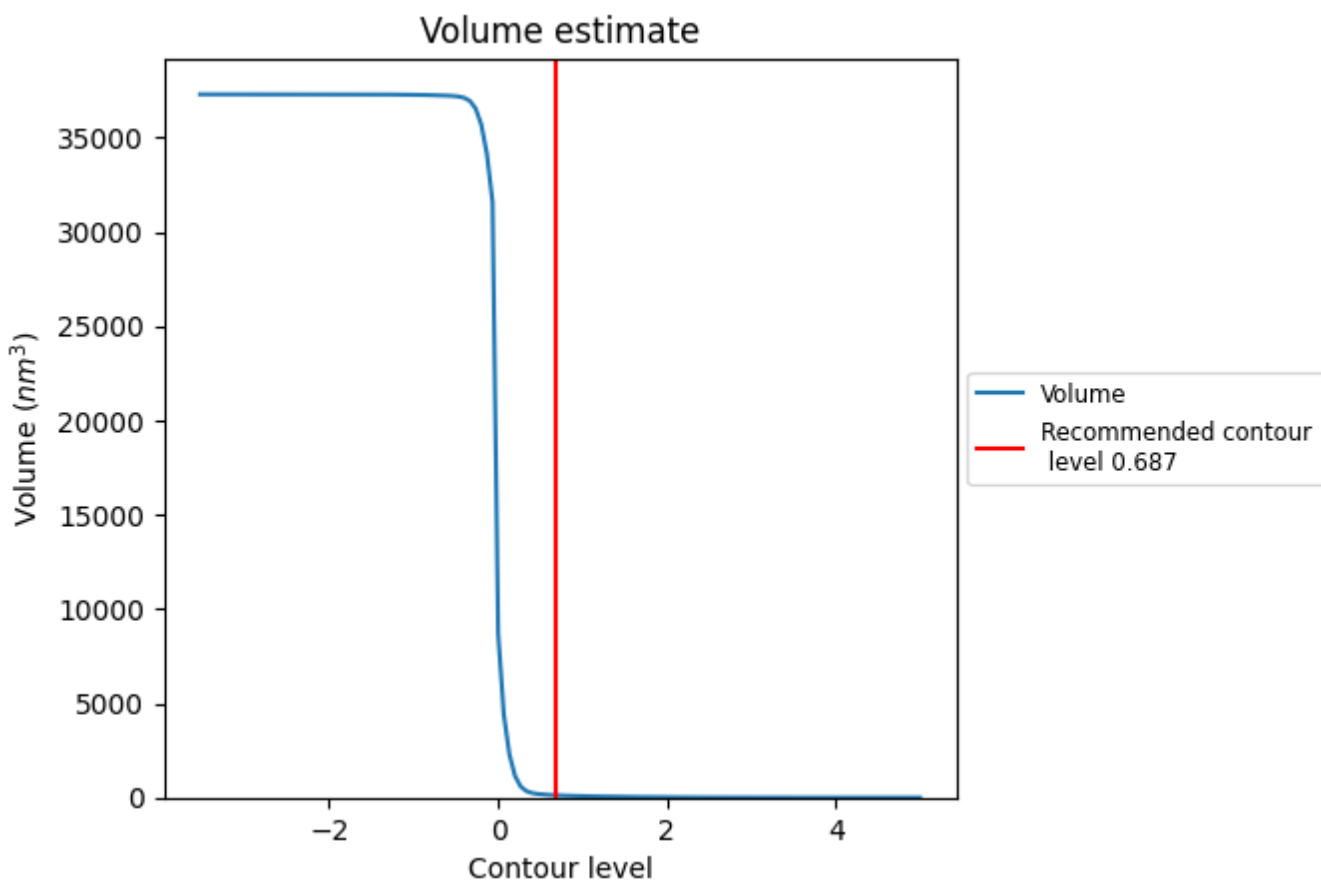
This section contains the results of statistical analysis of the map.

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.

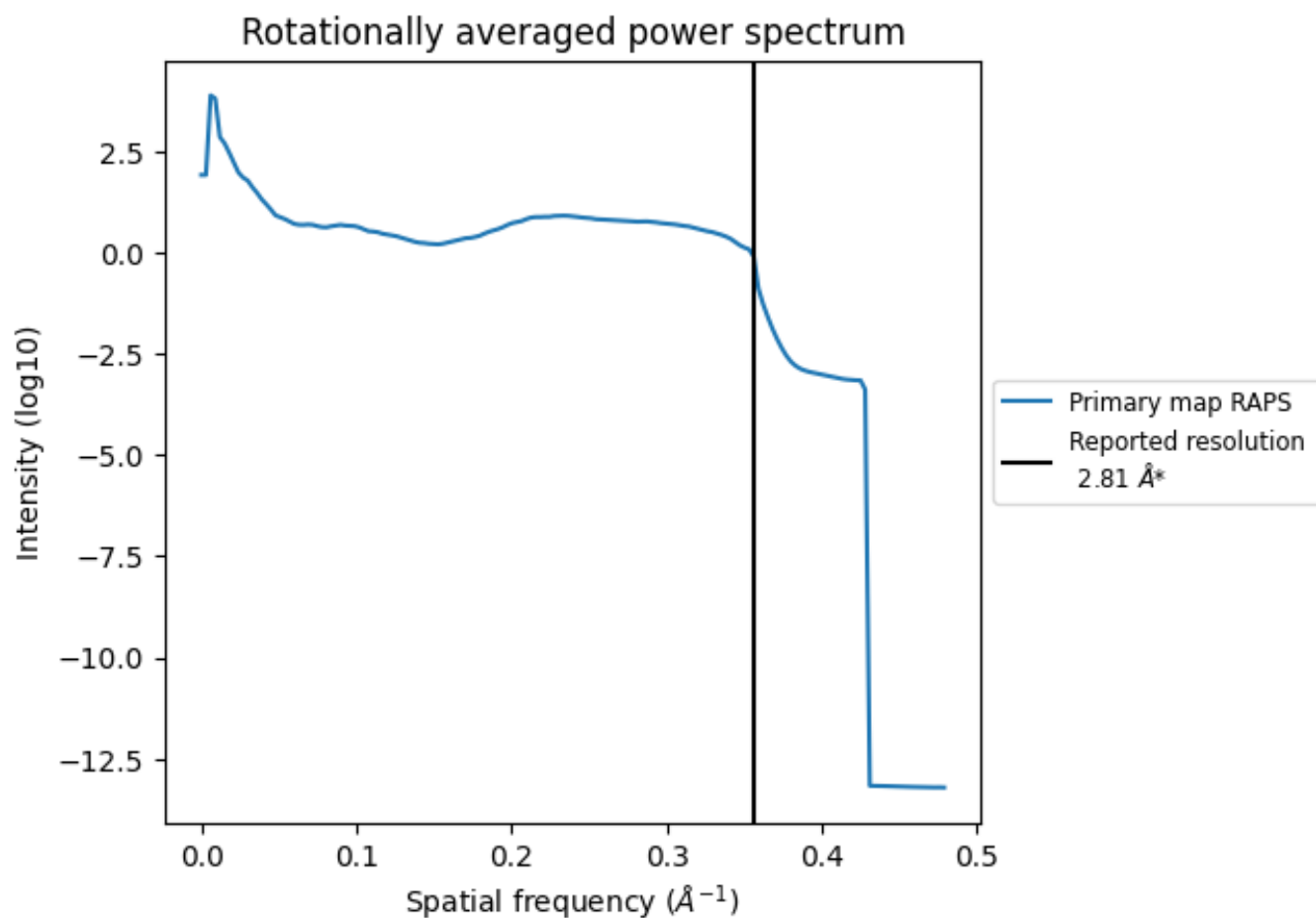
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm³; this corresponds to an approximate mass of 110 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 0.356 Å⁻¹

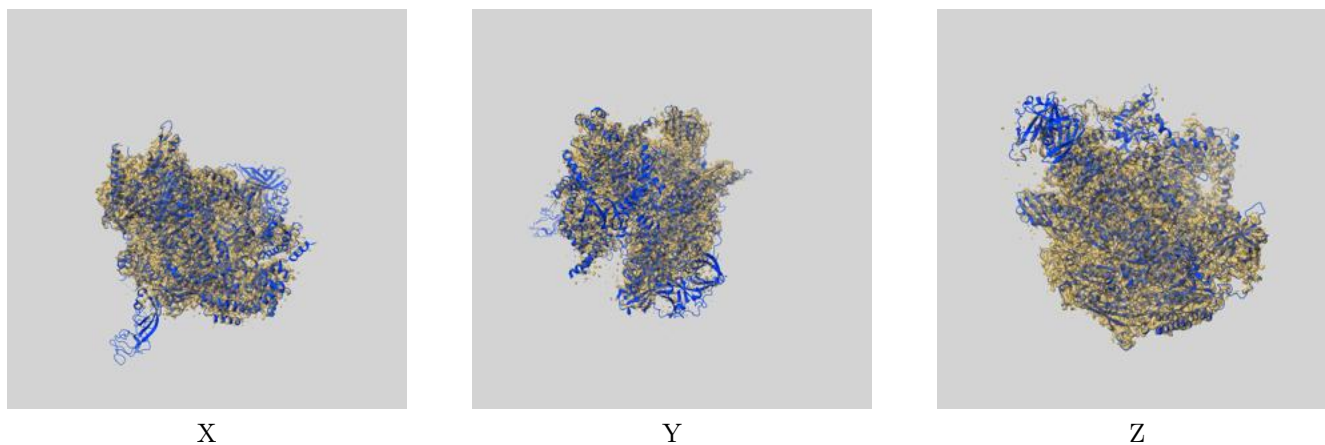
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

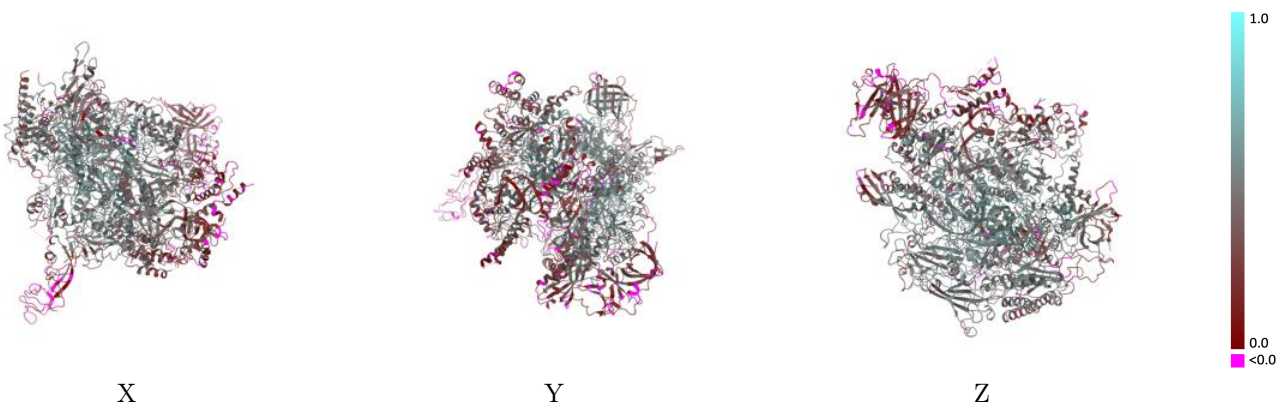
This section contains information regarding the fit between EMDB map EMD-31877 and PDB model 7VBB. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



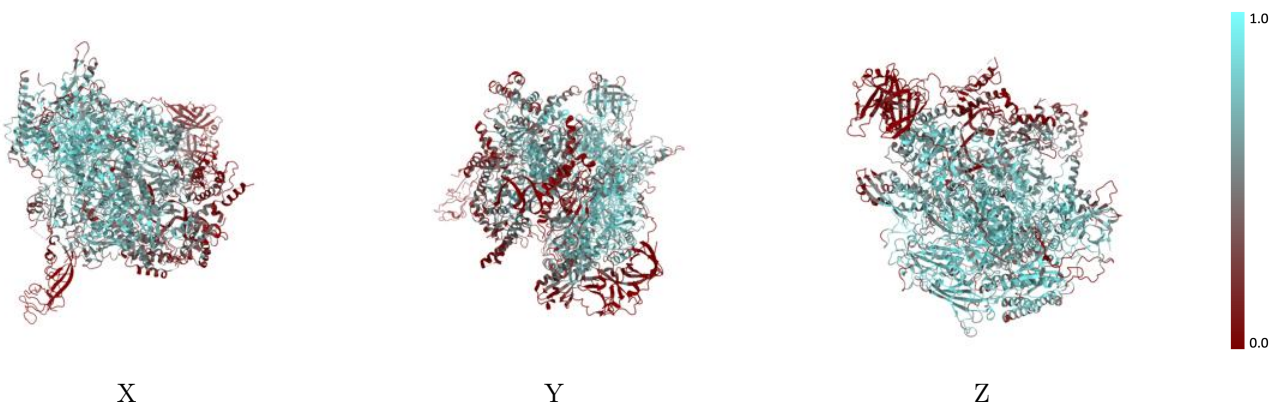
The images above show the 3D surface view of the map at the recommended contour level 0.687 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



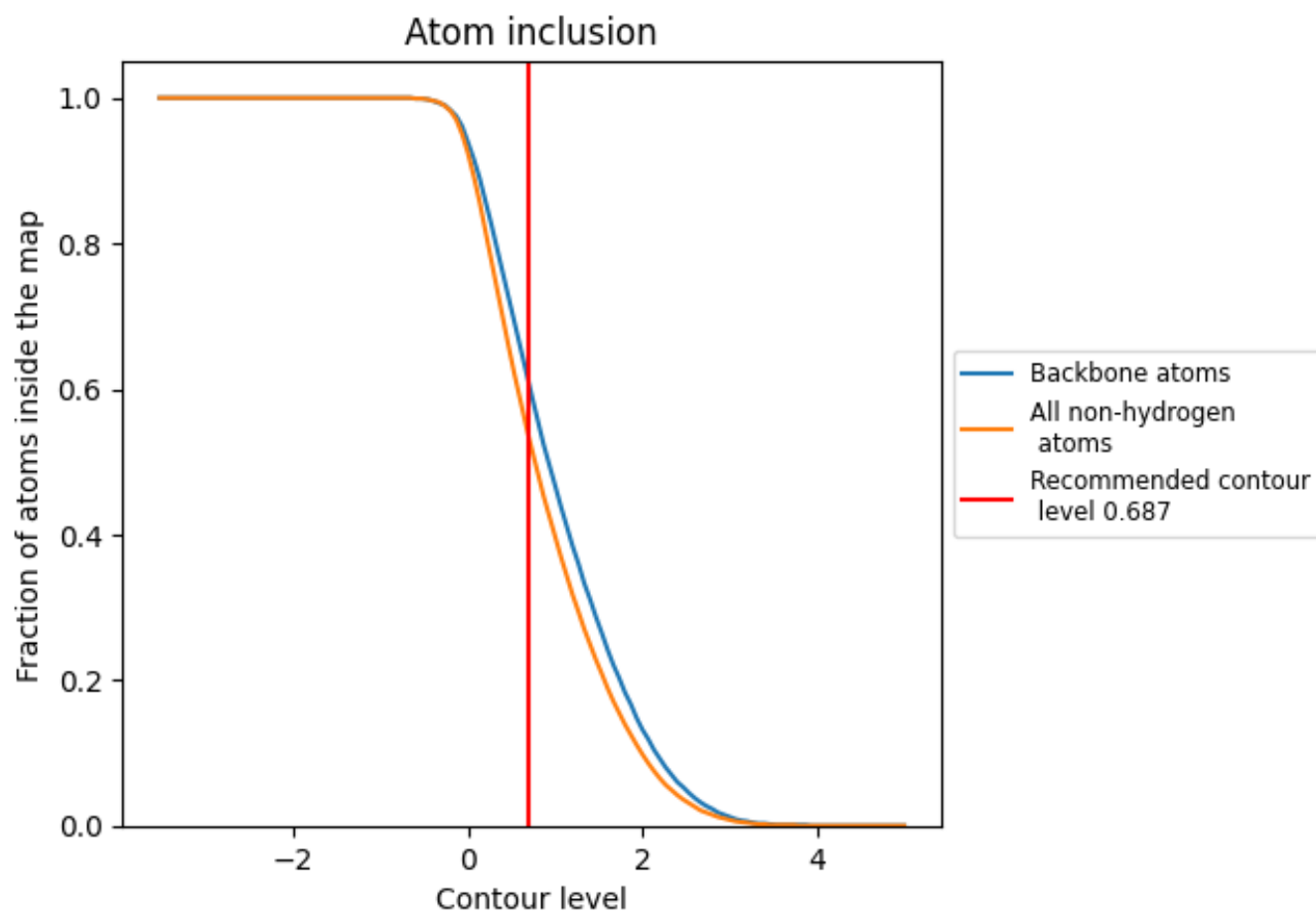
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.687).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 54% 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 (0.687) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5400	 0.4010
A	 0.5430	 0.4150
B	 0.6980	 0.4790
C	 0.6070	 0.4120
E	 0.5030	 0.3580
F	 0.5650	 0.4440
G	 0.0510	 0.1130
H	 0.5620	 0.3680
I	 0.1510	 0.1350
J	 0.8060	 0.5320
K	 0.6630	 0.4290
L	 0.7190	 0.4510
M	 0.0910	 0.1910
N	 0.0570	 0.1860
R	 0.6250	 0.5260
T	 0.3910	 0.3970
U	 0.0710	 0.2690

