



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:11 PM UTC

PDB ID : 8P4C / pdb_00008p4c
EMDB ID : EMD-17405
Title : Structural insights into human co-transcriptional capping - structure 3
Authors : Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on : 2023-05-20
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

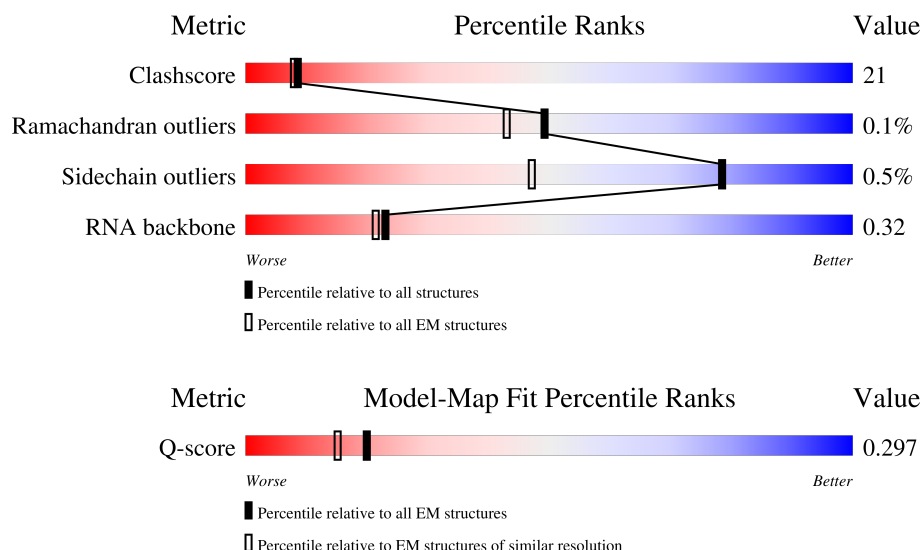
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	1970	
2	M	597	
3	N	32	

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Mol	Chain	Length	Quality of chain
4	T	41	
5	B	1174	
6	C	275	
7	E	210	
8	F	127	
9	H	150	
10	I	125	
11	J	67	
12	K	117	
13	L	58	
14	P	17	
15	D	142	
16	G	172	
17	Y	117	
18	Z	1087	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 41439 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1410	Total	C	N	O	S	0	0
			11166	7029	2001	2067	69		

- Molecule 2 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	493	Total	C	N	O	S	0	0
			3958	2524	687	718	29		

- Molecule 3 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	32	Total	C	N	O	P	0	0
			652	312	117	191	32		

- Molecule 4 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	41	Total	C	N	O	P	0	0
			847	403	155	248	41		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1132	Total	C	N	O	S	0	0
			9052	5725	1592	1671	64		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	263	Total	C	N	O	S	0	0
			2115	1324	365	420	6		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 13 is a protein called RNA polymerase II subunit K.

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

- Molecule 14 is a RNA chain called RNA (5'-R(P*CP*GP*GP*AP*GP*AP*GP*GP*GP*A

P*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	17	Total	C	N	O	P	0	0
			368	164	72	115	17		

- Molecule 15 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	458	Total	C	N	O	S	0	0
			3676	2342	651	667	16		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	Y	1	Total	Zn	0
			1	1	

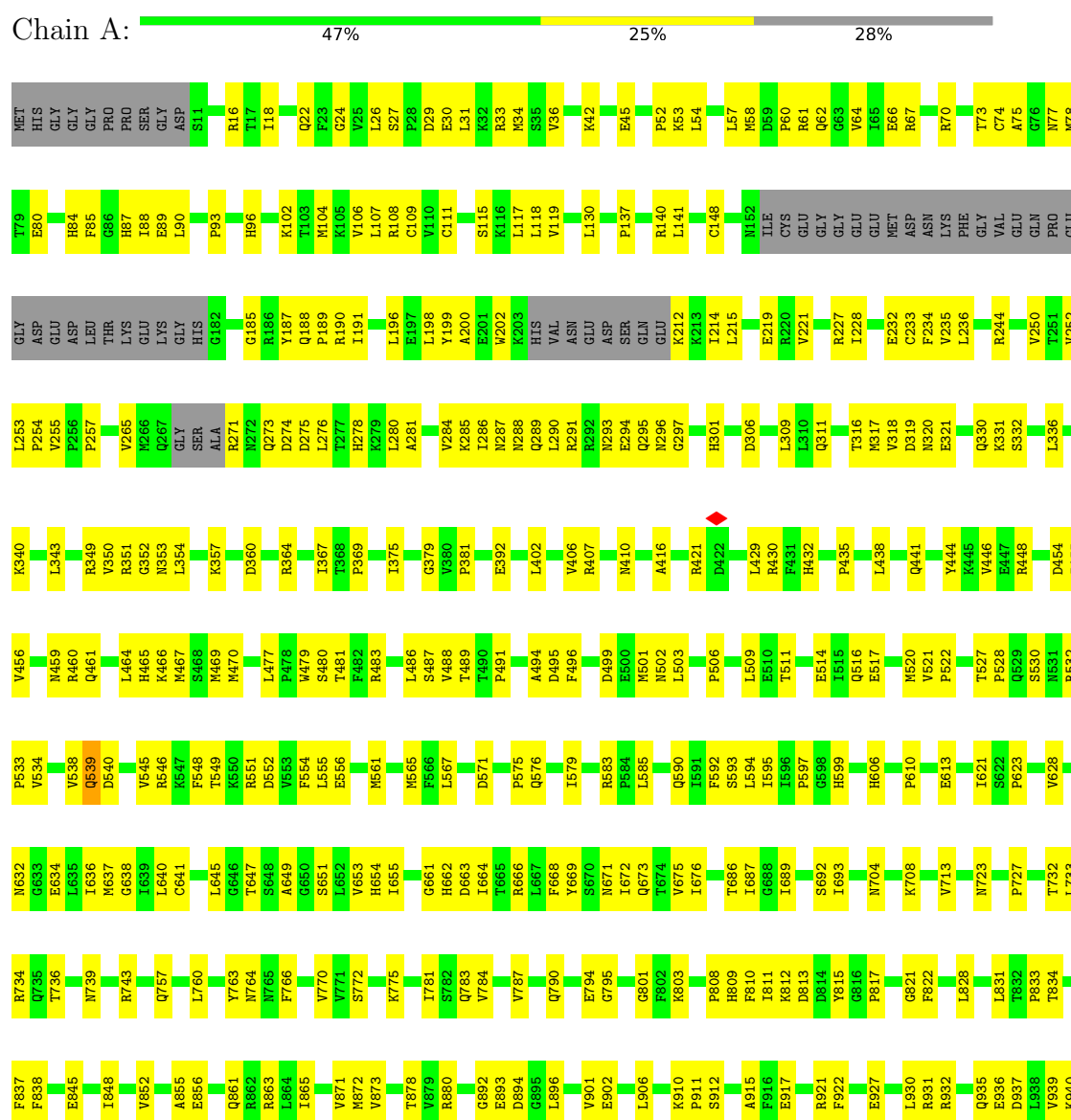
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

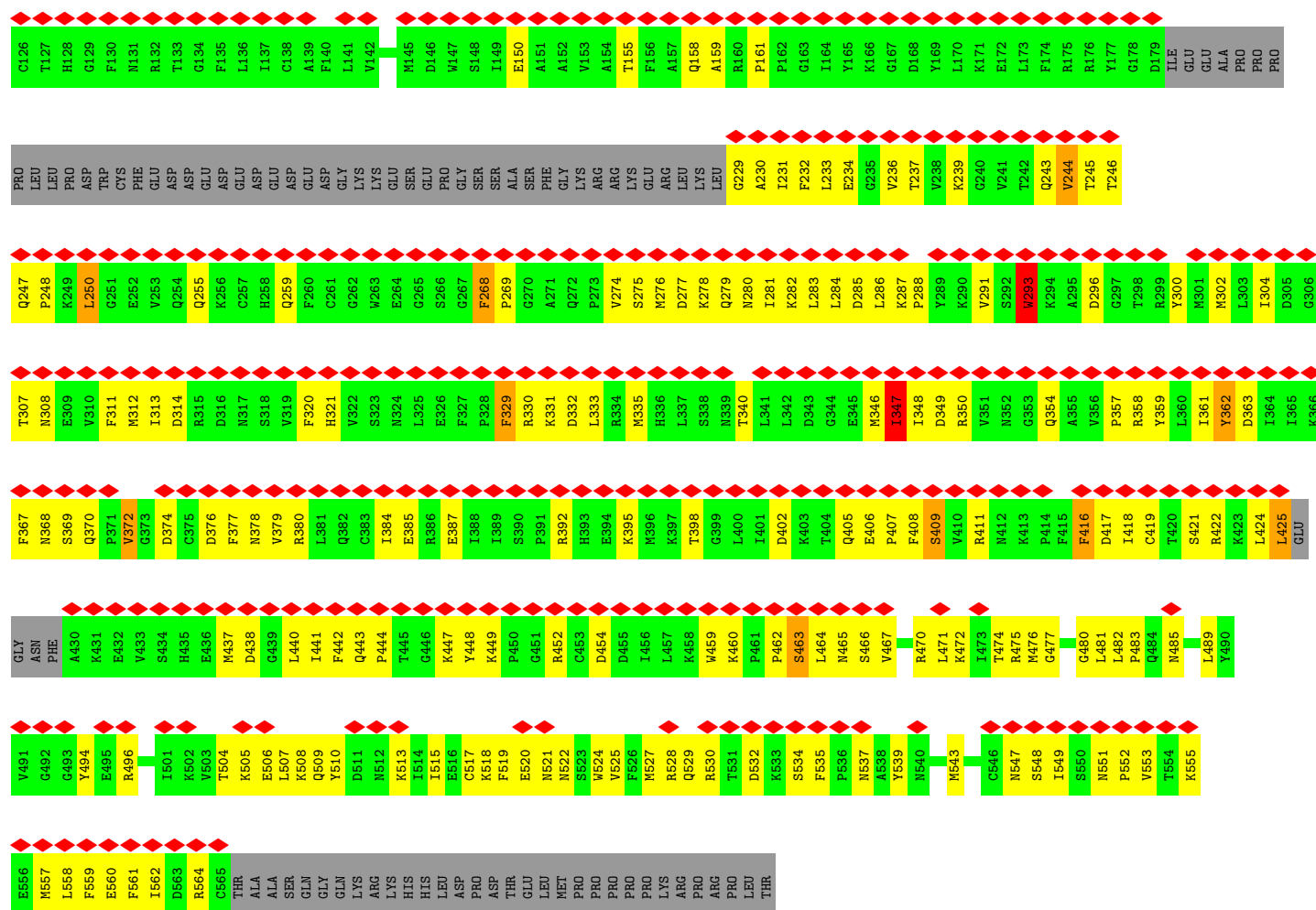
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

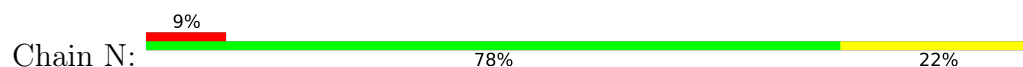
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

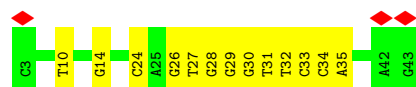




- Molecule 3: DNA (32-MER)

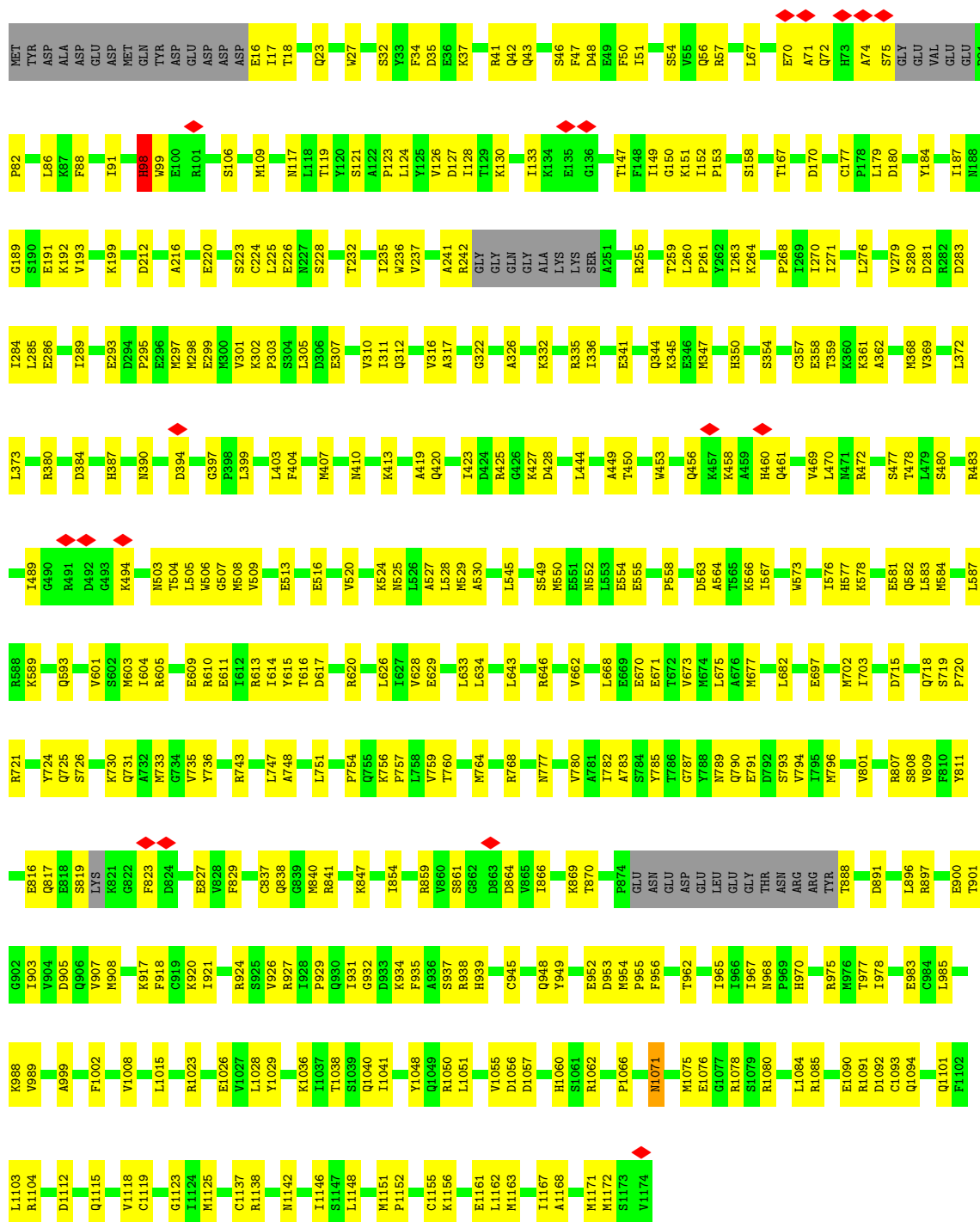


- Molecule 4: DNA (41-MER)



- Molecule 5: DNA-directed RNA polymerase subunit beta

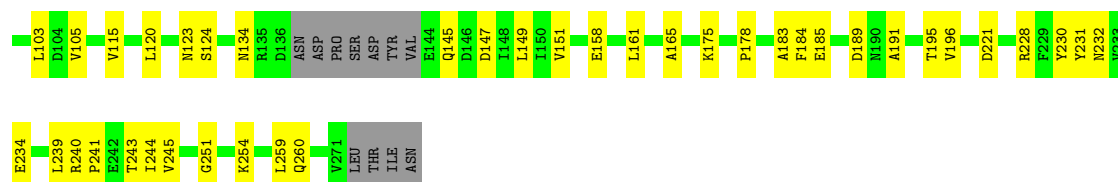




• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

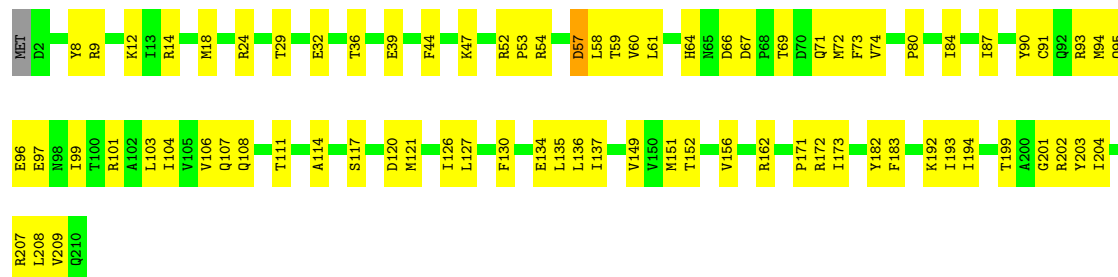
Chain C: 68% 27% •





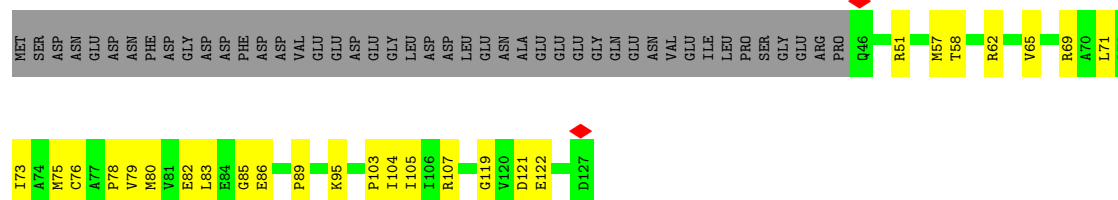
• Molecule 7: DNA-directed RNA polymerase II subunit E

Chain E: 62% 37%



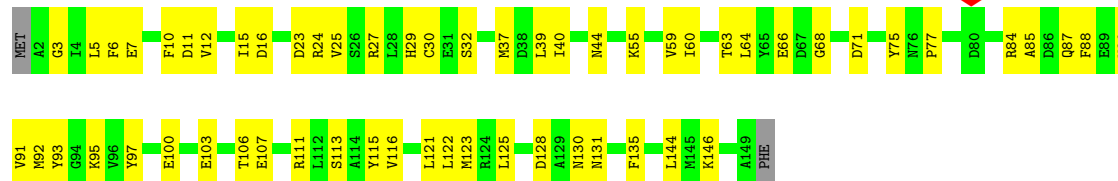
• Molecule 8: DNA-directed RNA polymerase II subunit F

Chain F: 44% 20% 35%



• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 60% 39%



• Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I: 65% 29% 6%

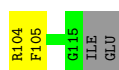
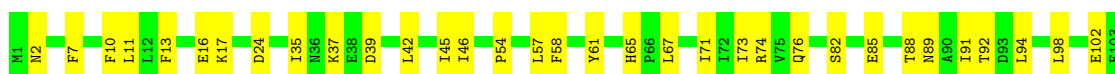




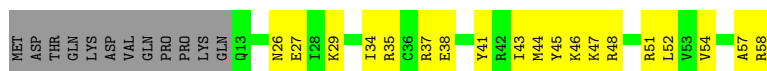
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11-a



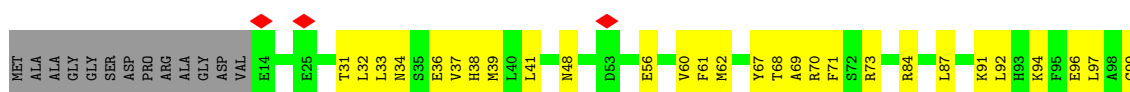
- Molecule 13: RNA polymerase II subunit K



- Molecule 14: RNA (5'-R(P*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3')

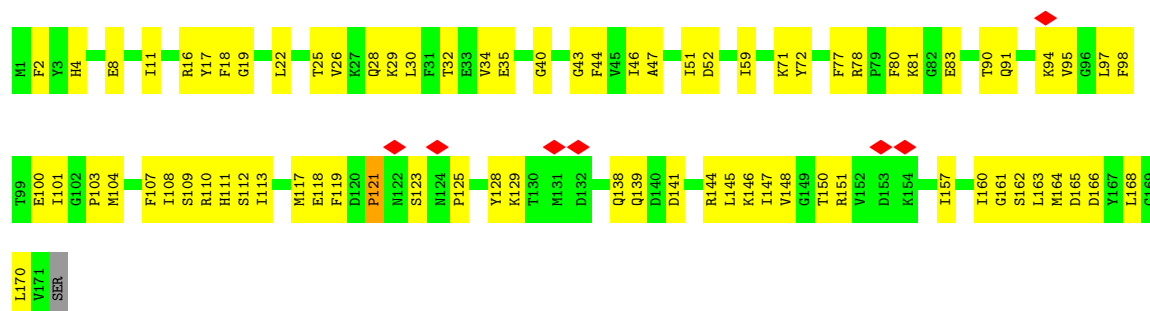


- Molecule 15: RNA polymerase II subunit D

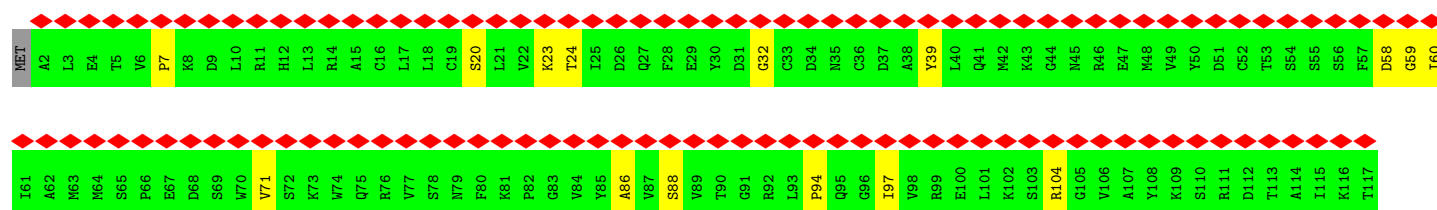
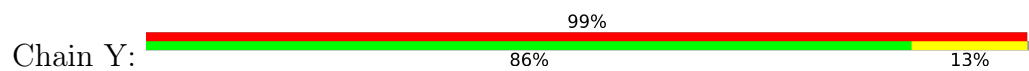


- Molecule 16: DNA-directed RNA polymerase II subunit RPB7

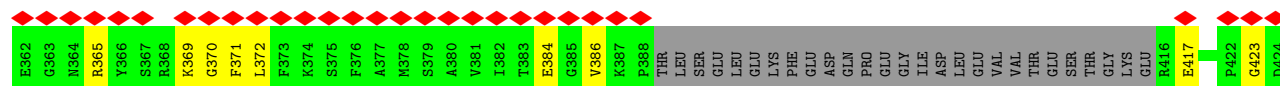
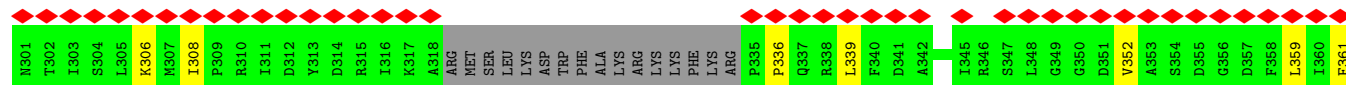
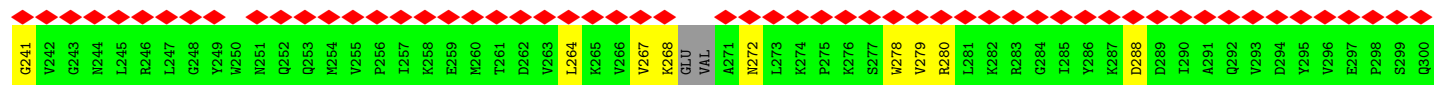
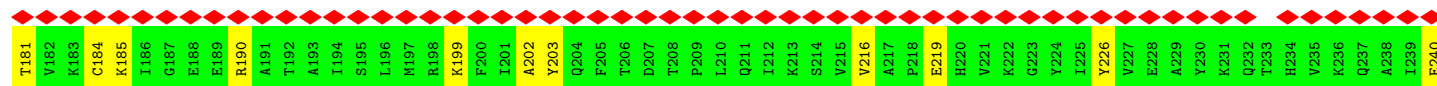
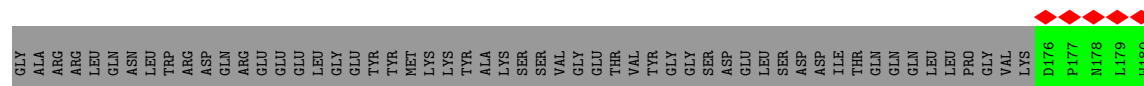
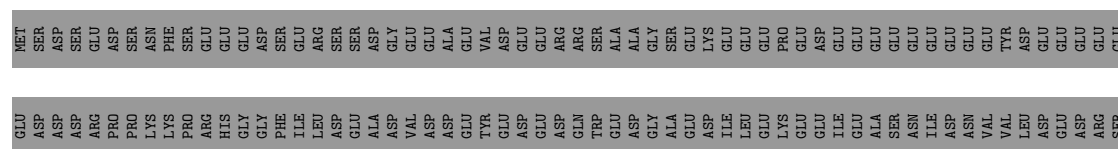
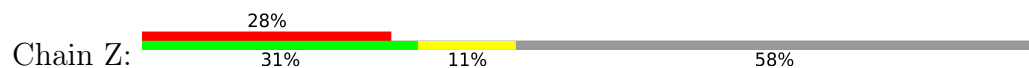


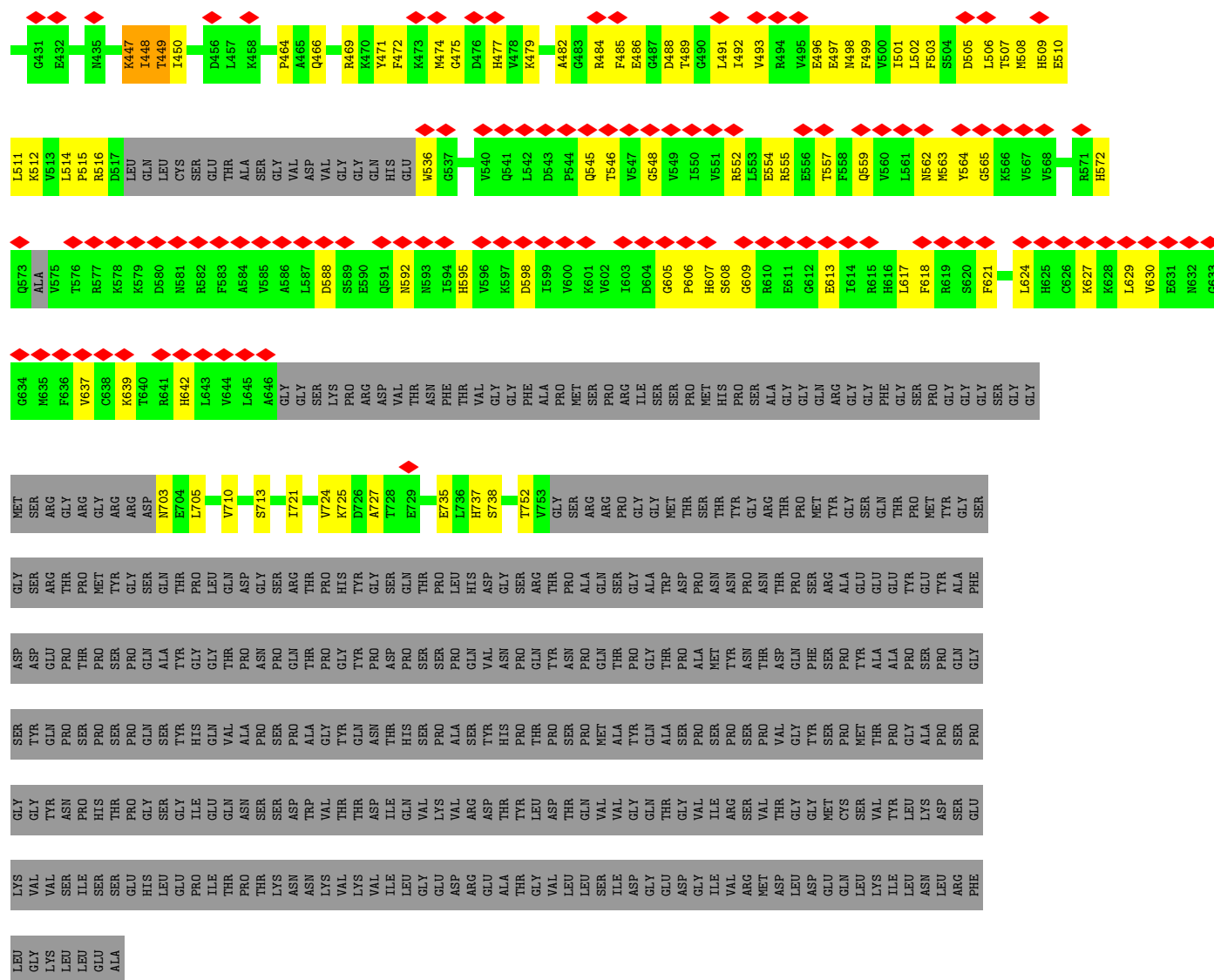


• Molecule 17: Transcription elongation factor SPT4



• Molecule 18: Transcription elongation factor SPT5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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	0.15	0/11369	0.40	0/15347
2	M	0.65	0/4043	1.06	10/5445 (0.2%)
3	N	0.25	0/729	0.47	0/1119
4	T	0.28	0/950	0.48	0/1466
5	B	0.16	0/9232	0.39	3/12462 (0.0%)
6	C	0.15	0/2158	0.35	0/2931
7	E	0.16	0/1751	0.47	0/2366
8	F	0.15	0/667	0.34	0/901
9	H	0.16	0/1207	0.38	0/1628
10	I	0.17	0/972	0.43	0/1316
11	J	0.14	0/542	0.39	1/730 (0.1%)
12	K	0.16	0/939	0.35	0/1271
13	L	0.19	0/394	0.61	0/524
14	P	0.27	0/412	0.64	2/641 (0.3%)
15	D	0.14	0/1017	0.37	0/1368
16	G	0.18	0/1364	0.44	1/1853 (0.1%)
17	Y	0.17	0/927	0.40	0/1250
18	Z	0.49	2/3739 (0.1%)	0.68	7/5030 (0.1%)
All	All	0.29	2/42412 (0.0%)	0.53	24/57648 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	M	0	1
5	B	0	1
7	E	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	450	ILE	CA-C	-6.41	1.45	1.52
18	Z	449	THR	CA-C	-5.98	1.46	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	449	THR	N-CA-C	-12.46	94.45	111.28
2	M	449	LYS	CA-C-N	11.33	131.08	120.21
2	M	449	LYS	C-N-CA	11.33	131.08	120.21
18	Z	450	ILE	N-CA-C	-11.07	94.16	109.21
18	Z	423	GLY	N-CA-C	10.35	127.01	114.69
18	Z	447	LYS	N-CA-C	-8.82	96.45	109.15
2	M	268	PHE	CA-C-N	8.54	128.18	119.56
2	M	268	PHE	C-N-CA	8.54	128.18	119.56
2	M	293	TRP	N-CA-C	7.70	121.78	108.76
2	M	362	TYR	CB-CA-C	7.43	122.59	109.65
14	P	36	G	C2'-C3'-O3'	6.80	119.70	109.50
18	Z	448	ILE	N-CA-C	-6.04	104.62	110.72
2	M	372	VAL	CB-CA-C	-5.95	103.36	112.05
5	B	98	HIS	CA-C-N	5.75	132.52	121.54
5	B	98	HIS	C-N-CA	5.75	132.52	121.54
18	Z	423	GLY	CA-C-N	5.49	130.50	121.39
18	Z	423	GLY	C-N-CA	5.49	130.50	121.39
2	M	362	TYR	CA-CB-CG	5.33	123.50	113.90
14	P	36	G	C4'-C3'-O3'	5.30	117.34	109.40
2	M	347	ILE	N-CA-C	5.22	115.49	107.77
2	M	296	ASP	N-CA-C	-5.17	102.00	109.59
11	J	14	VAL	N-CA-C	-5.16	108.26	113.47
5	B	99	TRP	N-CA-CB	5.08	119.08	110.49
16	G	121	PRO	CA-N-CD	-5.03	104.96	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
1	A	539	GLN	Peptide
5	B	98	HIS	Peptide
7	E	57	ASP	Peptide
2	M	23	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11166	0	11318	384	0
2	M	3958	0	3937	481	0
3	N	652	0	363	26	0
4	T	847	0	464	35	0
5	B	9052	0	9081	362	0
6	C	2115	0	2061	61	0
7	E	1720	0	1737	59	0
8	F	657	0	684	21	0
9	H	1186	0	1147	46	0
10	I	949	0	887	24	0
11	J	533	0	557	14	0
12	K	920	0	942	28	0
13	L	388	0	397	27	0
14	P	368	0	186	45	0
15	D	1004	0	980	55	0
16	G	1333	0	1315	186	0
17	Y	911	0	905	12	0
18	Z	3676	0	3736	306	0
19	A	2	0	0	0	0
19	Y	1	0	0	0	0
20	A	1	0	0	0	0
All	All	41439	0	40697	1750	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1750) 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)
2:M:419:CYS:HA	2:M:559:PHE:CE1	1.24	1.67
2:M:278:LYS:HG3	2:M:551:ASN:CB	1.19	1.64
5:B:859:ARG:HG3	18:Z:737:HIS:CG	1.32	1.62
18:Z:564:TYR:HA	18:Z:637:VAL:CG2	1.23	1.61
2:M:505:LYS:CE	15:D:56:GLU:HB2	1.25	1.60
2:M:481:LEU:HD23	16:G:17:TYR:CE2	1.32	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:278:LYS:CE	2:M:552:PRO:HD2	1.33	1.58
2:M:481:LEU:HA	16:G:17:TYR:CE2	1.10	1.58
18:Z:564:TYR:CA	18:Z:637:VAL:HG21	1.14	1.58
2:M:481:LEU:CD2	16:G:17:TYR:CZ	1.85	1.57
5:B:859:ARG:HG3	18:Z:737:HIS:CD2	1.34	1.57
2:M:462:PRO:CA	2:M:465:ASN:HB2	1.27	1.57
2:M:462:PRO:HA	2:M:465:ASN:CB	1.35	1.55
18:Z:564:TYR:C	18:Z:637:VAL:CG1	1.83	1.50
2:M:38:GLN:CD	2:M:243:GLN:HB3	1.18	1.50
2:M:481:LEU:CA	16:G:17:TYR:HE2	1.19	1.49
2:M:278:LYS:CG	2:M:551:ASN:HB2	1.06	1.49
18:Z:564:TYR:C	18:Z:637:VAL:HG11	1.09	1.49
2:M:278:LYS:CB	2:M:551:ASN:HB2	1.43	1.47
5:B:859:ARG:CG	18:Z:737:HIS:CD2	1.98	1.47
2:M:505:LYS:NZ	15:D:56:GLU:HB2	1.16	1.46
5:B:859:ARG:NH2	18:Z:738:SER:HA	1.30	1.45
18:Z:565:GLY:N	18:Z:637:VAL:HG11	1.21	1.39
2:M:419:CYS:CA	2:M:559:PHE:CE1	2.04	1.39
2:M:278:LYS:HG3	2:M:551:ASN:CA	1.51	1.39
3:N:24:DA:O5'	5:B:489:ILE:CD1	1.71	1.38
2:M:481:LEU:CA	16:G:17:TYR:CE2	1.95	1.37
2:M:418:ILE:HG22	2:M:559:PHE:CD1	1.60	1.36
2:M:462:PRO:HB3	2:M:549:ILE:CD1	1.53	1.35
5:B:72:GLN:CB	18:Z:203:TYR:OH	1.64	1.35
2:M:277:ASP:O	2:M:553:VAL:CG2	1.73	1.35
2:M:286:LEU:HD13	2:M:561:PHE:CZ	1.61	1.35
2:M:283:LEU:C	2:M:561:PHE:CE1	2.05	1.35
2:M:481:LEU:HB3	16:G:17:TYR:OH	1.24	1.35
2:M:285:ASP:N	2:M:561:PHE:CD1	1.88	1.34
2:M:276:MET:SD	2:M:553:VAL:CG1	2.16	1.33
2:M:276:MET:SD	2:M:553:VAL:HG12	1.66	1.33
2:M:38:GLN:OE1	2:M:243:GLN:CB	1.73	1.33
5:B:859:ARG:NH2	18:Z:738:SER:CA	1.88	1.33
18:Z:499:PHE:CD1	18:Z:555:ARG:HA	1.11	1.32
16:G:107:PHE:CZ	18:Z:508:MET:HA	1.12	1.32
2:M:38:GLN:CD	2:M:243:GLN:CB	2.02	1.32
2:M:422:ARG:CZ	2:M:559:PHE:CE2	2.12	1.31
18:Z:499:PHE:CD1	18:Z:555:ARG:CA	1.83	1.31
2:M:419:CYS:HA	2:M:559:PHE:CZ	1.65	1.31
2:M:482:LEU:HD21	16:G:25:THR:O	1.26	1.30
2:M:277:ASP:C	2:M:553:VAL:CG2	2.03	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:505:LYS:CE	15:D:56:GLU:CB	2.08	1.30
18:Z:512:LYS:CE	18:Z:557:THR:OG1	1.80	1.30
3:N:24:DA:O5'	5:B:489:ILE:HD11	1.13	1.29
2:M:277:ASP:O	2:M:553:VAL:HG21	1.16	1.28
3:N:10:DT:C2'	5:B:823:PHE:CZ	2.15	1.27
2:M:278:LYS:CG	2:M:551:ASN:CB	1.88	1.27
2:M:278:LYS:HE3	2:M:552:PRO:CD	1.66	1.25
3:N:10:DT:C3'	5:B:823:PHE:CZ	2.17	1.25
2:M:419:CYS:CA	2:M:559:PHE:HE1	1.38	1.25
16:G:107:PHE:CZ	18:Z:508:MET:CA	2.04	1.25
2:M:286:LEU:HD12	2:M:564:ARG:NH2	1.49	1.25
16:G:110:ARG:N	18:Z:510:GLU:OE2	1.69	1.24
18:Z:499:PHE:CE1	18:Z:555:ARG:HA	1.54	1.23
2:M:481:LEU:HD23	16:G:17:TYR:CZ	1.57	1.23
5:B:859:ARG:CG	18:Z:737:HIS:CG	2.16	1.23
2:M:150:GLU:CG	18:Z:336:PRO:HG3	1.69	1.22
3:N:24:DA:P	5:B:489:ILE:HD11	1.79	1.22
2:M:283:LEU:C	2:M:561:PHE:HE1	1.17	1.21
2:M:482:LEU:CD1	16:G:25:THR:HG23	1.71	1.21
18:Z:564:TYR:HE2	18:Z:618:PHE:CG	1.46	1.21
18:Z:564:TYR:CE2	18:Z:618:PHE:CG	2.14	1.21
2:M:505:LYS:NZ	15:D:56:GLU:CB	2.04	1.21
18:Z:496:GLU:HB2	18:Z:555:ARG:NE	1.54	1.21
2:M:286:LEU:CD1	2:M:564:ARG:NH2	2.04	1.20
2:M:285:ASP:HB3	2:M:564:ARG:NE	1.58	1.19
2:M:419:CYS:N	2:M:559:PHE:HE1	1.40	1.19
18:Z:564:TYR:CE2	18:Z:618:PHE:CD2	2.30	1.19
18:Z:564:TYR:O	18:Z:637:VAL:CG1	1.91	1.18
2:M:281:ILE:HD11	2:M:558:LEU:N	1.57	1.18
2:M:481:LEU:CD2	16:G:17:TYR:CE2	2.08	1.16
2:M:276:MET:CE	2:M:558:LEU:HD13	1.74	1.15
16:G:109:SER:HB2	18:Z:510:GLU:CG	1.75	1.15
2:M:278:LYS:HE2	2:M:552:PRO:HD2	1.18	1.14
2:M:281:ILE:CG1	2:M:558:LEU:HB3	1.76	1.14
2:M:481:LEU:HD22	16:G:17:TYR:CZ	1.55	1.14
2:M:481:LEU:CB	16:G:17:TYR:OH	1.96	1.14
5:B:859:ARG:HD2	18:Z:737:HIS:HA	1.16	1.14
2:M:281:ILE:HG13	2:M:558:LEU:CB	1.79	1.13
2:M:505:LYS:HE3	15:D:56:GLU:CB	1.73	1.13
18:Z:496:GLU:CB	18:Z:555:ARG:HE	1.60	1.13
3:N:10:DT:H2''	5:B:823:PHE:CZ	1.80	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:278:LYS:CE	2:M:552:PRO:CD	2.23	1.12
2:M:286:LEU:CD1	2:M:564:ARG:HH21	1.62	1.12
18:Z:564:TYR:O	18:Z:637:VAL:HG13	1.44	1.12
2:M:481:LEU:CD2	16:G:16:ARG:HH11	1.61	1.11
18:Z:563:MET:HE1	18:Z:617:LEU:C	1.75	1.11
2:M:90:GLN:OE1	2:M:535:PHE:CE1	2.02	1.11
18:Z:496:GLU:HB2	18:Z:555:ARG:HE	0.96	1.11
18:Z:512:LYS:HE3	18:Z:557:THR:CG2	1.80	1.11
2:M:462:PRO:HB3	2:M:549:ILE:HD11	1.28	1.11
2:M:281:ILE:HB	2:M:553:VAL:CG1	1.80	1.10
2:M:281:ILE:CD1	2:M:557:MET:HB3	1.81	1.10
2:M:284:LEU:N	2:M:561:PHE:CD1	2.19	1.10
2:M:505:LYS:HE3	15:D:56:GLU:CG	1.81	1.10
5:B:75:SER:HB2	18:Z:202:ALA:HA	1.20	1.10
5:B:859:ARG:CD	18:Z:737:HIS:HA	1.79	1.10
2:M:159:ALA:CB	18:Z:605:GLY:O	1.98	1.10
2:M:285:ASP:HA	2:M:562:ILE:HA	1.33	1.10
2:M:284:LEU:N	2:M:561:PHE:CE1	2.18	1.10
2:M:281:ILE:HB	2:M:553:VAL:HG13	1.20	1.09
5:B:75:SER:CB	18:Z:202:ALA:HA	1.81	1.09
1:A:301:HIS:CE1	18:Z:181:THR:HG21	1.87	1.09
2:M:34:ARG:HH11	2:M:231:ILE:HG13	0.91	1.08
2:M:150:GLU:HG2	18:Z:336:PRO:HG3	1.14	1.08
2:M:278:LYS:H	2:M:551:ASN:CG	1.60	1.08
18:Z:417:GLU:OE2	18:Z:516:ARG:NH1	1.84	1.08
2:M:276:MET:CG	2:M:553:VAL:HG11	1.83	1.07
2:M:505:LYS:HE3	15:D:56:GLU:HB2	1.28	1.07
2:M:34:ARG:HH11	2:M:231:ILE:CG1	1.57	1.07
2:M:462:PRO:CB	2:M:549:ILE:HD11	1.84	1.07
18:Z:308:ILE:HG12	18:Z:630:VAL:CG2	1.84	1.07
3:N:10:DT:H3'	5:B:823:PHE:CZ	1.88	1.07
4:T:32:DT:O4	14:P:39:A:N6	1.88	1.07
2:M:278:LYS:HE3	2:M:551:ASN:HA	1.28	1.06
2:M:422:ARG:HA	2:M:555:LYS:HE2	1.34	1.06
16:G:160:ILE:CG2	18:Z:491:LEU:HB2	1.85	1.06
18:Z:308:ILE:HG12	18:Z:630:VAL:HG21	1.08	1.06
2:M:69:ASN:OD1	2:M:535:PHE:CZ	2.07	1.06
18:Z:564:TYR:HA	18:Z:637:VAL:HG22	1.36	1.06
16:G:109:SER:HB2	18:Z:510:GLU:HG2	1.06	1.05
2:M:281:ILE:HD11	2:M:557:MET:C	1.80	1.05
3:N:10:DT:C2'	5:B:823:PHE:CE1	2.39	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:10:DT:H3'	5:B:823:PHE:CE1	1.91	1.05
16:G:148:VAL:HB	18:Z:475:GLY:HA2	1.35	1.05
2:M:418:ILE:CG2	2:M:559:PHE:CD1	2.40	1.04
2:M:482:LEU:HD23	16:G:29:LYS:HB2	1.33	1.04
4:T:34:DC:OP2	5:B:456:GLN:NE2	1.90	1.04
18:Z:512:LYS:HE2	18:Z:557:THR:OG1	1.50	1.04
2:M:278:LYS:HE3	2:M:552:PRO:HD2	1.10	1.03
6:C:91:GLU:OE1	18:Z:713:SER:OG	1.75	1.03
2:M:72:ARG:NH1	2:M:230:ALA:N	2.07	1.02
18:Z:512:LYS:HE3	18:Z:557:THR:HG23	1.37	1.02
2:M:150:GLU:HG2	18:Z:336:PRO:CG	1.89	1.02
2:M:481:LEU:HD22	16:G:17:TYR:OH	1.59	1.02
16:G:151:ARG:HD3	18:Z:505:ASP:HA	1.36	1.02
2:M:422:ARG:NE	2:M:559:PHE:CE2	2.26	1.01
2:M:38:GLN:OE1	2:M:243:GLN:HB3	0.84	1.00
2:M:422:ARG:CZ	2:M:559:PHE:HE2	1.61	1.00
2:M:481:LEU:CB	16:G:17:TYR:CE2	2.43	1.00
2:M:34:ARG:NH1	2:M:231:ILE:HG13	1.71	1.00
2:M:482:LEU:HD11	16:G:25:THR:HG23	1.40	1.00
2:M:277:ASP:C	2:M:553:VAL:HG21	1.73	1.00
2:M:285:ASP:HB3	2:M:564:ARG:CD	1.91	1.00
16:G:109:SER:CB	18:Z:510:GLU:HG2	1.91	1.00
18:Z:512:LYS:HE3	18:Z:557:THR:CB	1.91	0.99
5:B:75:SER:HA	18:Z:202:ALA:O	1.61	0.99
2:M:90:GLN:OE1	2:M:535:PHE:HE1	1.38	0.99
3:N:24:DA:P	5:B:489:ILE:CD1	2.47	0.99
2:M:285:ASP:HB2	2:M:561:PHE:CD2	1.97	0.99
2:M:278:LYS:CB	2:M:551:ASN:CB	2.32	0.99
2:M:278:LYS:HG3	2:M:551:ASN:C	1.86	0.98
2:M:505:LYS:HZ1	15:D:56:GLU:CB	1.69	0.98
2:M:462:PRO:CB	2:M:549:ILE:CD1	2.40	0.98
18:Z:564:TYR:N	18:Z:637:VAL:HG21	1.57	0.98
16:G:107:PHE:CE1	18:Z:508:MET:HA	1.90	0.97
2:M:482:LEU:HD11	16:G:25:THR:HA	1.45	0.97
2:M:69:ASN:OD1	2:M:535:PHE:HZ	1.46	0.97
5:B:859:ARG:HG2	18:Z:737:HIS:CD2	1.97	0.97
3:N:10:DT:H2''	5:B:823:PHE:HZ	1.17	0.97
2:M:481:LEU:HD23	16:G:17:TYR:CD2	2.00	0.97
2:M:481:LEU:HD21	16:G:16:ARG:HH11	1.29	0.97
18:Z:564:TYR:CZ	18:Z:618:PHE:CD2	2.44	0.97
2:M:38:GLN:NE2	2:M:243:GLN:CB	2.25	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:10:DT:C3'	5:B:823:PHE:CE1	2.48	0.96
1:A:301:HIS:HE1	18:Z:181:THR:CG2	1.79	0.96
2:M:38:GLN:NE2	2:M:243:GLN:HB3	1.79	0.96
2:M:278:LYS:HB2	2:M:551:ASN:HB2	1.44	0.96
2:M:286:LEU:HD12	2:M:564:ARG:HH21	0.81	0.96
16:G:107:PHE:CE2	18:Z:503:PHE:HB3	2.01	0.96
5:B:859:ARG:HH21	18:Z:738:SER:HA	1.21	0.95
2:M:422:ARG:HA	2:M:555:LYS:CE	1.96	0.95
2:M:150:GLU:CD	18:Z:336:PRO:HG3	1.91	0.95
5:B:72:GLN:HE21	18:Z:199:LYS:HG3	1.32	0.95
2:M:281:ILE:HD13	2:M:557:MET:CG	1.96	0.95
18:Z:565:GLY:N	18:Z:637:VAL:CG1	2.15	0.95
1:A:301:HIS:HE1	18:Z:181:THR:HG21	1.28	0.95
2:M:277:ASP:C	2:M:553:VAL:HG23	1.89	0.95
3:N:24:DA:O5'	5:B:489:ILE:HD12	1.67	0.94
2:M:278:LYS:CE	2:M:551:ASN:HA	1.96	0.94
2:M:159:ALA:HB2	18:Z:605:GLY:O	1.64	0.94
5:B:859:ARG:HH22	18:Z:738:SER:CA	1.77	0.94
2:M:90:GLN:HE22	2:M:534:SER:HB2	1.31	0.93
18:Z:564:TYR:CA	18:Z:637:VAL:CG2	2.00	0.93
2:M:276:MET:SD	2:M:553:VAL:HG11	2.00	0.93
2:M:72:ARG:HH11	2:M:230:ALA:N	1.65	0.93
13:L:54:VAL:HG21	18:Z:721:ILE:CG1	1.99	0.93
18:Z:512:LYS:HE3	18:Z:557:THR:OG1	1.67	0.93
18:Z:563:MET:CE	18:Z:618:PHE:HB2	1.98	0.93
2:M:481:LEU:CD2	16:G:17:TYR:OH	2.15	0.92
2:M:505:LYS:HZ1	15:D:56:GLU:HB2	1.14	0.92
4:T:31:DT:O4	14:P:40:A:N6	2.02	0.92
2:M:481:LEU:HD22	16:G:16:ARG:HH11	1.35	0.92
2:M:425:LEU:HD21	2:M:555:LYS:HB3	1.51	0.92
18:Z:471:TYR:O	18:Z:472:PHE:CG	2.23	0.91
2:M:281:ILE:CD1	2:M:557:MET:CB	2.49	0.91
2:M:418:ILE:HG22	2:M:559:PHE:CE1	2.06	0.91
2:M:482:LEU:CD2	16:G:25:THR:O	2.17	0.91
18:Z:308:ILE:CG1	18:Z:630:VAL:HG21	1.99	0.91
2:M:481:LEU:CB	16:G:17:TYR:CZ	2.53	0.90
2:M:285:ASP:HB2	2:M:561:PHE:CG	2.06	0.90
2:M:419:CYS:N	2:M:559:PHE:CE1	2.33	0.90
4:T:31:DT:N3	14:P:40:A:N1	2.17	0.90
5:B:75:SER:CA	18:Z:202:ALA:HA	2.01	0.90
2:M:286:LEU:CD1	2:M:561:PHE:CZ	2.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:278:LYS:CG	2:M:551:ASN:CA	2.35	0.90
2:M:462:PRO:C	2:M:465:ASN:HB2	1.96	0.90
5:B:859:ARG:HD2	18:Z:737:HIS:CA	2.00	0.89
18:Z:563:MET:HE2	18:Z:618:PHE:HB2	1.50	0.89
2:M:483:PRO:HD2	16:G:32:THR:OG1	1.73	0.89
2:M:282:LYS:HA	2:M:561:PHE:CD2	2.05	0.89
2:M:281:ILE:CB	2:M:553:VAL:HG13	2.01	0.89
5:B:549:SER:HG	5:B:577:HIS:HE2	1.19	0.89
5:B:71:ALA:O	18:Z:203:TYR:OH	1.91	0.88
17:Y:58:ASP:OD2	18:Z:268:LYS:NZ	2.06	0.88
5:B:859:ARG:NH2	18:Z:738:SER:N	1.93	0.88
2:M:72:ARG:NH1	2:M:230:ALA:H	1.70	0.88
2:M:284:LEU:CA	2:M:561:PHE:HD1	1.86	0.88
2:M:287:LYS:O	2:M:562:ILE:HG23	1.72	0.88
2:M:35:TYR:CE1	2:M:230:ALA:O	2.27	0.88
2:M:418:ILE:HG22	2:M:559:PHE:HD1	1.33	0.88
2:M:276:MET:HE1	2:M:558:LEU:HD13	1.54	0.88
2:M:286:LEU:HD13	2:M:561:PHE:HZ	1.32	0.88
2:M:422:ARG:CZ	2:M:559:PHE:CZ	2.55	0.88
1:A:301:HIS:CE1	18:Z:181:THR:CG2	2.54	0.88
2:M:462:PRO:HB3	2:M:549:ILE:HD12	1.54	0.87
2:M:276:MET:HG2	2:M:553:VAL:CB	2.05	0.87
2:M:464:LEU:H	2:M:465:ASN:N	1.72	0.87
2:M:278:LYS:HB2	2:M:551:ASN:CB	2.00	0.87
2:M:482:LEU:HD11	16:G:25:THR:CG2	2.04	0.87
16:G:148:VAL:O	18:Z:475:GLY:O	1.92	0.87
16:G:160:ILE:HG22	18:Z:491:LEU:HD12	1.56	0.87
2:M:281:ILE:HD13	2:M:557:MET:CB	2.04	0.87
2:M:286:LEU:HD11	2:M:564:ARG:NH2	1.88	0.86
2:M:285:ASP:HA	2:M:562:ILE:CA	1.95	0.86
16:G:111:HIS:N	18:Z:510:GLU:OE2	2.08	0.86
2:M:90:GLN:NE2	2:M:534:SER:HB2	1.89	0.86
3:N:10:DT:H2'	5:B:823:PHE:CE1	2.09	0.86
2:M:481:LEU:CG	16:G:17:TYR:CE2	2.57	0.86
2:M:482:LEU:HD22	16:G:29:LYS:N	1.89	0.86
2:M:505:LYS:CE	15:D:56:GLU:CG	2.47	0.86
2:M:285:ASP:OD1	2:M:560:GLU:O	1.93	0.85
2:M:418:ILE:CG2	2:M:559:PHE:HD1	1.86	0.85
2:M:481:LEU:HA	16:G:17:TYR:CD2	2.05	0.85
2:M:276:MET:CG	2:M:553:VAL:CG1	2.48	0.85
18:Z:370:GLY:C	18:Z:630:VAL:CG1	2.50	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:276:MET:HE1	2:M:558:LEU:HD22	1.56	0.85
5:B:819:SER:H	5:B:827:GLU:HB2	1.42	0.85
2:M:276:MET:HE1	2:M:558:LEU:CD1	2.07	0.85
2:M:422:ARG:NH2	2:M:559:PHE:CZ	2.44	0.85
2:M:481:LEU:HD21	16:G:16:ARG:HD3	1.59	0.85
16:G:110:ARG:CA	18:Z:510:GLU:OE2	2.25	0.85
2:M:277:ASP:O	2:M:553:VAL:HG22	1.74	0.84
2:M:462:PRO:O	2:M:465:ASN:O	1.95	0.84
2:M:482:LEU:CG	16:G:25:THR:HG23	2.07	0.84
2:M:285:ASP:N	2:M:561:PHE:HD1	1.76	0.83
5:B:859:ARG:HG3	18:Z:737:HIS:CB	2.07	0.83
6:C:19:VAL:HG23	6:C:241:PRO:HB2	1.60	0.83
18:Z:565:GLY:CA	18:Z:637:VAL:HG11	2.09	0.83
2:M:481:LEU:HD22	16:G:16:ARG:NH1	1.94	0.83
2:M:482:LEU:CD2	16:G:29:LYS:HB2	2.07	0.83
5:B:859:ARG:CZ	18:Z:737:HIS:ND1	2.34	0.82
16:G:95:VAL:CG1	18:Z:509:HIS:HA	2.09	0.82
5:B:864:ASP:OD1	18:Z:725:LYS:NZ	2.13	0.82
15:D:87:LEU:HD22	15:D:97:LEU:HG	1.61	0.82
2:M:276:MET:CE	2:M:558:LEU:CD1	2.58	0.82
16:G:151:ARG:HD3	18:Z:505:ASP:CA	1.53	0.82
16:G:11:ILE:HD11	16:G:26:VAL:HG13	1.60	0.82
2:M:284:LEU:N	2:M:561:PHE:HD1	1.75	0.82
16:G:148:VAL:HB	18:Z:475:GLY:CA	2.08	0.82
2:M:481:LEU:HB3	16:G:17:TYR:HH	1.42	0.81
2:M:481:LEU:CB	16:G:17:TYR:HE2	1.85	0.81
14:P:35:A:H3'	14:P:35:A:OP2	1.80	0.81
5:B:407:MET:HE1	5:B:444:LEU:HG	1.61	0.81
2:M:482:LEU:CD1	16:G:25:THR:CG2	2.57	0.81
14:P:37:G:H8	14:P:37:G:H5''	1.44	0.81
18:Z:485:PHE:HZ	18:Z:559:GLN:HE22	1.25	0.81
5:B:260:LEU:HD12	5:B:261:PRO:HD2	1.61	0.81
16:G:160:ILE:HG21	18:Z:491:LEU:HB2	1.60	0.81
2:M:276:MET:HE2	2:M:558:LEU:HD13	1.61	0.81
2:M:281:ILE:HG21	2:M:557:MET:SD	2.21	0.81
2:M:481:LEU:CD2	16:G:16:ARG:NH1	2.43	0.81
2:M:422:ARG:NE	2:M:559:PHE:CZ	2.48	0.80
18:Z:512:LYS:CE	18:Z:557:THR:CG2	2.58	0.80
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.62	0.80
1:A:42:LYS:O	1:A:288:ASN:ND2	2.14	0.80
2:M:281:ILE:HD13	2:M:557:MET:SD	2.22	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:285:ASP:CA	2:M:562:ILE:HA	2.06	0.80
2:M:402:ASP:HB3	2:M:405:GLN:HG2	1.64	0.80
5:B:74:ALA:C	18:Z:202:ALA:HB1	2.07	0.80
18:Z:496:GLU:HB2	18:Z:499:PHE:HB2	1.62	0.80
2:M:72:ARG:NH1	2:M:229:GLY:C	2.22	0.80
2:M:481:LEU:HD22	16:G:17:TYR:CE1	2.14	0.80
2:M:277:ASP:HB2	2:M:551:ASN:OD1	1.82	0.80
2:M:278:LYS:CD	2:M:551:ASN:CB	2.60	0.80
5:B:72:GLN:HB3	18:Z:203:TYR:OH	0.73	0.79
18:Z:339:LEU:HD11	18:Z:629:LEU:HD12	1.62	0.79
2:M:276:MET:HE1	2:M:558:LEU:CD2	2.10	0.79
2:M:278:LYS:HE3	2:M:551:ASN:CA	2.12	0.79
16:G:107:PHE:CZ	18:Z:503:PHE:HB3	2.16	0.79
2:M:281:ILE:CD1	2:M:558:LEU:N	2.42	0.79
2:M:425:LEU:HD21	2:M:555:LYS:CB	2.06	0.79
2:M:482:LEU:HD11	16:G:25:THR:CA	2.12	0.79
4:T:34:DC:N4	14:P:37:G:O6	2.15	0.79
2:M:281:ILE:CD1	2:M:557:MET:C	2.53	0.79
5:B:859:ARG:HG2	18:Z:737:HIS:NE2	1.96	0.79
2:M:281:ILE:HG21	2:M:557:MET:CE	2.12	0.79
13:L:26:ASN:HD21	13:L:44:MET:HE1	1.48	0.79
2:M:276:MET:HG2	2:M:553:VAL:HB	1.64	0.79
2:M:278:LYS:CD	2:M:551:ASN:HB2	2.12	0.79
2:M:418:ILE:C	2:M:559:PHE:HE1	1.91	0.79
2:M:481:LEU:CG	16:G:17:TYR:CZ	2.66	0.79
2:M:482:LEU:HG	16:G:25:THR:CG2	2.13	0.79
2:M:518:LYS:HD3	2:M:527:MET:HE2	1.65	0.79
18:Z:339:LEU:HD13	18:Z:629:LEU:HA	1.62	0.79
2:M:246:THR:HG22	2:M:248:PRO:HD2	1.65	0.78
2:M:284:LEU:C	2:M:561:PHE:CD1	2.62	0.78
2:M:419:CYS:CA	2:M:559:PHE:CZ	2.47	0.78
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.65	0.77
5:B:75:SER:HB2	18:Z:202:ALA:CA	2.10	0.77
1:A:770:VAL:HG21	1:A:781:ILE:HD11	1.64	0.77
2:M:158:GLN:HB3	18:Z:608:SER:N	1.99	0.77
18:Z:339:LEU:CD1	18:Z:629:LEU:HA	2.15	0.77
18:Z:563:MET:HE1	18:Z:618:PHE:N	1.99	0.77
5:B:403:LEU:HD23	5:B:407:MET:HE2	1.66	0.77
16:G:107:PHE:CE2	18:Z:508:MET:C	2.46	0.77
2:M:278:LYS:CG	2:M:551:ASN:C	2.58	0.76
5:B:861:SER:HB2	18:Z:735:GLU:OE2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:230:ALA:HB3	2:M:243:GLN:OE1	1.86	0.76
2:M:481:LEU:CA	16:G:17:TYR:CZ	2.67	0.76
2:M:38:GLN:NE2	2:M:243:GLN:HB2	1.99	0.76
5:B:179:LEU:HD22	5:B:768:ARG:HE	1.49	0.76
16:G:148:VAL:CB	18:Z:475:GLY:HA2	2.14	0.76
16:G:107:PHE:CE1	18:Z:508:MET:CA	2.46	0.76
3:N:10:DT:H3'	5:B:823:PHE:CD1	2.20	0.76
2:M:278:LYS:CD	2:M:551:ASN:HA	2.15	0.76
2:M:285:ASP:CG	2:M:564:ARG:HG2	2.11	0.75
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.51	0.75
1:A:686:THR:HG21	5:B:1041:ILE:HA	1.67	0.75
2:M:285:ASP:HB3	2:M:564:ARG:CG	2.15	0.75
18:Z:484:ARG:H	18:Z:552:ARG:HH12	1.33	0.75
1:A:64:VAL:HG11	1:A:78:MET:HA	1.67	0.75
2:M:281:ILE:HD13	2:M:557:MET:HB3	1.63	0.75
5:B:32:SER:HB3	5:B:643:LEU:HD21	1.68	0.75
2:M:286:LEU:HD11	2:M:564:ARG:HH22	1.52	0.75
2:M:291:VAL:HG11	2:M:421:SER:HB3	1.69	0.75
4:T:29:DG:O6	14:P:42:C:N4	2.18	0.75
2:M:276:MET:HA	2:M:280:ASN:HD22	1.52	0.75
2:M:422:ARG:NH2	2:M:559:PHE:CE2	2.54	0.75
16:G:107:PHE:CE2	18:Z:508:MET:O	2.39	0.75
18:Z:199:LYS:NZ	18:Z:240:GLU:O	2.18	0.75
5:B:380:ARG:HD2	5:B:609:GLU:HG3	1.68	0.75
5:B:603:MET:HG3	5:B:614:ILE:HG12	1.67	0.75
13:L:54:VAL:HG21	18:Z:721:ILE:HG12	1.67	0.75
2:M:462:PRO:HA	2:M:465:ASN:CG	2.10	0.74
5:B:72:GLN:HE21	18:Z:199:LYS:CG	2.00	0.74
5:B:268:PRO:HG2	5:B:271:ILE:HD12	1.67	0.74
18:Z:471:TYR:O	18:Z:472:PHE:CD2	2.40	0.74
2:M:483:PRO:CD	16:G:32:THR:OG1	2.34	0.74
5:B:480:SER:OG	5:B:525:ASN:ND2	2.18	0.74
16:G:112:SER:HG	18:Z:503:PHE:HZ	1.31	0.74
1:A:576:GLN:O	1:A:590:GLN:NE2	2.20	0.74
5:B:75:SER:HA	18:Z:202:ALA:C	2.12	0.74
15:D:33:LEU:HD11	15:D:101:ALA:HB3	1.70	0.74
2:M:281:ILE:HD11	2:M:557:MET:HB3	1.70	0.74
1:A:34:MET:HA	5:B:1138:ARG:HG3	1.69	0.74
2:M:159:ALA:CA	18:Z:605:GLY:O	2.35	0.74
2:M:481:LEU:CD2	16:G:17:TYR:CE1	2.64	0.73
16:G:112:SER:CB	18:Z:493:VAL:HG11	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:481:LEU:CG	16:G:17:TYR:OH	2.36	0.73
5:B:75:SER:HA	18:Z:202:ALA:CA	2.18	0.73
2:M:278:LYS:N	2:M:551:ASN:CG	2.44	0.73
18:Z:496:GLU:CB	18:Z:555:ARG:NE	2.31	0.73
1:A:576:GLN:HA	9:H:75:TYR:HB2	1.69	0.73
5:B:75:SER:CA	18:Z:202:ALA:CA	2.67	0.73
18:Z:499:PHE:CE1	18:Z:555:ARG:CA	2.37	0.73
18:Z:308:ILE:CG1	18:Z:630:VAL:CG2	2.64	0.73
2:M:281:ILE:HG13	2:M:558:LEU:HB3	0.86	0.73
2:M:281:ILE:HG21	2:M:557:MET:HE2	1.71	0.73
18:Z:496:GLU:CA	18:Z:555:ARG:HE	2.01	0.73
2:M:418:ILE:C	2:M:559:PHE:CE1	2.65	0.73
16:G:107:PHE:HE2	18:Z:503:PHE:CD1	2.06	0.73
18:Z:496:GLU:H	18:Z:555:ARG:NE	1.87	0.72
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.71	0.72
2:M:285:ASP:CB	2:M:561:PHE:CG	2.70	0.72
2:M:462:PRO:CA	2:M:465:ASN:CB	2.21	0.72
2:M:474:THR:HB	2:M:476:MET:HE3	1.70	0.72
2:M:518:LYS:HE3	2:M:525:VAL:HG23	1.70	0.72
1:A:931:ARG:HD2	1:A:939:VAL:HG11	1.72	0.72
2:M:38:GLN:CD	2:M:243:GLN:CA	2.62	0.72
5:B:847:LYS:HA	13:L:51:ARG:HH22	1.54	0.72
7:E:80:PRO:HA	7:E:107:GLN:HB2	1.71	0.72
2:M:482:LEU:CG	16:G:25:THR:CG2	2.68	0.72
5:B:907:VAL:HG22	5:B:921:ILE:HG12	1.71	0.72
2:M:38:GLN:CD	2:M:243:GLN:H	1.97	0.71
14:P:35:A:H3'	14:P:35:A:P	2.29	0.71
5:B:838:GLN:HE21	5:B:888:THR:N	1.88	0.71
5:B:896:LEU:HD21	5:B:900:GLU:HB3	1.72	0.71
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.72	0.71
4:T:28:DG:C2	14:P:44:A:C2	2.78	0.71
5:B:866:ILE:HD11	5:B:896:LEU:HD12	1.72	0.71
18:Z:545:GLN:O	18:Z:617:LEU:O	2.08	0.71
2:M:483:PRO:HG2	16:G:32:THR:OG1	1.90	0.71
4:T:29:DG:N1	14:P:42:C:N3	2.37	0.71
18:Z:370:GLY:C	18:Z:630:VAL:HG11	2.14	0.71
16:G:107:PHE:HE2	18:Z:503:PHE:HD1	1.39	0.71
2:M:482:LEU:CD2	16:G:29:LYS:N	2.54	0.70
5:B:91:ILE:HD11	5:B:124:LEU:HD12	1.73	0.70
5:B:344:GLN:NE2	5:B:354:SER:O	2.24	0.70
5:B:953:ASP:OD1	6:C:36:ARG:NH2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:564:TYR:C	18:Z:637:VAL:CG2	2.63	0.70
2:M:421:SER:HA	2:M:424:LEU:HD12	1.73	0.70
5:B:270:ILE:HG12	5:B:305:LEU:HD23	1.72	0.70
18:Z:565:GLY:CA	18:Z:637:VAL:CG1	2.69	0.70
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.23	0.70
18:Z:564:TYR:CZ	18:Z:618:PHE:HD2	2.05	0.70
5:B:119:THR:HG23	5:B:187:ILE:HG12	1.73	0.70
16:G:112:SER:OG	18:Z:503:PHE:CZ	2.40	0.70
18:Z:496:GLU:CA	18:Z:555:ARG:NE	2.54	0.70
2:M:276:MET:HG2	2:M:553:VAL:CG1	2.20	0.70
2:M:482:LEU:HG	16:G:25:THR:HG23	1.72	0.70
7:E:24:ARG:NE	7:E:183:PHE:O	2.25	0.70
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.65	0.70
2:M:285:ASP:CB	2:M:564:ARG:NE	2.48	0.69
5:B:387:HIS:NE2	5:B:671:GLU:OE2	2.26	0.69
2:M:38:GLN:CD	2:M:243:GLN:N	2.50	0.69
2:M:422:ARG:NH1	2:M:559:PHE:HE2	1.90	0.69
1:A:1372:GLU:HG3	7:E:193:ILE:HD13	1.75	0.69
2:M:38:GLN:OE1	2:M:243:GLN:CG	2.39	0.69
18:Z:496:GLU:H	18:Z:555:ARG:CZ	2.05	0.69
2:M:422:ARG:NH2	2:M:559:PHE:HZ	1.90	0.69
2:M:481:LEU:HD21	16:G:16:ARG:CD	2.22	0.69
6:C:47:ILE:HA	6:C:165:ALA:HA	1.75	0.69
1:A:381:PRO:HB3	1:A:480:SER:HA	1.75	0.69
2:M:459:TRP:CD1	2:M:553:VAL:O	2.44	0.69
5:B:458:LYS:HB2	5:B:461:GLN:HB2	1.74	0.69
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.75	0.69
2:M:293:TRP:HB3	2:M:440:LEU:HD23	1.75	0.69
5:B:311:ILE:HG23	5:B:316:VAL:HG23	1.74	0.69
14:P:37:G:H5"	14:P:37:G:C8	2.28	0.69
1:A:291:ARG:O	1:A:294:GLU:HG3	1.93	0.69
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.75	0.69
16:G:107:PHE:CE2	18:Z:503:PHE:CD1	2.81	0.69
1:A:196:LEU:HD22	1:A:311:GLN:HE22	1.58	0.68
1:A:902:GLU:OE2	1:A:985:ARG:NH2	2.25	0.68
5:B:748:ALA:HB3	5:B:811:TYR:HB2	1.75	0.68
5:B:859:ARG:CB	18:Z:737:HIS:CD2	2.76	0.68
2:M:462:PRO:HB2	2:M:549:ILE:HD11	1.73	0.68
5:B:298:MET:HA	5:B:301:VAL:HG12	1.76	0.68
13:L:54:VAL:CG2	18:Z:721:ILE:HG13	2.24	0.68
18:Z:370:GLY:O	18:Z:630:VAL:HG11	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:425:ARG:HG3	5:B:427:LYS:HG2	1.76	0.68
3:N:24:DA:OP1	5:B:489:ILE:HD11	1.93	0.68
14:P:35:A:H4'	14:P:36:G:H2'	1.74	0.68
18:Z:564:TYR:HE2	18:Z:618:PHE:CD1	2.08	0.68
1:A:487:SER:OG	1:A:673:GLN:NE2	2.27	0.68
16:G:111:HIS:H	18:Z:510:GLU:CD	2.00	0.68
2:M:246:THR:C	2:M:248:PRO:HD2	2.19	0.67
15:D:37:VAL:HG21	16:G:2:PHE:HD2	1.58	0.67
5:B:354:SER:HG	5:B:357:CYS:HG	1.38	0.67
10:I:65:LEU:O	10:I:122:ARG:NH1	2.28	0.67
10:I:115:THR:HG22	10:I:116:ALA:H	1.59	0.67
1:A:52:PRO:HB2	1:A:60:PRO:HD3	1.77	0.67
1:A:320:ASN:ND2	1:A:336:LEU:O	2.27	0.67
16:G:112:SER:HB3	18:Z:493:VAL:HG11	1.76	0.67
1:A:636:ILE:HG22	1:A:637:MET:HG2	1.75	0.67
1:A:808:PRO:HB2	5:B:675:LEU:HD13	1.76	0.67
5:B:939:HIS:NE2	5:B:983:GLU:OE1	2.26	0.67
18:Z:564:TYR:C	18:Z:637:VAL:CB	2.66	0.67
2:M:276:MET:HG2	2:M:553:VAL:HG11	1.74	0.67
5:B:153:PRO:HD2	5:B:444:LEU:HD13	1.77	0.67
18:Z:512:LYS:NZ	18:Z:557:THR:OG1	2.28	0.67
5:B:760:THR:OG1	5:B:764:MET:SD	2.49	0.67
2:M:286:LEU:HD13	2:M:561:PHE:CE2	2.27	0.67
18:Z:512:LYS:CE	18:Z:557:THR:CB	2.59	0.67
2:M:520:GLU:HG2	2:M:521:ASN:H	1.59	0.67
13:L:54:VAL:CG2	18:Z:721:ILE:CG1	2.72	0.67
2:M:387:GLU:HA	2:M:387:GLU:OE1	1.94	0.66
1:A:1212:LEU:HD22	1:A:1259:ILE:HD12	1.77	0.66
2:M:482:LEU:HD23	16:G:29:LYS:CB	2.18	0.66
5:B:483:ARG:HH12	5:B:528:LEU:HA	1.61	0.66
14:P:31:G:H2'	14:P:31:G:N3	2.10	0.66
2:M:285:ASP:HB3	2:M:564:ARG:HE	1.57	0.66
16:G:162:SER:CB	18:Z:493:VAL:HG13	2.26	0.66
1:A:296:ASN:OD1	1:A:297:GLY:N	2.28	0.66
7:E:120:ASP:OD1	7:E:121:MET:N	2.28	0.66
2:M:158:GLN:HG2	18:Z:609:GLY:HA3	1.76	0.66
2:M:284:LEU:CA	2:M:561:PHE:CD1	2.69	0.66
2:M:483:PRO:HD3	16:G:29:LYS:HD2	1.78	0.66
5:B:790:GLN:O	5:B:968:ASN:ND2	2.27	0.66
11:J:40:LEU:HD11	11:J:49:LEU:HD12	1.78	0.66
2:M:462:PRO:HB3	2:M:549:ILE:HD13	1.72	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:223:SER:HG	5:B:350:HIS:HD1	1.41	0.66
1:A:1170:THR:HA	1:A:1216:LEU:HA	1.77	0.66
2:M:278:LYS:CD	2:M:551:ASN:CA	2.72	0.66
7:E:24:ARG:HH11	7:E:72:MET:HE3	1.61	0.66
2:M:422:ARG:CA	2:M:555:LYS:CE	2.73	0.65
5:B:725:GLN:NE2	5:B:937:SER:O	2.30	0.65
1:A:111:CYS:HB2	1:A:118:LEU:HB3	1.78	0.65
5:B:861:SER:CB	18:Z:735:GLU:OE2	2.43	0.65
16:G:144:ARG:HB3	16:G:168:LEU:HD12	1.77	0.65
2:M:278:LYS:HE2	2:M:552:PRO:CD	2.07	0.65
2:M:281:ILE:HD12	2:M:553:VAL:HG13	1.78	0.65
2:M:463:SER:O	2:M:518:LYS:CG	2.44	0.65
1:A:517:GLU:OE1	8:F:62:ARG:NH1	2.29	0.65
4:T:28:DG:C6	14:P:44:A:N1	2.63	0.65
2:M:463:SER:O	2:M:518:LYS:HD2	1.97	0.65
18:Z:371:PHE:CA	18:Z:630:VAL:HG11	2.26	0.65
2:M:159:ALA:HA	18:Z:605:GLY:O	1.96	0.65
2:M:159:ALA:HB1	18:Z:605:GLY:O	1.95	0.65
6:C:69:GLY:HA3	13:L:57:ALA:HB1	1.77	0.65
1:A:763:TYR:OH	9:H:23:ASP:OD2	2.14	0.65
5:B:285:LEU:HD21	5:B:305:LEU:HD11	1.78	0.65
5:B:37:LYS:HD2	5:B:41:ARG:HG2	1.79	0.65
5:B:841:ARG:NE	14:P:34:G:H4'	2.11	0.65
2:M:284:LEU:C	2:M:561:PHE:HD1	2.00	0.65
5:B:718:GLN:HG2	5:B:720:PRO:HD2	1.78	0.65
7:E:9:ARG:HG3	7:E:136:LEU:HD21	1.77	0.65
5:B:809:VAL:HA	5:B:926:VAL:HA	1.79	0.64
13:L:54:VAL:HG21	18:Z:721:ILE:HG13	1.77	0.64
2:M:464:LEU:N	2:M:465:ASN:N	2.45	0.64
5:B:192:LYS:HE3	5:B:449:ALA:HA	1.79	0.64
1:A:692:SER:HB3	1:A:828:LEU:HD21	1.78	0.64
16:G:111:HIS:ND1	18:Z:510:GLU:CD	2.54	0.64
1:A:70:ARG:NH1	1:A:75:ALA:O	2.30	0.64
1:A:863:ARG:HG2	1:A:1414:ILE:HG22	1.78	0.64
1:A:1099:ALA:HA	1:A:1102:MET:HE3	1.78	0.64
1:A:406:VAL:HG13	1:A:429:LEU:HD21	1.79	0.64
2:M:483:PRO:CG	16:G:32:THR:OG1	2.45	0.64
2:M:285:ASP:N	2:M:561:PHE:CG	2.60	0.64
2:M:422:ARG:HH21	2:M:559:PHE:HZ	1.46	0.64
2:M:38:GLN:HE22	2:M:243:GLN:HB2	1.63	0.64
6:C:37:VAL:HG13	6:C:41:GLU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:67:ARG:NH1	11:J:3:ILE:O	2.29	0.64
7:E:61:LEU:HD11	7:E:71:GLN:HB3	1.79	0.64
18:Z:339:LEU:HD11	18:Z:629:LEU:CD1	2.28	0.64
5:B:509:VAL:HG11	5:B:524:LYS:HD3	1.79	0.63
16:G:18:PHE:HA	16:G:22:LEU:HD13	1.79	0.63
16:G:117:MET:HB3	16:G:128:TYR:HD1	1.62	0.63
2:M:277:ASP:CA	2:M:553:VAL:CG2	2.76	0.63
2:M:463:SER:O	2:M:518:LYS:CD	2.46	0.63
14:P:35:A:H5'	14:P:35:A:N3	2.12	0.63
4:T:27:DT:OP1	5:B:1085:ARG:HD3	1.98	0.63
4:T:30:DG:H5''	5:B:747:LEU:CD1	2.29	0.63
5:B:859:ARG:HH22	18:Z:738:SER:HG	1.45	0.63
18:Z:512:LYS:CE	18:Z:557:THR:HG23	2.19	0.63
1:A:36:VAL:HG21	1:A:73:THR:HG21	1.81	0.63
1:A:87:HIS:NE2	1:A:89:GLU:OE2	2.31	0.63
2:M:233:LEU:HD22	2:M:346:MET:HG3	1.79	0.63
1:A:704:ASN:O	1:A:708:LYS:HG2	1.98	0.63
2:M:467:VAL:HB	2:M:537:ASN:HD21	1.63	0.63
2:M:278:LYS:H	2:M:551:ASN:ND2	1.97	0.63
7:E:72:MET:SD	7:E:101:ARG:HG3	2.39	0.63
13:L:27:GLU:H	13:L:37:ARG:HH22	1.47	0.63
2:M:38:GLN:CG	2:M:243:GLN:N	2.62	0.63
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.80	0.62
2:M:38:GLN:CG	2:M:243:GLN:H	2.12	0.62
1:A:1476:ASP:HB2	8:F:105:ILE:HG23	1.80	0.62
2:M:419:CYS:CB	2:M:559:PHE:CZ	2.82	0.62
2:M:358:ARG:CG	2:M:409:SER:HB3	2.29	0.62
2:M:284:LEU:CB	2:M:558:LEU:HB2	2.23	0.62
2:M:312:MET:HE1	2:M:346:MET:HE1	1.79	0.62
18:Z:469:ARG:HD2	18:Z:515:PRO:CG	2.30	0.62
18:Z:496:GLU:N	18:Z:555:ARG:CZ	2.55	0.62
1:A:289:GLN:NE2	1:A:293:ASN:OD1	2.33	0.62
2:M:281:ILE:CG2	2:M:557:MET:HE2	2.30	0.62
5:B:629:GLU:HG2	5:B:634:LEU:HD21	1.82	0.62
2:M:53:TYR:OH	18:Z:642:HIS:CE1	2.53	0.62
5:B:859:ARG:CD	18:Z:737:HIS:CA	2.45	0.62
16:G:112:SER:HB2	18:Z:493:VAL:HG11	1.79	0.62
16:G:144:ARG:NH2	16:G:170:LEU:O	2.32	0.62
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.80	0.62
5:B:88:PHE:HB3	5:B:128:ILE:HG23	1.81	0.62
5:B:952:GLU:HB2	6:C:36:ARG:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:145:LEU:HD21	16:G:161:GLY:HA3	1.81	0.62
16:G:146:LYS:NZ	16:G:147:ILE:O	2.33	0.62
2:M:332:ASP:HB3	2:M:335:MET:HE3	1.80	0.61
17:Y:94:PRO:HD2	17:Y:97:ILE:HD12	1.81	0.61
18:Z:479:LYS:HG3	18:Z:489:THR:HG22	1.81	0.61
18:Z:496:GLU:N	18:Z:555:ARG:NE	2.47	0.61
2:M:284:LEU:HB2	2:M:558:LEU:HB2	1.82	0.61
1:A:689:ILE:HG21	5:B:985:LEU:HD22	1.82	0.61
2:M:281:ILE:HD11	2:M:557:MET:CB	2.26	0.61
2:M:287:LYS:HB2	2:M:288:PRO:CD	2.30	0.61
4:T:28:DG:C6	14:P:44:A:C6	2.88	0.61
5:B:289:ILE:HG12	5:B:297:MET:HB3	1.83	0.61
11:J:18:TRP:NE1	11:J:54:ASP:OD1	2.34	0.61
15:D:67:TYR:HA	15:D:70:ARG:HH12	1.66	0.61
1:A:54:LEU:O	1:A:61:ARG:NH2	2.34	0.61
18:Z:339:LEU:CD2	18:Z:630:VAL:HG22	2.30	0.61
5:B:298:MET:HB3	10:I:14:ILE:HD12	1.81	0.61
13:L:29:LYS:HA	13:L:29:LYS:HE3	1.82	0.61
2:M:278:LYS:NZ	2:M:552:PRO:HD2	2.14	0.61
6:C:32:ASN:OD1	6:C:35:ARG:NH2	2.33	0.61
1:A:470:MET:HE3	1:A:521:VAL:HG23	1.82	0.61
1:A:930:LEU:HD23	1:A:939:VAL:HG22	1.83	0.61
2:M:421:SER:O	2:M:424:LEU:HB2	2.00	0.61
5:B:549:SER:OG	5:B:577:HIS:NE2	2.25	0.61
15:D:100:LEU:HD11	15:D:118:LEU:HD11	1.83	0.61
16:G:95:VAL:HG11	18:Z:509:HIS:HA	1.83	0.61
2:M:38:GLN:NE2	2:M:243:GLN:H	1.98	0.60
7:E:24:ARG:NH2	7:E:182:TYR:O	2.29	0.60
16:G:110:ARG:HH22	16:G:118:GLU:HA	1.66	0.60
1:A:1189:ASP:HA	1:A:1192:TRP:HD1	1.66	0.60
2:M:281:ILE:HB	2:M:553:VAL:HG11	1.76	0.60
5:B:242:ARG:HA	5:B:242:ARG:HH11	1.66	0.60
14:P:34:G:C8	14:P:34:G:OP2	2.54	0.60
15:D:34:ASN:H	15:D:102:ASN:HD21	1.49	0.60
2:M:543:MET:O	2:M:547:ASN:ND2	2.34	0.60
6:C:9:VAL:HG22	6:C:23:ILE:HG12	1.83	0.60
6:C:67:ARG:NH2	6:C:149:LEU:O	2.32	0.60
1:A:556:GLU:OE1	1:A:583:ARG:NH1	2.34	0.60
1:A:623:PRO:HA	9:H:27:ARG:HH21	1.66	0.60
2:M:69:ASN:OD1	2:M:535:PHE:CE1	2.54	0.60
5:B:604:ILE:HG12	5:B:668:LEU:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:281:ILE:HD11	2:M:557:MET:CA	2.31	0.60
5:B:859:ARG:HG2	18:Z:737:HIS:CE1	2.37	0.60
9:H:106:THR:OG1	9:H:107:GLU:OE1	2.20	0.60
2:M:419:CYS:CB	2:M:559:PHE:HZ	2.13	0.60
8:F:82:GLU:O	8:F:95:LYS:NZ	2.35	0.60
18:Z:339:LEU:HD22	18:Z:630:VAL:H	1.66	0.60
2:M:90:GLN:CD	2:M:535:PHE:CE1	2.79	0.60
2:M:419:CYS:HB3	2:M:422:ARG:HH21	1.67	0.60
5:B:626:LEU:HD23	5:B:662:VAL:HG12	1.84	0.60
10:I:88:LYS:HE2	10:I:121:HIS:HB2	1.83	0.60
1:A:540:ASP:OD2	5:B:790:GLN:HG2	2.02	0.60
1:A:801:GLY:HA3	5:B:503:ASN:HB2	1.83	0.60
5:B:48:ASP:OD1	5:B:158:SER:OG	2.19	0.60
8:F:51:ARG:NH2	8:F:122:GLU:OE2	2.32	0.60
18:Z:371:PHE:N	18:Z:630:VAL:CG1	2.65	0.60
18:Z:484:ARG:H	18:Z:552:ARG:NH1	1.99	0.60
1:A:727:PRO:HA	1:A:736:THR:HG21	1.83	0.60
2:M:246:THR:HG22	2:M:248:PRO:CD	2.32	0.60
5:B:506:TRP:NE1	5:B:697:GLU:OE2	2.29	0.60
5:B:242:ARG:HA	5:B:242:ARG:NH1	2.17	0.59
6:C:183:ALA:HB3	6:C:232:ASN:HB3	1.84	0.59
18:Z:306:LYS:HA	18:Z:372:LEU:O	2.01	0.59
18:Z:371:PHE:HA	18:Z:630:VAL:HG11	1.83	0.59
1:A:22:GLN:HB3	5:B:1172:MET:HE1	1.83	0.59
1:A:912:SER:HB3	1:A:915:ALA:H	1.67	0.59
15:D:36:GLU:HA	15:D:39:MET:HG2	1.84	0.59
5:B:817:GLN:HB3	5:B:918:PHE:HD1	1.68	0.59
8:F:78:PRO:HG2	16:G:19:GLY:HA2	1.83	0.59
1:A:561:MET:HE2	12:K:58:PHE:HA	1.83	0.59
2:M:482:LEU:HD13	16:G:28:GLN:HB2	1.84	0.59
5:B:75:SER:CA	18:Z:202:ALA:O	2.45	0.59
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.85	0.59
2:M:276:MET:CE	2:M:558:LEU:HD22	2.31	0.59
5:B:117:ASN:HA	5:B:189:GLY:HA3	1.84	0.59
16:G:160:ILE:CG2	18:Z:491:LEU:HD12	2.29	0.59
1:A:514:GLU:OE1	5:B:1101:GLN:HB3	2.03	0.59
1:A:790:GLN:HA	1:A:822:PHE:HA	1.85	0.59
2:M:363:ASP:OD1	2:M:448:TYR:HD1	1.86	0.59
15:D:41:LEU:HD22	15:D:61:PHE:HE1	1.68	0.59
1:A:757:GLN:HA	1:A:760:LEU:HD12	1.84	0.59
2:M:281:ILE:CG1	2:M:558:LEU:CA	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:677:MET:H	5:B:682:LEU:HD22	1.68	0.59
1:A:552:ASP:HB2	9:H:24:ARG:HB2	1.85	0.58
1:A:610:PRO:HG2	1:A:613:GLU:HB2	1.85	0.58
1:A:1130:ILE:HG21	1:A:1411:LEU:HD13	1.85	0.58
2:M:276:MET:HG3	2:M:553:VAL:HG11	1.80	0.58
2:M:329:PHE:HD2	2:M:331:LYS:H	1.49	0.58
4:T:30:DG:C2	14:P:42:C:C2	2.91	0.58
6:C:44:ILE:HG21	6:C:178:PRO:HB3	1.84	0.58
1:A:369:PRO:HB3	1:A:486:LEU:HD21	1.85	0.58
2:M:276:MET:CG	2:M:553:VAL:CB	2.78	0.58
15:D:38:HIS:ND1	15:D:68:THR:HG23	2.17	0.58
2:M:277:ASP:C	2:M:553:VAL:HG22	2.20	0.58
2:M:505:LYS:HE2	15:D:56:GLU:CB	2.25	0.58
5:B:332:LYS:O	5:B:336:ILE:HG12	2.03	0.58
5:B:581:GLU:O	5:B:582:GLN:HG3	2.03	0.58
7:E:111:THR:HG23	7:E:114:ALA:H	1.67	0.58
17:Y:7:PRO:HG3	17:Y:23:LYS:HA	1.84	0.58
3:N:24:DA:C5'	5:B:489:ILE:HD11	2.27	0.58
4:T:30:DG:N1	14:P:42:C:N3	2.51	0.58
15:D:105:PRO:O	15:D:135:GLN:NE2	2.37	0.58
2:M:520:GLU:HG2	2:M:521:ASN:N	2.17	0.58
8:F:57:MET:HE3	8:F:62:ARG:HA	1.86	0.58
5:B:905:ASP:HB2	5:B:924:ARG:HG3	1.85	0.58
15:D:31:THR:O	15:D:84:ARG:NH2	2.30	0.58
1:A:927:GLU:O	1:A:931:ARG:HG2	2.03	0.58
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.37	0.58
6:C:2:PRO:HB3	12:K:54:PRO:HD2	1.85	0.58
17:Y:39:TYR:HA	17:Y:104:ARG:NH1	2.19	0.58
1:A:349:ARG:O	1:A:353:ASN:HB2	2.04	0.57
1:A:532:ARG:NH1	1:A:647:THR:O	2.36	0.57
5:B:954:MET:SD	5:B:955:PRO:HD2	2.45	0.57
5:B:1038:THR:HA	6:C:195:THR:HA	1.86	0.57
16:G:112:SER:OG	18:Z:503:PHE:HZ	1.84	0.57
2:M:285:ASP:CB	2:M:564:ARG:HG2	2.34	0.57
2:M:277:ASP:CA	2:M:553:VAL:HG21	2.34	0.57
2:M:422:ARG:C	2:M:555:LYS:NZ	2.61	0.57
5:B:903:ILE:O	5:B:924:ARG:N	2.37	0.57
7:E:47:LYS:H	7:E:53:PRO:HG3	1.69	0.57
9:H:66:GLU:HA	9:H:84:ARG:HH21	1.69	0.57
16:G:160:ILE:HG23	18:Z:491:LEU:HB2	1.82	0.57
1:A:111:CYS:HA	1:A:118:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ASN:HD22	1:A:430:ARG:HB3	1.70	0.57
2:M:71:SER:OG	2:M:532:ASP:O	2.20	0.57
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.85	0.57
4:T:28:DG:N1	14:P:44:A:C6	2.73	0.57
6:C:234:GLU:OE2	11:J:42:ARG:NH2	2.37	0.57
18:Z:279:VAL:HA	18:Z:386:VAL:HG21	1.87	0.57
2:M:280:ASN:O	2:M:283:LEU:HD12	2.04	0.57
4:T:31:DT:C4	14:P:40:A:N1	2.72	0.57
5:B:859:ARG:CG	18:Z:737:HIS:HA	2.33	0.57
16:G:163:LEU:HA	16:G:168:LEU:HD23	1.85	0.57
1:A:140:ARG:NH1	1:A:234:PHE:O	2.37	0.57
18:Z:496:GLU:N	18:Z:555:ARG:HE	2.03	0.57
1:A:432:HIS:HE1	18:Z:727:ALA:O	1.87	0.57
5:B:956:PHE:HB3	5:B:962:THR:HG22	1.87	0.57
11:J:40:LEU:HD22	11:J:45:CYS:HB3	1.87	0.57
13:L:54:VAL:O	18:Z:738:SER:OG	2.18	0.57
15:D:36:GLU:HB2	15:D:39:MET:HE2	1.87	0.57
5:B:302:LYS:HG3	5:B:303:PRO:HD3	1.87	0.57
5:B:369:VAL:O	5:B:373:LEU:HG	2.04	0.57
5:B:861:SER:HA	5:B:901:THR:HA	1.87	0.57
11:J:54:ASP:OD2	11:J:56:ILE:HG22	2.04	0.57
12:K:85:GLU:HA	12:K:88:THR:HG22	1.86	0.57
13:L:27:GLU:OE2	13:L:29:LYS:NZ	2.33	0.57
15:D:70:ARG:NH1	15:D:70:ARG:HB3	2.20	0.57
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.40	0.56
2:M:90:GLN:OE1	2:M:535:PHE:CD1	2.55	0.56
2:M:505:LYS:HE2	15:D:56:GLU:HB2	1.64	0.56
5:B:191:GLU:OE2	5:B:743:ARG:NH2	2.38	0.56
18:Z:564:TYR:CA	18:Z:637:VAL:CB	2.82	0.56
2:M:34:ARG:NH1	2:M:231:ILE:CG1	2.38	0.56
5:B:193:VAL:HG21	5:B:470:LEU:HD13	1.87	0.56
9:H:85:ALA:HB1	9:H:91:VAL:HG21	1.87	0.56
18:Z:639:LYS:HB2	18:Z:642:HIS:HD2	1.69	0.56
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.40	0.56
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.20	0.56
1:A:972:THR:HG22	1:A:1320:ILE:HG13	1.86	0.56
2:M:285:ASP:CB	2:M:564:ARG:CG	2.83	0.56
4:T:33:DC:H2"	4:T:34:DC:H5"	1.87	0.56
5:B:74:ALA:C	18:Z:202:ALA:CB	2.78	0.56
5:B:1151:MET:CE	5:B:1171:MET:HE1	2.35	0.56
16:G:44:PHE:CZ	16:G:104:MET:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:58:ASP:HB2	17:Y:88:SER:HB3	1.87	0.56
2:M:277:ASP:CA	2:M:553:VAL:HG23	2.36	0.56
5:B:310:VAL:HG23	5:B:311:ILE:HD12	1.86	0.56
7:E:97:GLU:HB2	7:E:99:ILE:HG12	1.88	0.56
8:F:105:ILE:HG22	8:F:119:GLY:HA2	1.86	0.56
1:A:1474:LEU:HB2	8:F:105:ILE:HG13	1.88	0.56
2:M:281:ILE:CG1	2:M:558:LEU:CB	2.58	0.56
2:M:505:LYS:NZ	15:D:56:GLU:CA	2.68	0.56
9:H:90:TYR:CE1	9:H:92:MET:HG3	2.41	0.56
16:G:160:ILE:HG22	18:Z:491:LEU:CD1	2.33	0.56
2:M:281:ILE:CD1	2:M:553:VAL:HG13	2.35	0.56
5:B:870:THR:HA	5:B:891:ASP:HA	1.87	0.56
5:B:1115:GLN:HB3	5:B:1148:LEU:HD11	1.88	0.56
18:Z:563:MET:CE	18:Z:618:PHE:N	2.69	0.56
1:A:1123:ARG:NH2	1:A:1360:ASN:OD1	2.39	0.56
7:E:74:VAL:HG12	7:E:103:LEU:HB2	1.88	0.56
1:A:375:ILE:HG12	1:A:666:ARG:HG3	1.87	0.56
5:B:780:VAL:HG12	5:B:965:ILE:HB	1.88	0.56
16:G:44:PHE:CE2	16:G:104:MET:HB2	2.41	0.56
1:A:301:HIS:HE1	18:Z:181:THR:HG23	1.65	0.55
1:A:1147:SER:HA	1:A:1153:ARG:HB2	1.86	0.55
2:M:278:LYS:HE3	2:M:552:PRO:HD3	1.79	0.55
4:T:30:DG:H5''	5:B:747:LEU:HD11	1.88	0.55
14:P:33:A:H3'	14:P:33:A:OP2	2.06	0.55
18:Z:448:ILE:O	18:Z:449:THR:OG1	2.23	0.55
1:A:331:LYS:HB2	4:T:35:DA:OP2	2.07	0.55
1:A:661:GLY:H	1:A:664:ILE:HD12	1.71	0.55
5:B:75:SER:CB	18:Z:202:ALA:CA	2.71	0.55
6:C:103:LEU:HD23	6:C:161:LEU:HD21	1.88	0.55
1:A:922:PHE:HD1	1:A:1052:ARG:HA	1.71	0.55
1:A:66:GLU:OE1	1:A:66:GLU:N	2.39	0.55
2:M:300:TYR:CE2	2:M:314:ASP:HB3	2.42	0.55
16:G:30:LEU:O	16:G:34:VAL:HG22	2.06	0.55
16:G:40:GLY:HA2	16:G:157:ILE:HD11	1.89	0.55
3:N:10:DT:H2'	5:B:823:PHE:HE1	1.69	0.55
5:B:470:LEU:HD11	5:B:478:THR:HG23	1.89	0.55
2:M:278:LYS:N	2:M:551:ASN:ND2	2.55	0.55
2:M:282:LYS:CB	2:M:561:PHE:CE2	2.84	0.55
2:M:376:ASP:HB3	2:M:379:VAL:HG23	1.88	0.55
5:B:286:GLU:HB3	5:B:558:PRO:HG2	1.88	0.55
1:A:104:MET:HG2	1:A:198:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:MET:HE2	7:E:134:GLU:HA	1.88	0.55
1:A:1429:LYS:HG3	1:A:1438:VAL:HG11	1.89	0.55
2:M:72:ARG:HH11	2:M:230:ALA:H	1.35	0.55
2:M:481:LEU:HD23	16:G:17:TYR:CE1	2.33	0.55
5:B:801:VAL:HG13	5:B:929:PRO:HD2	1.88	0.55
5:B:837:CYS:HB2	5:B:840:MET:HE3	1.87	0.55
6:C:47:ILE:HD11	6:C:68:LEU:HB3	1.89	0.55
16:G:91:GLN:HB3	16:G:98:PHE:HB2	1.88	0.55
18:Z:272:ASN:HD21	18:Z:384:GLU:HB2	1.70	0.55
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.88	0.55
2:M:155:THR:HG23	18:Z:606:PRO:O	2.06	0.55
5:B:628:VAL:HG22	5:B:633:LEU:HD23	1.89	0.55
13:L:46:LYS:O	13:L:47:LYS:HG2	2.07	0.55
2:M:284:LEU:HB3	2:M:558:LEU:O	2.07	0.55
2:M:422:ARG:NH1	2:M:559:PHE:CE2	2.68	0.55
2:M:481:LEU:HB3	16:G:17:TYR:CZ	2.22	0.55
5:B:721:ARG:HD2	5:B:975:ARG:HB3	1.89	0.55
5:B:816:GLU:OE2	5:B:869:LYS:NZ	2.25	0.55
18:Z:565:GLY:HA3	18:Z:637:VAL:CG1	2.37	0.55
2:M:333:LEU:O	2:M:395:LYS:HE3	2.06	0.55
9:H:10:PHE:CE1	9:H:32:SER:HB2	2.42	0.55
15:D:38:HIS:HE1	15:D:69:ALA:HB2	1.72	0.55
18:Z:471:TYR:C	18:Z:472:PHE:CG	2.85	0.55
1:A:441:GLN:NE2	1:A:444:TYR:OH	2.41	0.54
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.88	0.54
1:A:935:GLN:O	1:A:939:VAL:HG23	2.07	0.54
2:M:313:ILE:HD12	2:M:313:ILE:N	2.22	0.54
16:G:46:ILE:HD11	16:G:77:PHE:HB2	1.88	0.54
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.89	0.54
5:B:180:ASP:OD2	5:B:184:TYR:OH	2.25	0.54
7:E:149:VAL:O	7:E:192:LYS:N	2.39	0.54
1:A:1054:MET:HE1	1:A:1060:LEU:HD12	1.89	0.54
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.89	0.54
14:P:31:G:N3	14:P:31:G:C2'	2.70	0.54
5:B:841:ARG:HE	14:P:34:G:H4'	1.72	0.54
5:B:859:ARG:CD	18:Z:737:HIS:CG	2.89	0.54
16:G:111:HIS:CE1	18:Z:510:GLU:HB3	2.42	0.54
5:B:74:ALA:O	18:Z:202:ALA:HB1	2.07	0.54
16:G:148:VAL:C	18:Z:475:GLY:HA2	2.32	0.54
18:Z:370:GLY:O	18:Z:630:VAL:CG1	2.54	0.54
18:Z:498:ASN:O	18:Z:515:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:ARG:HH22	1:A:936:GLU:HG3	1.73	0.54
5:B:98:HIS:N	5:B:106:SER:O	2.39	0.54
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.89	0.54
1:A:1117:VAL:HG23	1:A:1119:LEU:HG	1.89	0.54
2:M:277:ASP:H	2:M:280:ASN:HB2	1.72	0.54
1:A:865:ILE:HG21	5:B:1092:ASP:CG	2.33	0.54
2:M:358:ARG:HD3	2:M:411:ARG:HD2	1.90	0.54
2:M:505:LYS:HE2	15:D:56:GLU:CG	2.37	0.54
2:M:505:LYS:HZ3	15:D:56:GLU:HB2	1.53	0.54
11:J:6:ARG:HG2	11:J:13:ILE:HD13	1.90	0.54
16:G:110:ARG:C	18:Z:510:GLU:OE2	2.51	0.54
2:M:422:ARG:CA	2:M:555:LYS:NZ	2.71	0.54
2:M:482:LEU:CD2	16:G:29:LYS:CB	2.81	0.54
5:B:86:LEU:HA	5:B:130:LYS:HA	1.90	0.54
5:B:584:MET:HE1	5:B:603:MET:HB3	1.90	0.54
14:P:32:G:N3	14:P:32:G:H5"	2.23	0.54
1:A:432:HIS:CE1	18:Z:727:ALA:O	2.61	0.53
2:M:291:VAL:HG13	2:M:416:PHE:CD1	2.43	0.53
10:I:54:TYR:CE2	10:I:56:ASN:HB2	2.43	0.53
18:Z:371:PHE:N	18:Z:630:VAL:HG12	2.24	0.53
1:A:546:ARG:HD3	1:A:772:SER:HB3	1.89	0.53
2:M:281:ILE:HD11	2:M:558:LEU:H	1.60	0.53
2:M:504:THR:HB	2:M:507:LEU:HG	1.89	0.53
7:E:67:ASP:OD1	7:E:69:THR:OG1	2.22	0.53
1:A:30:GLU:O	1:A:34:MET:HG2	2.08	0.53
2:M:358:ARG:HG3	2:M:409:SER:HB3	1.90	0.53
16:G:119:PHE:HB3	16:G:121:PRO:HD2	1.89	0.53
5:B:152:ILE:HG13	5:B:444:LEU:HD13	1.90	0.53
15:D:32:LEU:HD11	16:G:4:HIS:HB2	1.91	0.53
2:M:276:MET:CG	2:M:553:VAL:HB	2.36	0.53
2:M:285:ASP:CB	2:M:564:ARG:CD	2.78	0.53
2:M:358:ARG:HG2	2:M:409:SER:HB3	1.91	0.53
2:M:463:SER:O	2:M:518:LYS:HG2	2.07	0.53
7:E:64:HIS:ND1	7:E:66:ASP:OD1	2.41	0.53
16:G:162:SER:HB3	18:Z:493:VAL:HG13	1.90	0.53
1:A:130:LEU:HD11	1:A:235:VAL:HG13	1.91	0.53
1:A:1166:LEU:HD13	1:A:1292:MET:HE1	1.91	0.53
2:M:312:MET:HE3	2:M:346:MET:HE3	1.89	0.53
12:K:45:ILE:HB	12:K:94:LEU:HD21	1.90	0.53
5:B:859:ARG:HE	5:B:903:ILE:HD11	1.74	0.53
16:G:118:GLU:N	16:G:129:LYS:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:564:TYR:CE2	18:Z:621:PHE:CD2	2.88	0.53
13:L:26:ASN:ND2	13:L:44:MET:HE1	2.20	0.53
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.89	0.53
1:A:855:ALA:HB3	5:B:494:LYS:HZ2	1.74	0.53
2:M:281:ILE:HD13	2:M:557:MET:HG2	1.89	0.53
2:M:482:LEU:HD11	16:G:25:THR:CB	2.38	0.53
5:B:410:ASN:HA	5:B:413:LYS:HG2	1.90	0.53
16:G:150:THR:H	18:Z:491:LEU:HD21	1.74	0.53
1:A:1105:ASN:HB3	1:A:1107:PHE:CE2	2.44	0.53
2:M:230:ALA:CB	2:M:243:GLN:CD	2.82	0.53
2:M:276:MET:SD	2:M:553:VAL:CB	2.94	0.53
2:M:482:LEU:HD12	16:G:25:THR:HG23	1.78	0.53
5:B:70:GLU:HB2	18:Z:241:GLY:O	2.08	0.53
18:Z:488:ASP:OD1	18:Z:489:THR:N	2.42	0.53
8:F:73:ILE:HD12	8:F:79:VAL:HG12	1.91	0.52
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.90	0.52
18:Z:499:PHE:CE2	18:Z:572:HIS:HE1	2.28	0.52
2:M:291:VAL:HG13	2:M:416:PHE:CE1	2.44	0.52
1:A:460:ARG:HB2	1:A:501:MET:HE2	1.92	0.52
2:M:417:ASP:CG	2:M:418:ILE:H	2.16	0.52
2:M:482:LEU:HG	16:G:25:THR:HG22	1.91	0.52
6:C:175:LYS:HZ3	13:L:57:ALA:HB3	1.75	0.52
1:A:29:ASP:OD1	1:A:30:GLU:N	2.42	0.52
1:A:45:GLU:OE1	1:A:53:LYS:NZ	2.43	0.52
1:A:455:ILE:HD13	1:A:516:GLN:HB2	1.91	0.52
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.42	0.52
5:B:545:LEU:HB3	5:B:550:MET:SD	2.48	0.52
5:B:854:ILE:HD11	5:B:866:ILE:HA	1.90	0.52
1:A:448:ARG:NH2	1:A:454:ASP:OD1	2.37	0.52
2:M:346:MET:HE2	2:M:359:TYR:HD1	1.75	0.52
6:C:56:SER:OG	6:C:158:GLU:N	2.31	0.52
6:C:175:LYS:NZ	13:L:57:ALA:HB3	2.24	0.52
9:H:3:GLY:O	9:H:84:ARG:NH1	2.42	0.52
12:K:82:SER:HB3	12:K:85:GLU:HG2	1.92	0.52
18:Z:512:LYS:NZ	18:Z:557:THR:HG21	2.25	0.52
1:A:491:PRO:HG3	1:A:534:VAL:HG12	1.90	0.52
1:A:828:LEU:HD22	5:B:978:ILE:HG21	1.92	0.52
6:C:15:THR:HG22	6:C:17:GLU:H	1.74	0.52
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.90	0.52
1:A:734:ARG:NH1	1:A:815:TYR:OH	2.43	0.52
1:A:1344:MET:HE1	7:E:137:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:10:DT:H3'	5:B:823:PHE:CD2	2.41	0.52
1:A:364:ARG:HD2	5:B:1084:LEU:HD11	1.92	0.52
2:M:285:ASP:N	2:M:561:PHE:CE1	2.45	0.52
4:T:28:DG:O6	14:P:44:A:N6	2.43	0.52
5:B:283:ASP:OD1	5:B:284:ILE:N	2.42	0.52
3:N:10:DT:H3'	5:B:823:PHE:CG	2.45	0.52
1:A:496:PHE:CD2	5:B:791:GLU:HB3	2.45	0.52
1:A:502:ASN:HB2	5:B:1084:LEU:HG	1.92	0.52
2:M:286:LEU:CD1	2:M:561:PHE:CE2	2.90	0.52
2:M:464:LEU:N	2:M:465:ASN:O	2.33	0.52
7:E:91:CYS:O	7:E:94:MET:HB2	2.10	0.52
16:G:145:LEU:HD23	16:G:146:LYS:N	2.24	0.52
1:A:466:LYS:HA	5:B:1093:CYS:SG	2.50	0.51
1:A:861:GLN:NE2	1:A:1096:GLY:O	2.42	0.51
6:C:9:VAL:HG11	12:K:105:PHE:HD1	1.75	0.51
2:M:281:ILE:HD12	2:M:553:VAL:CG1	2.38	0.51
16:G:97:LEU:HB3	16:G:108:ILE:HG22	1.91	0.51
1:A:90:LEU:HA	1:A:287:ASN:HD21	1.74	0.51
1:A:107:LEU:HD21	1:A:221:VAL:HG13	1.91	0.51
1:A:367:ILE:HD13	1:A:501:MET:HE3	1.92	0.51
1:A:554:PHE:HB3	1:A:585:LEU:HD23	1.92	0.51
1:A:1005:HIS:HB3	1:A:1008:LYS:HG2	1.91	0.51
2:M:38:GLN:HE22	2:M:243:GLN:CB	2.15	0.51
2:M:245:THR:HG22	2:M:245:THR:O	2.11	0.51
18:Z:339:LEU:CD2	18:Z:630:VAL:H	2.21	0.51
18:Z:471:TYR:O	18:Z:472:PHE:CD1	2.63	0.51
18:Z:552:ARG:HB3	18:Z:559:GLN:HB2	1.92	0.51
1:A:496:PHE:HD2	5:B:791:GLU:HB3	1.75	0.51
1:A:556:GLU:CD	1:A:583:ARG:HH12	2.19	0.51
5:B:783:ALA:HB2	5:B:1041:ILE:HG23	1.92	0.51
5:B:1040:GLN:NE2	6:C:196:VAL:O	2.40	0.51
18:Z:184:CYS:SG	18:Z:185:LYS:N	2.83	0.51
18:Z:370:GLY:C	18:Z:630:VAL:HG12	2.35	0.51
5:B:427:LYS:HG3	5:B:428:ASP:H	1.76	0.51
7:E:152:THR:O	7:E:156:VAL:HG23	2.11	0.51
18:Z:512:LYS:NZ	18:Z:557:THR:CG2	2.73	0.51
18:Z:595:HIS:N	18:Z:598:ASP:OD2	2.29	0.51
1:A:18:ILE:HD12	5:B:1171:MET:HB2	1.92	0.51
1:A:74:CYS:SG	1:A:84:HIS:CE1	3.00	0.51
1:A:77:ASN:OD1	1:A:78:MET:N	2.35	0.51
2:M:275:SER:O	2:M:280:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:399:LEU:HB3	5:B:453:TRP:CZ2	2.45	0.51
5:B:1076:GLU:OE2	5:B:1080:ARG:NH2	2.44	0.51
12:K:46:ILE:HG21	12:K:73:ILE:HD13	1.93	0.51
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.46	0.51
1:A:275:ASP:HB3	1:A:336:LEU:HD22	1.92	0.51
4:T:28:DG:N1	14:P:44:A:N1	2.59	0.51
15:D:105:PRO:HB2	15:D:131:LEU:HD21	1.93	0.51
17:Y:7:PRO:HB3	17:Y:24:THR:HG23	1.92	0.51
1:A:1052:ARG:O	1:A:1056:GLU:HG2	2.11	0.51
2:M:244:VAL:O	2:M:250:LEU:HD13	2.11	0.51
7:E:24:ARG:HH12	7:E:103:LEU:HD11	1.74	0.51
1:A:350:VAL:HG11	1:A:1435:THR:HG21	1.91	0.51
5:B:789:ASN:HA	5:B:793:SER:HB2	1.91	0.51
18:Z:564:TYR:HA	18:Z:637:VAL:HG21	0.68	0.51
1:A:188:GLN:HE22	1:A:190:ARG:HA	1.77	0.50
1:A:790:GLN:HB2	1:A:822:PHE:HD1	1.75	0.50
2:M:481:LEU:HD21	16:G:16:ARG:CG	2.42	0.50
5:B:483:ARG:NH2	5:B:527:ALA:O	2.44	0.50
1:A:1189:ASP:HA	1:A:1192:TRP:CD1	2.47	0.50
6:C:134:ASN:OD1	6:C:145:GLN:NE2	2.44	0.50
7:E:117:SER:HB2	7:E:121:MET:HE1	1.93	0.50
2:M:438:ASP:O	2:M:460:LYS:HG3	2.11	0.50
2:M:463:SER:C	2:M:465:ASN:O	2.53	0.50
5:B:67:LEU:HB3	5:B:420:GLN:OE1	2.12	0.50
5:B:584:MET:SD	5:B:605:ARG:HB2	2.51	0.50
18:Z:474:MET:HA	18:Z:492:ILE:HG13	1.94	0.50
18:Z:564:TYR:HB3	18:Z:621:PHE:CE1	2.22	0.50
1:A:811:ILE:HD11	10:I:78:LEU:C	2.37	0.50
2:M:34:ARG:HD3	2:M:231:ILE:CG2	2.41	0.50
4:T:32:DT:H4'	5:B:450:THR:HG22	1.93	0.50
13:L:41:TYR:CE2	13:L:43:ILE:HB	2.46	0.50
1:A:375:ILE:HD13	1:A:669:TYR:HD2	1.76	0.50
1:A:910:LYS:HB3	1:A:1328:PHE:CE2	2.46	0.50
5:B:601:VAL:HG22	5:B:616:THR:HG23	1.92	0.50
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.42	0.50
5:B:35:ASP:OD2	5:B:646:ARG:NH2	2.45	0.50
5:B:956:PHE:CE2	6:C:184:PHE:HB3	2.46	0.50
9:H:111:ARG:HA	9:H:128:ASP:HA	1.94	0.50
16:G:35:GLU:OE2	16:G:47:ALA:HA	2.11	0.50
1:A:274:ASP:OD1	1:A:275:ASP:N	2.45	0.50
2:M:150:GLU:CG	18:Z:336:PRO:CG	2.61	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:350:ARG:HA	2:M:354:GLN:O	2.11	0.50
2:M:418:ILE:HG23	2:M:559:PHE:HD1	1.73	0.50
5:B:505:LEU:HD22	5:B:509:VAL:HB	1.93	0.50
5:B:931:ILE:HA	5:B:945:CYS:HB3	1.94	0.50
15:D:34:ASN:O	15:D:68:THR:OG1	2.29	0.50
18:Z:548:GLY:HA2	18:Z:562:ASN:HA	1.93	0.50
2:M:247:GLN:N	2:M:248:PRO:HD2	2.27	0.50
9:H:75:TYR:CZ	9:H:77:PRO:HG3	2.47	0.50
18:Z:369:LYS:O	18:Z:627:LYS:O	2.30	0.50
1:A:185:GLY:H	1:A:187:TYR:HE1	1.60	0.50
1:A:316:THR:HA	1:A:319:ASP:O	2.12	0.50
13:L:37:ARG:HG3	13:L:38:GLU:OE1	2.12	0.50
2:M:418:ILE:O	2:M:421:SER:OG	2.26	0.49
2:M:515:ILE:HG22	2:M:529:GLN:HG2	1.94	0.49
9:H:25:VAL:HG21	9:H:121:LEU:HD22	1.92	0.49
15:D:38:HIS:CE1	15:D:69:ALA:HB2	2.47	0.49
18:Z:361:PHE:O	18:Z:365:ARG:HB2	2.12	0.49
1:A:461:GLN:NE2	5:B:1090:GLU:OE2	2.45	0.49
1:A:533:PRO:O	1:A:647:THR:OG1	2.25	0.49
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.94	0.49
1:A:1139:LEU:HB3	1:A:1141:VAL:HG23	1.94	0.49
2:M:482:LEU:CD2	16:G:29:LYS:H	2.23	0.49
5:B:75:SER:N	18:Z:202:ALA:CB	2.75	0.49
5:B:726:SER:O	5:B:730:LYS:NZ	2.45	0.49
7:E:104:ILE:HD11	7:E:127:LEU:HD12	1.94	0.49
8:F:80:MET:HG3	8:F:103:PRO:HD3	1.94	0.49
9:H:7:GLU:OE1	9:H:59:VAL:HG22	2.12	0.49
15:D:103:LEU:HD13	15:D:114:LEU:HD13	1.94	0.49
1:A:460:ARG:NH2	14:P:46:U:O2'	2.43	0.49
2:M:471:LEU:HD13	2:M:489:LEU:HD23	1.94	0.49
5:B:589:LYS:O	5:B:593:GLN:HG3	2.11	0.49
9:H:130:ASN:OD1	9:H:131:ASN:N	2.45	0.49
1:A:330:GLN:HG2	1:A:331:LYS:H	1.75	0.49
1:A:983:LEU:HD12	1:A:1044:HIS:ND1	2.27	0.49
2:M:277:ASP:HB2	2:M:551:ASN:CG	2.37	0.49
2:M:312:MET:C	2:M:313:ILE:HD12	2.36	0.49
4:T:30:DG:H5''	5:B:747:LEU:HD12	1.93	0.49
5:B:513:GLU:OE2	5:B:525:ASN:ND2	2.46	0.49
17:Y:71:VAL:HG13	18:Z:264:LEU:HD11	1.94	0.49
18:Z:563:MET:HE1	18:Z:617:LEU:CA	2.40	0.49
2:M:466:SER:N	2:M:517:CYS:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:240:ARG:HB2	6:C:243:THR:HG22	1.95	0.49
13:L:54:VAL:CG2	18:Z:721:ILE:HB	2.42	0.49
1:A:1323:THR:OG1	1:A:1325:ASP:OD1	2.29	0.49
2:M:231:ILE:HG21	2:M:234:GLU:HG3	1.95	0.49
2:M:236:VAL:HG23	2:M:348:ILE:HD13	1.94	0.49
2:M:332:ASP:CB	2:M:335:MET:HE3	2.42	0.49
2:M:506:GLU:HA	2:M:509:GLN:HE22	1.76	0.49
16:G:162:SER:HB2	18:Z:493:VAL:HG13	1.95	0.49
1:A:340:LYS:HE3	1:A:1436:VAL:HG21	1.95	0.49
5:B:276:LEU:HD21	5:B:358:GLU:O	2.13	0.49
15:D:41:LEU:HD22	15:D:61:PHE:CE1	2.47	0.49
15:D:67:TYR:CE1	16:G:101:ILE:HD12	2.47	0.49
18:Z:466:GLN:OE1	18:Z:466:GLN:N	2.38	0.49
18:Z:471:TYR:CG	18:Z:472:PHE:N	2.81	0.49
2:M:300:TYR:HA	2:M:313:ILE:O	2.11	0.49
5:B:859:ARG:HH22	18:Z:738:SER:N	1.91	0.49
16:G:164:MET:HE1	18:Z:493:VAL:CG1	2.43	0.49
18:Z:280:ARG:HH21	18:Z:288:ASP:HB3	1.78	0.49
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.94	0.49
2:M:459:TRP:NE1	2:M:553:VAL:O	2.46	0.49
5:B:220:GLU:HB3	5:B:236:TRP:CD1	2.48	0.49
6:C:221:ASP:OD1	6:C:221:ASP:N	2.46	0.49
15:D:94:LYS:HA	15:D:97:LEU:HD13	1.95	0.49
5:B:260:LEU:HD11	5:B:347:MET:HB2	1.93	0.49
12:K:35:ILE:HB	12:K:71:ILE:HG22	1.94	0.49
1:A:1027:ASP:O	1:A:1031:ARG:HG2	2.13	0.48
2:M:281:ILE:O	2:M:561:PHE:CD1	2.66	0.48
5:B:1119:CYS:SG	5:B:1142:ASN:ND2	2.86	0.48
6:C:59:LEU:HD12	6:C:151:VAL:HG23	1.95	0.48
9:H:100:GLU:O	9:H:113:SER:N	2.45	0.48
1:A:1040:LEU:HB2	7:E:201:GLY:N	2.28	0.48
2:M:161:PRO:HD3	18:Z:608:SER:OG	2.13	0.48
2:M:276:MET:HG2	2:M:553:VAL:CG2	2.44	0.48
5:B:177:CYS:HB3	5:B:180:ASP:HB2	1.94	0.48
9:H:128:ASP:OD1	9:H:131:ASN:ND2	2.46	0.48
13:L:34:ILE:O	13:L:35:ARG:HD2	2.12	0.48
18:Z:471:TYR:C	18:Z:472:PHE:CD2	2.91	0.48
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.94	0.48
1:A:732:THR:HG22	1:A:733:LEU:H	1.77	0.48
1:A:1443:ALA:HB2	5:B:1167:ILE:HG23	1.94	0.48
2:M:462:PRO:C	2:M:465:ASN:CB	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:24:DA:OP1	5:B:489:ILE:CD1	2.58	0.48
5:B:587:LEU:HD13	5:B:603:MET:HG2	1.94	0.48
7:E:29:THR:HG23	7:E:32:GLU:H	1.79	0.48
7:E:117:SER:O	7:E:120:ASP:N	2.45	0.48
13:L:54:VAL:HB	18:Z:721:ILE:HB	1.95	0.48
15:D:105:PRO:HG3	15:D:114:LEU:HD12	1.95	0.48
16:G:150:THR:OG1	18:Z:477:HIS:CE1	2.66	0.48
17:Y:39:TYR:HA	17:Y:104:ARG:HH12	1.77	0.48
1:A:407:ARG:HG2	1:A:407:ARG:HH11	1.78	0.48
1:A:435:PRO:HA	1:A:438:LEU:HD23	1.94	0.48
1:A:1475:LEU:HG	16:G:59:ILE:HD11	1.96	0.48
10:I:83:ASP:OD1	10:I:84:HIS:N	2.47	0.48
15:D:37:VAL:O	15:D:41:LEU:HG	2.13	0.48
16:G:123:SER:OG	16:G:125:PRO:O	2.22	0.48
1:A:739:ASN:HB3	1:A:743:ARG:HH21	1.78	0.48
1:A:1030:SER:OG	7:E:162:ARG:NE	2.36	0.48
2:M:358:ARG:HG3	2:M:409:SER:CB	2.43	0.48
5:B:54:SER:HA	5:B:57:ARG:HG2	1.94	0.48
5:B:260:LEU:HD23	5:B:263:ILE:HG13	1.96	0.48
5:B:1071:ASN:HD22	5:B:1071:ASN:C	2.22	0.48
18:Z:371:PHE:N	18:Z:630:VAL:HG11	2.27	0.48
1:A:281:ALA:O	1:A:285:LYS:HG3	2.14	0.48
1:A:561:MET:HG2	12:K:58:PHE:CD1	2.49	0.48
1:A:651:SER:O	1:A:655:ILE:HG12	2.13	0.48
1:A:810:PHE:CZ	1:A:834:THR:HG21	2.48	0.48
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.13	0.48
2:M:475:ARG:HA	2:M:485:ASN:HA	1.94	0.48
1:A:932:ARG:HH12	9:H:103:GLU:HB2	1.77	0.48
2:M:159:ALA:HA	18:Z:608:SER:HB2	1.39	0.48
5:B:1029:TYR:HD2	6:C:184:PHE:HD2	1.62	0.48
9:H:71:ASP:OD1	9:H:71:ASP:N	2.46	0.48
11:J:35:LEU:HD11	11:J:50:LEU:HD12	1.95	0.48
1:A:488:VAL:O	1:A:491:PRO:HD2	2.14	0.48
9:H:6:PHE:HB3	9:H:60:ILE:HB	1.94	0.48
1:A:77:ASN:H	1:A:80:GLU:HB3	1.79	0.48
5:B:617:ASP:N	5:B:617:ASP:OD1	2.47	0.48
7:E:91:CYS:SG	7:E:95:GLN:NE2	2.85	0.48
2:M:278:LYS:HD2	2:M:551:ASN:CB	2.41	0.48
5:B:1163:MET:HA	5:B:1167:ILE:O	2.13	0.48
15:D:34:ASN:ND2	15:D:71:PHE:O	2.47	0.48
1:A:296:ASN:O	18:Z:267:VAL:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:HIS:HD2	1:A:467:MET:HB2	1.78	0.47
2:M:477:GLY:HA3	2:M:483:PRO:HA	1.96	0.47
5:B:50:PHE:HB2	5:B:397:GLY:HA2	1.96	0.47
5:B:751:LEU:HD12	5:B:808:SER:HB3	1.95	0.47
11:J:65:LEU:HD11	13:L:45:TYR:CG	2.49	0.47
1:A:1289:GLU:O	1:A:1292:MET:HG3	2.14	0.47
5:B:508:MET:HA	5:B:530:ALA:HB2	1.95	0.47
5:B:757:PRO:HA	5:B:777:ASN:HD21	1.78	0.47
5:B:956:PHE:HE2	6:C:184:PHE:HB3	1.78	0.47
1:A:109:CYS:HA	1:A:148:CYS:SG	2.54	0.47
1:A:812:LYS:HE2	10:I:77:THR:OG1	2.14	0.47
6:C:260:GLN:HB2	12:K:91:ILE:HG21	1.96	0.47
7:E:94:MET:HE3	7:E:99:ILE:HG13	1.96	0.47
15:D:112:LYS:HZ3	15:D:112:LYS:HB2	1.79	0.47
16:G:81:LYS:HG3	18:Z:475:GLY:HA3	1.96	0.47
18:Z:512:LYS:O	18:Z:554:GLU:HG2	2.14	0.47
1:A:1083:PRO:HD2	8:F:58:THR:HG21	1.96	0.47
1:A:1177:TYR:CD2	10:I:35:LEU:HD13	2.50	0.47
2:M:510:TYR:CE2	2:M:515:ILE:HG21	2.49	0.47
15:D:60:VAL:HG13	16:G:103:PRO:HB3	1.96	0.47
18:Z:564:TYR:OH	18:Z:621:PHE:N	2.37	0.47
1:A:1221:MET:HA	1:A:1221:MET:HE2	1.95	0.47
5:B:829:PHE:HD2	5:B:917:LYS:HD2	1.79	0.47
7:E:101:ARG:HB3	7:E:126:ILE:HG13	1.97	0.47
1:A:199:TYR:HB3	1:A:215:LEU:HA	1.96	0.47
2:M:347:ILE:HD12	2:M:349:ASP:HB2	1.96	0.47
5:B:859:ARG:CG	18:Z:737:HIS:CA	2.93	0.47
5:B:861:SER:HB2	18:Z:735:GLU:CD	2.40	0.47
7:E:54:ARG:O	7:E:58:LEU:HD23	2.15	0.47
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.95	0.47
1:A:351:ARG:NH1	4:T:24:DC:OP1	2.33	0.47
1:A:479:TRP:HB2	1:A:483:ARG:HH21	1.79	0.47
2:M:232:PHE:HB2	2:M:320:PHE:CE2	2.50	0.47
2:M:437:MET:HG3	2:M:437:MET:O	2.15	0.47
5:B:42:GLN:HG2	5:B:43:GLN:N	2.29	0.47
5:B:46:SER:HB3	5:B:397:GLY:H	1.79	0.47
5:B:264:LYS:HE3	5:B:326:ALA:HB2	1.97	0.47
7:E:194:ILE:HG13	7:E:204:ILE:HD12	1.97	0.47
12:K:10:PHE:HA	12:K:37:LYS:HB3	1.96	0.47
14:P:37:G:C8	14:P:37:G:C5'	2.95	0.47
18:Z:278:TRP:HZ3	18:Z:536:TRP:CZ3	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:499:PHE:CZ	18:Z:572:HIS:HE1	2.32	0.47
18:Z:512:LYS:HE2	18:Z:554:GLU:OE1	2.15	0.47
18:Z:563:MET:CE	18:Z:618:PHE:CB	2.84	0.47
1:A:117:LEU:HG	1:A:119:VAL:HG12	1.95	0.47
1:A:375:ILE:HG21	1:A:669:TYR:HD2	1.80	0.47
1:A:539:GLN:HE22	1:A:775:LYS:HE2	1.80	0.47
1:A:1473:LEU:HD12	8:F:104:ILE:HG21	1.96	0.47
2:M:346:MET:CE	2:M:359:TYR:HD1	2.27	0.47
3:N:39:DA:OP2	3:N:39:DA:H8	1.97	0.47
5:B:199:LYS:NZ	5:B:394:ASP:OD1	2.38	0.47
5:B:1119:CYS:HB2	5:B:1137:CYS:SG	2.55	0.47
9:H:64:LEU:O	9:H:84:ARG:N	2.32	0.47
16:G:52:ASP:N	16:G:71:LYS:O	2.47	0.47
18:Z:503:PHE:HD1	18:Z:508:MET:O	1.98	0.47
1:A:852:VAL:O	5:B:494:LYS:NZ	2.48	0.47
1:A:1030:SER:HG	7:E:162:ARG:HE	1.61	0.47
2:M:35:TYR:OH	2:M:230:ALA:N	2.48	0.47
2:M:281:ILE:CG1	2:M:553:VAL:HG13	2.45	0.47
2:M:281:ILE:HG12	2:M:558:LEU:CA	2.45	0.47
2:M:510:TYR:CD2	2:M:515:ILE:HG21	2.50	0.47
5:B:549:SER:HG	5:B:577:HIS:CD2	2.32	0.47
6:C:259:LEU:HD11	12:K:35:ILE:HD12	1.95	0.47
12:K:39:ASP:OD2	12:K:39:ASP:N	2.45	0.47
16:G:165:ASP:OD1	16:G:166:ASP:N	2.48	0.47
1:A:1401:LEU:HD11	1:A:1414:ILE:HD11	1.97	0.47
5:B:16:GLU:HG2	5:B:17:ILE:H	1.79	0.47
5:B:109:MET:HE2	5:B:109:MET:HA	1.97	0.47
5:B:1112:ASP:N	5:B:1112:ASP:OD1	2.45	0.47
16:G:111:HIS:ND1	18:Z:510:GLU:CG	2.78	0.47
1:A:599:HIS:ND1	1:A:632:ASN:OD1	2.48	0.46
1:A:962:ASP:OD2	1:A:1046:ARG:NH2	2.32	0.46
2:M:363:ASP:OD1	2:M:448:TYR:CD1	2.68	0.46
2:M:508:LYS:NZ	15:D:56:GLU:CG	2.77	0.46
5:B:216:ALA:N	5:B:241:ALA:HB2	2.30	0.46
5:B:477:SER:HB2	5:B:730:LYS:HA	1.98	0.46
1:A:62:GLN:HE22	1:A:255:VAL:HG13	1.81	0.46
1:A:379:GLY:HA3	1:A:477:LEU:HD12	1.96	0.46
1:A:551:ARG:HG2	9:H:25:VAL:HG11	1.97	0.46
1:A:1467:GLY:H	1:A:1470:CYS:HB2	1.81	0.46
2:M:255:GLN:O	2:M:259:GLN:HG3	2.14	0.46
2:M:293:TRP:N	2:M:293:TRP:CD1	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:532:ASP:OD2	2:M:532:ASP:N	2.48	0.46
5:B:126:VAL:HG12	5:B:149:ILE:HD11	1.97	0.46
1:A:290:LEU:HD13	1:A:306:ASP:HB3	1.98	0.46
1:A:653:VAL:HG21	1:A:669:TYR:CE1	2.50	0.46
16:G:52:ASP:H	16:G:72:TYR:HA	1.80	0.46
1:A:350:VAL:HA	1:A:354:LEU:HD12	1.97	0.46
1:A:528:PRO:HG2	1:A:1090:LEU:HD11	1.97	0.46
1:A:530:SER:O	1:A:532:ARG:HG3	2.16	0.46
1:A:871:VAL:HB	1:A:1088:GLY:HA3	1.96	0.46
2:M:230:ALA:CB	2:M:243:GLN:OE1	2.62	0.46
2:M:233:LEU:HD21	2:M:348:ILE:HG13	1.97	0.46
2:M:483:PRO:HG2	16:G:32:THR:CB	2.45	0.46
5:B:611:GLU:OE1	5:B:613:ARG:NH1	2.48	0.46
5:B:988:LYS:NZ	5:B:1026:GLU:OE2	2.47	0.46
6:C:259:LEU:HD22	12:K:42:LEU:HD21	1.97	0.46
10:I:86:CYS:HB2	10:I:114:CYS:SG	2.55	0.46
14:P:35:A:N3	14:P:35:A:C5'	2.78	0.46
18:Z:496:GLU:CB	18:Z:555:ARG:CZ	2.93	0.46
18:Z:710:VAL:HG12	18:Z:752:THR:HG22	1.96	0.46
1:A:937:ASP:HA	1:A:940:LYS:NZ	2.30	0.46
1:A:1040:LEU:HB2	7:E:201:GLY:H	1.80	0.46
5:B:1029:TYR:HE2	6:C:185:GLU:HA	1.80	0.46
15:D:32:LEU:CD1	16:G:4:HIS:HB2	2.45	0.46
1:A:552:ASP:HB3	9:H:25:VAL:HG12	1.98	0.46
1:A:813:ASP:OD1	10:I:100:HIS:NE2	2.48	0.46
2:M:482:LEU:CD2	16:G:29:LYS:CA	2.94	0.46
3:N:26:DC:H2'	3:N:27:DT:C6	2.50	0.46
5:B:425:ARG:HD3	5:B:427:LYS:HE3	1.98	0.46
5:B:908:MET:HE2	5:B:920:LYS:HB2	1.98	0.46
1:A:392:GLU:CD	1:A:448:ARG:HE	2.23	0.46
1:A:1290:SER:O	1:A:1293:LEU:HG	2.16	0.46
2:M:481:LEU:HD21	16:G:16:ARG:NH1	2.12	0.46
5:B:719:SER:OG	5:B:720:PRO:HD3	2.16	0.46
5:B:794:VAL:CG2	5:B:965:ILE:HG23	2.45	0.46
5:B:807:ARG:NH1	13:L:58:ARG:O	2.49	0.46
1:A:1221:MET:HE1	1:A:1226:LEU:HB2	1.97	0.46
2:M:53:TYR:OH	18:Z:642:HIS:HE1	1.99	0.46
2:M:312:MET:CE	2:M:346:MET:HE1	2.46	0.46
2:M:528:ARG:NH1	2:M:530:ARG:HG2	2.31	0.46
5:B:126:VAL:O	5:B:147:THR:N	2.46	0.46
5:B:276:LEU:HD22	5:B:362:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:573:TRP:HZ2	5:B:576:ILE:HD11	1.81	0.46
5:B:785:TYR:CZ	5:B:955:PRO:HD3	2.51	0.46
6:C:47:ILE:HG23	6:C:73:LEU:HD11	1.96	0.46
7:E:36:THR:OG1	7:E:39:GLU:OE1	2.21	0.46
16:G:151:ARG:CD	18:Z:505:ASP:HA	2.14	0.46
18:Z:447:LYS:HA	18:Z:464:PRO:HA	1.97	0.46
1:A:1368:VAL:HG12	1:A:1369:LEU:HD12	1.97	0.46
4:T:29:DG:N2	14:P:42:C:O2	2.46	0.46
5:B:34:PHE:HZ	5:B:528:LEU:HB3	1.79	0.46
5:B:780:VAL:HG11	5:B:1048:TYR:CE2	2.50	0.46
6:C:76:ASP:HA	6:C:239:LEU:HD23	1.97	0.46
17:Y:59:GLY:H	18:Z:219:GLU:HB2	1.81	0.46
18:Z:588:ASP:OD1	18:Z:592:ASN:N	2.46	0.46
1:A:57:LEU:HD21	1:A:284:VAL:HG21	1.96	0.46
1:A:85:PHE:CE1	1:A:257:PRO:HD3	2.50	0.46
1:A:495:ASP:N	1:A:499:ASP:OD2	2.43	0.46
2:M:425:LEU:HD22	2:M:555:LYS:HG2	1.45	0.46
7:E:171:PRO:HB2	7:E:207:ARG:HD3	1.97	0.46
10:I:80:ARG:HG2	10:I:95:VAL:HG22	1.98	0.46
14:P:36:G:H1'	14:P:37:G:OP2	2.16	0.46
18:Z:352:VAL:HG23	18:Z:359:LEU:HD21	1.98	0.46
1:A:479:TRP:HB2	5:B:931:ILE:HD11	1.98	0.45
1:A:506:PRO:HB2	1:A:511:THR:HG23	1.98	0.45
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.51	0.45
1:A:855:ALA:HB3	5:B:494:LYS:NZ	2.31	0.45
1:A:1439:LEU:HD13	5:B:1162:LEU:HD21	1.97	0.45
2:M:513:LYS:HE3	2:M:529:GLN:NE2	2.30	0.45
5:B:516:GLU:HG2	5:B:724:TYR:CE1	2.51	0.45
7:E:93:ARG:HA	7:E:96:GLU:HG3	1.98	0.45
8:F:83:LEU:HD12	8:F:85:GLY:H	1.81	0.45
16:G:148:VAL:CA	18:Z:475:GLY:HA2	2.46	0.45
17:Y:23:LYS:NZ	17:Y:32:GLY:O	2.44	0.45
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	1.98	0.45
1:A:1146:GLN:NE2	1:A:1150:ASP:OD2	2.49	0.45
1:A:1281:ASP:OD1	1:A:1282:ASP:N	2.47	0.45
5:B:460:HIS:CE1	5:B:461:GLN:HG3	2.51	0.45
6:C:105:VAL:HG11	6:C:115:VAL:HG22	1.97	0.45
15:D:62:MET:HE2	15:D:62:MET:HA	1.98	0.45
1:A:464:LEU:HD22	1:A:861:GLN:HE22	1.82	0.45
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.52	0.45
1:A:892:GLY:O	1:A:893:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:ASN:O	1:A:1183:SER:OG	2.26	0.45
1:A:1436:VAL:HG23	1:A:1437:ASP:H	1.81	0.45
2:M:281:ILE:HG12	2:M:558:LEU:HA	1.99	0.45
2:M:494:TYR:CZ	2:M:496:ARG:HB2	2.51	0.45
14:P:35:A:H5''	14:P:36:G:H2'	1.97	0.45
16:G:111:HIS:HD2	18:Z:501:ILE:HG21	1.22	0.45
1:A:432:HIS:HE1	18:Z:703:ASN:ND2	2.15	0.45
1:A:481:THR:HG21	5:B:932:GLY:HA3	1.99	0.45
1:A:927:GLU:OE2	1:A:931:ARG:HD3	2.16	0.45
1:A:1163:HIS:NE2	1:A:1302:GLU:OE1	2.49	0.45
2:M:230:ALA:HB3	2:M:243:GLN:CD	2.40	0.45
7:E:106:VAL:HG22	7:E:130:PHE:O	2.16	0.45
9:H:95:LYS:C	9:H:116:VAL:HG23	2.42	0.45
1:A:58:MET:HE3	1:A:58:MET:HB2	1.89	0.45
1:A:906:LEU:HD23	1:A:1044:HIS:HD2	1.81	0.45
2:M:281:ILE:CG1	2:M:558:LEU:N	2.78	0.45
2:M:521:ASN:CG	2:M:522:ASN:H	2.24	0.45
5:B:759:VAL:HG11	5:B:983:GLU:HG3	1.98	0.45
5:B:859:ARG:CG	18:Z:737:HIS:CE1	2.98	0.45
7:E:18:MET:SD	7:E:60:VAL:HG11	2.57	0.45
1:A:803:LYS:O	1:A:812:LYS:NZ	2.49	0.45
1:A:863:ARG:HG3	1:A:1432:PHE:CZ	2.51	0.45
1:A:1139:LEU:HD13	1:A:1359:SER:HA	1.97	0.45
1:A:1479:LYS:HE2	8:F:121:ASP:OD2	2.17	0.45
5:B:341:GLU:HG3	5:B:345:LYS:NZ	2.32	0.45
5:B:670:GLU:HA	5:B:673:VAL:HG12	1.99	0.45
12:K:89:ASN:HA	12:K:92:THR:HG22	1.98	0.45
1:A:480:SER:HB3	12:K:2:ASN:HD22	1.82	0.45
1:A:687:ILE:HD11	1:A:766:PHE:CE1	2.52	0.45
5:B:796:MET:HB2	5:B:948:GLN:HG2	1.99	0.45
5:B:1123:GLY:HA3	5:B:1171:MET:H	1.80	0.45
16:G:107:PHE:CE2	18:Z:503:PHE:CB	2.86	0.45
18:Z:484:ARG:HH11	18:Z:485:PHE:HE1	1.64	0.45
1:A:809:HIS:CD2	5:B:677:MET:HE1	2.52	0.45
1:A:1153:ARG:HH11	1:A:1153:ARG:HG3	1.82	0.45
2:M:284:LEU:CB	2:M:558:LEU:O	2.65	0.45
5:B:1075:MET:HG3	5:B:1076:GLU:H	1.81	0.45
7:E:173:ILE:O	7:E:209:VAL:HA	2.17	0.45
10:I:113:VAL:HG22	10:I:122:ARG:HG2	1.97	0.45
15:D:48:ASN:O	15:D:48:ASN:ND2	2.49	0.45
18:Z:514:LEU:HB3	18:Z:515:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ILE:HG13	9:H:92:MET:HG2	1.97	0.45
2:M:244:VAL:HG23	2:M:250:LEU:HB2	1.99	0.45
2:M:357:PRO:HB2	2:M:408:PHE:HB3	1.98	0.45
12:K:61:TYR:CD2	12:K:71:ILE:HD11	2.52	0.45
16:G:44:PHE:CE1	16:G:157:ILE:HB	2.51	0.45
16:G:107:PHE:HE2	18:Z:503:PHE:HB3	1.75	0.45
1:A:317:MET:HE2	1:A:318:VAL:HG13	1.98	0.45
1:A:343:LEU:HD23	5:B:1161:GLU:OE2	2.17	0.45
1:A:655:ILE:HG23	1:A:985:ARG:HD2	1.98	0.45
1:A:809:HIS:HE2	5:B:506:TRP:NE1	2.15	0.45
1:A:901:VAL:HG12	1:A:980:PRO:HA	1.99	0.45
1:A:1343:LEU:HD22	1:A:1359:SER:OG	2.17	0.45
2:M:284:LEU:CB	2:M:561:PHE:HD1	2.27	0.45
5:B:70:GLU:CB	18:Z:241:GLY:O	2.65	0.45
7:E:44:PHE:O	7:E:52:ARG:HG2	2.17	0.45
9:H:7:GLU:OE1	9:H:7:GLU:HA	2.17	0.45
18:Z:417:GLU:CD	18:Z:516:ARG:NH1	2.68	0.45
2:M:312:MET:CE	2:M:346:MET:CE	2.95	0.44
5:B:529:MET:HG3	5:B:702:MET:HB3	1.99	0.44
9:H:59:VAL:O	9:H:144:LEU:HB2	2.16	0.44
10:I:11:PHE:HA	10:I:55:VAL:HG11	1.99	0.44
11:J:10:CYS:HB2	11:J:44:CYS:SG	2.57	0.44
15:D:73:ARG:O	15:D:138:ARG:NH1	2.49	0.44
15:D:112:LYS:HD2	15:D:119:GLU:HA	1.99	0.44
16:G:90:THR:CG2	16:G:100:GLU:HB2	2.48	0.44
2:M:422:ARG:O	2:M:555:LYS:NZ	2.51	0.44
4:T:32:DT:C4	14:P:39:A:N6	2.65	0.44
6:C:42:VAL:HB	6:C:178:PRO:HG3	1.98	0.44
7:E:84:ILE:HA	7:E:87:ILE:HG12	1.98	0.44
9:H:88:PHE:HA	9:H:146:LYS:HD3	1.98	0.44
16:G:8:GLU:OE2	16:G:71:LYS:HG2	2.17	0.44
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.99	0.44
2:M:115:GLU:O	18:Z:507:THR:CG2	2.66	0.44
2:M:367:PHE:O	2:M:370:GLN:HB2	2.16	0.44
5:B:82:PRO:HB2	5:B:133:ILE:O	2.18	0.44
6:C:189:ASP:O	6:C:191:ALA:N	2.48	0.44
10:I:71:ASP:OD2	10:I:71:ASP:N	2.51	0.44
16:G:43:GLY:HA3	16:G:78:ARG:HB2	1.98	0.44
1:A:137:PRO:HB2	1:A:1445:HIS:HB3	1.98	0.44
1:A:402:LEU:HD22	1:A:446:VAL:HG11	2.00	0.44
1:A:480:SER:HB3	12:K:2:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:GLN:HB3	9:H:93:TYR:CE2	2.53	0.44
1:A:1172:ASN:OD1	1:A:1215:GLU:HB3	2.17	0.44
13:L:54:VAL:HG23	18:Z:721:ILE:HG13	1.97	0.44
18:Z:502:LEU:HD11	18:Z:511:LEU:HD12	1.98	0.44
1:A:24:GLY:O	5:B:1168:ALA:N	2.37	0.44
1:A:459:ASN:HB3	1:A:469:MET:HG2	1.99	0.44
1:A:723:ASN:HD21	10:I:109:ARG:HB2	1.82	0.44
1:A:996:ILE:HG13	1:A:1060:LEU:HD23	1.98	0.44
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.51	0.44
5:B:167:THR:HG23	5:B:170:ASP:H	1.83	0.44
5:B:962:THR:O	11:J:9:THR:HG23	2.17	0.44
10:I:74:GLN:OE1	10:I:74:GLN:N	2.50	0.44
11:J:10:CYS:SG	11:J:42:ARG:NH2	2.90	0.44
1:A:16:ARG:HG3	1:A:16:ARG:HH11	1.83	0.44
1:A:67:ARG:NH1	14:P:35:A:O2'	2.51	0.44
1:A:350:VAL:HG13	1:A:351:ARG:N	2.33	0.44
1:A:739:ASN:HB3	1:A:743:ARG:NH2	2.33	0.44
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	2.00	0.44
2:M:38:GLN:HG2	2:M:243:GLN:N	2.33	0.44
5:B:127:ASP:OD1	5:B:127:ASP:N	2.50	0.44
5:B:566:LYS:HA	5:B:576:ILE:HD13	2.00	0.44
1:A:108:ARG:NH2	1:A:191:ILE:O	2.50	0.44
1:A:545:VAL:HG23	1:A:676:ILE:HG21	2.00	0.44
1:A:775:LYS:HG2	5:B:970:HIS:O	2.18	0.44
2:M:277:ASP:N	2:M:553:VAL:HG21	2.33	0.44
4:T:29:DG:C6	14:P:42:C:N4	2.78	0.44
5:B:311:ILE:HG21	5:B:317:ALA:HB2	2.00	0.44
7:E:24:ARG:NH1	7:E:103:LEU:HD11	2.32	0.44
8:F:86:GLU:H	8:F:86:GLU:CD	2.24	0.44
9:H:39:LEU:HD13	9:H:125:LEU:HD13	1.99	0.44
9:H:63:THR:HG21	9:H:68:GLY:HA2	1.99	0.44
16:G:17:TYR:HB3	16:G:25:THR:HG21	1.99	0.44
16:G:164:MET:HE1	18:Z:493:VAL:HG12	2.00	0.44
18:Z:563:MET:HE3	18:Z:618:PHE:HB2	1.94	0.44
1:A:1325:ASP:OD1	1:A:1325:ASP:N	2.50	0.44
2:M:302:MET:HE3	2:M:302:MET:HB2	1.88	0.44
2:M:452:ARG:NH1	2:M:454:ASP:OD1	2.51	0.44
4:T:31:DT:H4'	5:B:469:VAL:HG21	2.00	0.44
5:B:934:LYS:HG2	5:B:1051:LEU:HD12	1.98	0.44
10:I:87:GLN:HE22	10:I:123:TRP:CB	2.31	0.44
18:Z:371:PHE:CA	18:Z:630:VAL:CG1	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:705:LEU:HG	18:Z:724:VAL:HG21	2.00	0.44
1:A:795:GLY:CA	1:A:1107:PHE:HB3	2.48	0.44
1:A:1247:PHE:HA	1:A:1257:LEU:HA	2.00	0.44
2:M:307:THR:HG23	2:M:308:ASN:N	2.32	0.44
5:B:293:GLU:O	5:B:295:PRO:HD3	2.18	0.44
9:H:88:PHE:CD2	9:H:144:LEU:HB3	2.53	0.44
1:A:539:GLN:NE2	1:A:775:LYS:HE2	2.33	0.43
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.47	0.43
1:A:1377:ALA:O	1:A:1381:GLU:HG2	2.18	0.43
2:M:505:LYS:HZ3	15:D:56:GLU:CA	2.31	0.43
5:B:344:GLN:O	5:B:361:LYS:NZ	2.51	0.43
5:B:563:ASP:O	5:B:610:ARG:NH1	2.51	0.43
5:B:1123:GLY:HA3	5:B:1171:MET:N	2.32	0.43
9:H:25:VAL:HA	9:H:44:ASN:HA	1.99	0.43
9:H:97:TYR:CZ	9:H:115:TYR:HB3	2.53	0.43
10:I:64:GLU:O	10:I:68:ILE:HG12	2.18	0.43
14:P:34:G:H3'	14:P:34:G:P	2.56	0.43
1:A:1020:LEU:HD21	1:A:1073:GLU:HA	1.99	0.43
6:C:123:ASN:OD1	6:C:124:SER:N	2.51	0.43
10:I:12:VAL:HG21	10:I:53:ILE:O	2.17	0.43
11:J:35:LEU:HD22	11:J:40:LEU:HD12	2.00	0.43
12:K:57:LEU:N	12:K:76:GLN:O	2.51	0.43
1:A:212:LYS:HB3	1:A:214:ILE:HG23	2.00	0.43
1:A:621:ILE:HA	9:H:122:LEU:HD13	2.00	0.43
1:A:848:ILE:HA	5:B:520:VAL:HG21	2.00	0.43
1:A:991:GLN:HA	1:A:996:ILE:HG12	1.99	0.43
1:A:1155:LYS:HD2	1:A:1158:LEU:HD23	2.00	0.43
5:B:1062:ARG:NH2	5:B:1066:PRO:O	2.48	0.43
9:H:11:ASP:OD1	9:H:55:LYS:HG3	2.19	0.43
18:Z:482:ALA:HA	18:Z:486:GLU:OE1	2.17	0.43
2:M:293:TRP:H	2:M:293:TRP:HD1	1.65	0.43
5:B:295:PRO:O	5:B:299:GLU:HG2	2.18	0.43
5:B:564:ALA:HB2	5:B:578:LYS:HD3	2.00	0.43
5:B:949:TYR:HB3	5:B:953:ASP:HB2	2.00	0.43
16:G:112:SER:HG	18:Z:503:PHE:HE2	1.50	0.43
16:G:150:THR:H	18:Z:477:HIS:CE1	2.37	0.43
1:A:783:GLN:HA	1:A:787:VAL:O	2.17	0.43
1:A:1036:ASN:OD1	7:E:202:ARG:NH1	2.50	0.43
5:B:50:PHE:HD2	5:B:51:ILE:HG23	1.83	0.43
5:B:359:THR:HG21	5:B:554:GLU:HG3	2.00	0.43
5:B:989:VAL:HG22	5:B:1015:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:66:ASP:OD1	7:E:66:ASP:N	2.51	0.43
16:G:117:MET:SD	16:G:128:TYR:HB3	2.58	0.43
17:Y:60:ILE:HD13	18:Z:190:ARG:HG3	1.99	0.43
1:A:291:ARG:O	1:A:295:GLN:OE1	2.36	0.43
1:A:477:LEU:HD13	1:A:483:ARG:HD2	2.01	0.43
1:A:713:VAL:HG11	1:A:817:PRO:HD3	2.01	0.43
1:A:837:PHE:HB2	5:B:506:TRP:HZ3	1.83	0.43
4:T:10:DT:H2'	4:T:10:DT:OP2	2.17	0.43
5:B:279:VAL:HG13	5:B:312:GLN:O	2.19	0.43
5:B:529:MET:SD	5:B:702:MET:HG3	2.59	0.43
18:Z:613:GLU:O	18:Z:624:LEU:HA	2.18	0.43
1:A:352:GLY:HA2	5:B:1085:ARG:HH22	1.84	0.43
1:A:1451:MET:HE3	1:A:1451:MET:HB3	1.93	0.43
5:B:735:VAL:HG23	5:B:754:PRO:HG2	2.01	0.43
12:K:65:HIS:HE1	12:K:67:LEU:HD12	1.83	0.43
16:G:107:PHE:CE2	18:Z:503:PHE:HD1	2.23	0.43
16:G:111:HIS:CE1	18:Z:510:GLU:HG2	2.53	0.43
18:Z:339:LEU:HD13	18:Z:629:LEU:CA	2.41	0.43
1:A:1177:TYR:OH	1:A:1282:ASP:OD2	2.36	0.43
2:M:268:PHE:HA	2:M:269:PRO:HD2	1.81	0.43
2:M:470:ARG:NH1	2:M:472:LYS:HE3	2.34	0.43
2:M:553:VAL:HA	2:M:557:MET:SD	2.59	0.43
5:B:384:ASP:O	5:B:390:ASN:ND2	2.51	0.43
5:B:387:HIS:CD2	5:B:504:THR:HG21	2.54	0.43
7:E:8:TYR:CZ	7:E:12:LYS:HD2	2.54	0.43
18:Z:469:ARG:HD2	18:Z:515:PRO:CB	2.49	0.43
18:Z:469:ARG:HD2	18:Z:515:PRO:HG3	1.99	0.43
1:A:27:SER:HB2	1:A:30:GLU:HB2	2.01	0.43
1:A:286:ILE:HD11	1:A:309:LEU:HB3	2.01	0.43
1:A:937:ASP:HA	1:A:940:LYS:HZ1	1.84	0.43
1:A:1112:VAL:HG21	1:A:1115:LYS:HB2	2.00	0.43
1:A:1430:CYS:C	1:A:1435:THR:HG22	2.44	0.43
1:A:1458:ILE:HD13	5:B:1091:ARG:HD3	2.00	0.43
2:M:69:ASN:CG	2:M:535:PHE:CZ	2.92	0.43
2:M:346:MET:HE2	2:M:346:MET:HB2	1.78	0.43
5:B:56:GLN:OE1	5:B:91:ILE:HG22	2.19	0.43
5:B:223:SER:OG	5:B:350:HIS:ND1	2.31	0.43
5:B:1101:GLN:HE22	5:B:1104:ARG:NH2	2.16	0.43
6:C:19:VAL:HG12	6:C:21:PHE:HD1	1.82	0.43
7:E:59:THR:HB	7:E:74:VAL:O	2.19	0.43
9:H:37:MET:HE2	9:H:125:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:147:ILE:HA	16:G:161:GLY:HA2	2.00	0.43
1:A:527:THR:HG23	1:A:530:SER:H	1.84	0.43
1:A:565:MET:HE3	1:A:565:MET:HB3	1.86	0.43
1:A:663:ASP:N	1:A:663:ASP:OD2	2.52	0.43
1:A:1040:LEU:HD23	7:E:199:THR:O	2.19	0.43
1:A:1243:LEU:HB2	1:A:1260:ARG:O	2.18	0.43
2:M:150:GLU:CD	2:M:150:GLU:H	2.27	0.43
2:M:278:LYS:HB2	2:M:551:ASN:HD22	1.84	0.43
2:M:417:ASP:CG	2:M:418:ILE:N	2.77	0.43
2:M:464:LEU:HB3	2:M:465:ASN:N	2.34	0.43
4:T:14:DG:OP2	4:T:14:DG:H8	2.01	0.43
5:B:75:SER:N	18:Z:202:ALA:HB1	2.32	0.43
5:B:237:VAL:HG12	5:B:372:LEU:HD22	2.01	0.43
1:A:872:MET:HE3	1:A:872:MET:HB2	1.90	0.42
1:A:1022:ILE:N	1:A:1034:GLN:OE1	2.33	0.42
4:T:28:DG:H1	14:P:43:C:H42	1.67	0.42
5:B:1151:MET:HG2	5:B:1152:PRO:O	2.18	0.42
6:C:8:THR:HG22	12:K:104:ARG:NH1	2.34	0.42
6:C:147:ASP:OD1	6:C:147:ASP:N	2.51	0.42
6:C:184:PHE:CD1	6:C:231:TYR:HE1	2.38	0.42
15:D:108:ALA:HB1	15:D:127:LEU:HD23	2.00	0.42
1:A:321:GLU:O	1:A:321:GLU:HG2	2.20	0.42
2:M:368:ASN:O	2:M:369:SER:HB2	2.20	0.42
2:M:377:PHE:HD1	2:M:380:ARG:HH21	1.67	0.42
5:B:47:PHE:O	5:B:51:ILE:HG12	2.20	0.42
6:C:103:LEU:HB2	6:C:120:LEU:HD23	2.01	0.42
15:D:96:GLU:HA	15:D:99:CYS:SG	2.59	0.42
16:G:117:MET:HE2	16:G:117:MET:HA	2.00	0.42
16:G:164:MET:CE	18:Z:493:VAL:HG12	2.49	0.42
1:A:276:LEU:O	1:A:280:LEU:HG	2.19	0.42
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.88	0.42
1:A:1321:ILE:HD13	1:A:1331:LEU:HD11	2.01	0.42
2:M:539:TYR:CE1	2:M:543:MET:HE3	2.55	0.42
5:B:123:PRO:HA	5:B:151:LYS:HA	2.01	0.42
5:B:731:GLN:NE2	14:P:44:A:O3'	2.52	0.42
5:B:1060:HIS:HB3	5:B:1078:ARG:HG3	2.02	0.42
7:E:14:ARG:O	7:E:18:MET:HG2	2.20	0.42
16:G:138:GLN:N	16:G:141:ASP:OD2	2.52	0.42
16:G:150:THR:N	18:Z:491:LEU:HD21	2.30	0.42
5:B:859:ARG:NE	18:Z:737:HIS:ND1	2.65	0.42
5:B:952:GLU:HG2	5:B:953:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1125:MET:HE1	5:B:1156:LYS:HD2	2.01	0.42
6:C:21:PHE:CZ	6:C:231:TYR:HD2	2.38	0.42
8:F:71:LEU:HG	8:F:75:MET:HE3	2.00	0.42
10:I:87:GLN:HE22	10:I:123:TRP:CG	2.37	0.42
16:G:94:LYS:HD3	16:G:94:LYS:N	2.34	0.42
1:A:22:GLN:HE22	1:A:1446:GLY:C	2.28	0.42
1:A:349:ARG:HA	1:A:349:ARG:HD3	1.89	0.42
1:A:693:ILE:HD11	5:B:1008:VAL:HG11	2.02	0.42
5:B:368:MET:HE2	5:B:368:MET:HB3	1.84	0.42
5:B:1029:TYR:HA	5:B:1036:LYS:HA	2.02	0.42
5:B:1118:VAL:HG21	5:B:1171:MET:HG3	2.02	0.42
5:B:1151:MET:HE1	5:B:1171:MET:HE1	2.01	0.42
7:E:80:PRO:HB3	7:E:108:GLN:HG3	2.02	0.42
14:P:35:A:P	14:P:35:A:C3'	3.04	0.42
1:A:416:ALA:HA	1:A:448:ARG:HA	2.02	0.42
1:A:794:GLU:N	1:A:845:GLU:OE2	2.40	0.42
1:A:833:PRO:HG3	5:B:1002:PHE:CG	2.55	0.42
1:A:1362:ILE:HG22	1:A:1411:LEU:HD11	2.01	0.42
2:M:419:CYS:HB3	2:M:559:PHE:HZ	1.82	0.42
2:M:422:ARG:CA	2:M:555:LYS:HE2	2.23	0.42
4:T:30:DG:C5'	5:B:747:LEU:HD11	2.48	0.42
6:C:51:GLN:OE1	13:L:52:LEU:HD22	2.19	0.42
8:F:69:ARG:O	8:F:73:ILE:HG12	2.19	0.42
16:G:160:ILE:CG2	18:Z:491:LEU:CB	2.76	0.42
18:Z:496:GLU:HB2	18:Z:555:ARG:CD	2.43	0.42
3:N:35:DC:H2'	3:N:35:DC:OP2	2.19	0.42
5:B:18:THR:O	5:B:18:THR:HG23	2.20	0.42
6:C:30:VAL:O	6:C:34:ILE:HG12	2.19	0.42
7:E:149:VAL:HB	7:E:192:LYS:HB2	2.02	0.42
7:E:172:ARG:HA	7:E:208:LEU:H	1.85	0.42
9:H:39:LEU:HD11	9:H:123:MET:SD	2.59	0.42
16:G:118:GLU:HG2	16:G:129:LYS:O	2.19	0.42
17:Y:20:SER:HB2	17:Y:86:ALA:HB3	2.02	0.42
1:A:106:VAL:HG13	1:A:236:LEU:HD21	2.02	0.42
1:A:910:LYS:HB3	1:A:1328:PHE:HE2	1.82	0.42
2:M:63:LEU:HD21	2:M:109:LEU:HD21	2.02	0.42
2:M:158:GLN:HB3	18:Z:607:HIS:C	2.44	0.42
2:M:480:GLY:O	16:G:17:TYR:HD2	2.03	0.42
4:T:31:DT:O4	14:P:40:A:C6	2.71	0.42
5:B:280:SER:OG	5:B:281:ASP:N	2.52	0.42
5:B:419:ALA:O	5:B:423:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1028:LEU:HG	5:B:1041:ILE:HB	2.02	0.42
7:E:130:PHE:CD1	7:E:135:LEU:HD21	2.55	0.42
9:H:15:ILE:HG13	9:H:16:ASP:H	1.84	0.42
18:Z:485:PHE:HZ	18:Z:559:GLN:NE2	2.03	0.42
18:Z:546:THR:HG23	18:Z:563:MET:HG2	2.02	0.42
1:A:957:GLU:O	1:A:961:GLU:HG2	2.20	0.42
1:A:1427:LEU:HA	1:A:1430:CYS:SG	2.60	0.42
1:A:1474:LEU:HD11	8:F:107:ARG:CZ	2.50	0.42
5:B:225:LEU:HG	5:B:226:GLU:H	1.84	0.42
6:C:27:ASP:HB2	6:C:30:VAL:HG23	2.01	0.42
9:H:12:VAL:HA	9:H:30:CYS:HB3	2.02	0.42
10:I:78:LEU:HD22	10:I:97:PHE:HB3	2.01	0.42
16:G:97:LEU:HB3	16:G:108:ILE:CG2	2.50	0.42
1:A:593:SER:HB3	1:A:634:GLU:HG3	2.01	0.42
1:A:878:THR:HG21	1:A:880:ARG:HE	1.85	0.42
1:A:1042:ASN:HB3	1:A:1046:ARG:NH1	2.35	0.42
1:A:1434:GLU:O	1:A:1435:THR:OG1	2.28	0.42
1:A:1473:LEU:HD11	8:F:65:VAL:HG22	2.01	0.42
2:M:22:GLY:H	18:Z:606:PRO:HG3	1.85	0.42
5:B:224:CYS:SG	5:B:232:THR:HG22	2.60	0.42
6:C:251:GLY:O	6:C:254:LYS:HG3	2.19	0.42
13:L:47:LYS:HD2	13:L:47:LYS:HA	1.84	0.42
15:D:92:LEU:HA	15:D:121:ARG:HH21	1.84	0.42
18:Z:492:ILE:HG13	18:Z:492:ILE:O	2.19	0.42
1:A:265:VAL:HA	1:A:271:ARG:HG2	2.03	0.41
1:A:375:ILE:HD13	1:A:669:TYR:CD2	2.54	0.41
1:A:481:THR:HG22	5:B:1055:VAL:HG21	2.02	0.41
6:C:38:PHE:HE1	6:C:245:VAL:HA	1.85	0.41
9:H:87:GLN:HG2	9:H:88:PHE:CD1	2.54	0.41
18:Z:308:ILE:HD11	18:Z:630:VAL:HG23	2.02	0.41
1:A:88:ILE:HB	1:A:253:LEU:HB3	2.03	0.41
1:A:532:ARG:HG2	1:A:649:ALA:HB2	2.02	0.41
1:A:653:VAL:HG21	1:A:669:TYR:HE1	1.85	0.41
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.55	0.41
1:A:1218:ARG:NH1	1:A:1252:ALA:O	2.47	0.41
2:M:442:PHE:CD2	2:M:558:LEU:HD11	2.55	0.41
2:M:462:PRO:HA	2:M:465:ASN:HB2	0.48	0.41
5:B:404:PHE:HA	5:B:407:MET:HE3	2.02	0.41
5:B:733:MET:CE	5:B:1050:ARG:HG2	2.50	0.41
6:C:38:PHE:CE1	6:C:245:VAL:HA	2.54	0.41
12:K:7:PHE:CD1	12:K:11:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.56	0.41
2:M:312:MET:HE3	2:M:346:MET:CE	2.51	0.41
5:B:270:ILE:HD12	5:B:270:ILE:H	1.85	0.41
5:B:759:VAL:HG22	5:B:999:ALA:HB2	2.01	0.41
6:C:10:ARG:HH22	6:C:228:ARG:HH22	1.66	0.41
7:E:87:ILE:HA	7:E:90:TYR:HD1	1.85	0.41
15:D:91:LYS:C	15:D:92:LEU:HD12	2.45	0.41
1:A:191:ILE:HA	1:A:200:ALA:HA	2.03	0.41
1:A:509:LEU:HD11	8:F:89:PRO:HG2	2.02	0.41
1:A:1167:ARG:HG3	1:A:1293:LEU:O	2.20	0.41
2:M:274:VAL:HG21	2:M:454:ASP:HA	2.01	0.41
6:C:22:ILE:HG12	6:C:230:TYR:CD1	2.55	0.41
9:H:60:ILE:HG21	9:H:135:PHE:HZ	1.84	0.41
1:A:130:LEU:HD21	1:A:235:VAL:HG22	2.03	0.41
1:A:548:PHE:HE1	1:A:555:LEU:HD11	1.85	0.41
1:A:893:GLU:HB2	7:E:203:TYR:CD1	2.55	0.41
2:M:480:GLY:O	16:G:17:TYR:CD2	2.72	0.41
2:M:482:LEU:CG	16:G:25:THR:HG22	2.47	0.41
4:T:26:DG:H1	14:P:45:C:H42	1.67	0.41
5:B:721:ARG:HG3	5:B:977:THR:HG22	2.02	0.41
5:B:859:ARG:HB2	18:Z:737:HIS:CD2	2.55	0.41
10:I:50:ASN:OD1	10:I:51:SER:N	2.54	0.41
10:I:82:GLU:HB3	10:I:92:LYS:HE3	2.02	0.41
12:K:13:PHE:HB2	12:K:16:GLU:HG3	2.03	0.41
14:P:36:G:N3	14:P:36:G:C2'	2.84	0.41
1:A:273:GLN:HB2	1:A:278:HIS:NE2	2.35	0.41
1:A:353:ASN:O	1:A:357:LYS:HE2	2.20	0.41
1:A:575:PRO:HD3	1:A:594:LEU:HD11	2.03	0.41
1:A:1370:GLY:O	1:A:1374:VAL:HG23	2.21	0.41
2:M:278:LYS:HB2	2:M:551:ASN:ND2	2.35	0.41
2:M:419:CYS:O	2:M:422:ARG:HB2	2.20	0.41
2:M:505:LYS:HZ1	15:D:56:GLU:HB3	1.71	0.41
5:B:235:ILE:HD12	5:B:347:MET:HG3	2.03	0.41
5:B:255:ARG:HD2	5:B:307:GLU:HG3	2.01	0.41
5:B:787:GLY:O	5:B:790:GLN:HG3	2.21	0.41
5:B:1094:GLN:HB2	5:B:1103:LEU:HD13	2.02	0.41
6:C:78:ILE:HA	6:C:81:LYS:HG2	2.03	0.41
9:H:116:VAL:HG11	9:H:123:MET:HE2	2.02	0.41
12:K:98:LEU:O	12:K:102:GLU:HG3	2.20	0.41
16:G:162:SER:HB2	16:G:164:MET:HE1	2.01	0.41
18:Z:216:VAL:HB	18:Z:226:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD21	5:B:1155:CYS:N	2.36	0.41
1:A:496:PHE:HB2	5:B:791:GLU:O	2.21	0.41
5:B:507:GLY:HA2	5:B:703:ILE:HA	2.02	0.41
5:B:756:LYS:O	11:J:51:ALA:HB1	2.21	0.41
7:E:47:LYS:H	7:E:53:PRO:CG	2.33	0.41
9:H:5:LEU:N	9:H:60:ILE:O	2.51	0.41
16:G:110:ARG:CB	18:Z:510:GLU:OE2	2.68	0.41
16:G:113:ILE:HG21	16:G:128:TYR:HE1	1.86	0.41
1:A:29:ASP:O	1:A:33:ARG:HG3	2.20	0.41
1:A:141:LEU:HD13	1:A:1445:HIS:CE1	2.56	0.41
1:A:360:ASP:OD1	5:B:1062:ARG:NE	2.32	0.41
1:A:1424:THR:HG21	1:A:1428:MET:HE2	2.03	0.41
2:M:462:PRO:C	2:M:465:ASN:O	2.63	0.41
2:M:519:PHE:HB2	2:M:524:TRP:CD1	2.56	0.41
5:B:23:GLN:O	5:B:27:TRP:HD1	2.04	0.41
9:H:29:HIS:ND1	9:H:40:ILE:HG12	2.35	0.41
15:D:37:VAL:HG21	16:G:2:PHE:CD2	2.47	0.41
16:G:125:PRO:HB2	16:G:138:GLN:CD	2.46	0.41
1:A:31:LEU:HD22	1:A:254:PRO:HB3	2.02	0.41
1:A:522:PRO:O	1:A:662:HIS:HB2	2.20	0.41
1:A:571:ASP:OD1	1:A:571:ASP:N	2.50	0.41
1:A:732:THR:HG22	1:A:733:LEU:N	2.35	0.41
1:A:831:LEU:HG	5:B:715:ASP:O	2.20	0.41
1:A:856:GLU:HG2	5:B:494:LYS:HD2	2.02	0.41
2:M:279:GLN:O	2:M:282:LYS:HB2	2.21	0.41
2:M:329:PHE:CE2	2:M:331:LYS:CG	3.04	0.41
2:M:374:ASP:OD2	2:M:447:LYS:HE3	2.20	0.41
2:M:406:GLU:HA	2:M:407:PRO:HD2	1.90	0.41
3:N:28:DT:OP2	3:N:28:DT:H2'	2.21	0.41
5:B:225:LEU:HD23	5:B:228:SER:HB2	2.01	0.41
5:B:615:TYR:HB3	5:B:620:ARG:HD3	2.03	0.41
5:B:896:LEU:HD23	5:B:897:ARG:O	2.20	0.41
5:B:927:ARG:HH12	5:B:1057:ASP:CG	2.29	0.41
5:B:935:PHE:HE1	5:B:1050:ARG:HG3	1.86	0.41
5:B:937:SER:OG	5:B:938:ARG:N	2.54	0.41
5:B:1056:ASP:O	5:B:1078:ARG:NH2	2.54	0.41
6:C:59:LEU:HD13	6:C:63:PHE:CE2	2.56	0.41
7:E:44:PHE:C	7:E:53:PRO:HB3	2.45	0.41
7:E:151:MET:HE3	7:E:192:LYS:HD2	2.03	0.41
9:H:60:ILE:HG21	9:H:135:PHE:CZ	2.56	0.41
12:K:7:PHE:HB2	12:K:11:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:O	1:A:332:SER:OG	2.35	0.41
1:A:545:VAL:HG11	1:A:645:LEU:HD12	2.02	0.41
1:A:671:ASN:O	1:A:675:VAL:HG12	2.20	0.41
1:A:693:ILE:HG21	5:B:1023:ARG:NH2	2.36	0.41
1:A:784:VAL:O	1:A:828:LEU:HD23	2.20	0.41
1:A:1411:LEU:HD23	1:A:1411:LEU:HA	1.86	0.41
2:M:304:ILE:HB	2:M:340:THR:HB	2.03	0.41
5:B:489:ILE:HD12	5:B:489:ILE:HA	1.88	0.41
5:B:552:ASN:HB2	5:B:555:GLU:OE2	2.22	0.41
5:B:567:ILE:HD11	5:B:577:HIS:HB2	2.03	0.41
16:G:107:PHE:CE1	18:Z:508:MET:N	2.86	0.41
1:A:102:LYS:O	1:A:106:VAL:HG23	2.21	0.40
5:B:121:SER:HA	5:B:153:PRO:HA	2.03	0.40
5:B:124:LEU:HD23	5:B:150:GLY:O	2.21	0.40
7:E:61:LEU:HD22	7:E:73:PHE:CZ	2.56	0.40
1:A:533:PRO:HD3	1:A:654:HIS:CG	2.56	0.40
1:A:548:PHE:CE1	1:A:555:LEU:HD11	2.56	0.40
1:A:873:VAL:HG23	1:A:1087:VAL:HG21	2.03	0.40
1:A:894:ASP:OD2	1:A:896:LEU:HB2	2.21	0.40
2:M:276:MET:HG2	2:M:553:VAL:HG21	2.03	0.40
2:M:311:PHE:HA	2:M:320:PHE:O	2.21	0.40
2:M:422:ARG:CD	2:M:559:PHE:CE2	3.04	0.40
5:B:212:ASP:OD1	5:B:212:ASP:N	2.46	0.40
5:B:1119:CYS:HA	5:B:1146:ILE:HD12	2.04	0.40
6:C:78:ILE:HG22	6:C:82:LEU:HG	2.03	0.40
12:K:17:LYS:HB3	12:K:17:LYS:HE3	1.84	0.40
16:G:51:ILE:HA	16:G:72:TYR:HA	2.03	0.40
16:G:90:THR:HG21	16:G:100:GLU:HB2	2.03	0.40
1:A:1163:HIS:NE2	1:A:1297:THR:HG22	2.36	0.40
1:A:1211:LEU:H	1:A:1211:LEU:HD23	1.86	0.40
2:M:287:LYS:O	2:M:562:ILE:CG2	2.58	0.40
2:M:330:ARG:NH2	2:M:331:LYS:NZ	2.70	0.40
2:M:361:ILE:HG22	2:M:384:ILE:HD13	2.02	0.40
2:M:380:ARG:NH1	2:M:448:TYR:N	2.70	0.40
2:M:392:ARG:NH2	2:M:406:GLU:OE1	2.55	0.40
4:T:30:DG:N2	14:P:42:C:C2	2.90	0.40
5:B:193:VAL:HG23	5:B:470:LEU:HB2	2.02	0.40
5:B:236:TRP:HB2	5:B:259:THR:HG22	2.03	0.40
16:G:151:ARG:HH22	18:Z:506:LEU:C	2.30	0.40
1:A:96:HIS:HE2	1:A:1440:MET:HE1	1.87	0.40
1:A:896:LEU:CD1	1:A:980:PRO:HG3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	2.03	0.40
1:A:1428:MET:HB2	1:A:1456:GLU:OE2	2.21	0.40
2:M:443:GLN:HA	2:M:444:PRO:HD3	1.97	0.40
3:N:35:DC:OP2	3:N:35:DC:H6	2.04	0.40
5:B:322:GLY:HA3	5:B:335:ARG:HB3	2.04	0.40
5:B:472:ARG:HG3	5:B:736:TYR:CD2	2.57	0.40
5:B:577:HIS:ND1	5:B:583:LEU:HD13	2.35	0.40
5:B:782:ILE:HG12	5:B:967:ILE:HD11	2.03	0.40
6:C:44:ILE:CG2	6:C:178:PRO:HB3	2.51	0.40
6:C:240:ARG:O	6:C:244:ILE:HG13	2.21	0.40
16:G:80:PHE:HB2	16:G:83:GLU:CG	2.52	0.40
16:G:90:THR:O	16:G:139:GLN:NE2	2.38	0.40
16:G:107:PHE:CD2	18:Z:508:MET:O	2.74	0.40
1:A:87:HIS:HB2	1:A:252:VAL:CG2	2.52	0.40
1:A:93:PRO:HD2	1:A:219:GLU:HB3	2.04	0.40
1:A:115:SER:OG	1:A:227:ARG:NE	2.24	0.40
1:A:188:GLN:NE2	1:A:189:PRO:O	2.55	0.40
1:A:521:VAL:N	1:A:522:PRO:HD2	2.36	0.40
2:M:277:ASP:HB3	2:M:548:SER:HA	2.03	0.40
6:C:61:ASP:OD2	13:L:48:ARG:NH2	2.53	0.40
8:F:76:CYS:SG	8:F:76:CYS:O	2.80	0.40
18:Z:308:ILE:CD1	18:Z:630:VAL:CG2	2.99	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	1398/1970 (71%)	1315 (94%)	82 (6%)	1 (0%)	48	79
2	M	484/597 (81%)	463 (96%)	21 (4%)	0	100	100
5	B	1122/1174 (96%)	1060 (94%)	62 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	259/275 (94%)	246 (95%)	13 (5%)	0	100	100
7	E	207/210 (99%)	198 (96%)	8 (4%)	1 (0%)	24	57
8	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
9	H	146/150 (97%)	137 (94%)	9 (6%)	0	100	100
10	I	115/125 (92%)	104 (90%)	11 (10%)	0	100	100
11	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
12	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
13	L	44/58 (76%)	37 (84%)	7 (16%)	0	100	100
15	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
16	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
17	Y	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
18	Z	442/1087 (41%)	425 (96%)	16 (4%)	1 (0%)	43	73
All	All	4882/6388 (76%)	4630 (95%)	249 (5%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	E	57	ASP
18	Z	497	GLU
1	A	911	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1241/1749 (71%)	1241 (100%)	0	100	100
2	M	434/534 (81%)	415 (96%)	19 (4%)	25	49
5	B	992/1027 (97%)	991 (100%)	1 (0%)	88	89
6	C	240/252 (95%)	240 (100%)	0	100	100
7	E	191/192 (100%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	71/111 (64%)	71 (100%)	0	100	100
9	H	129/131 (98%)	129 (100%)	0	100	100
10	I	105/112 (94%)	105 (100%)	0	100	100
11	J	56/56 (100%)	56 (100%)	0	100	100
12	K	104/106 (98%)	104 (100%)	0	100	100
13	L	43/55 (78%)	43 (100%)	0	100	100
15	D	109/126 (86%)	109 (100%)	0	100	100
16	G	146/153 (95%)	146 (100%)	0	100	100
17	Y	102/103 (99%)	102 (100%)	0	100	100
18	Z	405/940 (43%)	405 (100%)	0	100	100
All	All	4368/5647 (77%)	4348 (100%)	20 (0%)	78	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	27	LEU
2	M	237	THR
2	M	239	LYS
2	M	244	VAL
2	M	250	LEU
2	M	293	TRP
2	M	321	HIS
2	M	329	PHE
2	M	347	ILE
2	M	362	TYR
2	M	372	VAL
2	M	378	ASN
2	M	385	GLU
2	M	398	THR
2	M	409	SER
2	M	416	PHE
2	M	425	LEU
2	M	441	ILE
2	M	463	SER
5	B	1071	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	289	GLN
1	A	301	HIS
1	A	387	ASN
1	A	432	HIS
1	A	441	GLN
1	A	504	HIS
1	A	529	GLN
1	A	539	GLN
1	A	606	HIS
1	A	685	HIS
1	A	723	ASN
1	A	731	ASN
1	A	1044	HIS
2	M	90	GLN
2	M	94	HIS
2	M	128	HIS
2	M	280	ASN
2	M	443	GLN
2	M	537	ASN
2	M	547	ASN
5	B	197	GLN
5	B	315	ASN
5	B	460	HIS
5	B	525	ASN
5	B	593	GLN
5	B	725	GLN
5	B	797	ASN
5	B	980	HIS
6	C	145	GLN
10	I	46	GLN
10	I	98	GLN
10	I	118	HIS
10	I	121	HIS
12	K	29	ASN
12	K	55	GLN
15	D	48	ASN
15	D	102	ASN
17	Y	12	HIS
17	Y	41	GLN
17	Y	45	ASN
18	Z	272	ASN
18	Z	559	GLN

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Mol	Chain	Res	Type
18	Z	572	HIS
18	Z	642	HIS
18	Z	703	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	16/17 (94%)	9 (56%)	3 (18%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	31	G
14	P	32	G
14	P	33	A
14	P	34	G
14	P	35	A
14	P	36	G
14	P	37	G
14	P	38	G
14	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	36	G
14	P	37	G
14	P	38	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	M	2
3	N	1
18	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DT	O3'	24:DA	P	38.25
1	Z	580:ASP	C	581:ASN	N	14.51
1	M	465:ASN	C	466:SER	N	4.87
1	M	464:LEU	C	465:ASN	N	3.20

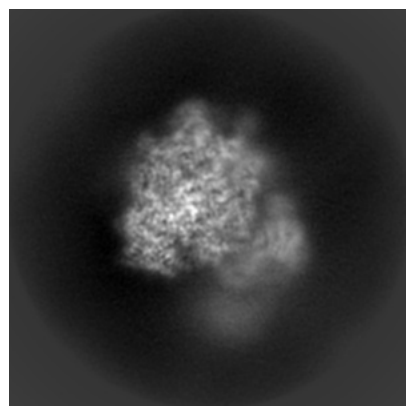
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17405. These allow visual inspection of the internal detail of the map and identification of artifacts.

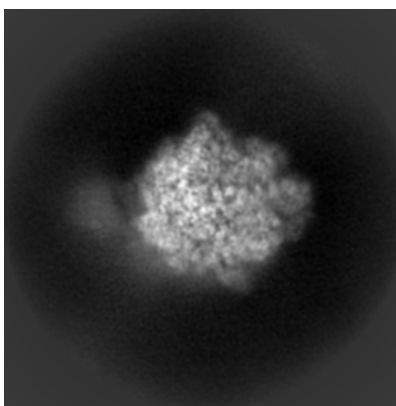
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

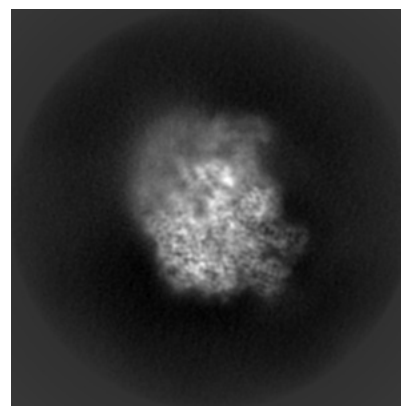
6.1.1 Primary map



X

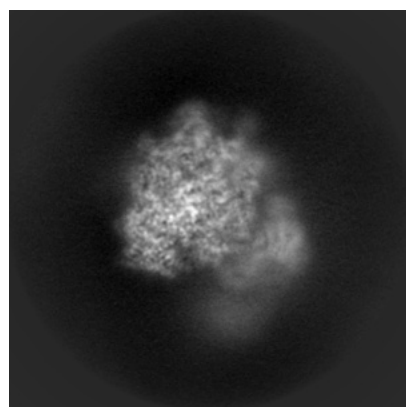


Y

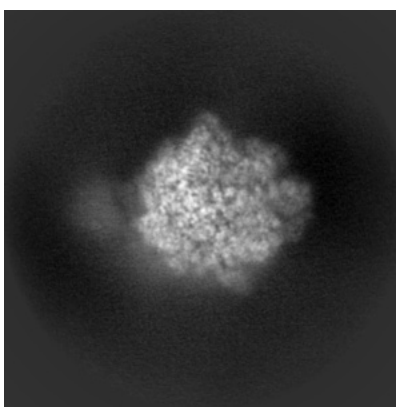


Z

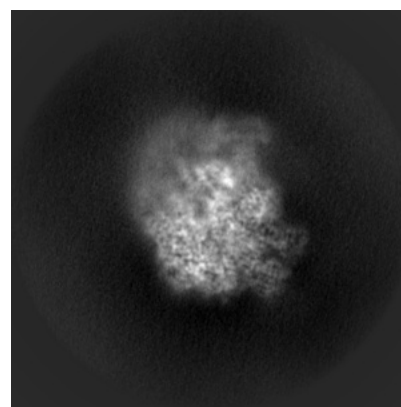
6.1.2 Raw map



X



Y

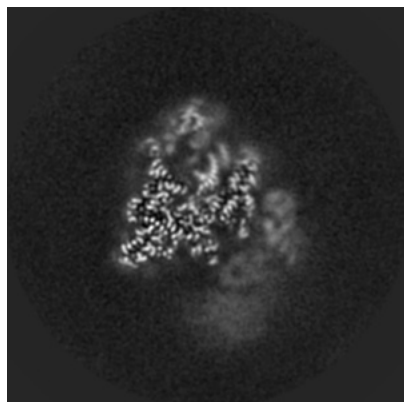


Z

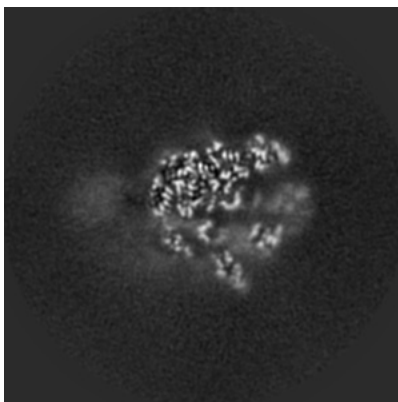
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

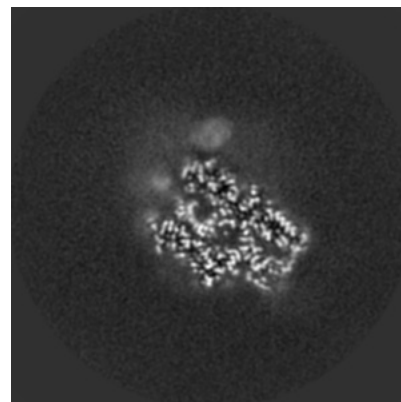
6.2.1 Primary map



X Index: 150

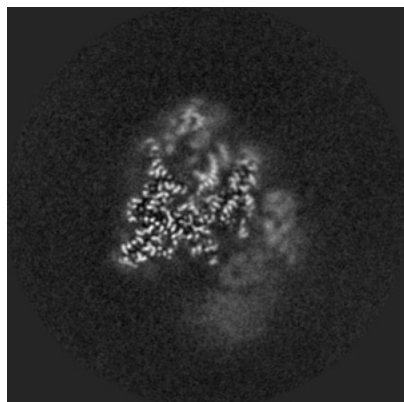


Y Index: 150

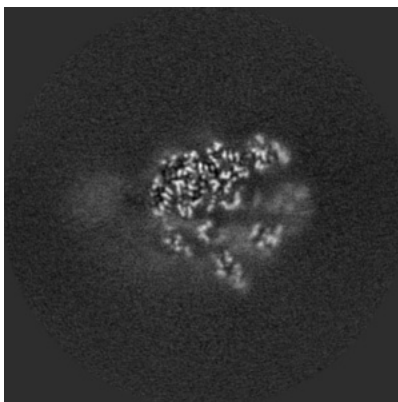


Z Index: 150

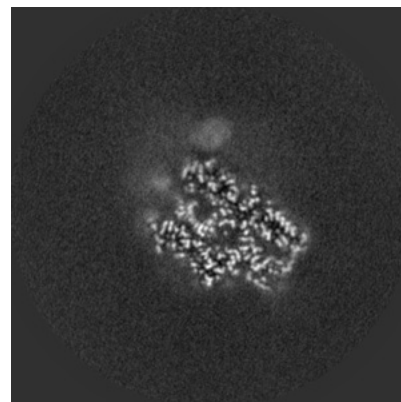
6.2.2 Raw map



X Index: 150



Y Index: 150

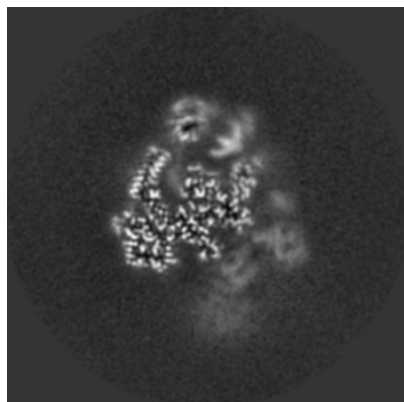


Z Index: 150

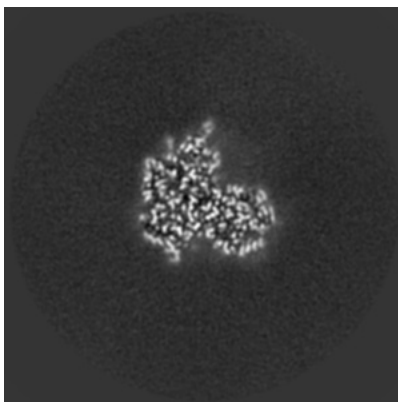
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

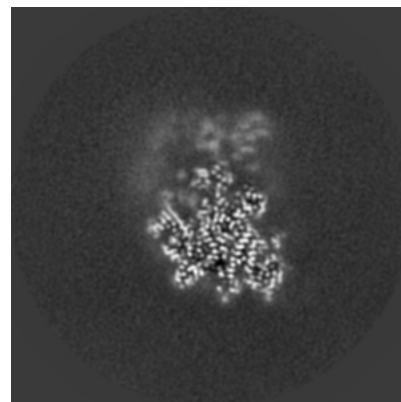
6.3.1 Primary map



X Index: 161

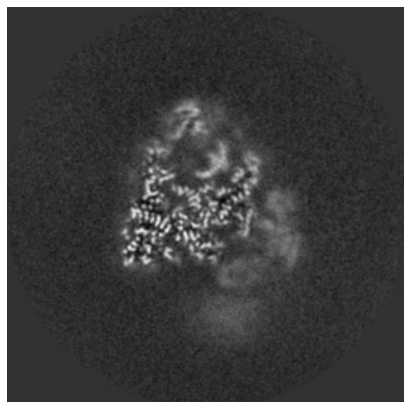


Y Index: 109

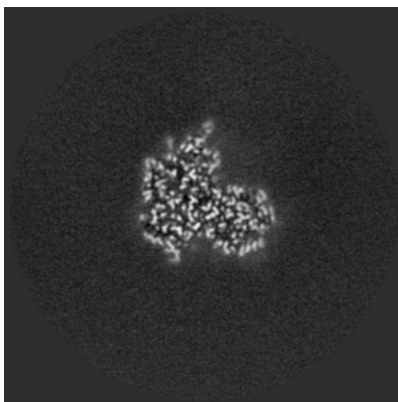


Z Index: 136

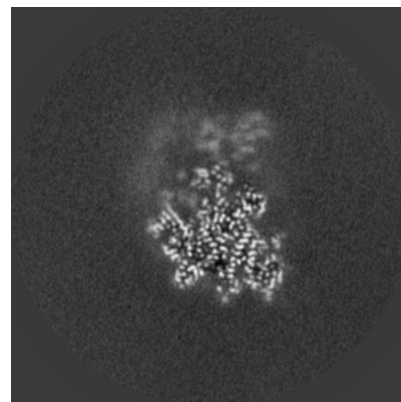
6.3.2 Raw map



X Index: 153



Y Index: 109

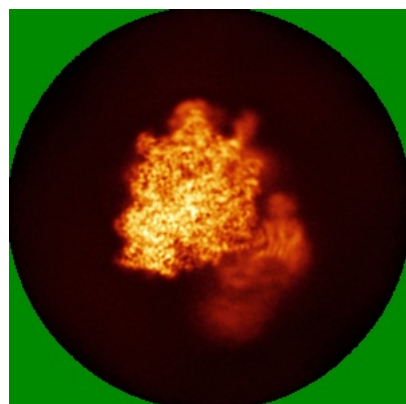


Z Index: 136

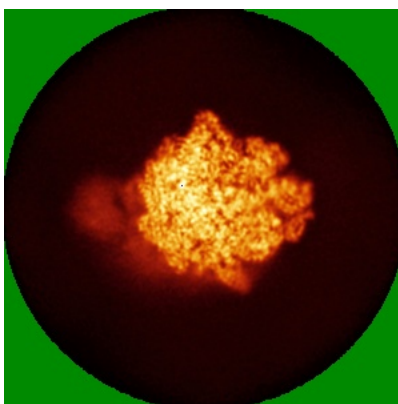
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

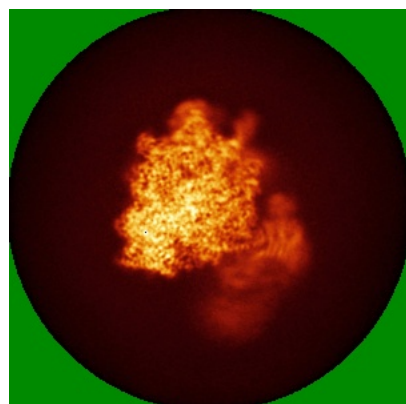


Y

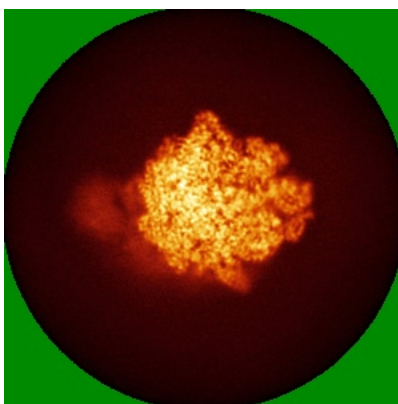


Z

6.4.2 Raw 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.

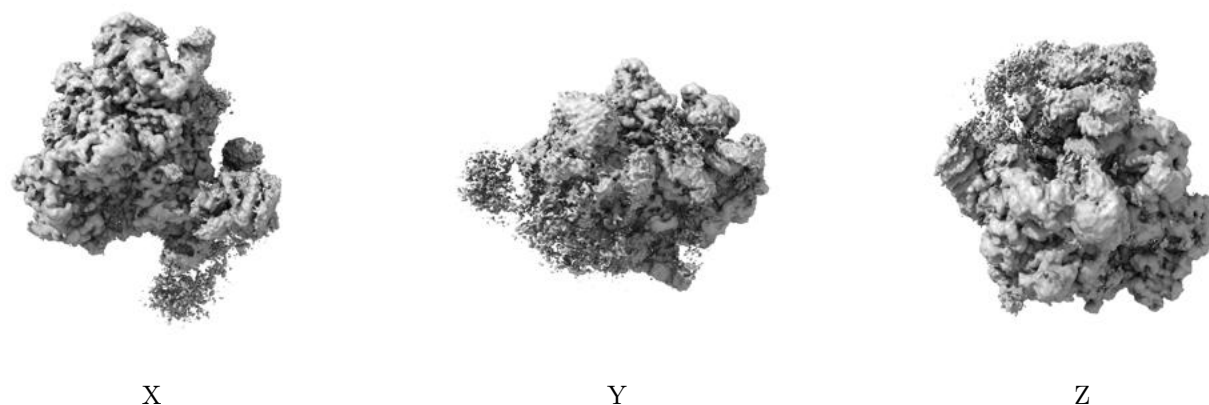
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

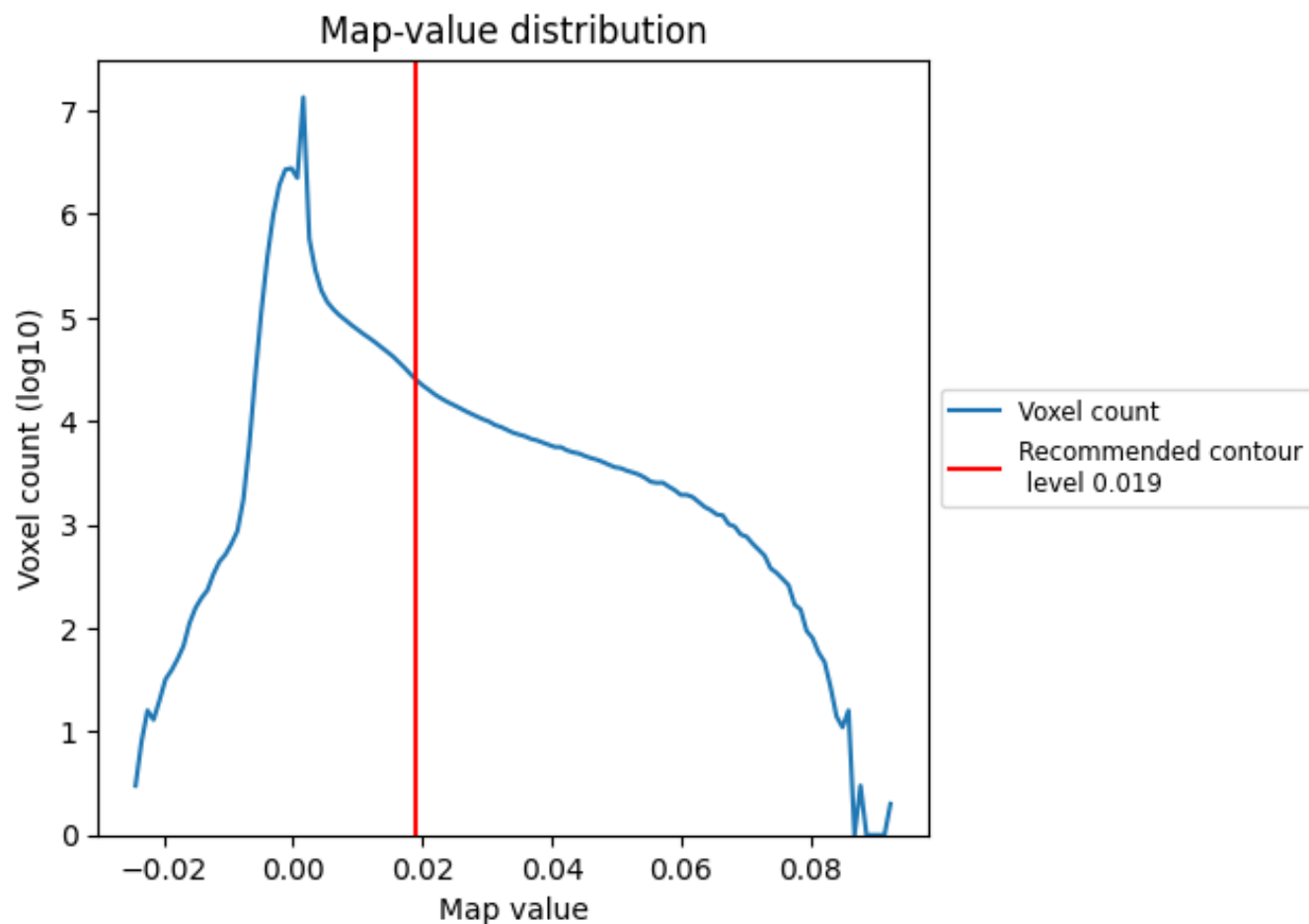
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

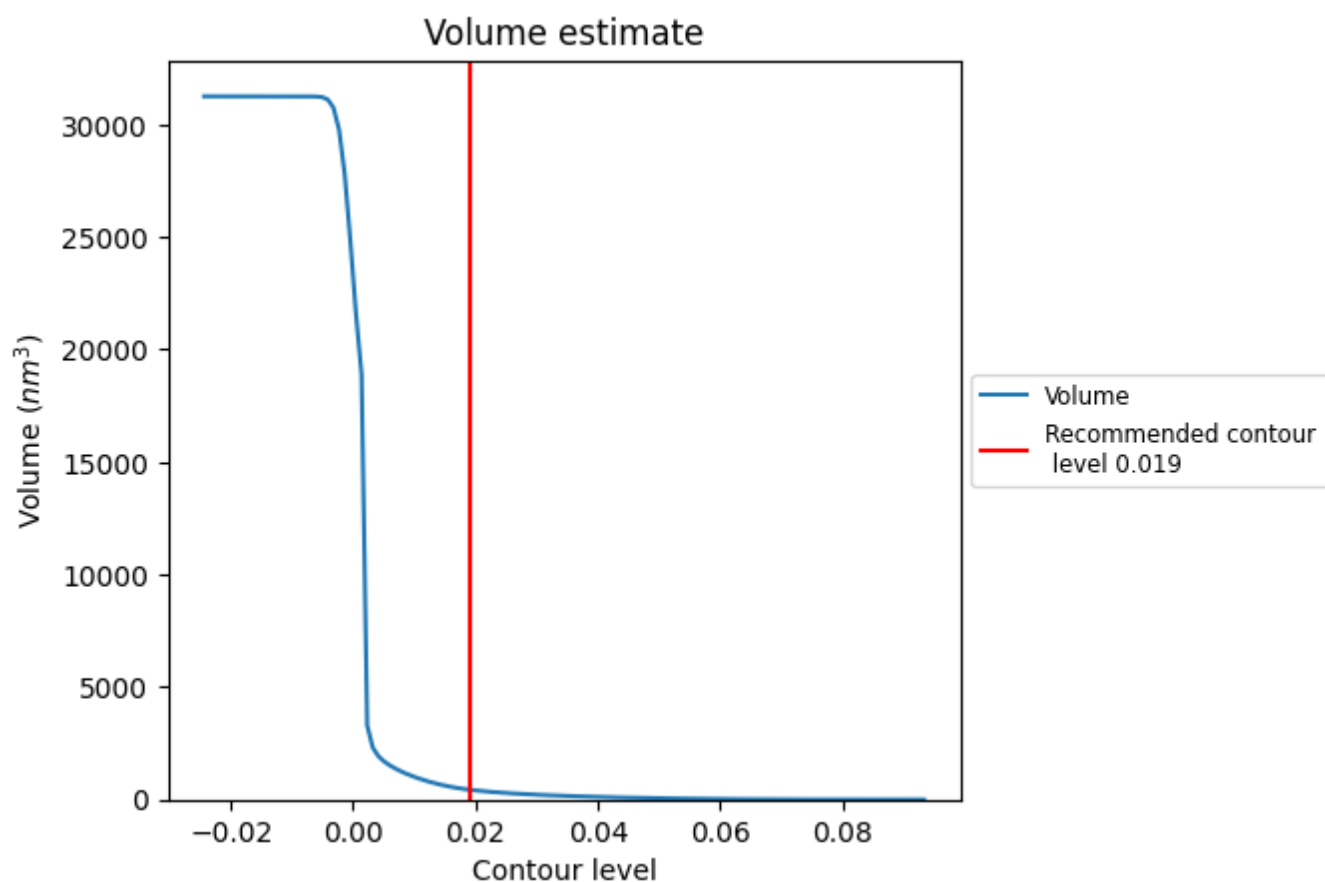
This section contains the results of statistical analysis of the map.

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.

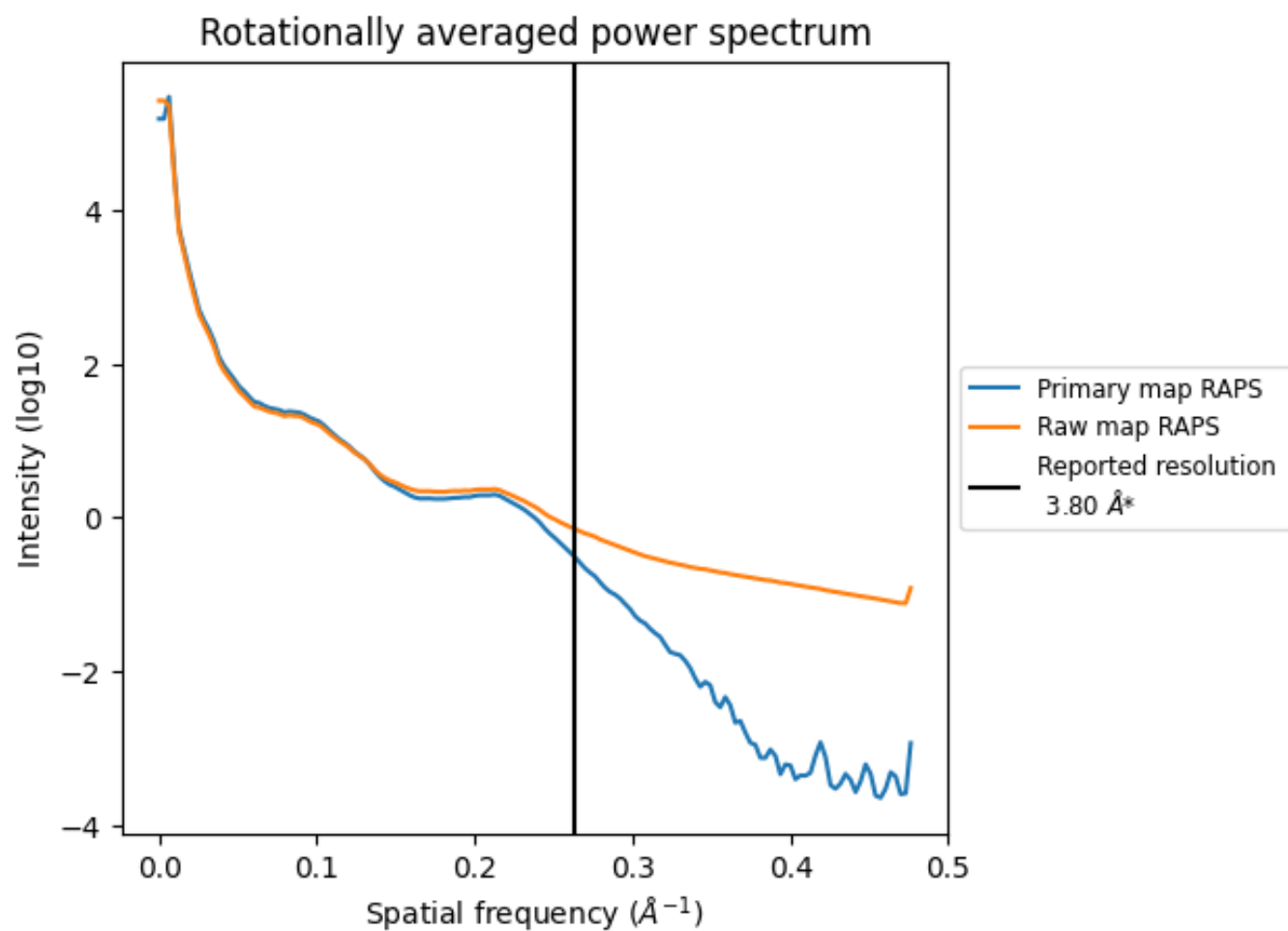
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 437 nm³; this corresponds to an approximate mass of 395 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

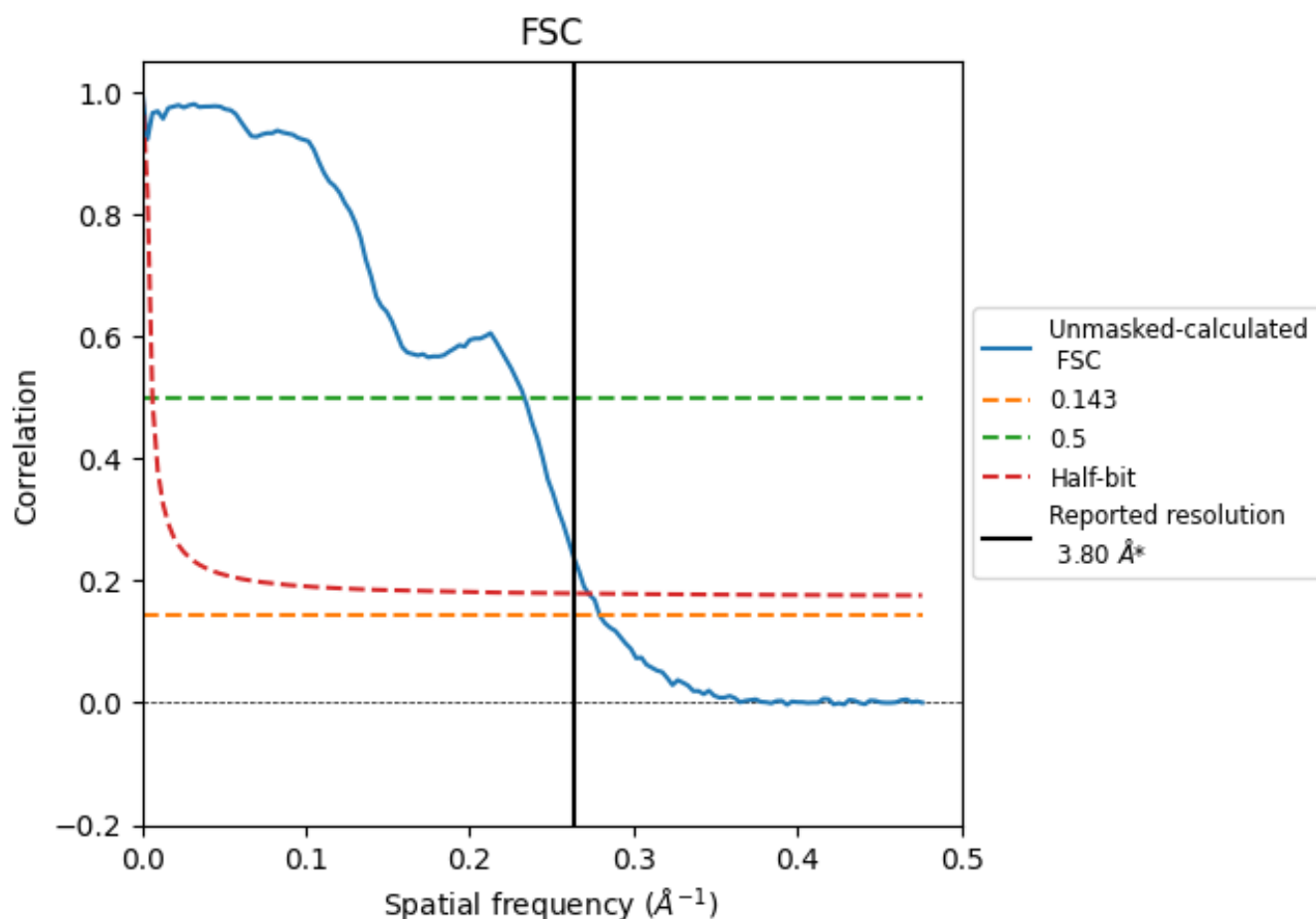


*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.29	3.67

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

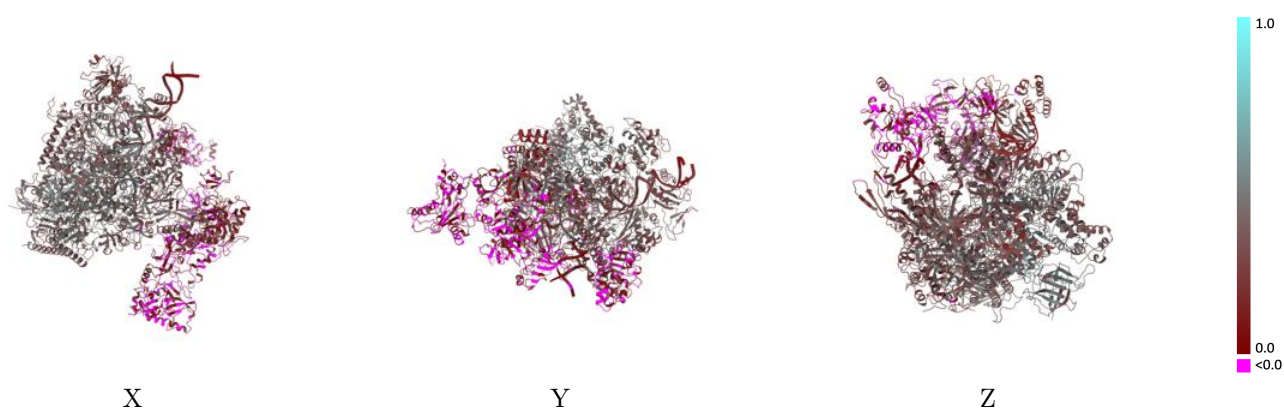
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-17405 and PDB model 8P4C. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

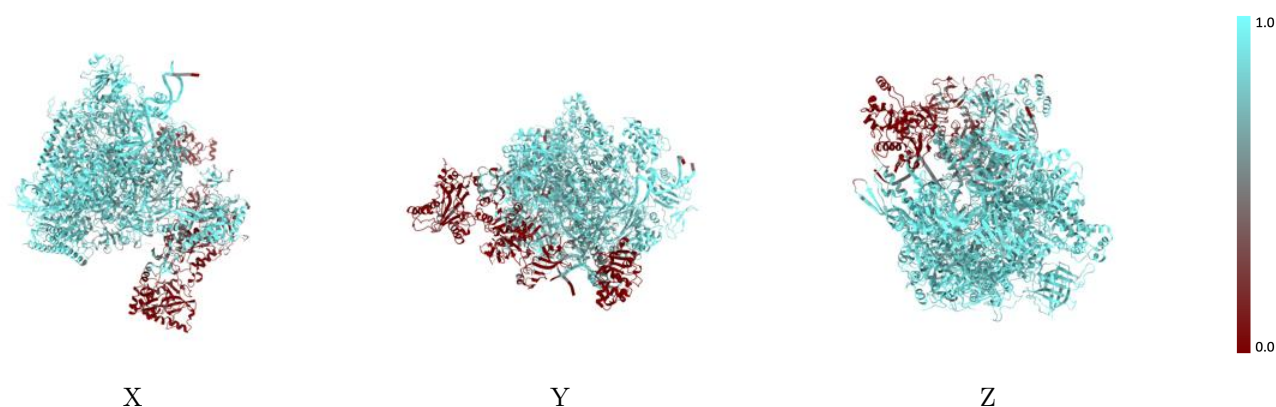
This section was not generated.

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



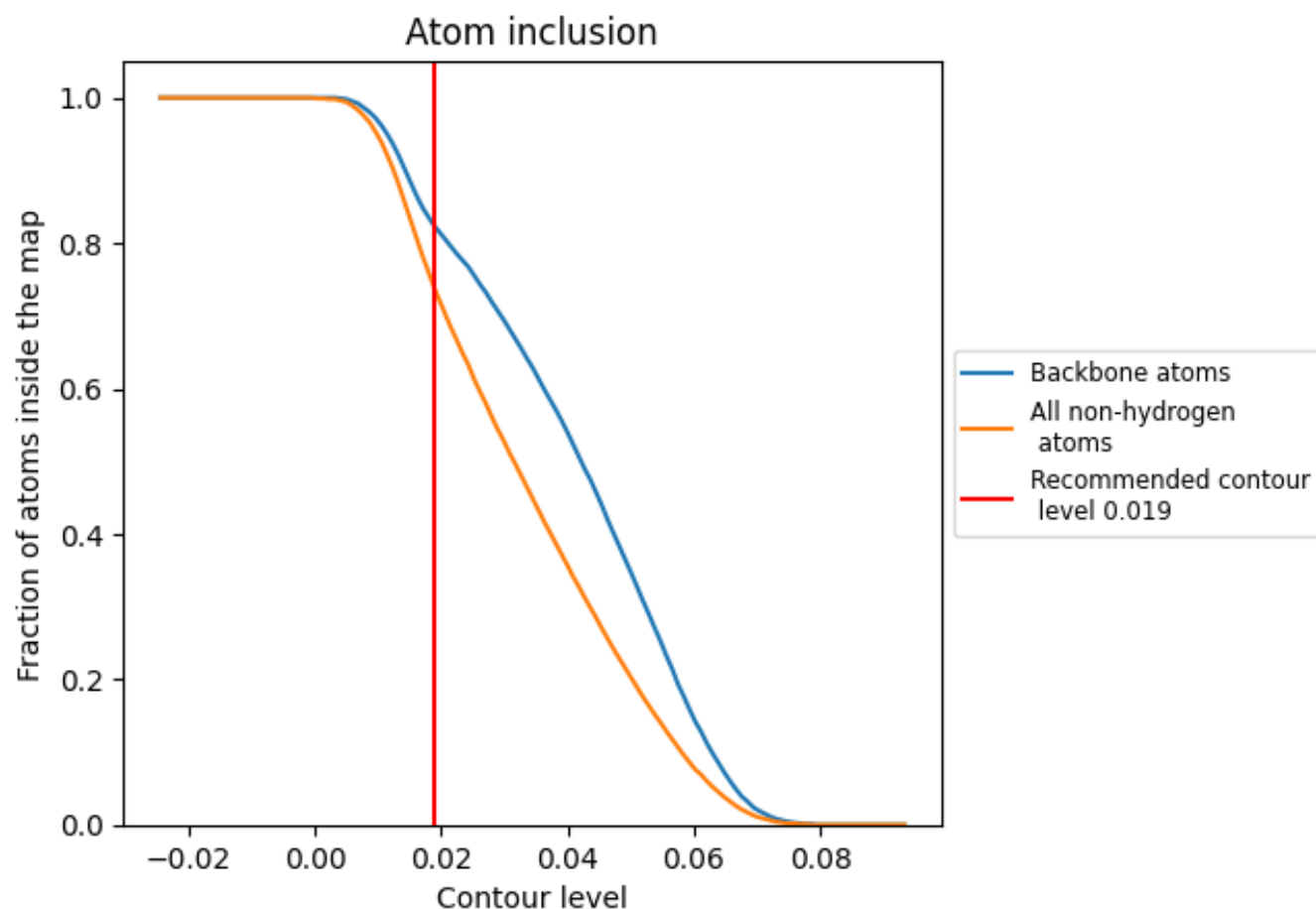
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.2970
A	 0.8860	 0.3960
B	 0.8680	 0.3480
C	 0.8840	 0.3590
D	 0.8150	 0.2130
E	 0.9090	 0.3910
F	 0.8760	 0.4180
G	 0.8320	 0.2690
H	 0.9270	 0.4400
I	 0.9050	 0.3310
J	 0.8750	 0.3400
K	 0.8970	 0.4180
L	 0.8680	 0.2910
M	 0.1530	 0.0390
N	 0.8070	 0.1850
P	 0.8780	 0.2880
T	 0.8680	 0.2470
Y	 0.0010	 0.0470
Z	 0.2910	 0.0840

