



Full wwPDB EM Validation Report ⓘ

Sep 3, 2026 – 01:25 PM EDT

PDB ID : 36AX / pdb_000036ax
EMDB ID : EMD-77338
Title : yeast 26S proteasome base assembly intermediate, base-Nas2-Rpn14-Hsm3-Nas6 with Rpt4-EQ
Authors : Hsieh, H.H.; Martin, A.
Deposited on : 2026-05-28
Resolution : 4.87 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:

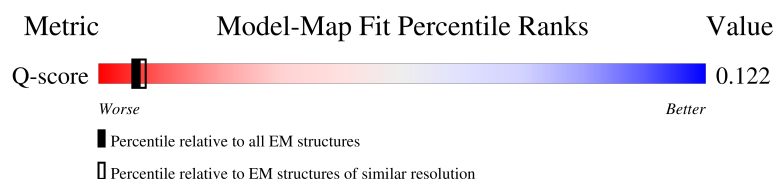
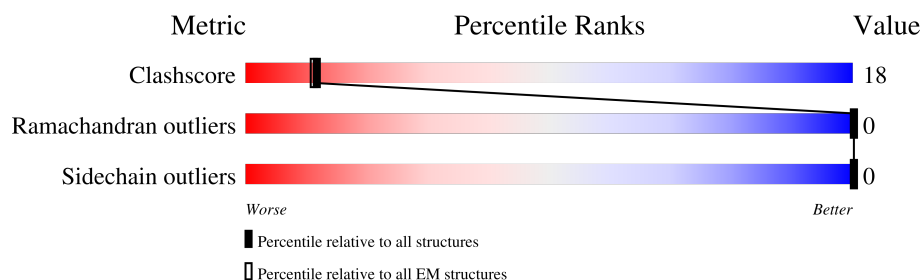
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



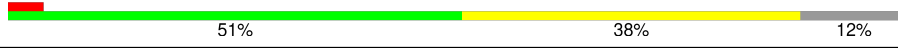
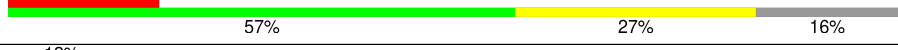
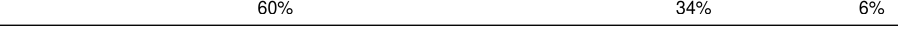
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1264 (4.37 - 5.36)

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	467	5% 49% 23% 28%
2	B	437	• 56% 34% 10%
3	C	993	7% 57% 28% 15%
4	D	480	77% 20% •

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Mol	Chain	Length	Quality of chain
5	I	405	
6	J	428	
7	K	437	
8	L	156	
9	M	417	
10	N	228	
11	P	434	
12	R	220	
13	Z	945	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ATP	K	501	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 43176 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 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2611	1638	466	492	15		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	392	Total	C	N	O	S	0	0
			3078	1937	516	608	17		

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	848	Total	C	N	O	S	0	0
			6584	4181	1077	1297	29		

- Molecule 4 is a protein called DNA mismatch repair protein HSM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	463	Total	C	N	O	S	0	0
			3783	2438	603	728	14		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	390	Total	C	N	O	S	0	0
			3063	1929	547	570	17		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	390	Total	C	N	O	S	0	0
			3088	1942	539	596	11		

- Molecule 7 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	385	Total	C	N	O	S	0	0
			3059	1930	545	572	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	282	GLN	GLU	engineered mutation	UNP P53549

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	131	Total	C	N	O	S	0	0
			1061	681	173	201	6		

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	417	Total	C	N	O	S	0	0
			3267	2049	557	650	11		

- Molecule 10 is a protein called Probable 26S proteasome regulatory subunit p28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	228	Total	C	N	O	S	0	0
			1808	1159	307	335	7		

- Molecule 11 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	410	Total	C	N	O	S	0	0
			3204	2003	556	631	14		

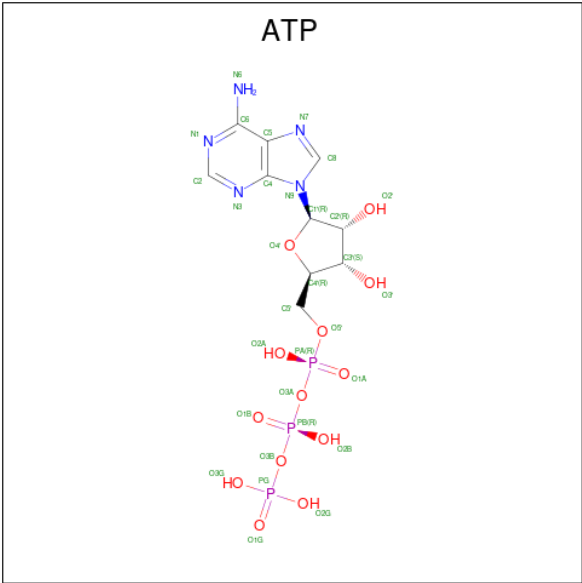
- Molecule 12 is a protein called Probable 26S proteasome regulatory subunit p27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	200	Total	C	N	O	S	0	0
			1577	989	275	304	9		

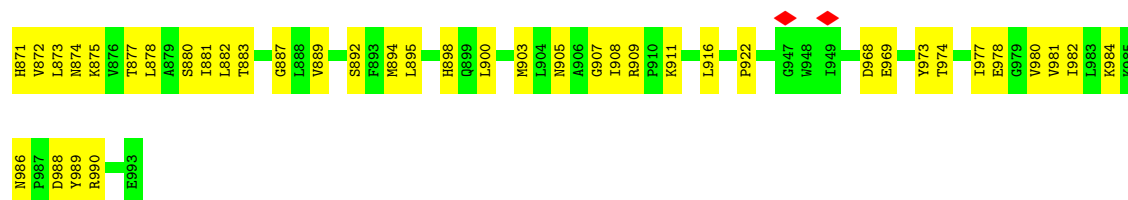
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	884	Total	C	N	O	S	0	0
			6807	4324	1145	1310	28		

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

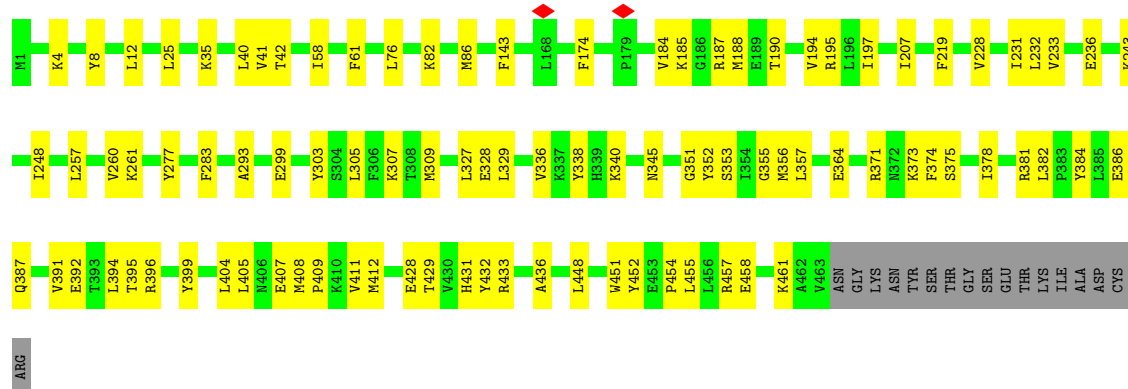


Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	P	1	Total	C	N	O	P	0
			31	10	5	13	3	



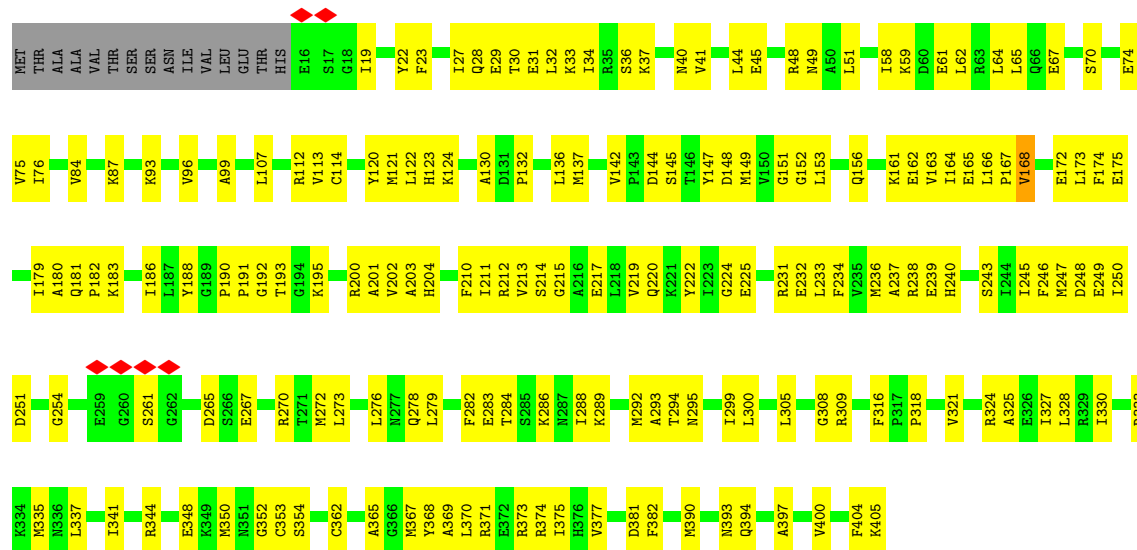
• Molecule 4: DNA mismatch repair protein HSM3

Chain D: 77% 20%



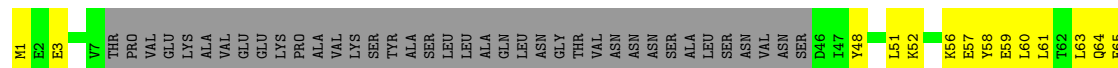
• Molecule 5: 26S proteasome regulatory subunit 8 homolog

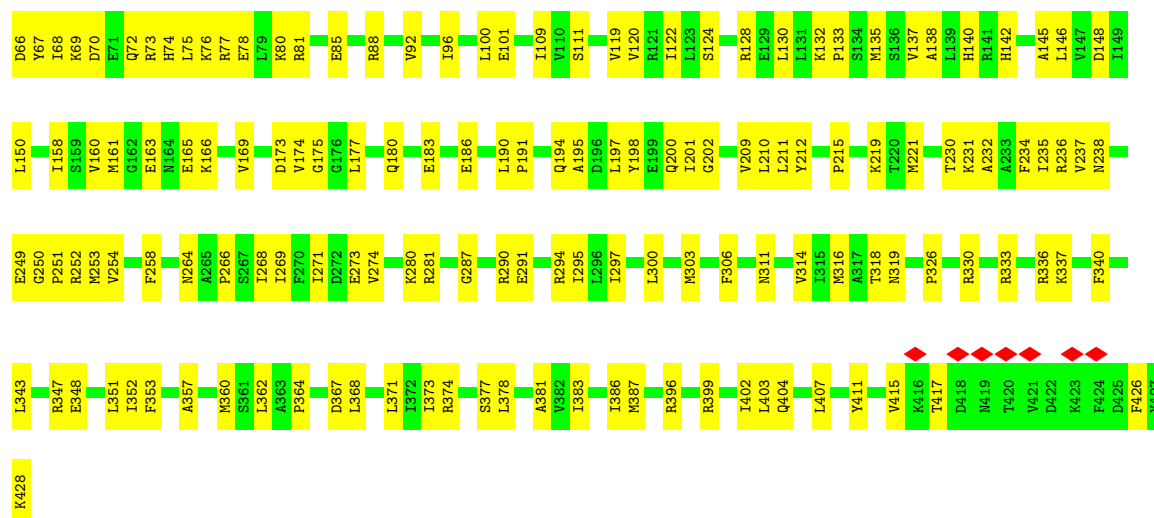
Chain I: 52% 44%



• Molecule 6: 26S proteasome regulatory subunit 6B homolog

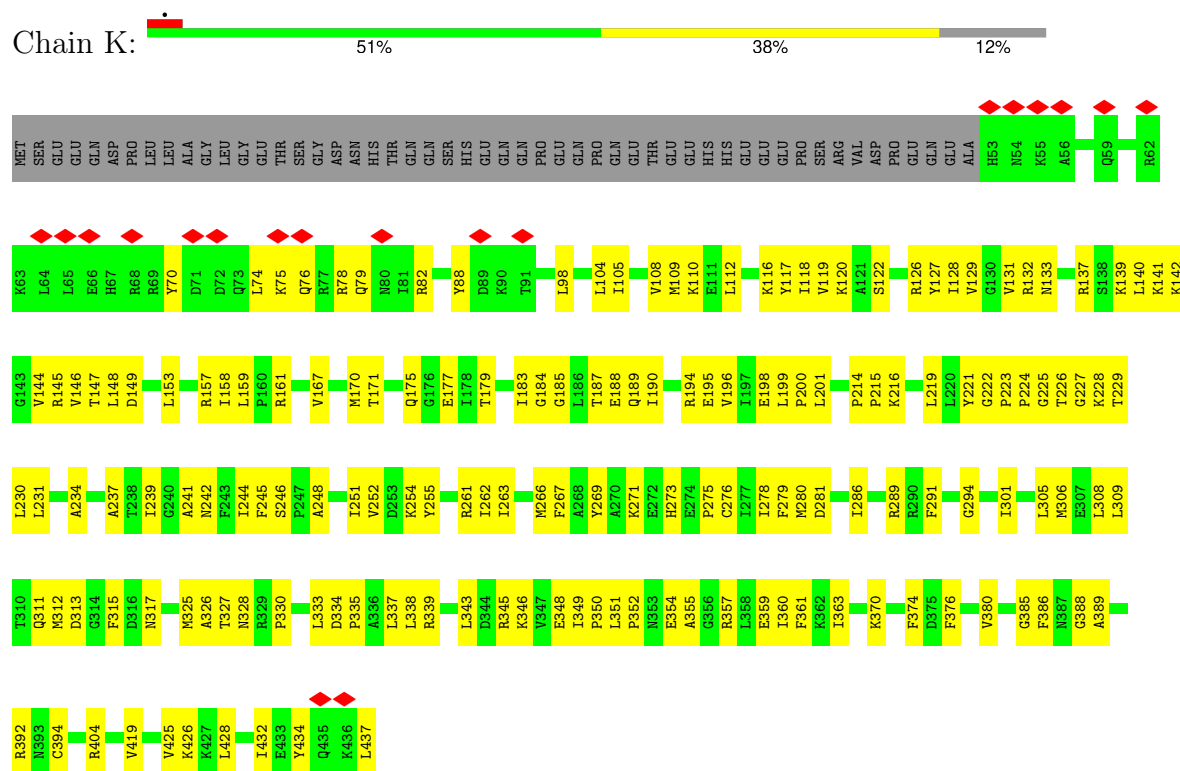
Chain J: 54% 37% 9%





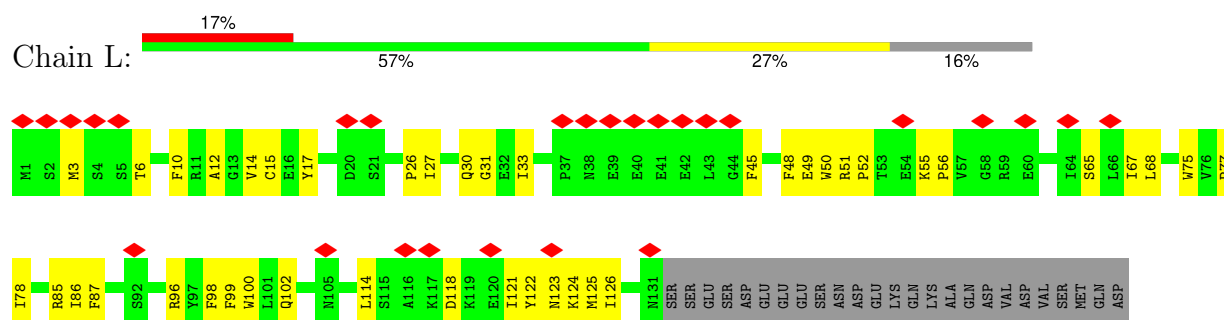
• Molecule 7: 26S proteasome subunit RPT4

Chain K:

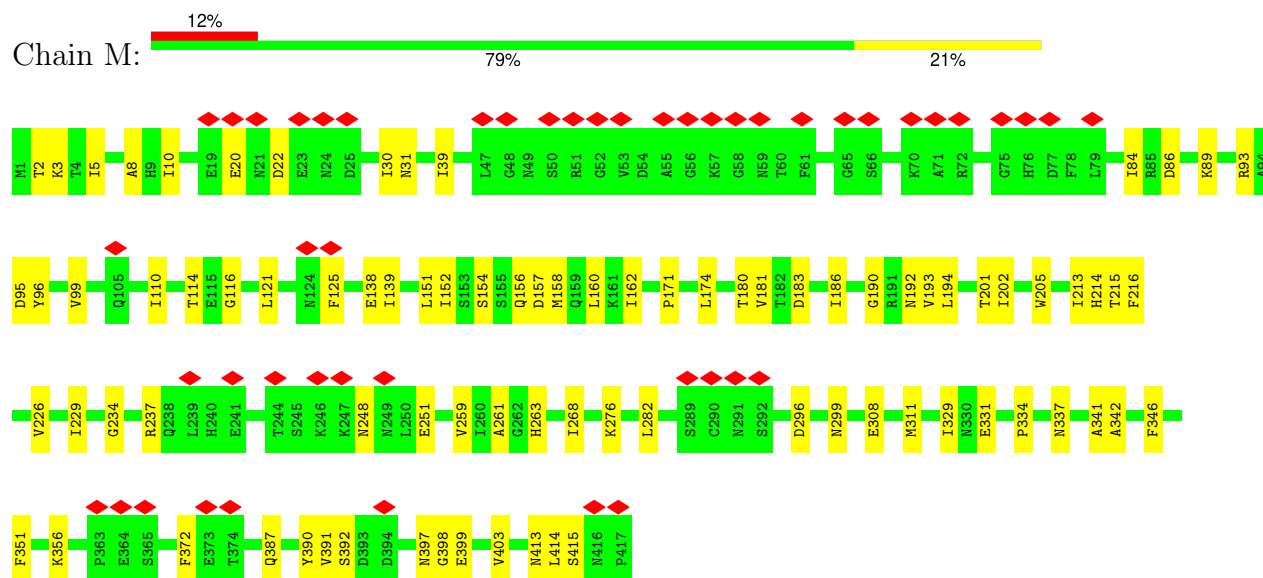


• Molecule 8: 26S proteasome regulatory subunit RPN13

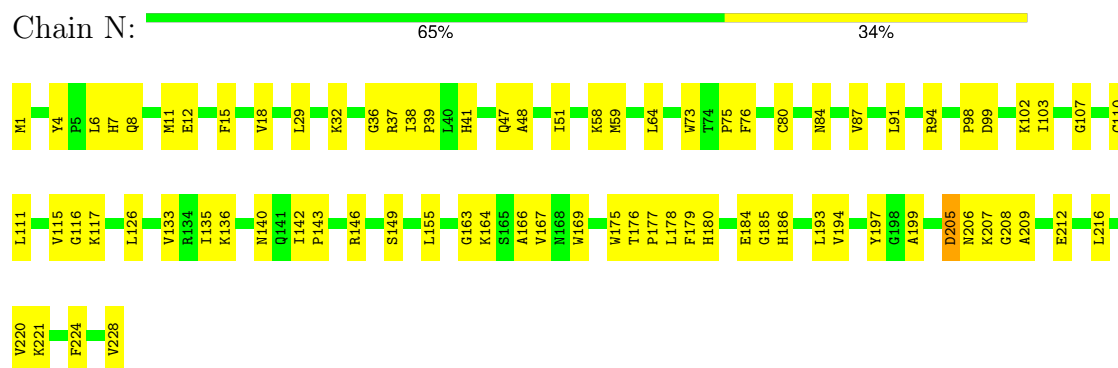
Chain L:



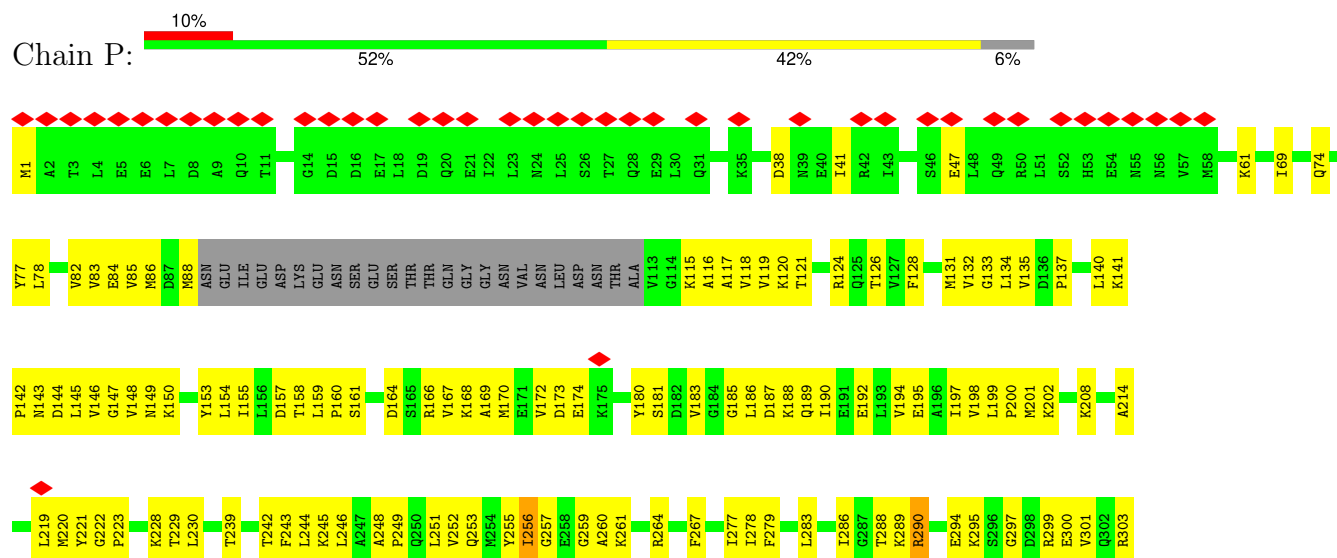
• Molecule 9: 26S proteasome regulatory subunit RPN14

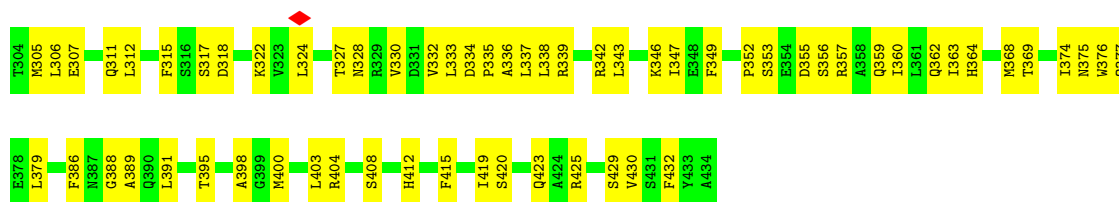


• Molecule 10: Probable 26S proteasome regulatory subunit p28



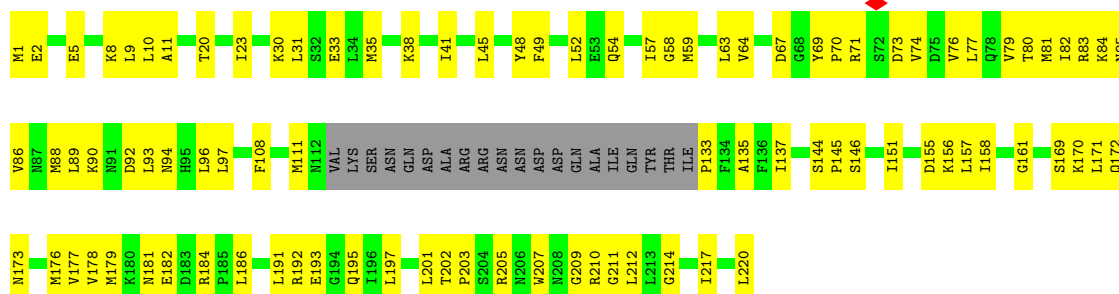
• Molecule 11: 26S proteasome regulatory subunit 6A





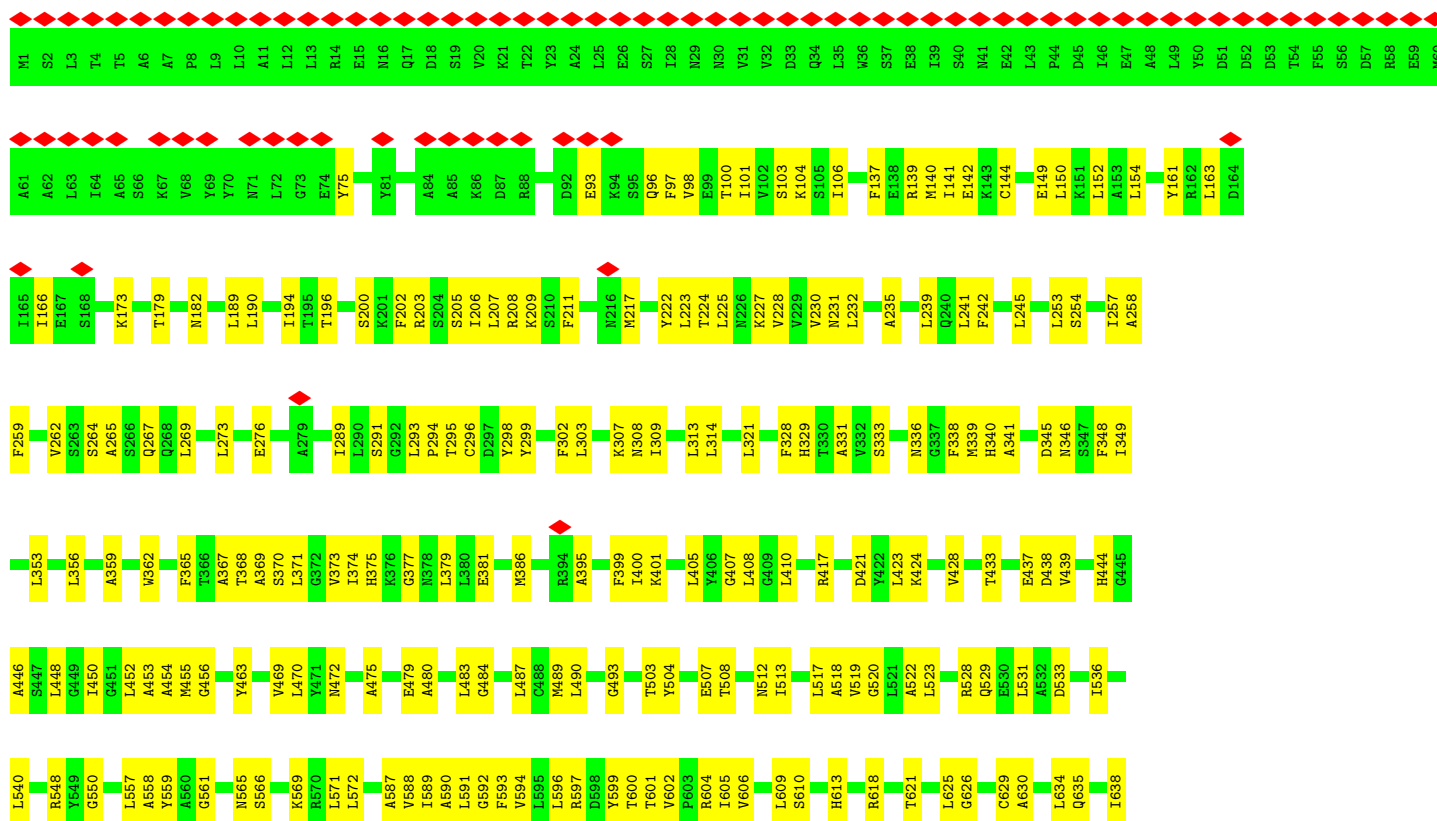
• Molecule 12: Probable 26S proteasome regulatory subunit p27

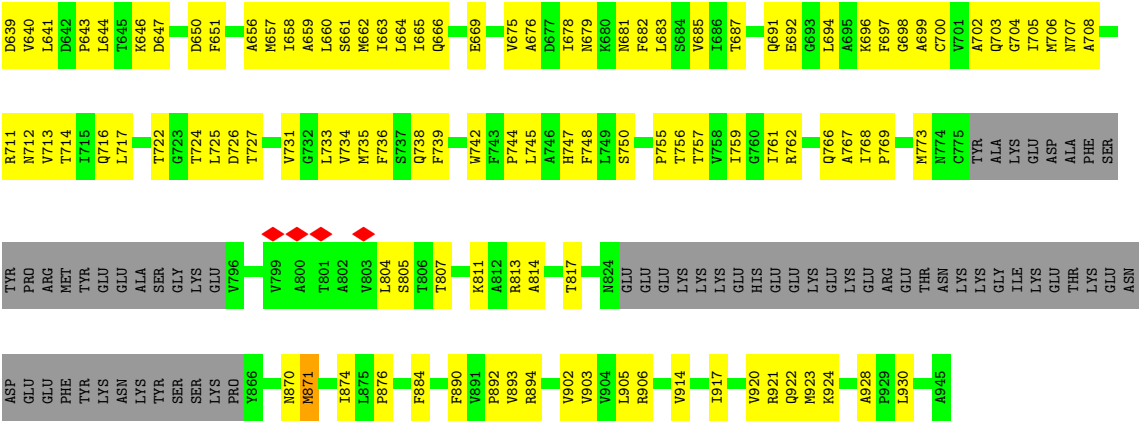
Chain R: 49% 42% 9%



• Molecule 13: 26S proteasome regulatory subunit RPN2

Chain Z: 10% 60% 34% 6%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.406	Depositor
Minimum map value	-0.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	536.576, 536.576, 536.576	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.14	0/2651	0.35	0/3563
2	B	0.16	0/3120	0.42	0/4204
3	C	0.14	0/6702	0.37	0/9090
4	D	0.14	0/3850	0.35	0/5214
5	I	0.21	0/3103	0.56	3/4166 (0.1%)
6	J	0.24	0/3130	0.48	0/4222
7	K	0.20	0/3105	0.44	0/4172
8	L	0.16	0/1087	0.46	0/1470
9	M	0.13	0/3328	0.35	0/4505
10	N	0.17	0/1851	0.40	0/2506
11	P	0.19	0/3242	0.45	0/4368
12	R	0.22	0/1598	0.44	0/2156
13	Z	0.21	0/6916	0.41	1/9358 (0.0%)
All	All	0.18	0/43683	0.42	4/58994 (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
10	N	0	1
11	P	0	3
13	Z	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	130	ALA	CA-C-N	12.79	141.78	121.83
5	I	130	ALA	C-N-CA	12.79	141.78	121.83
5	I	168	VAL	N-CA-C	-7.78	106.32	113.71
13	Z	871	MET	CA-CB-CG	5.38	124.85	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	N	205	ASP	Peptide
11	P	157	ASP	Peptide
11	P	256	ILE	Peptide
11	P	290	ARG	Peptide
13	Z	884	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2611	0	2648	104	0
2	B	3078	0	3148	134	0
3	C	6584	0	6535	210	0
4	D	3783	0	3818	80	0
5	I	3063	0	3201	157	0
6	J	3088	0	3156	150	0
7	K	3059	0	3145	161	0
8	L	1061	0	1050	38	0
9	M	3267	0	3175	62	0
10	N	1808	0	1792	71	0
11	P	3204	0	3266	185	0
12	R	1577	0	1614	106	0
13	Z	6807	0	6900	257	0
14	A	31	0	12	3	0
14	B	31	0	12	1	0
14	I	31	0	12	3	0
14	J	31	0	12	6	0
14	K	31	0	12	11	0
14	P	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	43176	0	43520	1528	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 18.

All (1528) 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)
11:P:147:GLY:H	11:P:159:LEU:HA	1.37	0.89
7:K:184:GLY:H	14:K:501:ATP:HN62	1.16	0.87
13:Z:150:LEU:HD22	13:Z:173:LYS:HD3	1.58	0.84
9:M:192:ASN:HD21	9:M:251:GLU:HA	1.43	0.83
7:K:145:ARG:HH12	11:P:299:ARG:HD2	1.44	0.82
12:R:137:ILE:HD12	12:R:155:ASP:HB2	1.61	0.82
11:P:169:ALA:HB1	11:P:251:LEU:HD23	1.61	0.82
1:A:45:TYR:HA	3:C:159:LEU:HD13	1.63	0.80
13:Z:230:VAL:HB	13:Z:724:THR:HG21	1.64	0.79
13:Z:518:ALA:HB1	13:Z:550:GLY:HA3	1.63	0.79
7:K:170:MET:HG2	7:K:244:ILE:HG23	1.64	0.79
11:P:246:LEU:HB3	11:P:251:LEU:HD11	1.63	0.78
6:J:92:VAL:HG21	7:K:153:LEU:HB2	1.66	0.78
5:I:214:SER:HA	5:I:248:ASP:HB2	1.67	0.78
7:K:144:VAL:HA	11:P:299:ARG:HH22	1.49	0.77
10:N:37:ARG:HE	10:N:41:HIS:HB3	1.49	0.77
13:Z:339:MET:HG2	13:Z:707:ASN:HB2	1.66	0.77
5:I:250:ILE:HG22	5:I:294:THR:HB	1.67	0.77
4:D:378:ILE:HG12	4:D:381:ARG:HH21	1.48	0.76
3:C:809:MET:HB3	3:C:847:ILE:HD12	1.66	0.76
13:Z:211:PHE:HB2	13:Z:228:VAL:HG11	1.68	0.76
13:Z:679:ASN:HA	13:Z:682:PHE:CE1	2.20	0.76
1:A:238:LEU:HD22	4:D:4:LYS:HB3	1.66	0.75
3:C:422:ILE:HB	3:C:436:LEU:HD21	1.66	0.75
11:P:82:VAL:HG21	11:P:140:LEU:HD11	1.66	0.75
13:Z:528:ARG:HB3	13:Z:531:LEU:HB2	1.69	0.75
7:K:171:THR:HG22	7:K:244:ILE:HG12	1.68	0.75
6:J:357:ALA:HA	6:J:387:MET:HE1	1.69	0.74
7:K:139:LYS:HD2	7:K:158:ILE:HG21	1.69	0.74
6:J:161:MET:HE1	6:J:166:LYS:HA	1.67	0.74
13:Z:606:VAL:HB	13:Z:621:THR:HG23	1.69	0.74
11:P:267:PHE:HD1	11:P:311:GLN:HB3	1.52	0.74
3:C:547:MET:HE3	3:C:587:THR:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:759:ILE:HB	13:Z:902:VAL:HG22	1.69	0.74
4:D:188:MET:HE1	4:D:233:VAL:HG11	1.70	0.74
3:C:407:VAL:HG12	3:C:415:MET:HE3	1.70	0.73
9:M:213:ILE:HG23	9:M:248:ASN:HD22	1.52	0.73
6:J:138:ALA:HB3	6:J:148:ASP:HB2	1.68	0.73
11:P:244:LEU:HD22	11:P:278:ILE:HG23	1.70	0.73
10:N:136:LYS:HB3	10:N:140:ASN:HA	1.71	0.73
1:A:43:ALA:HB3	2:B:54:ARG:HB2	1.70	0.73
11:P:88:MET:HE2	11:P:116:ALA:HB2	1.71	0.73
2:B:275:ALA:HB1	2:B:321:ASP:HB2	1.70	0.72
7:K:251:ILE:HG12	7:K:266:MET:HE1	1.69	0.72
1:A:199:THR:HB	1:A:273:ARG:HB3	1.70	0.72
6:J:177:LEU:HG	6:J:180:GLN:HB2	1.70	0.72
5:I:28:GLN:HE22	13:Z:96:GLN:HE21	1.34	0.72
7:K:286:ILE:HA	7:K:301:ILE:HG23	1.70	0.72
6:J:211:LEU:HB3	6:J:219:LYS:HD3	1.69	0.72
2:B:395:MET:HE3	2:B:420:LYS:HB2	1.71	0.72
6:J:300:LEU:HA	6:J:303:MET:HE2	1.72	0.71
4:D:305:LEU:HG	4:D:309:MET:HE1	1.72	0.71
7:K:109:MET:HE3	7:K:118:ILE:HG22	1.70	0.71
11:P:400:MET:HE1	11:P:404:ARG:HH21	1.55	0.71
12:R:20:THR:HA	12:R:23:ILE:HD12	1.70	0.71
7:K:388:GLY:HA3	14:K:501:ATP:C8	2.25	0.71
13:Z:407:GLY:HA2	13:Z:410:LEU:HD12	1.72	0.71
2:B:119:ILE:HG12	2:B:129:TYR:HB2	1.73	0.71
5:I:142:VAL:HG11	5:I:200:ARG:HB3	1.73	0.71
2:B:290:LYS:HE2	2:B:303:GLN:HA	1.72	0.71
10:N:1:MET:HE2	10:N:4:TYR:HB2	1.72	0.71
7:K:98:LEU:HA	11:P:154:LEU:HD13	1.73	0.70
7:K:281:ASP:HA	7:K:326:ALA:HB3	1.72	0.70
6:J:396:ARG:HH21	7:K:195:GLU:HG3	1.56	0.70
13:Z:717:LEU:HD21	13:Z:733:LEU:HD11	1.74	0.70
1:A:234:ARG:HH12	4:D:42:THR:HG21	1.57	0.70
13:Z:163:LEU:HD22	13:Z:209:LYS:HZ3	1.55	0.70
12:R:181:ASN:HB3	12:R:184:ARG:HB2	1.74	0.70
2:B:219:VAL:HG12	2:B:346:ARG:HB2	1.74	0.70
7:K:184:GLY:H	14:K:501:ATP:N6	1.88	0.70
7:K:262:ILE:HG22	7:K:266:MET:HE3	1.74	0.70
13:Z:540:LEU:HA	13:Z:548:ARG:HG2	1.74	0.70
11:P:83:VAL:HG21	11:P:120:LYS:HG3	1.73	0.69
10:N:212:GLU:HB2	10:N:221:LYS:HE3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:328:GLU:HG2	4:D:355:GLY:HA3	1.75	0.69
8:L:31:GLY:HA3	8:L:50:TRP:HE1	1.56	0.69
12:R:84:LYS:HG2	12:R:88:MET:HE1	1.75	0.69
2:B:284:ILE:HG12	2:B:326:MET:HE3	1.74	0.69
4:D:375:SER:H	4:D:378:ILE:HB	1.56	0.69
7:K:120:LYS:HE2	7:K:122:SER:HA	1.74	0.69
12:R:63:LEU:HD13	12:R:76:VAL:HG13	1.75	0.69
5:I:247:MET:HG2	5:I:250:ILE:HD13	1.75	0.68
2:B:282:ASP:HA	2:B:327:ALA:HB3	1.76	0.68
3:C:256:LEU:HD13	3:C:260:GLU:HB3	1.74	0.68
12:R:181:ASN:HA	12:R:184:ARG:HD2	1.75	0.68
12:R:80:THR:HA	12:R:83:ARG:HB2	1.74	0.68
2:B:358:LYS:HB3	2:B:381:VAL:HG11	1.75	0.68
4:D:336:VAL:HA	4:D:340:LYS:HE3	1.76	0.68
3:C:285:ALA:HA	3:C:293:MET:HE3	1.76	0.68
12:R:77:LEU:HG	12:R:81:MET:HE2	1.74	0.68
3:C:406:TRP:HA	3:C:409:LYS:HD3	1.76	0.67
6:J:353:PHE:HB3	6:J:368:LEU:HD13	1.76	0.67
9:M:114:THR:HA	9:M:138:GLU:HG3	1.76	0.67
5:I:76:ILE:HD11	5:I:87:LYS:HB2	1.76	0.67
2:B:75:PHE:HB2	3:C:621:LEU:HD22	1.76	0.67
10:N:64:LEU:HD22	10:N:76:PHE:HD2	1.59	0.67
6:J:122:ILE:HG23	6:J:146:LEU:HD23	1.74	0.67
5:I:390:MET:HB3	5:I:394:GLN:HG3	1.77	0.67
6:J:371:LEU:HD11	6:J:407:LEU:HD21	1.77	0.67
11:P:174:GLU:HA	11:P:242:THR:HG23	1.76	0.67
1:A:63:ILE:HG12	2:B:73:GLU:HB2	1.76	0.67
5:I:163:VAL:HA	5:I:182:PRO:HG2	1.77	0.67
6:J:132:LYS:H	6:J:135:MET:HE2	1.59	0.67
1:A:45:TYR:CZ	3:C:226:GLU:HG3	2.30	0.67
5:I:75:VAL:HG21	5:I:107:LEU:HD11	1.76	0.67
7:K:392:ARG:HD3	14:K:501:ATP:H4'	1.75	0.67
8:L:49:GLU:HB3	8:L:65:SER:HB3	1.77	0.67
3:C:812:ILE:HA	3:C:815:MET:HE2	1.77	0.67
1:A:311:ILE:HG12	1:A:355:THR:HB	1.76	0.66
7:K:389:ALA:HB2	14:K:501:ATP:H5'1	1.77	0.66
3:C:883:THR:HG21	3:C:903:MET:HG3	1.77	0.66
1:A:226:GLU:HG2	1:A:267:THR:HG22	1.77	0.66
13:Z:190:LEU:HD13	13:Z:227:LYS:HG2	1.77	0.66
7:K:194:ARG:O	7:K:198:GLU:HG2	1.96	0.66
8:L:85:ARG:HD3	8:L:114:LEU:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:GLY:HA3	2:B:258:GLY:HA3	1.78	0.66
2:B:203:THR:HG23	2:B:240:THR:HG22	1.78	0.66
11:P:376:TRP:HA	11:P:379:LEU:HD12	1.77	0.66
5:I:190:PRO:HD2	5:I:193:THR:HG21	1.78	0.65
5:I:375:ILE:HG23	6:J:200:GLN:HB3	1.78	0.65
11:P:135:VAL:HG21	11:P:158:THR:H	1.62	0.65
13:Z:307:LYS:HD2	13:Z:309:ILE:HD11	1.77	0.65
13:Z:661:SER:HA	13:Z:706:MET:HE3	1.77	0.65
1:A:357:ARG:HH22	4:D:431:HIS:CE1	2.15	0.65
1:A:410:LEU:HD11	4:D:232:LEU:HG	1.79	0.65
7:K:404:ARG:HH21	11:P:195:GLU:HG3	1.62	0.65
8:L:121:ILE:HA	8:L:124:LYS:HE2	1.79	0.65
7:K:222:GLY:HA3	7:K:349:ILE:HG23	1.78	0.65
13:Z:433:THR:HG23	13:Z:439:VAL:HG11	1.78	0.65
13:Z:920:VAL:HA	13:Z:923:MET:HE2	1.79	0.65
9:M:397:ASN:HA	9:M:415:SER:HB3	1.78	0.65
10:N:48:ALA:HB1	10:N:51:ILE:HD13	1.79	0.65
5:I:231:ARG:HG2	5:I:278:GLN:HE21	1.62	0.64
6:J:221:MET:HB2	14:J:501:ATP:H2'	1.78	0.64
13:Z:470:LEU:HD11	13:Z:517:LEU:HD21	1.80	0.64
11:P:267:PHE:CD1	11:P:311:GLN:HB3	2.32	0.64
13:Z:702:ALA:HA	13:Z:705:ILE:HD12	1.80	0.64
5:I:283:GLU:HB2	5:I:286:LYS:HE3	1.79	0.64
5:I:337:LEU:HB3	5:I:341:ILE:HD12	1.79	0.64
2:B:366:THR:HB	2:B:371:LEU:HD11	1.78	0.64
3:C:968:ASP:HB2	3:C:990:ARG:H	1.62	0.64
6:J:347:ARG:HH11	10:N:216:LEU:HD22	1.61	0.64
3:C:741:LEU:HG	3:C:775:MET:HE2	1.80	0.64
6:J:52:LYS:HD2	13:Z:196:THR:HG21	1.80	0.64
13:Z:768:ILE:HB	13:Z:917:ILE:HB	1.79	0.64
13:Z:892:PRO:HA	13:Z:905:LEU:HA	1.79	0.64
7:K:141:LYS:HD2	7:K:161:ARG:HH12	1.62	0.64
7:K:360:ILE:HG12	14:K:501:ATP:C6	2.32	0.64
2:B:246:ARG:HG3	2:B:280:PHE:HD2	1.62	0.63
3:C:510:LEU:HA	3:C:530:LEU:HD11	1.81	0.63
11:P:82:VAL:HA	11:P:119:VAL:HG12	1.78	0.63
3:C:93:ARG:HH21	3:C:126:TYR:HA	1.62	0.63
5:I:167:PRO:HG2	5:I:289:LYS:HD2	1.79	0.63
6:J:74:HIS:CE1	6:J:81:ARG:HH12	2.16	0.63
12:R:203:PRO:HB3	12:R:212:LEU:HB3	1.80	0.63
2:B:177:PRO:HB2	2:B:238:ASN:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:116:GLY:HA2	9:M:139:ILE:HG13	1.80	0.63
3:C:338:HIS:HE1	3:C:922:PRO:HD3	1.62	0.63
3:C:761:PHE:CD2	3:C:780:MET:HB3	2.33	0.63
5:I:234:PHE:HA	5:I:237:ALA:HB3	1.80	0.63
5:I:236:MET:HA	5:I:239:GLU:HG3	1.80	0.63
5:I:192:GLY:HA3	5:I:354:SER:HB2	1.79	0.63
7:K:184:GLY:HA3	7:K:360:ILE:HG13	1.81	0.63
3:C:453:LEU:HB2	3:C:488:ALA:HB1	1.81	0.63
2:B:101:GLY:HA3	2:B:151:HIS:HE1	1.64	0.63
3:C:491:LEU:HD13	3:C:903:MET:HE3	1.81	0.63
7:K:140:LEU:HD22	7:K:146:VAL:HG11	1.81	0.63
11:P:141:LYS:HB2	11:P:252:VAL:HG12	1.80	0.63
1:A:200:VAL:HG22	1:A:272:ILE:HG23	1.80	0.63
12:R:158:ILE:HD11	12:R:191:LEU:HB2	1.81	0.63
2:B:79:SER:HA	3:C:626:PRO:HG2	1.81	0.63
3:C:338:HIS:CE1	3:C:922:PRO:HD3	2.33	0.63
3:C:401:VAL:HG22	3:C:422:ILE:HG23	1.80	0.63
3:C:82:MET:HG3	3:C:152:GLU:HG2	1.81	0.62
3:C:812:ILE:HG21	3:C:848:THR:HA	1.80	0.62
1:A:200:VAL:HG13	1:A:272:ILE:HG12	1.81	0.62
11:P:338:LEU:HB3	11:P:346:LYS:HZ1	1.62	0.62
1:A:79:SER:HA	1:A:82:TRP:CE2	2.34	0.62
7:K:196:VAL:HG13	7:K:215:PRO:HB2	1.81	0.62
3:C:225:LEU:HD11	3:C:256:LEU:HD21	1.81	0.62
6:J:186:GLU:HB2	6:J:336:ARG:HH22	1.63	0.62
12:R:137:ILE:HD13	12:R:151:ILE:HG23	1.82	0.62
6:J:60:LEU:HD22	13:Z:601:THR:HB	1.80	0.62
3:C:124:MET:HE3	3:C:156:HIS:HB3	1.82	0.62
11:P:327:THR:HG21	11:P:333:LEU:HD11	1.81	0.62
3:C:570:LEU:HD11	3:C:584:VAL:HG21	1.81	0.62
5:I:325:ALA:HB2	5:I:344:ARG:HG3	1.82	0.62
10:N:115:VAL:HB	10:N:155:LEU:HD21	1.82	0.62
3:C:809:MET:HG2	3:C:844:ALA:HA	1.81	0.62
4:D:184:VAL:HG22	4:D:187:ARG:HH21	1.63	0.61
13:Z:713:VAL:HG12	13:Z:755:PRO:HA	1.82	0.61
1:A:396:MET:HA	2:B:211:MET:O	2.00	0.61
3:C:905:ASN:HA	3:C:908:ILE:HD12	1.81	0.61
2:B:130:VAL:HG11	2:B:154:MET:HG3	1.82	0.61
3:C:133:ASP:HA	3:C:136:ARG:HB3	1.81	0.61
7:K:108:VAL:HG22	7:K:119:VAL:HG12	1.82	0.61
3:C:761:PHE:HB3	3:C:776:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:84:ILE:HD11	9:M:413:ASN:HB2	1.83	0.61
10:N:175:TRP:CD2	10:N:179:PHE:HB3	2.36	0.61
2:B:47:PRO:HB3	3:C:755:GLU:HB2	1.82	0.61
2:B:119:ILE:HA	2:B:129:TYR:HA	1.82	0.61
3:C:460:SER:HA	3:C:496:ALA:HA	1.83	0.61
6:J:60:LEU:HD21	13:Z:604:ARG:HB2	1.83	0.61
7:K:354:GLU:HG2	7:K:357:ARG:NH2	2.15	0.61
2:B:370:ASN:HD22	2:B:409:MET:HG3	1.65	0.61
4:D:351:GLY:HA2	4:D:386:GLU:CD	2.25	0.61
6:J:371:LEU:HA	6:J:374:ARG:NH2	2.16	0.61
6:J:100:LEU:HD11	6:J:111:SER:HB3	1.83	0.61
12:R:144:SER:HB2	12:R:214:GLY:HA3	1.82	0.61
13:Z:362:TRP:HH2	13:Z:444:HIS:CD2	2.18	0.61
3:C:452:LEU:HD13	3:C:489:ALA:HB2	1.80	0.61
5:I:137:MET:HB2	6:J:281:ARG:HH12	1.65	0.61
11:P:295:LYS:HE2	12:R:67:ASP:HA	1.83	0.61
13:Z:353:LEU:HD23	13:Z:356:LEU:HD12	1.81	0.61
2:B:106:ILE:HG13	5:I:93:LYS:HB2	1.83	0.61
3:C:288:LEU:HD12	3:C:293:MET:HE1	1.82	0.61
3:C:575:MET:HA	3:C:607:ALA:HA	1.83	0.61
2:B:331:ILE:HA	2:B:334:LEU:HD23	1.83	0.60
9:M:308:GLU:HG3	9:M:334:PRO:HB3	1.83	0.60
11:P:164:ASP:HB3	11:P:167:VAL:HG23	1.82	0.60
13:Z:484:GLY:HA2	13:Z:487:LEU:HB2	1.83	0.60
3:C:282:ILE:HD11	3:C:314:LEU:HD11	1.83	0.60
8:L:102:GLN:HA	13:Z:928:ALA:HB3	1.82	0.60
7:K:104:LEU:HB2	7:K:148:LEU:HB2	1.82	0.60
11:P:147:GLY:N	11:P:159:LEU:HA	2.12	0.60
12:R:57:ILE:HD11	12:R:74:VAL:HG11	1.83	0.60
11:P:124:ARG:HA	12:R:69:TYR:CD1	2.36	0.60
3:C:224:LEU:HB3	3:C:230:ILE:HA	1.84	0.60
5:I:247:MET:HB3	5:I:292:MET:HA	1.83	0.60
13:Z:356:LEU:HD22	13:Z:367:ALA:HB1	1.83	0.60
7:K:183:ILE:HG23	7:K:231:LEU:HG	1.83	0.60
3:C:621:LEU:HD23	3:C:624:LEU:HD12	1.84	0.60
5:I:19:ILE:HD11	13:Z:141:ILE:HG12	1.83	0.60
7:K:144:VAL:HA	11:P:299:ARG:NH2	2.15	0.60
5:I:19:ILE:HG12	13:Z:140:MET:HG3	1.83	0.59
11:P:364:HIS:HB2	11:P:395:THR:HG21	1.84	0.59
2:B:362:LEU:HD22	2:B:381:VAL:HG23	1.82	0.59
3:C:745:LEU:HD21	3:C:882:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:179:ILE:HG22	5:I:181:GLN:H	1.66	0.59
7:K:327:THR:HG21	7:K:333:LEU:HD11	1.84	0.59
10:N:84:ASN:HB3	10:N:87:VAL:HG22	1.83	0.59
13:Z:493:GLY:HA3	13:Z:528:ARG:NE	2.17	0.59
6:J:221:MET:HE3	14:J:501:ATP:H2'	1.83	0.59
5:I:330:ILE:HA	5:I:333:ARG:HE	1.66	0.59
6:J:360:MET:HE3	6:J:402:ILE:HD11	1.83	0.59
6:J:426:PHE:HB2	10:N:207:LYS:HB2	1.84	0.59
10:N:103:ILE:HB	10:N:107:GLY:HA2	1.84	0.59
4:D:405:LEU:HD12	4:D:412:MET:HE3	1.83	0.59
7:K:148:LEU:HD13	7:K:153:LEU:HD12	1.85	0.59
13:Z:93:GLU:HB3	13:Z:98:VAL:HG21	1.84	0.59
13:Z:227:LYS:HA	13:Z:722:THR:HA	1.84	0.59
2:B:101:GLY:HA3	2:B:151:HIS:CE1	2.37	0.59
2:B:194:ILE:HD13	2:B:232:LEU:HG	1.85	0.59
6:J:132:LYS:H	6:J:135:MET:CE	2.15	0.59
10:N:94:ARG:HH12	10:N:98:PRO:HD3	1.67	0.59
2:B:220:ILE:HG12	2:B:326:MET:HB2	1.85	0.59
3:C:610:GLY:HA3	3:C:873:LEU:HD22	1.83	0.59
7:K:244:ILE:HB	7:K:278:ILE:HA	1.84	0.59
11:P:69:ILE:HD11	11:P:134:LEU:HB3	1.84	0.59
11:P:78:LEU:HB2	11:P:150:LYS:HA	1.85	0.59
5:I:59:LYS:HB3	13:Z:613:HIS:CE1	2.37	0.58
5:I:238:ARG:HA	5:I:288:ILE:HD11	1.84	0.58
5:I:367:MET:SD	6:J:183:GLU:HG2	2.43	0.58
6:J:67:TYR:CD1	13:Z:572:LEU:HD22	2.37	0.58
6:J:367:ASP:HB3	10:N:117:LYS:HE3	1.85	0.58
13:Z:566:SER:HA	13:Z:569:LYS:HE3	1.85	0.58
13:Z:626:GLY:HA2	13:Z:663:ILE:HD11	1.85	0.58
7:K:221:TYR:HB2	7:K:330:PRO:HG3	1.85	0.58
13:Z:683:LEU:O	13:Z:687:THR:HG23	2.03	0.58
3:C:127:SER:HB2	3:C:133:ASP:HB2	1.85	0.58
13:Z:208:ARG:HH21	13:Z:232:LEU:HB3	1.68	0.58
5:I:166:LEU:HD21	9:M:158:MET:HE2	1.84	0.58
11:P:74:GLN:HG2	12:R:10:LEU:HB3	1.86	0.58
11:P:403:LEU:HD11	12:R:31:LEU:HD12	1.85	0.58
12:R:45:LEU:HB3	12:R:49:PHE:CE2	2.39	0.58
13:Z:811:LYS:HA	13:Z:814:ALA:HB3	1.86	0.58
1:A:36:VAL:HA	3:C:125:THR:HB	1.84	0.58
7:K:105:ILE:HD11	11:P:128:PHE:HB2	1.85	0.58
11:P:220:MET:HB2	11:P:349:PHE:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ARG:HA	2:B:347:LYS:HZ2	1.69	0.58
3:C:208:VAL:HG13	3:C:220:ALA:HB1	1.85	0.58
2:B:220:ILE:HG13	2:B:344:ILE:HG21	1.85	0.58
3:C:64:TYR:HD2	3:C:111:LEU:HD13	1.69	0.58
7:K:223:PRO:HD2	7:K:226:THR:HG21	1.84	0.58
3:C:620:LEU:HD22	3:C:739:ALA:HA	1.85	0.58
5:I:232:GLU:HB3	5:I:236:MET:HE1	1.86	0.58
1:A:198:MET:HE1	1:A:274:VAL:HG22	1.85	0.57
11:P:290:ARG:HD2	11:P:332:VAL:HG12	1.86	0.57
13:Z:235:ALA:HB2	13:Z:269:LEU:HA	1.85	0.57
3:C:591:ILE:HG22	3:C:593:HIS:H	1.69	0.57
11:P:77:TYR:HB2	12:R:77:LEU:HD13	1.86	0.57
4:D:382:LEU:HD13	4:D:386:GLU:HG3	1.86	0.57
6:J:96:ILE:HG12	7:K:126:ARG:H	1.68	0.57
1:A:307:PHE:HD1	1:A:352:MET:HE3	1.68	0.57
5:I:330:ILE:HG12	5:I:333:ARG:HH21	1.68	0.57
2:B:106:ILE:HG13	5:I:93:LYS:HE2	1.86	0.57
7:K:361:PHE:HB3	7:K:376:PHE:CD1	2.40	0.57
10:N:37:ARG:HE	10:N:41:HIS:CB	2.15	0.57
2:B:221:LEU:HD13	2:B:325:ILE:HG23	1.86	0.57
3:C:969:GLU:HA	3:C:989:TYR:HD1	1.70	0.57
10:N:11:MET:SD	10:N:12:GLU:HG3	2.44	0.57
13:Z:773:MET:HE1	13:Z:870:ASN:HA	1.86	0.57
2:B:143:PRO:HD3	2:B:304:ARG:HD3	1.86	0.57
1:A:225:VAL:HG11	1:A:305:ILE:HD11	1.87	0.57
3:C:249:MET:HE2	3:C:268:ALA:HB2	1.87	0.57
5:I:327:ILE:HG12	14:I:501:ATP:C6	2.39	0.57
3:C:282:ILE:HB	3:C:297:VAL:HG11	1.86	0.57
3:C:439:TYR:HB2	3:C:451:ALA:HB2	1.86	0.57
9:M:214:HIS:CG	9:M:276:LYS:HD2	2.40	0.57
13:Z:203:ARG:NH1	13:Z:597:ARG:HH12	2.02	0.57
13:Z:349:ILE:HD11	13:Z:374:ILE:HD12	1.87	0.57
2:B:332:GLU:HB2	4:D:429:THR:HG21	1.85	0.57
3:C:319:THR:HG23	3:C:321:PHE:H	1.69	0.57
1:A:311:ILE:HG21	1:A:353:PHE:HB3	1.86	0.56
9:M:356:LYS:HE3	9:M:414:LEU:HD22	1.87	0.56
12:R:108:PHE:HA	12:R:111:MET:HE3	1.86	0.56
3:C:385:PHE:HZ	3:C:898:HIS:HB3	1.70	0.56
3:C:772:ILE:O	3:C:776:VAL:HG23	2.05	0.56
3:C:774:ARG:HA	3:C:807:VAL:HG22	1.85	0.56
7:K:119:VAL:HG23	7:K:127:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:289:LYS:HG3	11:P:334:ASP:HA	1.86	0.56
3:C:624:LEU:HD23	3:C:736:LEU:HD22	1.86	0.56
4:D:353:SER:O	4:D:357:LEU:HG	2.05	0.56
6:J:234:PHE:HE2	6:J:236:ARG:HB2	1.70	0.56
11:P:117:ALA:HB2	11:P:132:VAL:HG22	1.87	0.56
11:P:288:THR:HA	11:P:333:LEU:HA	1.87	0.56
13:Z:230:VAL:HG11	13:Z:264:SER:HB2	1.88	0.56
13:Z:745:LEU:O	13:Z:748:PHE:HD1	1.88	0.56
5:I:211:ILE:HG21	5:I:233:LEU:HD11	1.86	0.56
13:Z:331:ALA:HB2	13:Z:697:PHE:CD1	2.40	0.56
13:Z:571:LEU:HD12	13:Z:587:ALA:HA	1.87	0.56
1:A:197:MET:HE1	1:A:278:GLU:HB2	1.86	0.56
5:I:166:LEU:HD22	9:M:157:ASP:HA	1.88	0.56
5:I:166:LEU:HD11	5:I:173:LEU:HD12	1.87	0.56
12:R:173:ASN:O	12:R:176:MET:HG3	2.06	0.56
13:Z:807:THR:HA	13:Z:811:LYS:HB2	1.87	0.56
2:B:200:LEU:HG	2:B:208:TYR:HE1	1.70	0.56
7:K:360:ILE:HA	7:K:363:ILE:HD12	1.87	0.56
8:L:3:MET:HE1	8:L:6:THR:H	1.69	0.56
2:B:186:GLY:HA3	2:B:357:THR:HG23	1.88	0.56
7:K:74:LEU:HD11	11:P:47:GLU:HB3	1.88	0.56
13:Z:242:PHE:HA	13:Z:245:LEU:HD12	1.86	0.56
2:B:290:LYS:HD3	2:B:292:TYR:CE1	2.40	0.56
4:D:261:LYS:HG2	4:D:305:LEU:HD22	1.87	0.56
6:J:186:GLU:O	6:J:191:PRO:HD3	2.06	0.56
11:P:160:PRO:HB2	12:R:84:LYS:HD3	1.87	0.56
2:B:66:LYS:HE3	13:Z:805:SER:HB3	1.88	0.56
6:J:291:GLU:O	6:J:295:ILE:HG13	2.06	0.56
5:I:44:LEU:HB3	6:J:68:ILE:HG21	1.88	0.55
6:J:212:TYR:HA	6:J:318:THR:O	2.06	0.55
12:R:48:TYR:HB3	12:R:82:ILE:HG23	1.87	0.55
4:D:353:SER:O	4:D:356:MET:HB2	2.06	0.55
5:I:214:SER:HA	5:I:248:ASP:CB	2.34	0.55
2:B:177:PRO:HB3	2:B:234:LYS:HE3	1.87	0.55
2:B:227:THR:OG1	2:B:350:PHE:HB3	2.07	0.55
6:J:169:VAL:HG11	6:J:221:MET:HG3	1.88	0.55
6:J:190:LEU:HD12	6:J:194:GLN:HB2	1.89	0.55
6:J:294:ARG:HA	6:J:297:ILE:HD12	1.86	0.55
11:P:158:THR:OG1	11:P:160:PRO:HA	2.05	0.55
12:R:1:MET:HG3	12:R:2:GLU:N	2.21	0.55
12:R:45:LEU:HD21	12:R:89:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:267:GLN:HB3	13:Z:455:MET:O	2.06	0.55
3:C:977:ILE:HG23	3:C:981:VAL:HG21	1.86	0.55
11:P:173:ASP:HB3	11:P:243:PHE:HB3	1.88	0.55
13:Z:533:ASP:HA	13:Z:536:ILE:HD12	1.88	0.55
3:C:93:ARG:HA	3:C:96:TYR:HB2	1.89	0.55
6:J:92:VAL:HG12	7:K:127:TYR:HB3	1.88	0.55
6:J:280:LYS:HE2	6:J:326:PRO:HD3	1.88	0.55
6:J:404:GLN:HG2	10:N:73:TRP:CZ2	2.42	0.55
11:P:201:MET:HE3	11:P:322:LYS:HG2	1.88	0.55
13:Z:463:TYR:HB2	13:Z:489:MET:HE3	1.89	0.55
2:B:237:ALA:HB2	2:B:278:ILE:HD12	1.89	0.55
6:J:120:VAL:HB	6:J:145:ALA:HA	1.88	0.55
13:Z:520:GLY:HA2	13:Z:523:LEU:HD12	1.89	0.55
13:Z:659:ALA:O	13:Z:663:ILE:HG12	2.07	0.55
3:C:916:LEU:HB2	3:C:982:ILE:HG12	1.87	0.55
4:D:194:VAL:HG13	4:D:236:GLU:HG2	1.88	0.55
5:I:162:GLU:HB2	9:M:180:THR:OG1	2.07	0.55
5:I:183:LYS:HG2	5:I:284:THR:HG22	1.87	0.55
13:Z:208:ARG:HE	13:Z:232:LEU:HD13	1.72	0.55
8:L:33:ILE:HD13	8:L:48:PHE:CZ	2.42	0.55
5:I:273:LEU:HD23	5:I:276:LEU:HD12	1.89	0.55
2:B:104:LEU:HD22	2:B:157:VAL:HG21	1.88	0.54
3:C:457:ILE:HG12	3:C:495:ILE:HD13	1.88	0.54
5:I:367:MET:HE1	6:J:336:ARG:CZ	2.37	0.54
7:K:145:ARG:NH1	11:P:299:ARG:HD2	2.17	0.54
7:K:351:LEU:HD13	7:K:385:GLY:HA2	1.89	0.54
13:Z:231:ASN:ND2	13:Z:724:THR:HG22	2.22	0.54
3:C:812:ILE:HG12	3:C:834:LEU:HD13	1.90	0.54
7:K:149:ASP:H	7:K:153:LEU:HA	1.73	0.54
1:A:454:TYR:HE2	1:A:462:ARG:H	1.55	0.54
7:K:146:VAL:HG12	7:K:158:ILE:HG23	1.89	0.54
10:N:15:PHE:HD1	10:N:51:ILE:HG13	1.72	0.54
10:N:51:ILE:HD12	10:N:51:ILE:H	1.73	0.54
13:Z:298:TYR:OH	13:Z:766:GLN:HB3	2.06	0.54
1:A:265:ASN:HA	3:C:364:ASN:ND2	2.21	0.54
3:C:87:LYS:HA	3:C:90:LYS:HZ3	1.72	0.54
4:D:407:GLU:O	4:D:408:MET:HE2	2.08	0.54
11:P:257:GLY:H	11:P:261:LYS:NZ	2.05	0.54
13:Z:589:ILE:HG22	13:Z:593:PHE:CE1	2.43	0.54
1:A:444:LEU:HD21	4:D:232:LEU:HD12	1.89	0.54
11:P:83:VAL:HB	11:P:118:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:405:LEU:HD11	4:D:451:TRP:CD1	2.43	0.54
11:P:85:VAL:HB	11:P:255:TYR:CG	2.43	0.54
11:P:219:LEU:HB2	11:P:343:LEU:HD13	1.89	0.54
11:P:430:VAL:HG11	12:R:49:PHE:CE1	2.43	0.54
13:Z:339:MET:HG3	13:Z:704:GLY:HA2	1.88	0.54
2:B:248:VAL:HG22	2:B:282:ASP:HB3	1.88	0.54
7:K:88:TYR:CE1	11:P:61:LYS:HB3	2.43	0.54
7:K:267:PHE:CD1	7:K:311:GLN:HB3	2.42	0.54
13:Z:190:LEU:HB3	13:Z:227:LYS:HE2	1.90	0.54
1:A:204:PRO:HD2	3:C:364:ASN:ND2	2.23	0.54
1:A:403:ARG:HH21	4:D:232:LEU:HD13	1.73	0.54
3:C:72:LYS:HB3	3:C:76:LYS:HE3	1.89	0.54
5:I:163:VAL:HG13	5:I:182:PRO:HB2	1.89	0.54
10:N:184:GLU:HG3	10:N:186:HIS:CE1	2.43	0.54
10:N:207:LYS:HE3	10:N:207:LYS:HA	1.90	0.54
11:P:84:GLU:HA	11:P:142:PRO:HG3	1.90	0.54
1:A:432:ARG:HH12	2:B:195:LYS:HB3	1.73	0.54
4:D:454:PRO:HA	4:D:457:ARG:NE	2.22	0.54
7:K:141:LYS:HD3	7:K:142:LYS:N	2.23	0.54
10:N:149:SER:O	10:N:184:GLU:HG2	2.08	0.54
13:Z:762:ARG:HH21	13:Z:769:PRO:HB3	1.71	0.54
3:C:895:LEU:HA	3:C:898:HIS:CE1	2.43	0.54
11:P:85:VAL:HG23	11:P:142:PRO:HD3	1.89	0.54
11:P:190:ILE:HD13	12:R:205:ARG:HH12	1.73	0.54
6:J:73:ARG:HG3	6:J:74:HIS:N	2.23	0.53
7:K:201:LEU:HD12	7:K:239:ILE:HD13	1.89	0.53
12:R:192:ARG:HB3	12:R:195:GLN:HE21	1.73	0.53
1:A:52:THR:HG23	2:B:66:LYS:HE2	1.91	0.53
1:A:299:ARG:HA	1:A:349:ILE:HD11	1.91	0.53
13:Z:349:ILE:HG23	13:Z:356:LEU:HD11	1.90	0.53
13:Z:529:GLN:HA	13:Z:558:ALA:HB1	1.89	0.53
13:Z:588:VAL:HA	13:Z:591:LEU:HD12	1.90	0.53
1:A:196:THR:HG21	2:B:290:LYS:NZ	2.23	0.53
5:I:19:ILE:HB	13:Z:144:CYS:SG	2.48	0.53
5:I:164:ILE:HD12	5:I:289:LYS:HB3	1.90	0.53
5:I:353:CYS:SG	5:I:390:MET:HE1	2.49	0.53
6:J:343:LEU:HB2	6:J:377:SER:HB2	1.90	0.53
10:N:4:TYR:HB3	10:N:7:HIS:ND1	2.24	0.53
11:P:425:ARG:HB3	11:P:432:PHE:CD1	2.44	0.53
2:B:201:PRO:HB2	2:B:323:LYS:HE3	1.90	0.53
6:J:85:GLU:HA	6:J:88:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:339:ARG:HD2	11:P:342:ARG:NH1	2.23	0.53
11:P:430:VAL:HG13	12:R:59:MET:HG2	1.90	0.53
8:L:55:LYS:HE2	8:L:56:PRO:HD2	1.91	0.53
3:C:754:LYS:HB3	3:C:783:VAL:HG13	1.90	0.53
7:K:370:LYS:HB2	7:K:374:PHE:CE1	2.43	0.53
9:M:152:ILE:HD13	9:M:193:VAL:HG11	1.90	0.53
11:P:245:LYS:HA	11:P:279:PHE:HB3	1.91	0.53
12:R:192:ARG:HB3	12:R:195:GLN:NE2	2.23	0.53
13:Z:258:ALA:O	13:Z:262:VAL:HG23	2.09	0.53
5:I:153:LEU:HB3	5:I:156:GLN:HB2	1.90	0.53
6:J:269:ILE:HB	6:J:314:VAL:HG22	1.88	0.53
12:R:63:LEU:HG	12:R:83:ARG:CZ	2.39	0.53
1:A:431:ILE:HD11	2:B:211:MET:HG3	1.91	0.53
3:C:381:LEU:HD22	3:C:414:GLY:HA3	1.91	0.53
5:I:37:LYS:O	5:I:41:VAL:HG23	2.08	0.53
5:I:180:ALA:O	5:I:284:THR:HG21	2.09	0.53
7:K:254:LYS:HZ1	11:P:290:ARG:HG2	1.74	0.53
11:P:201:MET:HE3	11:P:322:LYS:HE2	1.90	0.53
13:Z:664:LEU:HD21	13:Z:675:VAL:HG13	1.90	0.53
5:I:144:ASP:HA	5:I:204:HIS:ND1	2.24	0.53
6:J:72:GLN:HA	6:J:75:LEU:HD12	1.92	0.53
12:R:5:GLU:HA	12:R:8:LYS:HB2	1.91	0.53
11:P:141:LYS:NZ	11:P:249:PRO:HB3	2.24	0.52
13:Z:664:LEU:O	13:Z:664:LEU:HD23	2.09	0.52
3:C:407:VAL:HG12	3:C:415:MET:CE	2.38	0.52
4:D:378:ILE:HG12	4:D:381:ARG:NH2	2.20	0.52
13:Z:307:LYS:HA	13:Z:712:ASN:HD21	1.73	0.52
13:Z:386:MET:HE2	13:Z:386:MET:HA	1.91	0.52
13:Z:408:LEU:HD23	13:Z:423:LEU:HD21	1.91	0.52
8:L:48:PHE:HB2	8:L:68:LEU:HD11	1.90	0.52
12:R:156:LYS:HB2	12:R:191:LEU:HB3	1.92	0.52
13:Z:682:PHE:CE2	13:Z:703:GLN:HG2	2.45	0.52
3:C:306:MET:SD	3:C:973:TYR:HD1	2.32	0.52
3:C:474:LEU:O	3:C:478:VAL:HG23	2.10	0.52
6:J:57:GLU:HG3	13:Z:604:ARG:HH22	1.75	0.52
11:P:260:ALA:O	11:P:307:GLU:HG2	2.08	0.52
11:P:369:THR:H	12:R:108:PHE:HB3	1.74	0.52
12:R:85:ASN:HA	12:R:88:MET:SD	2.49	0.52
13:Z:469:VAL:HA	13:Z:472:ASN:OD1	2.10	0.52
3:C:124:MET:HE1	3:C:153:TYR:HA	1.91	0.52
5:I:203:ALA:HB2	5:I:210:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:373:VAL:HG21	13:Z:747:HIS:HD1	1.74	0.52
3:C:320:SER:HA	3:C:500:SER:HA	1.92	0.52
3:C:572:ILE:HA	3:C:575:MET:HG3	1.92	0.52
3:C:765:MET:HG2	3:C:799:PHE:CE1	2.44	0.52
6:J:411:TYR:O	6:J:415:VAL:HG23	2.08	0.52
12:R:135:ALA:HB3	12:R:157:LEU:HB2	1.92	0.52
13:Z:592:GLY:O	13:Z:596:LEU:HD23	2.10	0.52
8:L:15:CYS:HG	8:L:100:TRP:CD1	2.27	0.52
11:P:243:PHE:CE2	11:P:245:LYS:HB2	2.45	0.52
12:R:41:ILE:O	12:R:45:LEU:HD23	2.09	0.52
13:Z:259:PHE:CE1	13:Z:294:PRO:HB2	2.45	0.52
4:D:82:LYS:O	4:D:86:MET:HG3	2.09	0.52
7:K:141:LYS:HZ1	7:K:261:ARG:HB2	1.74	0.52
11:P:246:LEU:HD22	11:P:251:LEU:HD21	1.92	0.52
1:A:329:VAL:O	1:A:333:MET:HG3	2.10	0.52
1:A:396:MET:O	1:A:398:VAL:HG23	2.10	0.52
11:P:137:PRO:O	11:P:255:TYR:HE1	1.92	0.52
13:Z:241:LEU:HD21	13:Z:257:ILE:HG21	1.92	0.52
3:C:279:THR:HG21	3:C:974:THR:HA	1.92	0.52
5:I:32:LEU:HD22	13:Z:75:TYR:OH	2.10	0.52
5:I:350:MET:HE3	5:I:353:CYS:CB	2.40	0.52
11:P:168:LYS:HG3	11:P:170:MET:H	1.75	0.52
12:R:93:LEU:HA	12:R:96:LEU:HD12	1.92	0.52
13:Z:475:ALA:HB1	13:Z:512:ASN:HD21	1.75	0.52
10:N:29:LEU:HD21	10:N:58:LYS:HB3	1.91	0.51
13:Z:163:LEU:HD23	13:Z:166:ILE:HD12	1.92	0.51
13:Z:302:PHE:CZ	13:Z:712:ASN:HB3	2.44	0.51
13:Z:450:ILE:HA	13:Z:453:ALA:HB3	1.92	0.51
13:Z:643:PRO:HA	13:Z:646:LYS:HG2	1.91	0.51
1:A:224:VAL:HG21	1:A:246:ILE:HB	1.93	0.51
4:D:408:MET:HB3	4:D:411:VAL:HG21	1.91	0.51
13:Z:267:GLN:HE22	13:Z:454:ALA:HA	1.76	0.51
13:Z:630:ALA:HA	13:Z:663:ILE:HD13	1.91	0.51
1:A:198:MET:CE	1:A:294:LEU:HD13	2.40	0.51
3:C:563:VAL:HA	3:C:566:LEU:HD12	1.92	0.51
9:M:202:ILE:HB	9:M:216:PHE:HB2	1.93	0.51
3:C:87:LYS:HA	3:C:90:LYS:NZ	2.25	0.51
3:C:416:THR:HG23	3:C:450:GLY:HA2	1.92	0.51
3:C:452:LEU:HD21	3:C:477:TYR:HD2	1.74	0.51
5:I:174:PHE:CG	5:I:181:GLN:HG2	2.46	0.51
7:K:425:VAL:O	7:K:428:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:85:ARG:HD2	8:L:118:ASP:OD2	2.10	0.51
11:P:208:LYS:HD2	11:P:208:LYS:N	2.24	0.51
13:Z:635:GLN:HA	13:Z:638:ILE:HG12	1.91	0.51
5:I:137:MET:HB2	6:J:281:ARG:NH1	2.25	0.51
5:I:172:GLU:HA	5:I:175:GLU:HG2	1.92	0.51
5:I:212:ARG:HA	5:I:246:PHE:HB3	1.93	0.51
7:K:161:ARG:HA	11:P:299:ARG:CZ	2.40	0.51
13:Z:664:LEU:HD22	13:Z:678:ILE:HD11	1.92	0.51
1:A:409:ARG:NH2	4:D:195:ARG:HG2	2.26	0.51
3:C:864:MET:HE3	3:C:877:THR:HG23	1.92	0.51
5:I:240:HIS:HD2	5:I:243:SER:HB3	1.76	0.51
7:K:219:LEU:HD23	7:K:346:LYS:HG2	1.93	0.51
9:M:10:ILE:HG13	9:M:30:ILE:HG12	1.93	0.51
4:D:448:LEU:HD21	4:D:455:LEU:HD12	1.92	0.51
7:K:105:ILE:HB	11:P:126:THR:HG22	1.93	0.51
7:K:170:MET:HE3	7:K:246:SER:HB3	1.93	0.51
7:K:305:LEU:HD11	7:K:337:LEU:HD11	1.92	0.51
13:Z:259:PHE:HD1	13:Z:295:THR:HG1	1.59	0.51
4:D:373:LYS:O	4:D:378:ILE:HG21	2.11	0.51
7:K:184:GLY:HA2	7:K:359:GLU:HB3	1.93	0.51
7:K:219:LEU:HD13	7:K:343:LEU:HD13	1.93	0.51
10:N:1:MET:HB2	10:N:8:GLN:HB2	1.93	0.51
11:P:131:MET:HE3	11:P:133:GLY:H	1.76	0.51
13:Z:329:HIS:CE1	13:Z:359:ALA:HB2	2.46	0.51
1:A:431:ILE:HG22	2:B:200:LEU:HD11	1.93	0.51
3:C:796:LEU:HB3	3:C:815:MET:SD	2.51	0.51
10:N:37:ARG:HH21	10:N:41:HIS:C	2.19	0.51
13:Z:893:VAL:HG22	13:Z:906:ARG:HG3	1.93	0.51
3:C:230:ILE:HG12	3:C:264:PHE:CE1	2.46	0.51
7:K:139:LYS:HZ3	7:K:161:ARG:HB2	1.76	0.51
10:N:29:LEU:HG	10:N:59:MET:HE3	1.93	0.51
2:B:247:ILE:HD11	2:B:267:ILE:HG21	1.93	0.50
2:B:287:ILE:HG22	2:B:306:MET:HB3	1.94	0.50
3:C:158:ALA:HB1	3:C:223:LEU:HD13	1.94	0.50
5:I:23:PHE:HE2	13:Z:149:GLU:HB3	1.77	0.50
6:J:236:ARG:HH22	7:K:339:ARG:HG2	1.75	0.50
7:K:117:TYR:CZ	7:K:140:LEU:HD12	2.47	0.50
7:K:273:HIS:O	7:K:276:CYS:HB2	2.11	0.50
8:L:33:ILE:HG12	8:L:50:TRP:HA	1.92	0.50
13:Z:610:SER:HB3	13:Z:621:THR:HG21	1.92	0.50
3:C:381:LEU:HD21	3:C:898:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:145:ARG:HE	7:K:159:LEU:HB3	1.76	0.50
13:Z:456:GLY:HA2	13:Z:490:LEU:HB2	1.93	0.50
6:J:100:LEU:HD12	6:J:109:ILE:HG22	1.93	0.50
7:K:289:ARG:HG2	7:K:334:ASP:HA	1.93	0.50
11:P:388:GLY:HA3	14:P:501:ATP:C8	2.46	0.50
2:B:57:LEU:HB2	3:C:252:CYS:SG	2.51	0.50
5:I:276:LEU:HB3	5:I:309:ARG:CZ	2.41	0.50
7:K:105:ILE:HD12	11:P:118:VAL:HG13	1.93	0.50
11:P:360:ILE:HA	11:P:363:ILE:HD12	1.94	0.50
7:K:132:ARG:HG2	7:K:133:ASN:H	1.76	0.50
1:A:196:THR:HG21	2:B:290:LYS:HZ2	1.76	0.50
2:B:125:MET:HE1	2:B:149:LEU:HD12	1.92	0.50
3:C:861:THR:C	3:C:911:LYS:HG2	2.37	0.50
5:I:152:GLY:HA3	9:M:351:PHE:CD2	2.47	0.50
8:L:26:PRO:HB2	13:Z:930:LEU:HD11	1.93	0.50
12:R:207:TRP:CH2	12:R:209:GLY:HA3	2.45	0.50
1:A:227:LEU:HD21	1:A:234:ARG:HH11	1.77	0.50
4:D:197:ILE:HG21	4:D:236:GLU:HG3	1.93	0.50
13:Z:200:SER:HB3	13:Z:529:GLN:HG3	1.94	0.50
1:A:301:LYS:HB2	1:A:304:CYS:HB2	1.93	0.50
1:A:398:VAL:HG13	1:A:402:ILE:HD12	1.93	0.50
2:B:207:LEU:O	2:B:211:MET:HG2	2.11	0.50
3:C:135:LEU:HD23	3:C:164:VAL:HG21	1.94	0.50
6:J:163:GLU:HA	6:J:166:LYS:HG3	1.92	0.50
6:J:428:LYS:HB2	10:N:209:ALA:H	1.77	0.50
10:N:116:GLY:HA3	10:N:146:ARG:HH11	1.76	0.50
11:P:160:PRO:HB2	12:R:84:LYS:CD	2.41	0.50
13:Z:235:ALA:HA	13:Z:269:LEU:HG	1.93	0.50
6:J:251:PRO:HD3	6:J:295:ILE:HG12	1.94	0.50
7:K:167:VAL:O	7:K:170:MET:HB3	2.11	0.50
13:Z:75:TYR:HB3	13:Z:104:LYS:HE2	1.94	0.50
13:Z:504:TYR:O	13:Z:508:THR:HG22	2.12	0.50
1:A:244:LYS:HE2	1:A:345:PRO:HD3	1.94	0.49
3:C:93:ARG:N	3:C:94:PRO:HD2	2.27	0.49
3:C:283:ALA:HA	3:C:872:VAL:HG22	1.94	0.49
5:I:23:PHE:HE1	6:J:48:TYR:HB2	1.77	0.49
6:J:66:ASP:HA	6:J:69:LYS:HD2	1.94	0.49
12:R:63:LEU:HD11	12:R:79:VAL:HG12	1.93	0.49
13:Z:331:ALA:HB1	13:Z:700:CYS:HB3	1.94	0.49
13:Z:405:LEU:HD13	13:Z:446:ALA:HB2	1.94	0.49
1:A:245:GLY:HA2	1:A:351:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:NH1	4:D:190:THR:HG21	2.27	0.49
2:B:148:LEU:HD12	2:B:158:GLY:HA3	1.94	0.49
3:C:562:TRP:CH2	3:C:900:LEU:HD11	2.46	0.49
5:I:335:MET:HA	6:J:202:GLY:HA3	1.93	0.49
6:J:190:LEU:HD23	6:J:198:TYR:CE2	2.47	0.49
10:N:206:ASN:O	10:N:207:LYS:HD2	2.12	0.49
11:P:374:ILE:HA	11:P:412:HIS:HB2	1.94	0.49
12:R:161:GLY:HA3	12:R:177:VAL:HG11	1.93	0.49
13:Z:202:PHE:CE2	13:Z:206:ILE:HD11	2.47	0.49
1:A:412:PRO:HG3	4:D:243:LYS:HE2	1.95	0.49
2:B:142:GLU:HB3	2:B:143:PRO:HD2	1.95	0.49
2:B:335:ASP:HB3	2:B:338:LEU:HD23	1.94	0.49
3:C:257:PRO:HG2	13:Z:813:ARG:HH12	1.78	0.49
4:D:382:LEU:HB2	4:D:387:GLN:HG3	1.93	0.49
6:J:65:GLU:HG2	6:J:69:LYS:HE3	1.93	0.49
11:P:146:VAL:HB	11:P:155:ILE:HG23	1.93	0.49
11:P:377:GLN:HG3	12:R:170:LYS:HD3	1.93	0.49
1:A:46:ALA:HA	1:A:49:LEU:HD12	1.93	0.49
2:B:358:LYS:HG2	2:B:392:ILE:HD11	1.95	0.49
2:B:105:SER:O	2:B:148:LEU:HA	2.13	0.49
3:C:254:PRO:O	3:C:612:GLY:HA3	2.12	0.49
3:C:258:PRO:HG2	3:C:579:GLU:H	1.77	0.49
4:D:405:LEU:HD11	4:D:451:TRP:CG	2.47	0.49
11:P:386:PHE:HZ	11:P:423:GLN:HB3	1.78	0.49
13:Z:597:ARG:NH2	13:Z:725:LEU:HG	2.27	0.49
3:C:161:ILE:HG23	3:C:200:THR:CG2	2.42	0.49
4:D:428:GLU:HG2	4:D:432:TYR:CE2	2.47	0.49
5:I:166:LEU:HD13	9:M:157:ASP:HA	1.93	0.49
6:J:330:ARG:HB3	6:J:333:ARG:HD2	1.95	0.49
7:K:216:LYS:HD3	7:K:315:PHE:HD2	1.78	0.49
9:M:5:ILE:HD12	9:M:329:ILE:HG12	1.94	0.49
11:P:85:VAL:O	11:P:86:MET:HE2	2.13	0.49
1:A:379:LEU:HD13	1:A:413:ASN:HA	1.94	0.49
10:N:115:VAL:HG21	10:N:143:PRO:HB3	1.94	0.49
11:P:74:GLN:HG3	12:R:11:ALA:HB3	1.94	0.49
13:Z:762:ARG:HG2	13:Z:767:ALA:O	2.13	0.49
4:D:448:LEU:HD23	4:D:452:TYR:HA	1.94	0.49
5:I:121:MET:SD	5:I:123:HIS:HB3	2.53	0.49
6:J:249:GLU:O	6:J:253:MET:HG2	2.13	0.49
7:K:105:ILE:HA	7:K:147:THR:HA	1.94	0.49
8:L:50:TRP:CZ3	8:L:56:PRO:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:2:THR:HG23	9:M:311:MET:HE1	1.94	0.49
10:N:184:GLU:HG3	10:N:186:HIS:ND1	2.28	0.49
11:P:186:LEU:HB3	11:P:189:GLN:HB2	1.94	0.49
13:Z:154:LEU:HD23	13:Z:189:LEU:HD13	1.94	0.49
13:Z:762:ARG:NH2	13:Z:769:PRO:HB3	2.28	0.49
1:A:247:LEU:HD11	1:A:355:THR:HG22	1.94	0.49
3:C:301:THR:HG21	3:C:306:MET:HG3	1.95	0.49
13:Z:365:PHE:HB2	13:Z:399:PHE:HB3	1.95	0.49
3:C:248:TYR:HD2	3:C:249:MET:HB3	1.77	0.49
3:C:491:LEU:HB3	3:C:903:MET:HE1	1.94	0.49
3:C:585:LEU:HA	3:C:588:ILE:HD12	1.95	0.49
3:C:588:ILE:HG23	3:C:591:ILE:HD12	1.94	0.49
6:J:209:VAL:HA	6:J:336:ARG:HB2	1.95	0.49
6:J:353:PHE:CE1	6:J:383:ILE:HG23	2.47	0.49
7:K:157:ARG:HG2	7:K:158:ILE:H	1.78	0.49
9:M:160:LEU:HB2	9:M:174:LEU:HB2	1.95	0.49
11:P:248:ALA:O	11:P:252:VAL:HG23	2.13	0.49
2:B:407:ARG:HD3	2:B:407:ARG:N	2.27	0.48
3:C:527:SER:HB3	3:C:546:ILE:HG12	1.94	0.48
3:C:748:LEU:HD21	3:C:866:VAL:HG21	1.95	0.48
7:K:149:ASP:O	7:K:153:LEU:HA	2.12	0.48
9:M:234:GLY:O	9:M:237:ARG:HG3	2.13	0.48
11:P:243:PHE:HE2	11:P:245:LYS:HB2	1.77	0.48
6:J:1:MET:HE3	6:J:3:GLU:HG2	1.95	0.48
6:J:158:ILE:HA	7:K:306:MET:SD	2.53	0.48
6:J:165:GLU:HB3	7:K:313:ASP:HB3	1.95	0.48
6:J:219:LYS:HG2	6:J:340:PHE:CZ	2.48	0.48
7:K:149:ASP:HB3	7:K:153:LEU:N	2.27	0.48
4:D:327:LEU:HB2	4:D:356:MET:SD	2.53	0.48
5:I:220:GLN:HG3	5:I:225:GLU:HB3	1.94	0.48
6:J:174:VAL:HG13	14:J:501:ATP:N6	2.28	0.48
9:M:156:GLN:HG3	9:M:180:THR:OG1	2.14	0.48
1:A:466:TYR:HD2	14:A:501:ATP:H4'	1.78	0.48
2:B:232:LEU:HD23	2:B:350:PHE:HZ	1.78	0.48
2:B:357:THR:HA	2:B:360:LYS:HD2	1.96	0.48
3:C:454:GLY:HA2	3:C:457:ILE:HD12	1.94	0.48
6:J:271:ILE:HG22	6:J:274:VAL:HG12	1.94	0.48
7:K:230:LEU:HD22	14:K:501:ATP:C2	2.48	0.48
8:L:30:GLN:HA	8:L:102:GLN:HE22	1.78	0.48
3:C:230:ILE:HG13	3:C:267:THR:HG21	1.95	0.48
3:C:512:ILE:HG23	3:C:518:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:236:MET:HA	5:I:239:GLU:CG	2.43	0.48
11:P:188:LYS:HE3	11:P:189:GLN:NE2	2.27	0.48
11:P:222:GLY:O	11:P:328:ASN:HA	2.13	0.48
11:P:362:GLN:HB3	12:R:176:MET:HB3	1.95	0.48
12:R:59:MET:HE1	12:R:83:ARG:HA	1.96	0.48
3:C:278:LEU:HB3	3:C:297:VAL:HG13	1.95	0.48
7:K:105:ILE:O	11:P:126:THR:HB	2.13	0.48
11:P:149:ASN:HB3	11:P:153:TYR:H	1.79	0.48
11:P:257:GLY:H	11:P:261:LYS:HZ3	1.61	0.48
1:A:418:GLU:OE2	1:A:450:VAL:HG12	2.14	0.48
2:B:68:HIS:HB3	3:C:756:MET:HE2	1.96	0.48
3:C:312:TYR:HB3	3:C:980:VAL:HB	1.96	0.48
4:D:184:VAL:HG22	4:D:187:ARG:NH2	2.29	0.48
4:D:340:LYS:HE2	4:D:340:LYS:HA	1.94	0.48
5:I:145:SER:O	5:I:201:ALA:HA	2.14	0.48
11:P:420:SER:HA	11:P:423:GLN:NE2	2.29	0.48
13:Z:759:ILE:O	13:Z:761:ILE:HG13	2.14	0.48
1:A:31:GLU:HB2	1:A:35:GLN:NE2	2.28	0.48
3:C:93:ARG:HG3	3:C:125:THR:OG1	2.14	0.48
5:I:29:GLU:CD	5:I:33:LYS:HZ1	2.22	0.48
5:I:161:LYS:NZ	9:M:114:THR:HB	2.27	0.48
6:J:221:MET:HE3	14:J:501:ATP:C2'	2.44	0.48
10:N:32:LYS:HB3	10:N:36:GLY:HA2	1.95	0.48
11:P:170:MET:SD	11:P:172:VAL:HG23	2.54	0.48
11:P:388:GLY:HA2	11:P:391:LEU:HD12	1.95	0.48
12:R:195:GLN:HE22	12:R:197:LEU:HG	1.79	0.48
13:Z:590:ALA:HA	13:Z:593:PHE:CD1	2.49	0.48
2:B:290:LYS:HE3	2:B:306:MET:SD	2.54	0.48
4:D:409:PRO:C	4:D:411:VAL:H	2.20	0.48
5:I:279:LEU:HD13	5:I:309:ARG:HB3	1.96	0.48
11:P:248:ALA:HA	11:P:251:LEU:HD12	1.96	0.48
13:Z:106:ILE:HG12	13:Z:137:PHE:HD2	1.79	0.48
3:C:491:LEU:HD22	3:C:903:MET:SD	2.54	0.48
3:C:578:GLY:O	3:C:581:VAL:HG12	2.13	0.48
6:J:219:LYS:HG2	6:J:340:PHE:CE2	2.49	0.48
11:P:120:LYS:HB3	12:R:69:TYR:CD1	2.49	0.48
13:Z:298:TYR:HB3	13:Z:759:ILE:HG21	1.95	0.48
13:Z:561:GLY:O	13:Z:597:ARG:HD2	2.13	0.48
13:Z:650:ASP:HB3	13:Z:692:GLU:OE1	2.14	0.48
1:A:253:GLY:H	14:A:501:ATP:PB	2.37	0.47
3:C:230:ILE:HD11	3:C:233:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:248:ILE:HG21	4:D:257:LEU:HG	1.96	0.47
9:M:214:HIS:CD2	9:M:276:LYS:HD2	2.49	0.47
10:N:216:LEU:HD23	10:N:220:VAL:HG21	1.96	0.47
11:P:419:ILE:HG22	11:P:423:GLN:OE1	2.14	0.47
13:Z:373:VAL:HG13	13:Z:750:SER:HB3	1.96	0.47
3:C:775:MET:SD	3:C:889:VAL:HG22	2.54	0.47
6:J:234:PHE:CE2	6:J:236:ARG:HB2	2.48	0.47
10:N:194:VAL:HA	10:N:199:ALA:HB3	1.95	0.47
12:R:9:LEU:HD11	12:R:82:ILE:HG13	1.96	0.47
13:Z:871:MET:O	13:Z:871:MET:SD	2.72	0.47
5:I:161:LYS:HZ2	9:M:114:THR:HB	1.79	0.47
5:I:211:ILE:HD12	5:I:245:ILE:HG12	1.95	0.47
6:J:177:LEU:H	6:J:348:GLU:CD	2.22	0.47
7:K:161:ARG:HG3	11:P:299:ARG:NH2	2.29	0.47
7:K:228:LYS:HE3	7:K:327:THR:N	2.29	0.47
11:P:288:THR:HG22	11:P:333:LEU:HD23	1.96	0.47
12:R:145:PRO:HB3	12:R:202:THR:O	2.13	0.47
1:A:244:LYS:HD2	1:A:369:GLY:O	2.15	0.47
2:B:247:ILE:HD13	2:B:267:ILE:HD13	1.96	0.47
3:C:778:LEU:HG	3:C:810:ASN:HB3	1.95	0.47
3:C:892:SER:HA	3:C:895:LEU:HD12	1.97	0.47
5:I:41:VAL:O	5:I:45:GLU:HG3	2.15	0.47
6:J:274:VAL:HG11	6:J:316:MET:HE3	1.97	0.47
6:J:291:GLU:N	6:J:294:ARG:HH21	2.12	0.47
7:K:305:LEU:O	7:K:309:LEU:HD23	2.14	0.47
9:M:194:LEU:HD13	9:M:259:VAL:HG21	1.97	0.47
10:N:167:VAL:HG21	10:N:197:TYR:HB3	1.96	0.47
12:R:64:VAL:HA	12:R:70:PRO:HA	1.95	0.47
13:Z:589:ILE:HG22	13:Z:593:PHE:HE1	1.80	0.47
1:A:307:PHE:CD1	1:A:352:MET:HE3	2.48	0.47
3:C:880:SER:HB2	3:C:903:MET:O	2.14	0.47
3:C:973:TYR:CZ	3:C:984:LYS:HB2	2.50	0.47
8:L:17:TYR:CD2	8:L:96:ARG:HB2	2.50	0.47
11:P:429:SER:O	12:R:58:GLY:HA3	2.14	0.47
13:Z:738:GLN:HE21	13:Z:745:LEU:HD13	1.79	0.47
1:A:311:ILE:HD13	1:A:353:PHE:HB3	1.95	0.47
2:B:284:ILE:HG23	2:B:334:LEU:HD11	1.95	0.47
5:I:328:LEU:HD23	5:I:362:CYS:SG	2.55	0.47
9:M:96:TYR:HB2	9:M:403:VAL:HB	1.96	0.47
11:P:197:ILE:C	11:P:200:PRO:HD2	2.40	0.47
13:Z:224:THR:O	13:Z:227:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:HE1	1:A:294:LEU:HD13	1.95	0.47
1:A:220:LYS:HG2	4:D:41:VAL:HG11	1.96	0.47
2:B:200:LEU:HG	2:B:208:TYR:CE1	2.48	0.47
3:C:225:LEU:HD13	3:C:264:PHE:CZ	2.50	0.47
3:C:838:TYR:O	3:C:845:LEU:HB2	2.15	0.47
3:C:864:MET:HG3	3:C:881:ILE:HD11	1.96	0.47
5:I:45:GLU:HA	5:I:48:ARG:HB3	1.97	0.47
5:I:188:TYR:HE2	5:I:405:LYS:HE3	1.78	0.47
5:I:350:MET:HE3	5:I:353:CYS:HB2	1.95	0.47
11:P:368:MET:HE1	11:P:395:THR:HG22	1.97	0.47
13:Z:302:PHE:CZ	13:Z:757:THR:HB	2.50	0.47
1:A:203:LYS:HG3	3:C:364:ASN:HD22	1.80	0.47
2:B:151:HIS:CD2	2:B:152:LYS:HG2	2.50	0.47
3:C:765:MET:HE1	3:C:807:VAL:HG11	1.96	0.47
6:J:74:HIS:CE1	6:J:81:ARG:NH1	2.83	0.47
11:P:264:ARG:HG3	11:P:311:GLN:NE2	2.30	0.47
12:R:133:PRO:HA	12:R:158:ILE:HA	1.97	0.47
13:Z:362:TRP:CE2	13:Z:742:TRP:HZ2	2.32	0.47
2:B:51:PRO:HD3	2:B:57:LEU:HD23	1.96	0.47
3:C:520:ILE:HB	3:C:557:GLU:HB3	1.96	0.47
3:C:815:MET:CG	3:C:827:LEU:HD11	2.44	0.47
5:I:33:LYS:O	5:I:37:LYS:HG2	2.15	0.47
5:I:195:LYS:HG2	5:I:316:PHE:CD2	2.49	0.47
5:I:295:ASN:O	5:I:404:PHE:HA	2.14	0.47
5:I:353:CYS:SG	5:I:397:ALA:HB2	2.55	0.47
8:L:15:CYS:HB2	8:L:98:PHE:HB3	1.97	0.47
11:P:220:MET:HE2	11:P:349:PHE:CE1	2.50	0.47
11:P:221:TYR:CD2	11:P:330:VAL:HB	2.50	0.47
13:Z:139:ARG:O	13:Z:142:GLU:HG2	2.14	0.47
13:Z:231:ASN:CG	13:Z:724:THR:HG22	2.40	0.47
13:Z:259:PHE:HE1	13:Z:294:PRO:HB2	1.80	0.47
13:Z:291:SER:HB2	13:Z:417:ARG:CZ	2.44	0.47
13:Z:479:GLU:OE2	13:Z:512:ASN:HB2	2.15	0.47
13:Z:762:ARG:HH22	13:Z:914:VAL:HG21	1.80	0.47
2:B:383:THR:HG21	4:D:345:ASN:HB3	1.97	0.47
3:C:316:ALA:HB1	3:C:909:ARG:HB2	1.97	0.47
3:C:784:SER:O	3:C:818:CYS:HA	2.15	0.47
3:C:877:THR:HA	3:C:907:GLY:HA3	1.97	0.47
5:I:28:GLN:HE22	13:Z:96:GLN:NE2	2.09	0.47
5:I:224:GLY:H	5:I:267:GLU:CD	2.23	0.47
6:J:169:VAL:HG13	6:J:173:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:228:LYS:HE3	7:K:327:THR:H	1.80	0.47
11:P:141:LYS:HB3	11:P:253:GLN:HA	1.96	0.47
11:P:230:LEU:HD22	14:P:501:ATP:H2'	1.96	0.47
11:P:256:ILE:HD12	11:P:300:GLU:HG3	1.96	0.47
12:R:1:MET:HG3	12:R:2:GLU:H	1.79	0.47
13:Z:293:LEU:HG	13:Z:417:ARG:HH22	1.79	0.47
3:C:143:VAL:HG12	3:C:145:ASP:H	1.80	0.46
3:C:433:LEU:HD13	3:C:469:PRO:HB2	1.97	0.46
10:N:6:LEU:HD23	10:N:39:PRO:HG2	1.96	0.46
12:R:63:LEU:HA	12:R:71:ARG:HD3	1.97	0.46
1:A:409:ARG:CZ	4:D:195:ARG:HG2	2.45	0.46
2:B:229:LYS:HB2	14:B:501:ATP:O2B	2.15	0.46
7:K:196:VAL:O	7:K:200:PRO:HG2	2.16	0.46
9:M:183:ASP:HB3	9:M:229:ILE:HG12	1.98	0.46
10:N:115:VAL:HG12	10:N:155:LEU:HD11	1.97	0.46
11:P:120:LYS:HA	11:P:126:THR:HA	1.96	0.46
13:Z:242:PHE:HE2	13:Z:273:LEU:HD21	1.79	0.46
13:Z:529:GLN:HB3	13:Z:559:TYR:CE1	2.50	0.46
13:Z:602:VAL:O	13:Z:606:VAL:HG22	2.15	0.46
3:C:382:ALA:HB1	3:C:849:ARG:HB2	1.96	0.46
4:D:307:LYS:HD3	4:D:338:TYR:OH	2.16	0.46
4:D:327:LEU:HB2	4:D:356:MET:HE1	1.96	0.46
5:I:231:ARG:HH12	5:I:270:ARG:NH2	2.14	0.46
6:J:215:PRO:HB3	6:J:319:ASN:ND2	2.29	0.46
13:Z:194:ILE:HG23	13:Z:597:ARG:CZ	2.44	0.46
2:B:171:MET:SD	2:B:267:ILE:HG23	2.54	0.46
2:B:330:LYS:HE3	2:B:332:GLU:OE2	2.15	0.46
5:I:137:MET:HA	6:J:281:ARG:HH22	1.80	0.46
9:M:5:ILE:HG12	9:M:372:PHE:HB2	1.98	0.46
11:P:208:LYS:HE2	11:P:318:ASP:HA	1.96	0.46
12:R:84:LYS:HG2	12:R:88:MET:CE	2.44	0.46
13:Z:106:ILE:HG12	13:Z:137:PHE:CD2	2.51	0.46
13:Z:289:ILE:HA	13:Z:294:PRO:HG2	1.96	0.46
3:C:135:LEU:HD22	3:C:161:ILE:HA	1.98	0.46
5:I:213:VAL:HG12	5:I:246:PHE:O	2.15	0.46
7:K:171:THR:HG21	7:K:269:TYR:CE1	2.49	0.46
7:K:222:GLY:O	7:K:328:ASN:HA	2.15	0.46
7:K:231:LEU:HD11	14:K:501:ATP:N6	2.30	0.46
13:Z:600:THR:HA	13:Z:634:LEU:HD21	1.97	0.46
13:Z:727:THR:O	13:Z:731:VAL:HG12	2.16	0.46
1:A:464:MET:SD	2:B:339:ILE:HG13	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:PRO:HD2	2:B:388:SER:HA	1.97	0.46
3:C:230:ILE:HG21	3:C:264:PHE:CD1	2.51	0.46
5:I:114:CYS:SG	5:I:124:LYS:HB3	2.55	0.46
5:I:210:PHE:CZ	5:I:246:PHE:HB2	2.51	0.46
6:J:137:VAL:HA	6:J:150:LEU:HG	1.98	0.46
7:K:214:PRO:HD2	7:K:317:ASN:HB3	1.97	0.46
7:K:306:MET:HA	7:K:309:LEU:HB2	1.96	0.46
9:M:3:LYS:HD3	9:M:372:PHE:CE1	2.50	0.46
9:M:110:ILE:HG21	9:M:151:LEU:HD22	1.98	0.46
10:N:76:PHE:CZ	10:N:98:PRO:HG3	2.51	0.46
11:P:208:LYS:HD2	11:P:208:LYS:H	1.80	0.46
13:Z:733:LEU:O	13:Z:736:PHE:HB3	2.16	0.46
4:D:433:ARG:HH22	4:D:458:GLU:HG2	1.81	0.46
7:K:177:GLU:HA	7:K:237:ALA:HB1	1.98	0.46
2:B:195:LYS:HG2	2:B:199:GLU:OE1	2.14	0.46
7:K:348:GLU:OE2	7:K:350:PRO:HB3	2.16	0.46
8:L:14:VAL:HG12	8:L:27:ILE:HD12	1.97	0.46
12:R:176:MET:HA	12:R:179:MET:HG2	1.98	0.46
2:B:398:GLU:HB2	2:B:422:ARG:HH21	1.80	0.46
3:C:218:GLU:HG2	3:C:219:ASP:N	2.30	0.46
3:C:228:GLU:HG2	3:C:260:GLU:OE2	2.16	0.46
5:I:30:THR:O	5:I:34:ILE:HG23	2.16	0.46
7:K:267:PHE:HE2	7:K:271:LYS:HE3	1.81	0.46
10:N:178:LEU:HD22	10:N:193:LEU:HD13	1.98	0.46
11:P:187:ASP:OD2	12:R:210:ARG:HB2	2.15	0.46
11:P:289:LYS:HD2	11:P:335:PRO:HD3	1.98	0.46
13:Z:222:TYR:HA	13:Z:225:LEU:HD12	1.98	0.46
13:Z:245:LEU:HB3	13:Z:254:SER:OG	2.16	0.46
13:Z:599:TYR:HB2	13:Z:629:CYS:SG	2.56	0.46
1:A:393:SER:HB2	1:A:398:VAL:CG2	2.46	0.46
1:A:456:LYS:HE2	4:D:329:LEU:HD11	1.98	0.46
5:I:41:VAL:HG22	6:J:65:GLU:HB2	1.98	0.46
5:I:337:LEU:HD22	5:I:377:VAL:HB	1.97	0.46
6:J:140:HIS:CD2	6:J:142:HIS:HB2	2.51	0.46
10:N:64:LEU:HD22	10:N:76:PHE:CD2	2.44	0.46
11:P:199:LEU:HB3	11:P:200:PRO:HD3	1.97	0.46
13:Z:444:HIS:ND1	13:Z:480:ALA:HB2	2.31	0.46
3:C:456:GLY:HA2	3:C:496:ALA:HB2	1.98	0.45
5:I:248:ASP:C	5:I:293:ALA:HB3	2.41	0.45
7:K:185:GLY:HA3	7:K:355:ALA:O	2.16	0.45
11:P:149:ASN:HB3	11:P:153:TYR:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:364:HIS:CB	11:P:395:THR:HG21	2.46	0.45
12:R:20:THR:O	12:R:23:ILE:HB	2.16	0.45
2:B:66:LYS:HE3	13:Z:805:SER:CB	2.46	0.45
2:B:103:PRO:HG3	5:I:120:TYR:CG	2.51	0.45
3:C:258:PRO:HG2	3:C:579:GLU:N	2.32	0.45
3:C:578:GLY:N	3:C:611:THR:HG21	2.31	0.45
3:C:986:ASN:ND2	3:C:988:ASP:HB2	2.31	0.45
4:D:307:LYS:HD3	4:D:338:TYR:CZ	2.51	0.45
5:I:113:VAL:HG11	5:I:122:LEU:HD11	1.97	0.45
5:I:181:GLN:CD	5:I:284:THR:HB	2.41	0.45
6:J:138:ALA:HB2	6:J:150:LEU:HD21	1.98	0.45
7:K:222:GLY:HA2	7:K:434:TYR:CZ	2.50	0.45
8:L:87:PHE:CE2	8:L:122:TYR:HB2	2.51	0.45
9:M:186:ILE:HG23	9:M:190:GLY:HA2	1.97	0.45
10:N:38:ILE:HG12	10:N:41:HIS:CE1	2.51	0.45
10:N:80:CYS:SG	10:N:110:CYS:HB3	2.56	0.45
11:P:220:MET:HE2	11:P:349:PHE:CZ	2.50	0.45
11:P:286:ILE:HA	11:P:301:VAL:HG13	1.98	0.45
2:B:115:ASP:HB3	2:B:138:LYS:HD3	1.98	0.45
2:B:116:ASP:HA	2:B:132:ILE:HB	1.98	0.45
3:C:743:ILE:HG22	3:C:757:SER:HB2	1.98	0.45
5:I:151:GLY:H	14:I:501:ATP:N6	2.14	0.45
5:I:251:ASP:HB2	5:I:299:ILE:HD11	1.97	0.45
5:I:261:SER:HB2	5:I:265:ASP:HB3	1.98	0.45
5:I:367:MET:HE1	6:J:336:ARG:NH2	2.30	0.45
7:K:117:TYR:C	7:K:128:ILE:HD12	2.42	0.45
7:K:117:TYR:O	7:K:129:VAL:HG12	2.17	0.45
7:K:404:ARG:NH2	11:P:194:VAL:HG12	2.32	0.45
11:P:336:ALA:HA	11:P:339:ARG:HG3	1.99	0.45
11:P:377:GLN:HA	12:R:172:GLN:HE22	1.81	0.45
13:Z:308:ASN:CG	13:Z:711:ARG:HH11	2.24	0.45
13:Z:338:PHE:O	13:Z:708:ALA:HA	2.16	0.45
13:Z:444:HIS:NE2	13:Z:448:LEU:HD11	2.31	0.45
13:Z:606:VAL:HG21	13:Z:625:LEU:HG	1.98	0.45
1:A:77:ALA:HB1	1:A:81:LEU:HD12	1.99	0.45
3:C:374:LEU:HD11	3:C:839:SER:HB2	1.98	0.45
6:J:234:PHE:HD1	6:J:268:ILE:HB	1.80	0.45
7:K:110:LYS:HB2	7:K:118:ILE:HD12	1.99	0.45
7:K:194:ARG:HB3	7:K:198:GLU:CD	2.42	0.45
9:M:174:LEU:HD13	9:M:205:TRP:CG	2.52	0.45
11:P:142:PRO:O	11:P:143:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:189:GLN:HG3	11:P:347:ILE:HG22	1.98	0.45
3:C:52:LEU:HD22	3:C:67:SER:HA	1.98	0.45
6:J:378:LEU:HD23	6:J:417:THR:HG21	1.99	0.45
7:K:75:LYS:O	7:K:78:ARG:HG2	2.16	0.45
7:K:105:ILE:HG12	7:K:147:THR:HA	1.97	0.45
13:Z:368:THR:HG21	13:Z:400:ILE:O	2.16	0.45
13:Z:522:ALA:HB1	13:Z:557:LEU:HD13	1.98	0.45
13:Z:657:MET:HE1	13:Z:698:GLY:C	2.41	0.45
1:A:464:MET:HE2	1:A:466:TYR:HA	1.99	0.45
3:C:392:LEU:HD22	3:C:862:MET:SD	2.56	0.45
4:D:58:ILE:HG23	4:D:76:LEU:HG	1.98	0.45
4:D:371:ARG:HA	4:D:374:PHE:HD2	1.82	0.45
5:I:27:ILE:HG13	6:J:51:LEU:HD13	1.97	0.45
5:I:324:ARG:HA	5:I:327:ILE:HD12	1.98	0.45
7:K:170:MET:CG	7:K:244:ILE:HG23	2.41	0.45
7:K:187:THR:HA	7:K:190:ILE:HD12	1.99	0.45
7:K:227:GLY:HA3	7:K:231:LEU:HD13	1.98	0.45
7:K:335:PRO:HA	7:K:338:LEU:HB2	1.99	0.45
10:N:166:ALA:HB3	10:N:169:TRP:HE1	1.81	0.45
11:P:220:MET:HE1	11:P:228:LYS:HA	1.97	0.45
13:Z:200:SER:HB3	13:Z:529:GLN:CG	2.47	0.45
1:A:295:PHE:CD1	1:A:339:GLN:HB3	2.52	0.45
2:B:64:ARG:HH22	3:C:255:LEU:HA	1.82	0.45
4:D:364:GLU:HA	4:D:399:TYR:CE1	2.52	0.45
5:I:84:VAL:HG11	5:I:107:LEU:HD21	1.98	0.45
6:J:78:GLU:HA	6:J:81:ARG:HB2	1.99	0.45
7:K:199:LEU:HB3	7:K:200:PRO:HD3	1.99	0.45
9:M:337:ASN:ND2	9:M:387:GLN:HA	2.31	0.45
11:P:186:LEU:HD13	11:P:349:PHE:HD2	1.81	0.45
12:R:182:GLU:HG3	12:R:212:LEU:HD21	1.98	0.45
13:Z:569:LYS:HA	13:Z:572:LEU:HD12	1.97	0.45
13:Z:590:ALA:HA	13:Z:593:PHE:HD1	1.81	0.45
13:Z:700:CYS:O	13:Z:703:GLN:HB2	2.17	0.45
1:A:462:ARG:O	2:B:347:LYS:HG2	2.16	0.45
2:B:128:TYR:CE1	12:R:54:GLN:HB3	2.52	0.45
3:C:136:ARG:HG3	3:C:193:PHE:CG	2.51	0.45
4:D:299:GLU:HG2	4:D:303:TYR:CE1	2.51	0.45
6:J:347:ARG:NH1	10:N:185:GLY:HA3	2.32	0.45
7:K:175:GLN:OE1	7:K:242:ASN:HA	2.17	0.45
7:K:188:GLU:HG2	7:K:189:GLN:N	2.32	0.45
9:M:214:HIS:NE2	9:M:276:LYS:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:163:GLY:O	10:N:164:LYS:HG3	2.17	0.45
11:P:38:ASP:HA	11:P:41:ILE:HD12	1.98	0.45
11:P:183:VAL:HG22	11:P:230:LEU:HG	1.98	0.45
13:Z:610:SER:O	13:Z:618:ARG:HD2	2.16	0.45
5:I:99:ALA:HB2	5:I:121:MET:HE1	1.98	0.45
5:I:147:TYR:OH	5:I:202:VAL:HA	2.17	0.45
9:M:226:VAL:HG22	9:M:263:HIS:CE1	2.51	0.45
11:P:161:SER:O	12:R:84:LYS:HD2	2.17	0.45
13:Z:227:LYS:HA	13:Z:722:THR:CA	2.47	0.45
13:Z:731:VAL:HA	13:Z:734:VAL:HG22	1.99	0.45
1:A:260:ALA:HB1	1:A:352:MET:CE	2.47	0.45
3:C:265:LEU:HD13	3:C:288:LEU:HG	1.98	0.45
3:C:382:ALA:HB2	3:C:846:PHE:CD1	2.52	0.45
4:D:394:LEU:HD13	4:D:404:LEU:HD13	1.99	0.45
7:K:145:ARG:HE	7:K:159:LEU:CB	2.30	0.45
7:K:289:ARG:NE	7:K:335:PRO:HD3	2.32	0.45
8:L:15:CYS:HB2	8:L:98:PHE:CB	2.47	0.45
11:P:283:LEU:HD21	11:P:337:LEU:HD13	1.99	0.45
1:A:39:SER:OG	3:C:124:MET:HG2	2.18	0.44
2:B:103:PRO:HB3	5:I:96:VAL:HG12	1.98	0.44
3:C:419:VAL:HG12	3:C:436:LEU:HD22	1.99	0.44
3:C:491:LEU:HG	3:C:525:MET:SD	2.57	0.44
5:I:148:ASP:HB3	9:M:95:ASP:OD1	2.17	0.44
6:J:85:GLU:HG2	6:J:88:ARG:HH21	1.83	0.44
6:J:130:LEU:O	6:J:135:MET:HE1	2.17	0.44
6:J:166:LYS:NZ	6:J:231:LYS:HA	2.32	0.44
7:K:157:ARG:HG2	7:K:158:ILE:N	2.32	0.44
7:K:224:PRO:HG3	7:K:432:ILE:HD12	1.99	0.44
7:K:309:LEU:HD21	7:K:337:LEU:HG	1.98	0.44
8:L:77:PRO:HD3	8:L:122:TYR:CE1	2.52	0.44
9:M:216:PHE:HE2	9:M:276:LYS:HA	1.82	0.44
9:M:226:VAL:HG13	9:M:261:ALA:HB1	2.00	0.44
11:P:187:ASP:HA	11:P:190:ILE:HD12	1.99	0.44
11:P:188:LYS:HE3	11:P:189:GLN:CD	2.42	0.44
13:Z:657:MET:O	13:Z:660:LEU:HB2	2.17	0.44
13:Z:890:PHE:HZ	13:Z:914:VAL:HG21	1.81	0.44
3:C:478:VAL:HG21	3:C:493:LEU:HD11	1.99	0.44
3:C:516:THR:HA	3:C:553:ARG:NH2	2.32	0.44
4:D:328:GLU:HG2	4:D:355:GLY:CA	2.46	0.44
5:I:164:ILE:HG23	5:I:289:LYS:HB3	1.99	0.44
5:I:324:ARG:NH1	5:I:352:GLY:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:245:PHE:HD1	7:K:279:PHE:HD2	1.65	0.44
9:M:121:LEU:HB3	9:M:125:PHE:HA	2.00	0.44
9:M:337:ASN:HD22	9:M:387:GLN:HA	1.83	0.44
10:N:58:LYS:O	10:N:59:MET:HE2	2.17	0.44
11:P:141:LYS:HB3	11:P:253:GLN:CA	2.47	0.44
11:P:338:LEU:HB3	11:P:346:LYS:NZ	2.32	0.44
12:R:9:LEU:HD13	12:R:81:MET:HB2	1.99	0.44
13:Z:395:ALA:O	13:Z:401:LYS:HE3	2.18	0.44
5:I:58:ILE:O	5:I:61:GLU:HB3	2.17	0.44
6:J:404:GLN:HG2	10:N:73:TRP:CE2	2.52	0.44
8:L:122:TYR:O	8:L:126:ILE:HG13	2.16	0.44
9:M:341:ALA:HB3	9:M:346:PHE:CE2	2.52	0.44
11:P:115:LYS:HD3	11:P:255:TYR:HE2	1.83	0.44
12:R:30:LYS:HB2	12:R:33:GLU:OE1	2.17	0.44
12:R:92:ASP:O	12:R:96:LEU:HG	2.17	0.44
12:R:181:ASN:HB2	12:R:186:LEU:HD11	1.99	0.44
13:Z:638:ILE:HG13	13:Z:639:ASP:N	2.32	0.44
3:C:463:HIS:ND1	3:C:500:SER:HB3	2.33	0.44
3:C:535:VAL:HG11	3:C:875:LYS:HB3	1.99	0.44
6:J:130:LEU:O	6:J:132:LYS:HG2	2.17	0.44
6:J:210:LEU:HG	6:J:212:TYR:HD1	1.82	0.44
6:J:212:TYR:CE1	6:J:337:LYS:HB3	2.53	0.44
7:K:187:THR:HA	7:K:190:ILE:HB	1.99	0.44
7:K:226:THR:HA	7:K:388:GLY:H	1.83	0.44
8:L:50:TRP:CZ3	8:L:52:PRO:HA	2.52	0.44
12:R:181:ASN:ND2	12:R:186:LEU:HD21	2.33	0.44
12:R:192:ARG:HG2	12:R:193:GLU:OE1	2.18	0.44
13:Z:493:GLY:HA3	13:Z:528:ARG:CZ	2.48	0.44
13:Z:813:ARG:O	13:Z:817:THR:HG23	2.17	0.44
4:D:391:VAL:O	4:D:395:THR:HG23	2.17	0.44
5:I:353:CYS:SG	5:I:393:ASN:HB3	2.58	0.44
5:I:367:MET:HG3	5:I:371:ARG:CZ	2.47	0.44
6:J:300:LEU:HD23	6:J:303:MET:HE2	2.00	0.44
6:J:403:LEU:HD11	10:N:37:ARG:HH12	1.83	0.44
7:K:79:GLN:OE1	7:K:82:ARG:HD2	2.18	0.44
7:K:241:ALA:HA	7:K:275:PRO:HG2	2.00	0.44
10:N:166:ALA:HB3	10:N:169:TRP:NE1	2.32	0.44
12:R:205:ARG:NH1	12:R:211:GLY:HA2	2.33	0.44
13:Z:606:VAL:O	13:Z:609:LEU:HB2	2.17	0.44
1:A:393:SER:HB2	1:A:398:VAL:HG21	1.98	0.44
1:A:441:LYS:HG2	1:A:444:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:SER:OG	2:B:412:THR:HA	2.18	0.44
4:D:40:LEU:HD13	4:D:82:LYS:HB2	2.00	0.44
5:I:183:LYS:HD2	5:I:308:GLY:O	2.18	0.44
7:K:229:THR:HA	7:K:279:PHE:CE2	2.52	0.44
7:K:267:PHE:CE1	7:K:311:GLN:HB3	2.53	0.44
10:N:6:LEU:HD11	10:N:18:VAL:HG13	2.00	0.44
12:R:79:VAL:O	12:R:83:ARG:N	2.50	0.44
13:Z:179:THR:HG23	13:Z:217:MET:HE3	1.99	0.44
4:D:293:ALA:HB2	4:D:329:LEU:HB3	1.99	0.44
6:J:250:GLY:HA3	6:J:295:ILE:HD13	2.00	0.44
7:K:139:LYS:NZ	7:K:161:ARG:HB2	2.33	0.44
7:K:376:PHE:O	7:K:380:VAL:HG23	2.17	0.44
8:L:10:PHE:CE1	8:L:12:ALA:HB2	2.53	0.44
10:N:76:PHE:CZ	10:N:91:LEU:HB3	2.53	0.44
10:N:176:THR:HB	10:N:177:PRO:HD2	2.00	0.44
2:B:365:HIS:HA	2:B:368:LYS:NZ	2.32	0.44
3:C:265:LEU:HA	3:C:284:LEU:HD13	1.99	0.44
3:C:513:ALA:O	3:C:523:ALA:HB1	2.17	0.44
3:C:800:SER:HA	3:C:808:SER:HA	2.00	0.44
4:D:174:PHE:CE2	4:D:207:ILE:HD11	2.52	0.44
4:D:185:LYS:HE3	4:D:219:PHE:CD2	2.53	0.44
5:I:191:PRO:HG2	5:I:400:VAL:HG13	1.99	0.44
5:I:348:GLU:CD	9:M:39:ILE:H	2.26	0.44
6:J:219:LYS:HB2	14:J:501:ATP:O2B	2.18	0.44
12:R:176:MET:SD	12:R:177:VAL:HG23	2.58	0.44
13:Z:307:LYS:HA	13:Z:712:ASN:ND2	2.32	0.44
1:A:221:LEU:HD21	1:A:248:LEU:HD11	2.00	0.44
2:B:351:GLU:HG3	4:D:351:GLY:HA3	2.00	0.44
5:I:190:PRO:HB3	5:I:400:VAL:O	2.18	0.44
5:I:279:LEU:HA	5:I:282:PHE:CD2	2.53	0.44
6:J:77:ARG:HH12	6:J:80:LYS:HB3	1.83	0.44
6:J:266:PRO:HA	6:J:311:ASN:O	2.18	0.44
7:K:230:LEU:HD13	14:K:501:ATP:H2'	2.00	0.44
7:K:330:PRO:HB2	7:K:437:LEU:HG	1.99	0.44
9:M:296:ASP:HB3	9:M:299:ASN:O	2.18	0.44
10:N:111:LEU:HA	10:N:126:LEU:HD13	2.00	0.44
10:N:175:TRP:HE3	10:N:180:HIS:CD2	2.36	0.44
11:P:141:LYS:HB3	11:P:253:GLN:N	2.33	0.44
11:P:220:MET:HA	11:P:347:ILE:O	2.18	0.44
11:P:228:LYS:HE3	11:P:327:THR:O	2.18	0.44
11:P:256:ILE:HA	11:P:259:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:182:ASN:HB2	13:Z:217:MET:HE1	2.00	0.44
13:Z:369:ALA:O	13:Z:373:VAL:HG23	2.18	0.44
1:A:196:THR:OG1	2:B:307:LEU:HD21	2.18	0.43
2:B:332:GLU:CD	4:D:384:TYR:HB3	2.43	0.43
4:D:327:LEU:HB2	4:D:356:MET:CE	2.48	0.43
6:J:235:ILE:HG22	6:J:237:VAL:HG23	2.00	0.43
11:P:83:VAL:HG12	11:P:297:GLY:HA3	2.00	0.43
11:P:120:LYS:HG2	11:P:126:THR:OG1	2.18	0.43
13:Z:299:TYR:CG	13:Z:755:PRO:HG2	2.53	0.43
13:Z:381:GLU:CD	13:Z:924:LYS:HD3	2.43	0.43
13:Z:669:GLU:CD	13:Z:676:ALA:HB2	2.43	0.43
2:B:71:LEU:HD21	13:Z:804:LEU:HD21	2.00	0.43
3:C:358:TYR:CE1	3:C:849:ARG:HD2	2.53	0.43
5:I:168:VAL:HB	5:I:289:LYS:HG3	2.00	0.43
6:J:161:MET:SD	6:J:234:PHE:HB3	2.58	0.43
6:J:399:ARG:HD3	6:J:403:LEU:HD23	1.99	0.43
7:K:219:LEU:HD12	7:K:325:MET:HB2	2.00	0.43
7:K:251:ILE:HD13	7:K:263:ILE:HD11	1.99	0.43
9:M:194:LEU:HD13	9:M:259:VAL:CG2	2.48	0.43
10:N:176:THR:O	10:N:179:PHE:HB2	2.18	0.43
11:P:121:THR:C	12:R:70:PRO:HD2	2.43	0.43
13:Z:678:ILE:HA	13:Z:681:ASN:HB3	2.00	0.43
1:A:78:PRO:HD2	1:A:81:LEU:HD12	1.99	0.43
2:B:181:TYR:OH	2:B:236:VAL:HG22	2.18	0.43
2:B:266:GLN:O	2:B:269:LYS:HG3	2.18	0.43
3:C:887:GLY:HA3	3:C:894:MET:SD	2.58	0.43
4:D:336:VAL:HA	4:D:340:LYS:CE	2.46	0.43
5:I:279:LEU:HA	5:I:282:PHE:HD2	1.83	0.43
7:K:308:LEU:O	7:K:312:MET:HG2	2.18	0.43
7:K:404:ARG:CZ	11:P:199:LEU:HD13	2.49	0.43
11:P:166:ARG:NH2	12:R:88:MET:HB2	2.33	0.43
13:Z:307:LYS:HZ3	13:Z:345:ASP:HB2	1.83	0.43
13:Z:682:PHE:HB2	13:Z:699:ALA:HB1	2.00	0.43
1:A:45:TYR:CE2	3:C:222:ASP:HB3	2.53	0.43
4:D:58:ILE:HG12	4:D:76:LEU:HD11	2.00	0.43
11:P:181:SER:HA	12:R:205:ARG:HH21	1.84	0.43
11:P:214:ALA:HB3	11:P:317:SER:HB2	2.00	0.43
13:Z:333:SER:O	13:Z:336:ASN:HB3	2.18	0.43
13:Z:665:ILE:HG23	13:Z:714:THR:HG23	1.99	0.43
1:A:45:TYR:HE2	3:C:222:ASP:HB3	1.84	0.43
1:A:63:ILE:HG23	2:B:73:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:GLU:HB2	2:B:422:ARG:NH2	2.33	0.43
5:I:368:TYR:HA	5:I:371:ARG:HD2	2.00	0.43
6:J:160:VAL:HG21	6:J:264:ASN:ND2	2.34	0.43
6:J:347:ARG:HG2	10:N:184:GLU:OE1	2.18	0.43
7:K:223:PRO:HD3	7:K:434:TYR:CZ	2.53	0.43
10:N:64:LEU:HD11	10:N:75:PRO:HB2	2.01	0.43
11:P:145:LEU:HD21	12:R:64:VAL:HG22	2.00	0.43
11:P:180:TYR:HB2	12:R:205:ARG:HD2	1.99	0.43
11:P:375:ASN:HA	12:R:169:SER:OG	2.18	0.43
13:Z:475:ALA:HA	13:Z:513:ILE:HD11	2.00	0.43
1:A:278:GLU:HA	1:A:281:GLN:HE21	1.84	0.43
5:I:62:LEU:HA	5:I:65:LEU:HD12	2.00	0.43
6:J:254:VAL:HG13	6:J:258:PHE:HE2	1.82	0.43
8:L:45:PHE:HE1	8:L:67:ILE:HG23	1.83	0.43
10:N:94:ARG:NH1	10:N:98:PRO:HD3	2.34	0.43
10:N:135:ILE:O	10:N:142:ILE:HA	2.18	0.43
11:P:353:SER:O	11:P:357:ARG:HG3	2.19	0.43
12:R:52:LEU:HD22	12:R:79:VAL:HG13	2.00	0.43
13:Z:314:LEU:HB2	13:Z:339:MET:SD	2.58	0.43
13:Z:424:LYS:O	13:Z:428:VAL:HG23	2.19	0.43
13:Z:661:SER:HB3	13:Z:702:ALA:HB1	2.00	0.43
1:A:411:CYS:HA	1:A:451:ILE:HG21	2.01	0.43
1:A:431:ILE:HG23	2:B:207:LEU:HB3	2.00	0.43
2:B:194:ILE:HG21	2:B:232:LEU:HD11	2.01	0.43
3:C:392:LEU:HD21	3:C:427:GLN:CD	2.43	0.43
3:C:831:LEU:HD12	3:C:855:LEU:HD22	2.00	0.43
5:I:236:MET:O	5:I:239:GLU:HG3	2.19	0.43
7:K:352:PRO:HD2	7:K:386:PHE:O	2.18	0.43
8:L:12:ALA:HB3	8:L:33:ILE:HD12	1.99	0.43
8:L:75:TRP:HH2	8:L:99:PHE:HB2	1.83	0.43
9:M:162:ILE:O	9:M:171:PRO:HD2	2.19	0.43
10:N:111:LEU:O	10:N:115:VAL:HG22	2.19	0.43
11:P:115:LYS:HD3	11:P:255:TYR:CE2	2.54	0.43
11:P:159:LEU:HD22	12:R:80:THR:HB	2.01	0.43
13:Z:227:LYS:HG3	13:Z:722:THR:O	2.18	0.43
13:Z:522:ALA:C	13:Z:557:LEU:HD22	2.44	0.43
1:A:234:ARG:HB2	4:D:8:TYR:CZ	2.54	0.43
2:B:177:PRO:HB3	2:B:234:LYS:HG3	2.00	0.43
2:B:380:LEU:HA	2:B:417:LYS:NZ	2.33	0.43
3:C:869:ASP:HB3	3:C:978:GLU:HG2	2.01	0.43
5:I:212:ARG:HB2	5:I:246:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:124:SER:HA	6:J:128:ARG:HH22	1.84	0.43
9:M:8:ALA:HA	9:M:31:ASN:O	2.19	0.43
11:P:355:ASP:O	11:P:359:GLN:HG3	2.19	0.43
12:R:157:LEU:HD11	12:R:217:ILE:HD12	2.00	0.43
13:Z:205:SER:C	13:Z:209:LYS:HZ2	2.27	0.43
1:A:388:ILE:HG12	14:A:501:ATP:N1	2.34	0.43
2:B:177:PRO:HG2	2:B:237:ALA:HB3	2.01	0.43
2:B:246:ARG:HG3	2:B:280:PHE:CD2	2.49	0.43
3:C:438:LYS:HE3	3:C:439:TYR:CE2	2.53	0.43
4:D:231:ILE:HG12	4:D:283:PHE:HB2	2.01	0.43
6:J:175:GLY:HA3	6:J:351:LEU:O	2.19	0.43
6:J:190:LEU:HD11	6:J:197:LEU:HD12	2.00	0.43
6:J:364:PRO:CB	10:N:47:GLN:HE22	2.31	0.43
7:K:251:ILE:HG21	7:K:263:ILE:HD11	1.99	0.43
9:M:268:ILE:HB	9:M:282:LEU:HB2	2.00	0.43
9:M:342:ALA:HB2	9:M:390:TYR:CZ	2.54	0.43
11:P:352:PRO:HG2	11:P:357:ARG:HG2	2.00	0.43
13:Z:207:LEU:HB2	13:Z:232:LEU:HD21	1.99	0.43
13:Z:685:VAL:HA	13:Z:691:GLN:NE2	2.34	0.43
13:Z:756:THR:HB	13:Z:874:ILE:O	2.19	0.43
1:A:52:THR:HG22	2:B:62:MET:HG3	2.01	0.43
2:B:200:LEU:HB3	2:B:201:PRO:HD3	2.01	0.43
3:C:208:VAL:HG23	3:C:223:LEU:HD23	2.01	0.43
4:D:12:LEU:HD21	4:D:35:LYS:HE2	1.99	0.43
4:D:458:GLU:OE2	4:D:461:LYS:HD3	2.18	0.43
6:J:61:LEU:HA	6:J:64:GLN:OE1	2.19	0.43
6:J:70:ASP:HA	6:J:73:ARG:HG2	2.01	0.43
6:J:374:ARG:HH21	6:J:411:TYR:HE2	1.60	0.43
11:P:78:LEU:O	11:P:148:VAL:HG22	2.19	0.43
11:P:194:VAL:O	11:P:198:VAL:HB	2.18	0.43
12:R:57:ILE:HD11	12:R:74:VAL:HG21	2.01	0.43
13:Z:223:LEU:HD11	13:Z:894:ARG:HB2	2.01	0.43
1:A:426:ALA:O	1:A:442:ASP:HB3	2.19	0.42
2:B:75:PHE:CZ	3:C:764:LEU:HA	2.54	0.42
2:B:165:ASP:OD1	2:B:166:PRO:HD2	2.19	0.42
3:C:165:TYR:CD1	3:C:227:ILE:HA	2.54	0.42
3:C:866:VAL:HG13	3:C:878:LEU:HB2	2.01	0.42
5:I:31:GLU:HA	5:I:34:ILE:HG12	2.00	0.42
5:I:188:TYR:HA	5:I:294:THR:O	2.18	0.42
7:K:120:LYS:HG3	7:K:126:ARG:HG2	2.01	0.42
7:K:394:CYS:SG	7:K:419:VAL:HA	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:190:ILE:O	11:P:194:VAL:HG23	2.19	0.42
13:Z:739:PHE:HA	13:Z:742:TRP:O	2.19	0.42
13:Z:742:TRP:CG	13:Z:744:PRO:HD2	2.54	0.42
13:Z:921:ARG:HH21	13:Z:922:GLN:NE2	2.17	0.42
3:C:392:LEU:HG	3:C:424:SER:O	2.20	0.42
3:C:563:VAL:HG11	3:C:595:MET:HG2	1.99	0.42
5:I:36:SER:O	5:I:40:ASN:HB2	2.19	0.42
5:I:64:LEU:HA	5:I:67:GLU:HB2	2.01	0.42
5:I:341:ILE:HD13	5:I:382:PHE:CE2	2.54	0.42
9:M:86:ASP:HB3	9:M:89:LYS:NZ	2.34	0.42
11:P:286:ILE:O	11:P:305:MET:HB2	2.19	0.42
12:R:45:LEU:HD12	12:R:49:PHE:CZ	2.54	0.42
12:R:135:ALA:HB2	12:R:171:LEU:HD21	2.01	0.42
12:R:146:SER:HA	12:R:201:LEU:HD12	1.99	0.42
12:R:178:VAL:HG13	12:R:203:PRO:HB3	2.02	0.42
13:Z:239:LEU:HD21	13:Z:276:GLU:CG	2.50	0.42
13:Z:293:LEU:HA	13:Z:379:LEU:HD12	2.01	0.42
1:A:35:GLN:HA	1:A:38:LYS:HE3	2.02	0.42
1:A:84:ILE:HG22	1:A:85:MET:HE2	2.01	0.42
1:A:454:TYR:OH	1:A:462:ARG:HB2	2.19	0.42
2:B:310:LEU:HD22	2:B:343:ARG:HD3	2.01	0.42
3:C:254:PRO:HG3	3:C:871:HIS:NE2	2.35	0.42
3:C:558:LEU:HD13	3:C:593:HIS:CD2	2.54	0.42
3:C:565:PHE:CZ	3:C:900:LEU:HD13	2.55	0.42
4:D:228:VAL:HG11	4:D:277:TYR:CD1	2.54	0.42
6:J:287:GLY:HA2	6:J:290:ARG:HD2	2.02	0.42
7:K:141:LYS:HZ2	7:K:261:ARG:HD3	1.84	0.42
11:P:142:PRO:HD2	11:P:252:VAL:HG12	2.01	0.42
2:B:395:MET:CE	2:B:420:LYS:HB2	2.46	0.42
3:C:132:HIS:HB2	3:C:195:PHE:CZ	2.54	0.42
5:I:214:SER:HB3	5:I:217:GLU:HG3	2.01	0.42
5:I:404:PHE:CD2	5:I:405:LYS:HG3	2.55	0.42
6:J:48:TYR:CE1	13:Z:152:LEU:HD13	2.54	0.42
6:J:348:GLU:HG2	6:J:351:LEU:HD12	2.02	0.42
6:J:381:ALA:HA	14:J:501:ATP:O4'	2.18	0.42
7:K:196:VAL:HG22	7:K:345:ARG:CZ	2.49	0.42
7:K:248:ALA:O	7:K:252:VAL:HG23	2.20	0.42
10:N:224:PHE:CE1	10:N:228:VAL:HG21	2.54	0.42
1:A:407:ILE:HD11	1:A:440:GLU:HG3	2.00	0.42
1:A:427:GLY:O	1:A:431:ILE:HG13	2.18	0.42
3:C:581:VAL:HG22	3:C:585:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:327:ILE:HG23	14:I:501:ATP:N3	2.34	0.42
5:I:369:ALA:HA	5:I:374:ARG:NH2	2.34	0.42
6:J:238:ASN:OD1	6:J:273:GLU:HG3	2.19	0.42
7:K:146:VAL:HA	7:K:158:ILE:HA	2.01	0.42
10:N:99:ASP:HB3	10:N:102:LYS:HB2	2.02	0.42
11:P:229:THR:HG22	11:P:279:PHE:CZ	2.53	0.42
12:R:86:VAL:O	12:R:90:LYS:N	2.52	0.42
13:Z:293:LEU:HD23	13:Z:379:LEU:HB2	2.01	0.42
13:Z:321:LEU:HB3	13:Z:328:PHE:HB3	2.01	0.42
13:Z:340:HIS:HE1	13:Z:348:PHE:H	1.66	0.42
13:Z:519:VAL:O	13:Z:523:LEU:HG	2.18	0.42
1:A:308:PHE:HB3	1:A:311:ILE:HG22	2.01	0.42
3:C:780:MET:HE1	3:C:792:VAL:HG13	2.02	0.42
5:I:249:GLU:OE1	5:I:294:THR:C	2.62	0.42
5:I:254:GLY:HA2	5:I:272:MET:CG	2.50	0.42
7:K:70:TYR:CD2	11:P:41:ILE:HG23	2.55	0.42
9:M:391:VAL:O	9:M:399:GLU:HB2	2.19	0.42
12:R:205:ARG:NE	12:R:212:LEU:HG	2.34	0.42
13:Z:559:TYR:O	13:Z:594:VAL:HA	2.19	0.42
13:Z:640:VAL:O	13:Z:644:LEU:HD23	2.19	0.42
13:Z:651:PHE:HB3	13:Z:694:LEU:HD13	2.02	0.42
1:A:447:VAL:HG13	1:A:451:ILE:HG13	2.01	0.42
4:D:392:GLU:O	4:D:396:ARG:HG3	2.19	0.42
5:I:70:SER:HB2	6:J:119:VAL:HB	2.01	0.42
7:K:225:GLY:H	14:K:501:ATP:PG	2.42	0.42
9:M:214:HIS:CE1	9:M:276:LYS:HB3	2.55	0.42
11:P:135:VAL:HG11	11:P:158:THR:HG23	2.02	0.42
13:Z:161:TYR:HA	13:Z:202:PHE:CZ	2.55	0.42
13:Z:303:LEU:O	13:Z:307:LYS:HB3	2.20	0.42
13:Z:329:HIS:NE2	13:Z:359:ALA:HB2	2.35	0.42
13:Z:609:LEU:O	13:Z:618:ARG:HG2	2.20	0.42
3:C:156:HIS:CE1	3:C:159:LEU:HD23	2.54	0.42
3:C:381:LEU:HG	3:C:846:PHE:CE1	2.54	0.42
3:C:505:VAL:HG11	3:C:533:VAL:HG21	2.01	0.42
4:D:257:LEU:HA	4:D:260:VAL:HG12	2.02	0.42
6:J:347:ARG:HG2	10:N:184:GLU:CD	2.45	0.42
6:J:362:LEU:HD11	6:J:387:MET:HE1	2.02	0.42
6:J:386:ILE:HD13	6:J:411:TYR:HD1	1.84	0.42
9:M:20:GLU:HB3	9:M:22:ASP:OD1	2.20	0.42
9:M:201:THR:HB	9:M:215:THR:HG23	2.00	0.42
11:P:277:ILE:HG21	11:P:324:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:290:ARG:HD2	11:P:332:VAL:HA	2.02	0.42
13:Z:299:TYR:CD1	13:Z:755:PRO:HG2	2.55	0.42
13:Z:313:LEU:HD23	13:Z:707:ASN:HD21	1.84	0.42
1:A:462:ARG:HB3	2:B:347:LYS:O	2.20	0.42
3:C:321:PHE:CE2	3:C:323:TYR:HB2	2.54	0.42
13:Z:230:VAL:HG13	13:Z:265:ALA:HA	2.02	0.42
13:Z:368:THR:O	13:Z:371:LEU:HB2	2.19	0.42
1:A:204:PRO:HB3	1:A:261:ARG:HB3	2.01	0.42
2:B:85:PHE:CG	2:B:86:GLU:N	2.88	0.42
2:B:109:LEU:HD12	2:B:147:VAL:HG11	2.02	0.42
3:C:317:GLN:HA	3:C:874:ASN:ND2	2.34	0.42
3:C:547:MET:HE1	3:C:588:ILE:HA	2.02	0.42
5:I:186:ILE:HA	5:I:292:MET:O	2.20	0.42
5:I:321:VAL:HG11	9:M:39:ILE:HD12	2.01	0.42
6:J:77:ARG:HB3	6:J:81:ARG:NH1	2.35	0.42
7:K:222:GLY:HA2	7:K:434:TYR:OH	2.20	0.42
11:P:303:ARG:HA	11:P:306:LEU:HD12	2.01	0.42
13:Z:588:VAL:O	13:Z:591:LEU:HB2	2.20	0.42
2:B:215:PRO:HG2	2:B:318:ASP:O	2.20	0.41
2:B:281:ILE:HG21	2:B:284:ILE:HD13	2.02	0.41
3:C:820:ALA:HA	3:C:854:LEU:O	2.20	0.41
5:I:222:TYR:HB2	5:I:225:GLU:HG3	2.01	0.41
7:K:112:LEU:HD11	7:K:118:ILE:HD11	2.02	0.41
7:K:179:THR:O	7:K:234:ALA:HB1	2.20	0.41
7:K:389:ALA:CB	14:K:501:ATP:H5'1	2.47	0.41
9:M:154:SER:HB2	9:M:181:VAL:HB	2.02	0.41
13:Z:340:HIS:CE1	13:Z:348:PHE:H	2.38	0.41
13:Z:490:LEU:HD23	13:Z:523:LEU:HB3	2.02	0.41
13:Z:519:VAL:O	13:Z:522:ALA:HB3	2.19	0.41
13:Z:523:LEU:HD21	13:Z:735:MET:HE3	2.01	0.41
13:Z:656:ALA:O	13:Z:659:ALA:HB3	2.20	0.41
1:A:393:SER:HA	1:A:396:MET:HB3	2.02	0.41
2:B:232:LEU:O	2:B:236:VAL:HG23	2.20	0.41
7:K:404:ARG:NH1	11:P:199:LEU:HD13	2.35	0.41
8:L:10:PHE:HZ	8:L:125:MET:HE3	1.86	0.41
11:P:223:PRO:HD2	11:P:349:PHE:O	2.21	0.41
11:P:415:PHE:O	11:P:419:ILE:HG13	2.19	0.41
12:R:45:LEU:HB3	12:R:49:PHE:CZ	2.55	0.41
1:A:276:GLY:HA2	1:A:279:LEU:HD12	2.02	0.41
1:A:357:ARG:NH2	4:D:431:HIS:CE1	2.86	0.41
2:B:109:LEU:HA	2:B:120:VAL:HG12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:ALA:HA	2:B:340:ARG:NE	2.35	0.41
2:B:419:ALA:O	2:B:422:ARG:HG3	2.20	0.41
5:I:22:TYR:HE2	13:Z:103:SER:HA	1.85	0.41
5:I:34:ILE:HG22	6:J:58:TYR:HD1	1.85	0.41
6:J:77:ARG:NH1	6:J:80:LYS:HB3	2.36	0.41
6:J:191:PRO:O	6:J:195:ALA:HB2	2.20	0.41
6:J:258:PHE:HB3	6:J:306:PHE:CE2	2.55	0.41
7:K:228:LYS:HD2	7:K:326:ALA:HA	2.03	0.41
7:K:262:ILE:O	7:K:266:MET:HG3	2.19	0.41
12:R:71:ARG:HB3	12:R:73:ASP:OD1	2.20	0.41
13:Z:97:PHE:CE1	13:Z:101:ILE:HG13	2.55	0.41
13:Z:321:LEU:HD21	13:Z:696:LYS:HB3	2.03	0.41
13:Z:437:GLU:HG2	13:Z:438:ASP:N	2.35	0.41
13:Z:452:LEU:HD21	13:Z:748:PHE:CE2	2.56	0.41
13:Z:483:LEU:O	13:Z:487:LEU:HG	2.20	0.41
13:Z:529:GLN:HG2	13:Z:558:ALA:O	2.20	0.41
1:A:405:GLU:O	1:A:409:ARG:HG3	2.20	0.41
2:B:329:ASN:C	2:B:330:LYS:HD2	2.45	0.41
3:C:597:SER:O	3:C:601:VAL:HG23	2.20	0.41
3:C:845:LEU:HD21	3:C:849:ARG:NH2	2.35	0.41
5:I:74:GLU:HB3	5:I:112:ARG:HD3	2.02	0.41
6:J:250:GLY:HA3	6:J:295:ILE:CD1	2.50	0.41
7:K:109:MET:O	7:K:142:LYS:HG2	2.21	0.41
7:K:185:GLY:N	7:K:359:GLU:HB3	2.35	0.41
11:P:389:ALA:HB2	14:P:501:ATP:H5'1	2.03	0.41
11:P:400:MET:HE3	12:R:38:LYS:HE2	2.02	0.41
12:R:93:LEU:O	12:R:97:LEU:HG	2.20	0.41
1:A:265:ASN:HA	3:C:364:ASN:HD21	1.82	0.41
2:B:339:ILE:HD12	2:B:344:ILE:O	2.20	0.41
2:B:349:LEU:HB3	4:D:352:TYR:CZ	2.55	0.41
2:B:386:ASP:H	2:B:424:MET:HE1	1.84	0.41
3:C:165:TYR:CG	3:C:227:ILE:HA	2.55	0.41
3:C:513:ALA:HB1	3:C:527:SER:OG	2.21	0.41
3:C:536:GLY:HA3	3:C:875:LYS:NZ	2.36	0.41
5:I:300:LEU:HB2	5:I:305:LEU:HD11	2.02	0.41
6:J:56:LYS:HG3	6:J:59:GLU:OE1	2.20	0.41
6:J:212:TYR:HE1	6:J:337:LYS:HB3	1.86	0.41
7:K:117:TYR:CE2	7:K:140:LEU:HD12	2.55	0.41
7:K:279:PHE:O	7:K:280:MET:HE2	2.21	0.41
9:M:268:ILE:HB	9:M:282:LEU:HD12	2.03	0.41
13:Z:346:ASN:HD21	13:Z:375:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:520:GLY:O	13:Z:523:LEU:HB2	2.21	0.41
13:Z:894:ARG:NH2	13:Z:903:VAL:HG22	2.35	0.41
1:A:45:TYR:H	3:C:159:LEU:HB2	1.85	0.41
1:A:440:GLU:O	1:A:444:LEU:HG	2.20	0.41
2:B:194:ILE:HG12	2:B:236:VAL:HG21	2.02	0.41
2:B:290:LYS:HD3	2:B:292:TYR:HE1	1.85	0.41
3:C:445:PRO:HA	3:C:485:ILE:HD11	2.03	0.41
5:I:51:LEU:HD21	6:J:76:LYS:HG3	2.01	0.41
5:I:318:PRO:HD3	5:I:404:PHE:CE1	2.56	0.41
6:J:101:GLU:HB3	6:J:109:ILE:HD13	2.02	0.41
7:K:141:LYS:HD2	7:K:161:ARG:HH22	1.86	0.41
7:K:386:PHE:HA	7:K:426:LYS:HZ2	1.86	0.41
8:L:51:ARG:NE	8:L:52:PRO:HD2	2.35	0.41
9:M:99:VAL:HA	9:M:110:ILE:O	2.20	0.41
11:P:192:GLU:OE1	11:P:347:ILE:HG12	2.21	0.41
12:R:156:LYS:HE2	12:R:191:LEU:O	2.21	0.41
13:Z:716:GLN:HE22	13:Z:726:ASP:HB2	1.85	0.41
1:A:242:PRO:HD2	1:A:346:ARG:HG2	2.02	0.41
2:B:332:GLU:HG2	2:B:333:THR:HG23	2.03	0.41
5:I:240:HIS:CD2	5:I:243:SER:HB3	2.54	0.41
6:J:73:ARG:HG3	6:J:74:HIS:H	1.86	0.41
8:L:10:PHE:CZ	8:L:125:MET:HE3	2.56	0.41
10:N:194:VAL:HG22	10:N:199:ALA:HB3	2.03	0.41
11:P:408:SER:HA	12:R:111:MET:SD	2.61	0.41
12:R:45:LEU:O	12:R:48:TYR:HB2	2.21	0.41
13:Z:100:THR:HA	13:Z:103:SER:OG	2.21	0.41
2:B:253:ILE:HD11	2:B:287:ILE:HA	2.03	0.41
6:J:249:GLU:HA	6:J:252:ARG:CD	2.50	0.41
7:K:131:VAL:HG11	7:K:137:ARG:HG2	2.02	0.41
10:N:175:TRP:CE3	10:N:179:PHE:HB3	2.56	0.41
11:P:84:GLU:H	11:P:118:VAL:HB	1.85	0.41
13:Z:208:ARG:NE	13:Z:232:LEU:HD22	2.35	0.41
13:Z:370:SER:HA	13:Z:373:VAL:HB	2.02	0.41
13:Z:717:LEU:HD11	13:Z:733:LEU:HD12	2.02	0.41
13:Z:742:TRP:HD1	13:Z:745:LEU:HG	1.86	0.41
1:A:464:MET:HE1	2:B:341:PRO:HD3	2.02	0.41
2:B:355:LEU:HD22	2:B:383:THR:HG22	2.03	0.41
2:B:421:GLU:O	2:B:425:LYS:HB2	2.21	0.41
3:C:135:LEU:O	3:C:139:LEU:HG	2.21	0.41
3:C:303:ASP:HB3	3:C:306:MET:HG2	2.03	0.41
3:C:487:SER:HB3	3:C:525:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:490:ILE:HD11	3:C:512:ILE:HG21	2.03	0.41
4:D:371:ARG:HA	4:D:374:PHE:CD2	2.56	0.41
4:D:392:GLU:HA	4:D:436:ALA:HB2	2.03	0.41
5:I:370:LEU:C	5:I:373:ARG:H	2.29	0.41
6:J:64:GLN:HG3	13:Z:605:ILE:HG12	2.03	0.41
6:J:249:GLU:HA	6:J:252:ARG:HD3	2.02	0.41
7:K:291:PHE:HB3	7:K:294:GLY:H	1.85	0.41
9:M:331:GLU:H	9:M:331:GLU:CD	2.28	0.41
11:P:120:LYS:NZ	11:P:295:LYS:HG2	2.36	0.41
11:P:141:LYS:HG2	11:P:144:ASP:CG	2.45	0.41
11:P:159:LEU:HD13	12:R:80:THR:HG21	2.01	0.41
11:P:337:LEU:HB3	11:P:343:LEU:HD12	2.03	0.41
11:P:398:ALA:HB2	11:P:415:PHE:HA	2.02	0.41
12:R:202:THR:O	12:R:202:THR:HG23	2.21	0.41
13:Z:303:LEU:HD23	13:Z:303:LEU:HA	1.96	0.41
1:A:285:GLY:H	1:A:328:GLU:CD	2.29	0.41
2:B:75:PHE:CE1	3:C:764:LEU:HD23	2.56	0.41
3:C:812:ILE:HA	3:C:815:MET:CE	2.48	0.41
5:I:45:GLU:O	5:I:49:ASN:N	2.48	0.41
5:I:149:MET:HE3	9:M:93:ARG:NH2	2.36	0.41
6:J:186:GLU:HA	6:J:190:LEU:HB2	2.02	0.41
6:J:428:LYS:HB2	10:N:208:GLY:HA3	2.03	0.41
7:K:76:GLN:HG2	11:P:1:MET:HE3	2.03	0.41
9:M:216:PHE:CE2	9:M:276:LYS:HA	2.55	0.41
11:P:145:LEU:O	11:P:159:LEU:HB2	2.21	0.41
11:P:376:TRP:H	12:R:169:SER:HB3	1.86	0.41
12:R:94:ASN:HA	12:R:97:LEU:HD12	2.03	0.41
13:Z:211:PHE:CE1	13:Z:225:LEU:HD22	2.56	0.41
13:Z:267:GLN:NE2	13:Z:454:ALA:HA	2.36	0.41
13:Z:503:THR:HG22	13:Z:507:GLU:CD	2.46	0.41
1:A:406:LEU:HB3	4:D:232:LEU:HD21	2.04	0.40
2:B:140:LEU:HD13	2:B:161:GLN:HE22	1.86	0.40
3:C:290:GLU:O	3:C:294:ILE:HG13	2.22	0.40
5:I:254:GLY:HA2	5:I:272:MET:HG2	2.03	0.40
10:N:133:VAL:O	10:N:143:PRO:HD2	2.21	0.40
10:N:205:ASP:O	10:N:206:ASN:C	2.64	0.40
12:R:31:LEU:O	12:R:35:MET:HG3	2.21	0.40
12:R:38:LYS:HE3	12:R:38:LYS:HB3	1.94	0.40
13:Z:203:ARG:HH12	13:Z:597:ARG:HH12	1.67	0.40
13:Z:296:CYS:HB3	13:Z:377:GLY:O	2.21	0.40
2:B:142:GLU:OE1	2:B:262:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:TYR:HB2	3:C:227:ILE:HG22	2.03	0.40
3:C:357:ILE:HG21	3:C:852:GLN:HB3	2.02	0.40
3:C:365:SER:HB3	3:C:367:SER:OG	2.21	0.40
3:C:623:ARG:HD3	3:C:735:GLU:CG	2.51	0.40
5:I:165:GLU:O	5:I:168:VAL:HG12	2.22	0.40
5:I:215:GLY:O	5:I:219:VAL:HG23	2.21	0.40
5:I:330:ILE:HG23	5:I:333:ARG:HH21	1.86	0.40
5:I:365:ALA:O	5:I:381:ASP:HB3	2.20	0.40
6:J:132:LYS:HB3	6:J:133:PRO:HD2	2.03	0.40
6:J:169:VAL:HG11	6:J:221:MET:CG	2.52	0.40
6:J:348:GLU:O	6:J:352:ILE:HG13	2.21	0.40
7:K:255:TYR:HA	11:P:294:GLU:HG2	2.03	0.40
8:L:45:PHE:CE1	8:L:67:ILE:HG23	2.56	0.40
8:L:51:ARG:HE	8:L:52:PRO:HD2	1.86	0.40
8:L:123:ASN:HA	8:L:126:ILE:HD12	2.03	0.40
11:P:312:LEU:O	11:P:315:PHE:HB2	2.22	0.40
13:Z:222:TYR:CD2	13:Z:253:LEU:HD21	2.56	0.40
13:Z:339:MET:HA	13:Z:707:ASN:O	2.21	0.40
13:Z:641:LEU:C	13:Z:641:LEU:HD12	2.46	0.40
13:Z:761:ILE:HG23	13:Z:767:ALA:O	2.22	0.40
13:Z:894:ARG:HH21	13:Z:903:VAL:HG22	1.86	0.40
2:B:57:LEU:HD22	3:C:248:TYR:O	2.22	0.40
3:C:154:ILE:HD12	3:C:210:TYR:CE1	2.56	0.40
3:C:374:LEU:HA	3:C:842:GLN:HE22	1.86	0.40
3:C:864:MET:HE2	3:C:881:ILE:HG13	2.04	0.40
4:D:25:LEU:HD21	4:D:61:PHE:CZ	2.56	0.40
5:I:377:VAL:HG23	6:J:201:ILE:HG22	2.02	0.40
6:J:63:LEU:HD21	13:Z:565:ASN:HB3	2.03	0.40
6:J:373:ILE:HD11	10:N:180:HIS:ND1	2.36	0.40
7:K:108:VAL:HG22	7:K:119:VAL:CG1	2.50	0.40
7:K:116:LYS:HB3	7:K:128:ILE:HD11	2.02	0.40
8:L:15:CYS:HG	8:L:100:TRP:HD1	1.69	0.40
11:P:146:VAL:HA	11:P:159:LEU:N	2.37	0.40
11:P:180:TYR:HB2	12:R:205:ARG:CD	2.52	0.40
11:P:185:GLY:HA3	11:P:356:SER:OG	2.20	0.40
12:R:146:SER:HA	12:R:151:ILE:HD12	2.04	0.40
13:Z:658:ILE:HG22	13:Z:662:MET:HE2	2.03	0.40
13:Z:666:GLN:OE1	13:Z:876:PRO:HD3	2.22	0.40
2:B:70:LEU:HD13	13:Z:804:LEU:HA	2.03	0.40
3:C:506:LEU:HB2	3:C:534:PHE:CE1	2.56	0.40
3:C:900:LEU:HA	3:C:903:MET:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:PHE:CD2	4:D:184:VAL:HG21	2.56	0.40
5:I:132:PRO:O	5:I:136:LEU:HG	2.22	0.40
5:I:167:PRO:O	5:I:289:LYS:HE3	2.21	0.40
8:L:48:PHE:HB2	8:L:68:LEU:HD21	2.03	0.40
8:L:55:LYS:HE2	8:L:55:LYS:HA	2.04	0.40
9:M:392:SER:HB2	9:M:398:GLY:HA2	2.04	0.40
11:P:202:LYS:HE3	11:P:239:THR:HA	2.02	0.40
12:R:135:ALA:C	12:R:220:LEU:HG	2.47	0.40
13:Z:239:LEU:HD21	13:Z:276:GLU:HG2	2.03	0.40
13:Z:303:LEU:HD13	13:Z:341:ALA:O	2.21	0.40
13:Z:421:ASP:HA	13:Z:424:LYS:HB3	2.04	0.40
3:C:524:ALA:HB1	3:C:566:LEU:HG	2.03	0.40
6:J:230:THR:HG22	6:J:232:ALA:H	1.86	0.40
7:K:194:ARG:HB3	7:K:198:GLU:OE2	2.21	0.40
8:L:33:ILE:HG23	8:L:49:GLU:O	2.22	0.40
8:L:78:ILE:HB	8:L:86:ILE:O	2.22	0.40
11:P:166:ARG:HH21	12:R:88:MET:HB2	1.87	0.40
12:R:48:TYR:CD1	12:R:82:ILE:HG12	2.56	0.40
13:Z:644:LEU:HA	13:Z:647:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/467 (70%)	322 (98%)	6 (2%)	0	100	100
2	B	390/437 (89%)	371 (95%)	19 (5%)	0	100	100
3	C	842/993 (85%)	812 (96%)	30 (4%)	0	100	100
4	D	461/480 (96%)	452 (98%)	9 (2%)	0	100	100
5	I	388/405 (96%)	366 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	J	386/428 (90%)	366 (95%)	20 (5%)	0	100	100
7	K	383/437 (88%)	359 (94%)	24 (6%)	0	100	100
8	L	129/156 (83%)	122 (95%)	7 (5%)	0	100	100
9	M	415/417 (100%)	403 (97%)	12 (3%)	0	100	100
10	N	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
11	P	406/434 (94%)	391 (96%)	15 (4%)	0	100	100
12	R	196/220 (89%)	186 (95%)	10 (5%)	0	100	100
13	Z	878/945 (93%)	849 (97%)	29 (3%)	0	100	100
All	All	5428/6047 (90%)	5220 (96%)	208 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	279/399 (70%)	279 (100%)	0	100	100
2	B	349/385 (91%)	349 (100%)	0	100	100
3	C	724/850 (85%)	724 (100%)	0	100	100
4	D	431/445 (97%)	431 (100%)	0	100	100
5	I	339/352 (96%)	339 (100%)	0	100	100
6	J	342/374 (91%)	342 (100%)	0	100	100
7	K	330/377 (88%)	330 (100%)	0	100	100
8	L	120/144 (83%)	120 (100%)	0	100	100
9	M	364/364 (100%)	364 (100%)	0	100	100
10	N	198/198 (100%)	198 (100%)	0	100	100
11	P	354/375 (94%)	354 (100%)	0	100	100
12	R	184/202 (91%)	184 (100%)	0	100	100
13	Z	741/797 (93%)	741 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4755/5262 (90%)	4755 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	89	GLN
2	B	95	GLN
2	B	312	GLN
2	B	370	ASN
3	C	338	HIS
3	C	364	ASN
3	C	379	GLN
3	C	391	ASN
3	C	842	GLN
3	C	898	HIS
4	D	39	ASN
4	D	359	ASN
4	D	431	HIS
5	I	28	GLN
5	I	220	GLN
5	I	331	HIS
6	J	74	HIS
6	J	264	ASN
6	J	319	ASN
7	K	93	ASN
9	M	192	ASN
9	M	248	ASN
10	N	47	GLN
13	Z	240	GLN
13	Z	306	ASN
13	Z	340	HIS
13	Z	346	ASN
13	Z	510	HIS
13	Z	712	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	ATP	J	501	-	32,33,33	0.54	1 (3%)	48,52,52	0.38	0
14	ATP	I	501	-	32,33,33	0.39	0	48,52,52	0.36	0
14	ATP	A	501	-	32,33,33	0.36	0	48,52,52	0.35	0
14	ATP	P	501	-	32,33,33	0.55	1 (3%)	48,52,52	0.34	0
14	ATP	B	501	-	32,33,33	0.35	0	48,52,52	0.42	0
14	ATP	K	501	-	32,33,33	0.42	0	48,52,52	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ATP	J	501	-	-	6/22/38/38	0/3/3/3
14	ATP	I	501	-	-	5/22/38/38	0/3/3/3
14	ATP	A	501	-	-	0/22/38/38	0/3/3/3
14	ATP	P	501	-	-	4/22/38/38	0/3/3/3
14	ATP	B	501	-	-	5/22/38/38	0/3/3/3
14	ATP	K	501	-	-	3/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	501	ATP	PA-O3A	-2.05	1.57	1.59
14	P	501	ATP	PA-O3A	-2.03	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	501	ATP	PB-O3B-PG-O2G
14	B	501	ATP	C5'-O5'-PA-O2A
14	I	501	ATP	C5'-O5'-PA-O1A
14	I	501	ATP	C5'-O5'-PA-O3A
14	J	501	ATP	C5'-O5'-PA-O2A
14	J	501	ATP	C5'-O5'-PA-O3A
14	K	501	ATP	C5'-O5'-PA-O3A
14	P	501	ATP	C5'-O5'-PA-O1A
14	P	501	ATP	C5'-O5'-PA-O2A
14	P	501	ATP	C5'-O5'-PA-O3A
14	J	501	ATP	PB-O3B-PG-O1G
14	B	501	ATP	C5'-O5'-PA-O1A
14	B	501	ATP	C5'-O5'-PA-O3A
14	I	501	ATP	C5'-O5'-PA-O2A
14	K	501	ATP	C5'-O5'-PA-O1A
14	J	501	ATP	C4'-C5'-O5'-PA
14	K	501	ATP	C4'-C5'-O5'-PA
14	B	501	ATP	PB-O3B-PG-O3G
14	J	501	ATP	PB-O3B-PG-O2G
14	J	501	ATP	PB-O3B-PG-O3G
14	I	501	ATP	PG-O3B-PB-O3A
14	I	501	ATP	PG-O3B-PB-O1B
14	P	501	ATP	PG-O3B-PB-O1B

There are no ring outliers.

6 monomers are involved in 27 short contacts:

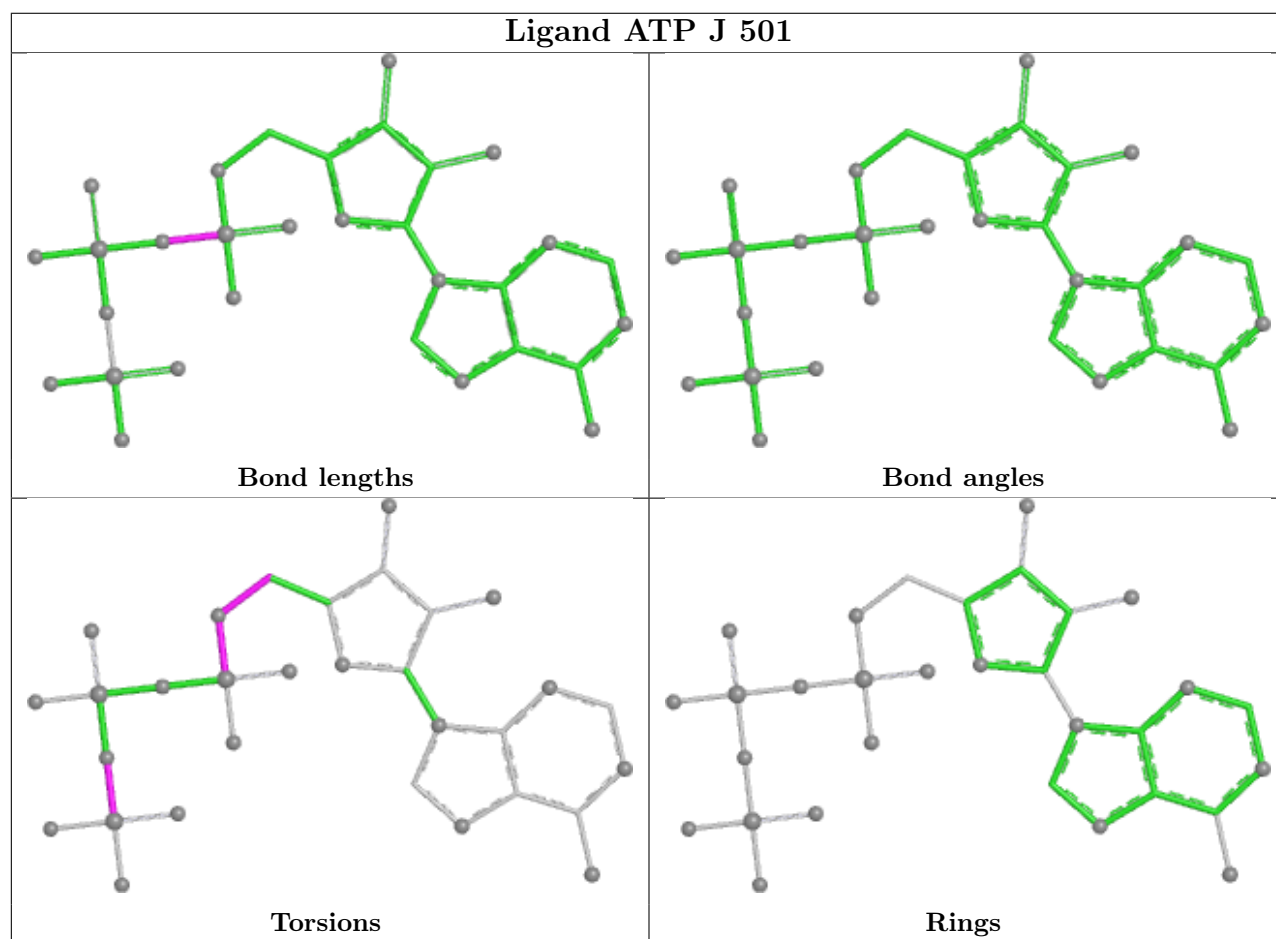
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	J	501	ATP	6	0
14	I	501	ATP	3	0
14	A	501	ATP	3	0
14	P	501	ATP	3	0

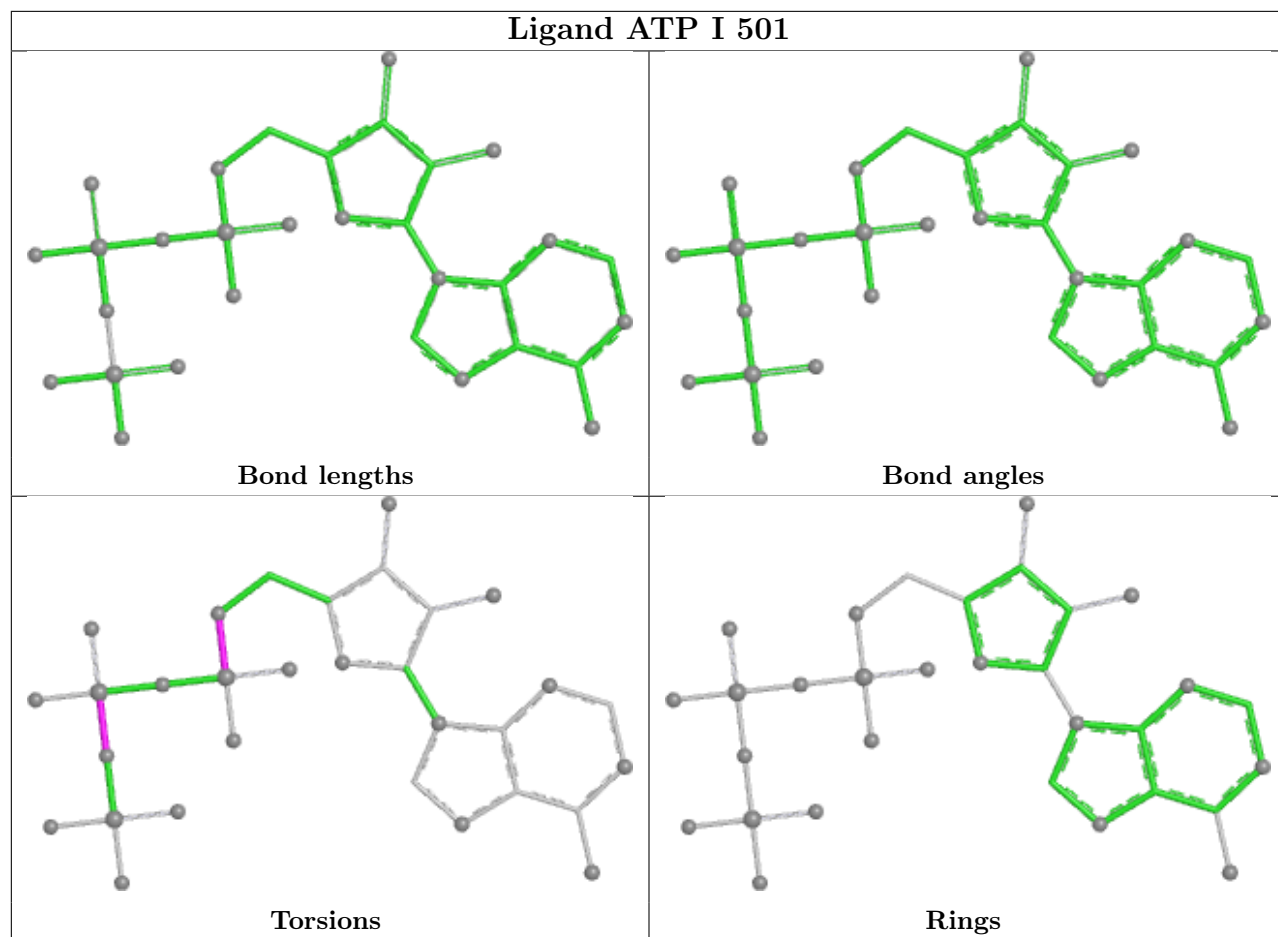
Continued on next page...

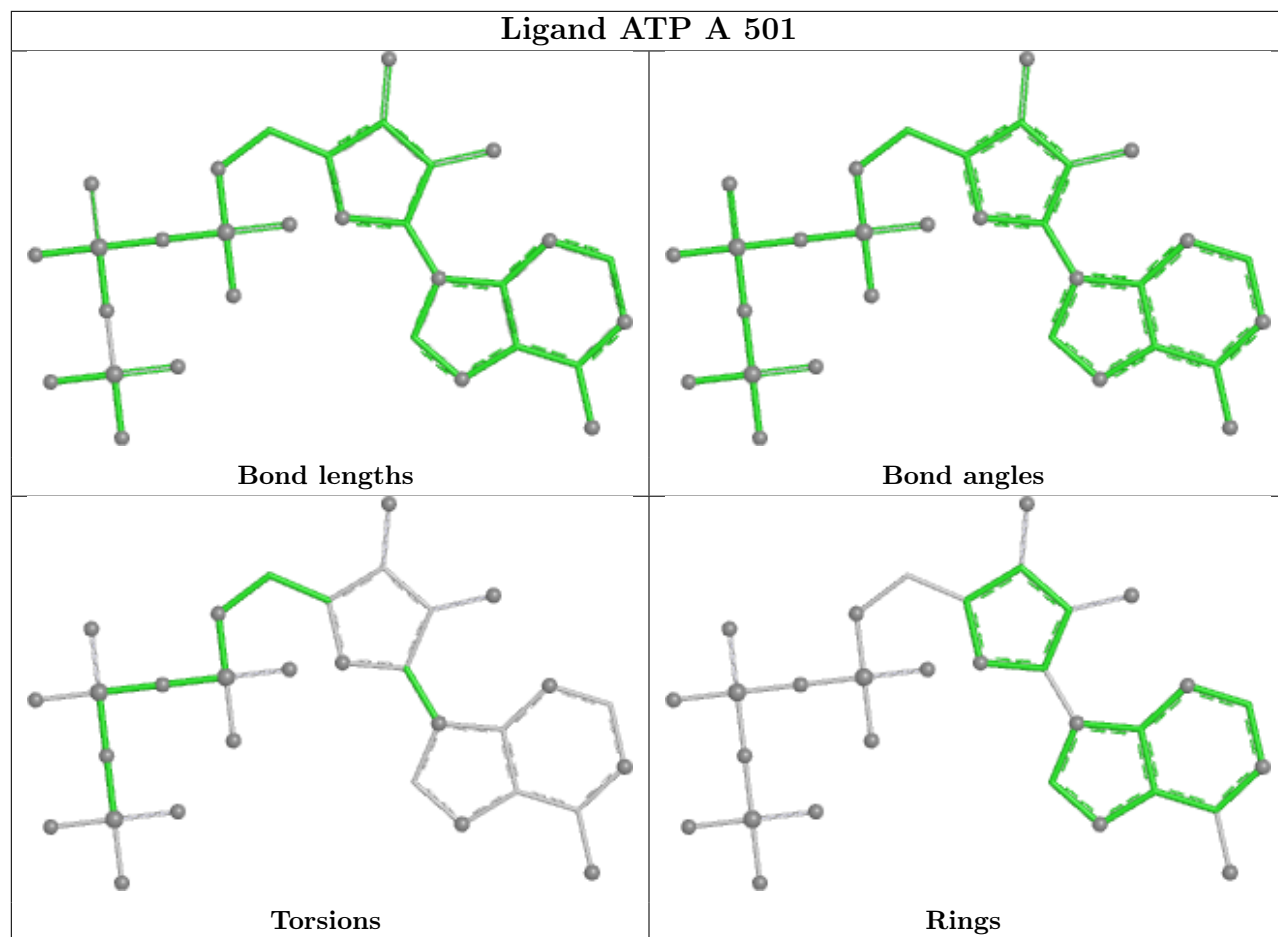
Continued from previous page...

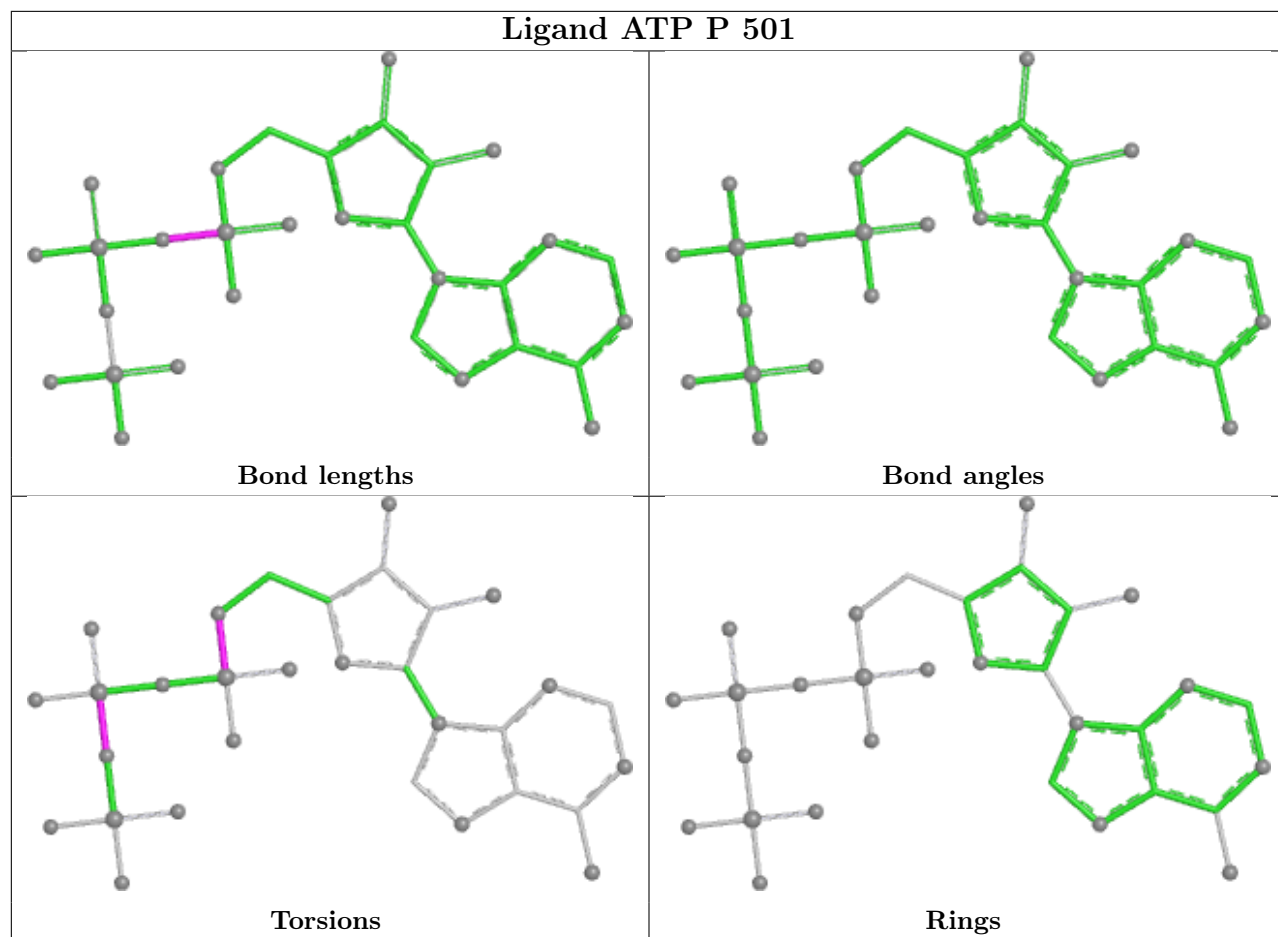
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	501	ATP	1	0
14	K	501	ATP	11	0

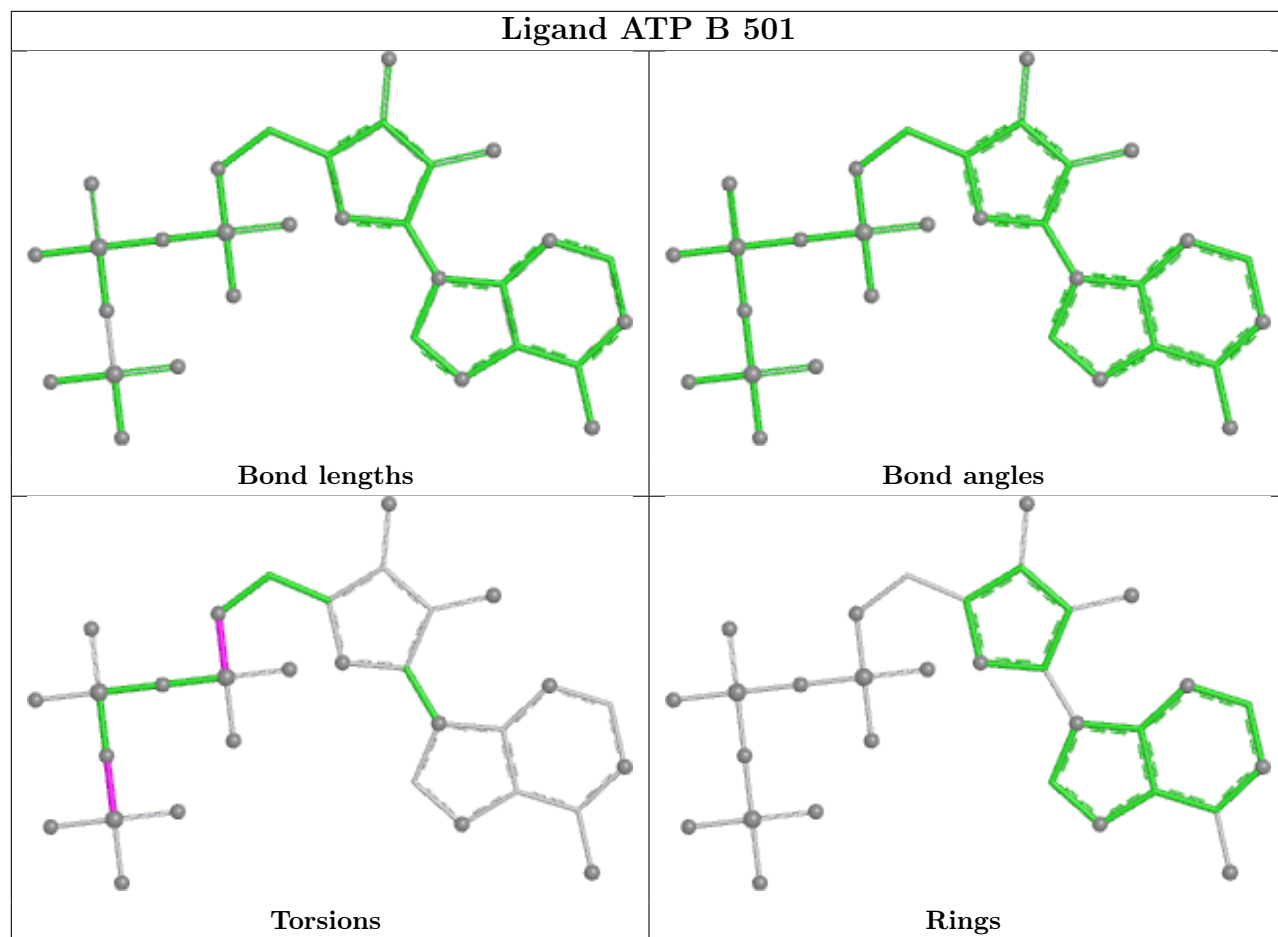
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

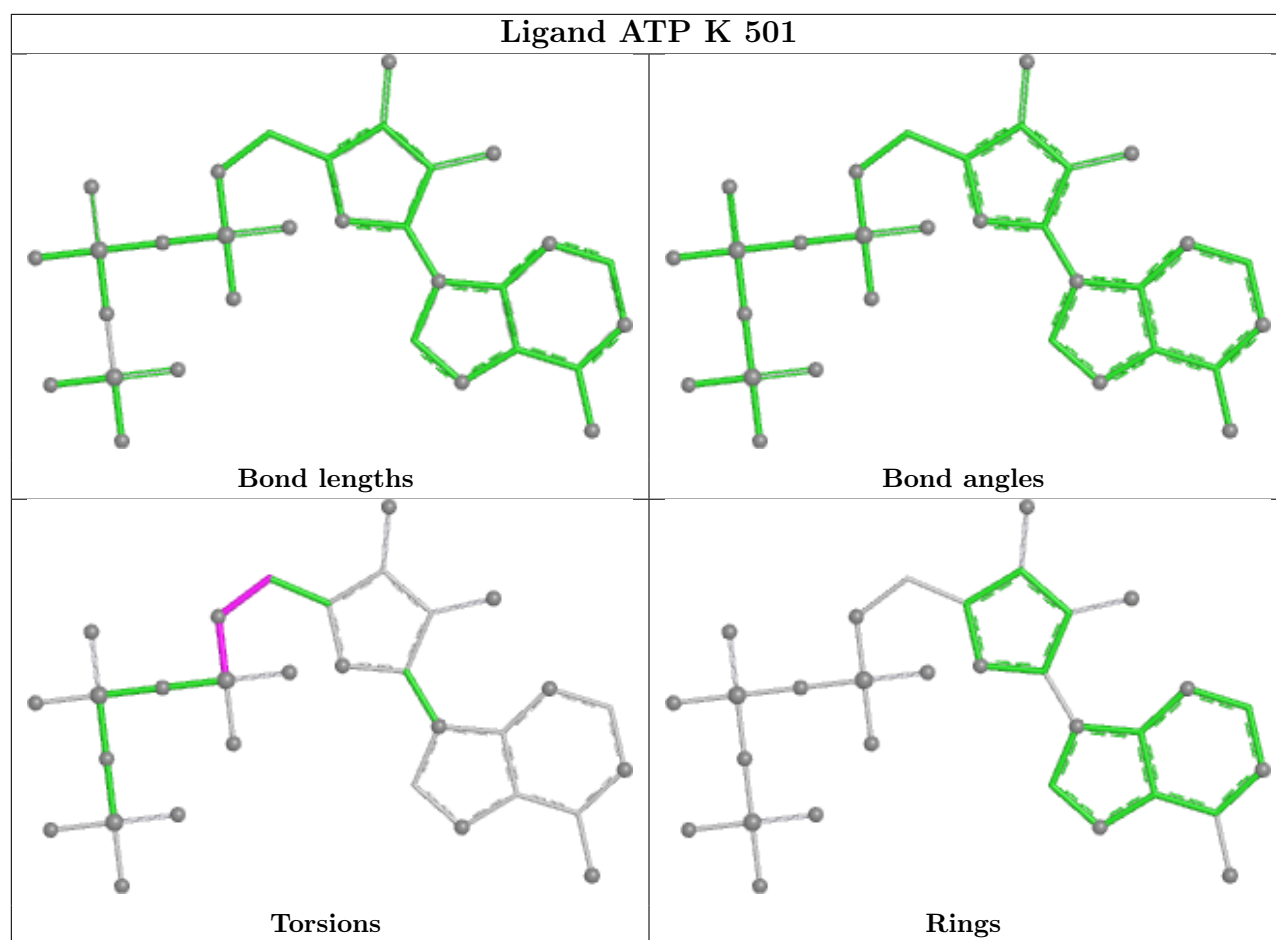












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

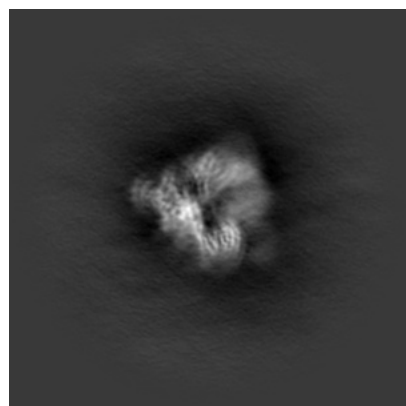
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77338. These allow visual inspection of the internal detail of the map and identification of artifacts.

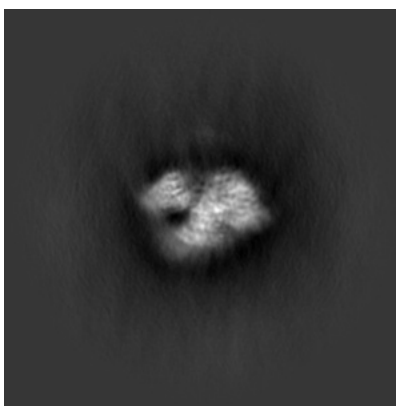
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

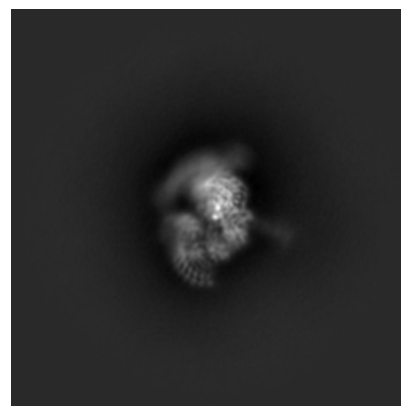
6.1.1 Primary map



X

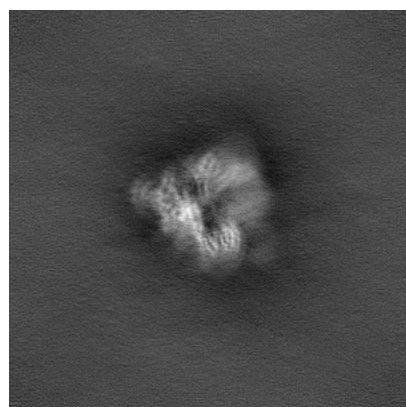


Y

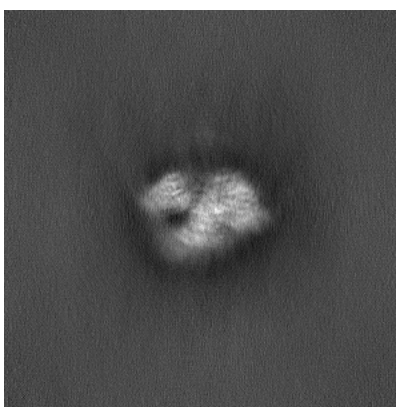


Z

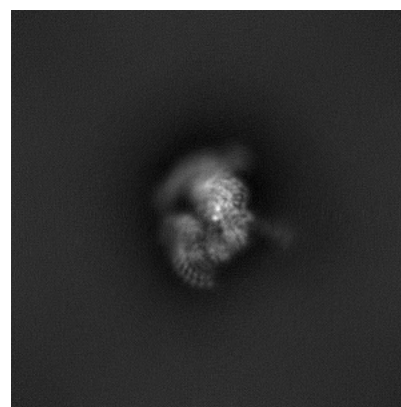
6.1.2 Raw map



X



Y

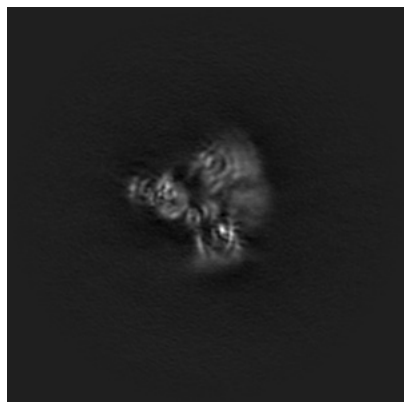


Z

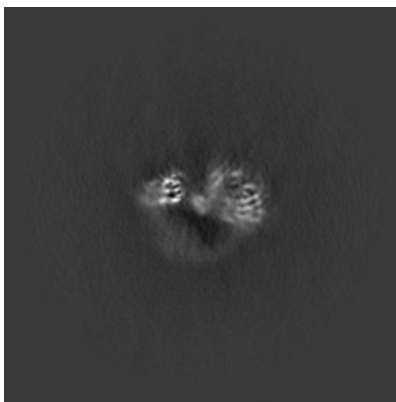
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

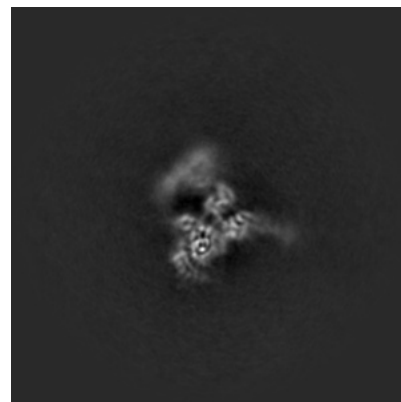
6.2.1 Primary map



X Index: 256

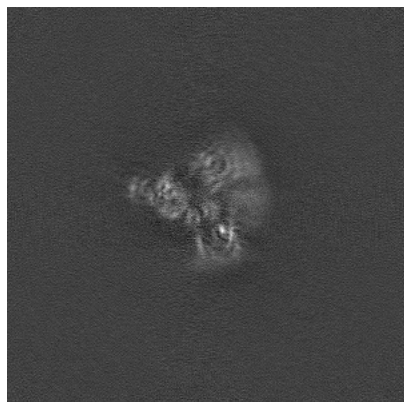


Y Index: 256



Z Index: 256

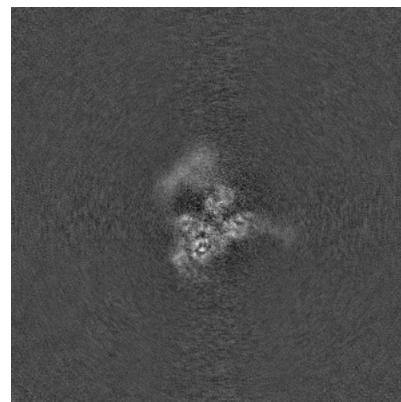
6.2.2 Raw map



X Index: 256



Y Index: 256

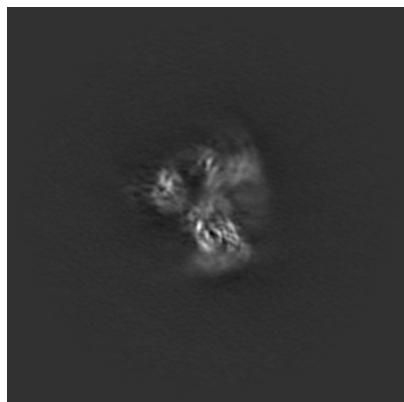


Z Index: 256

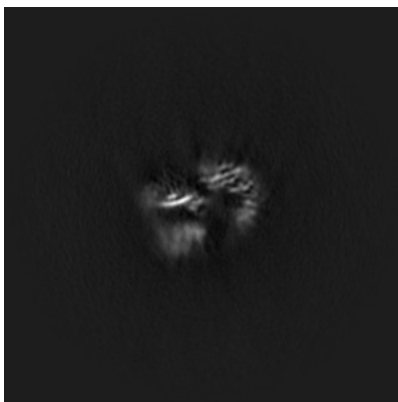
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

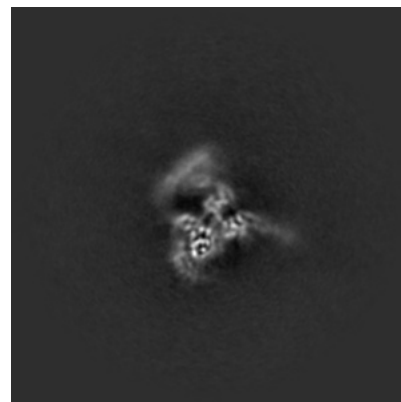
6.3.1 Primary map



X Index: 265

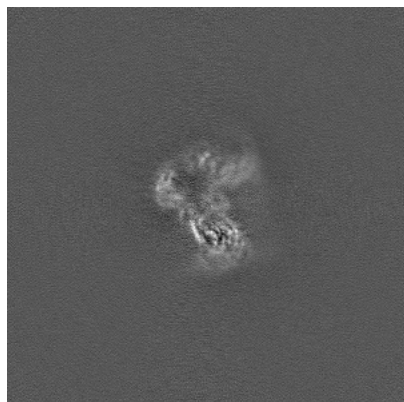


Y Index: 245

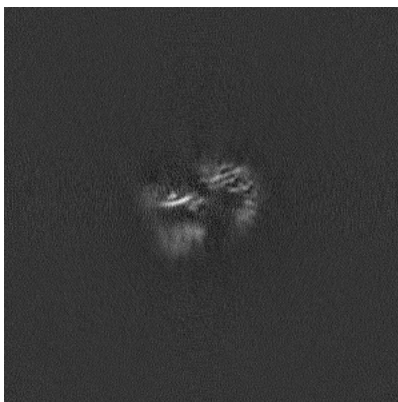


Z Index: 254

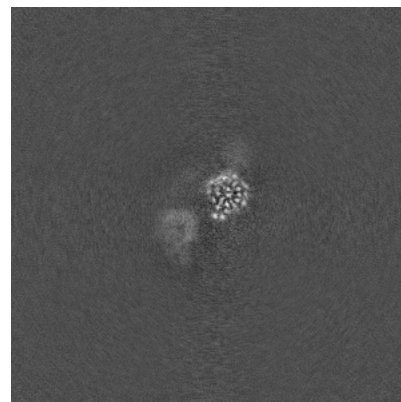
6.3.2 Raw map



X Index: 270



Y Index: 245

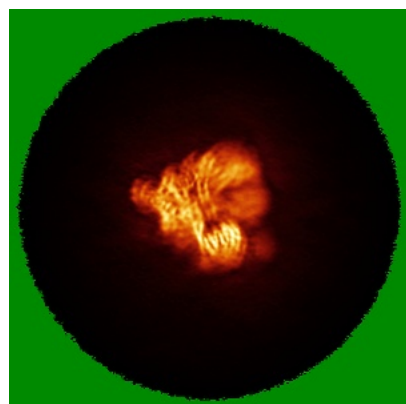


Z Index: 219

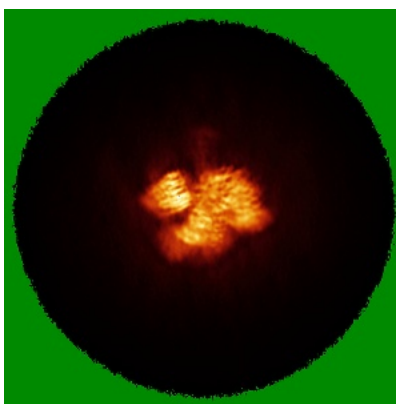
The images above show the largest variance slices of the map in three orthogonal directions.

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

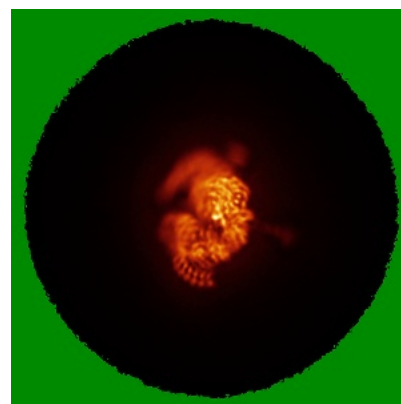
6.4.1 Primary map



X

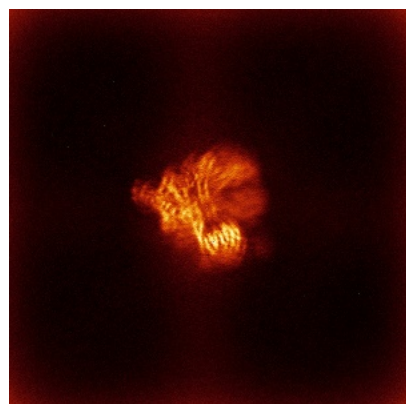


Y

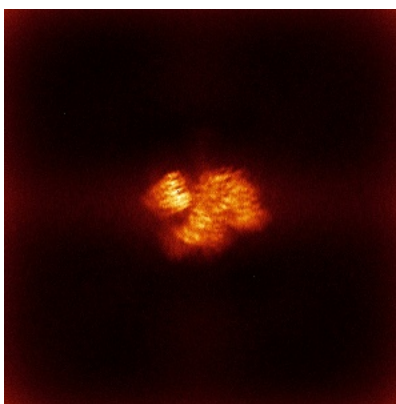


Z

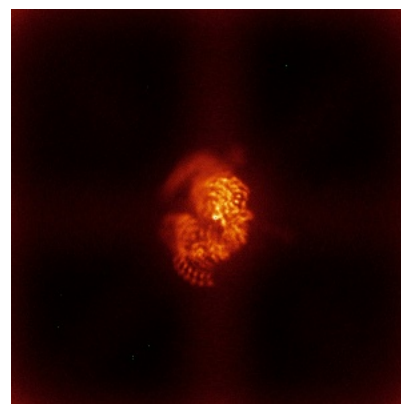
6.4.2 Raw map



X



Y

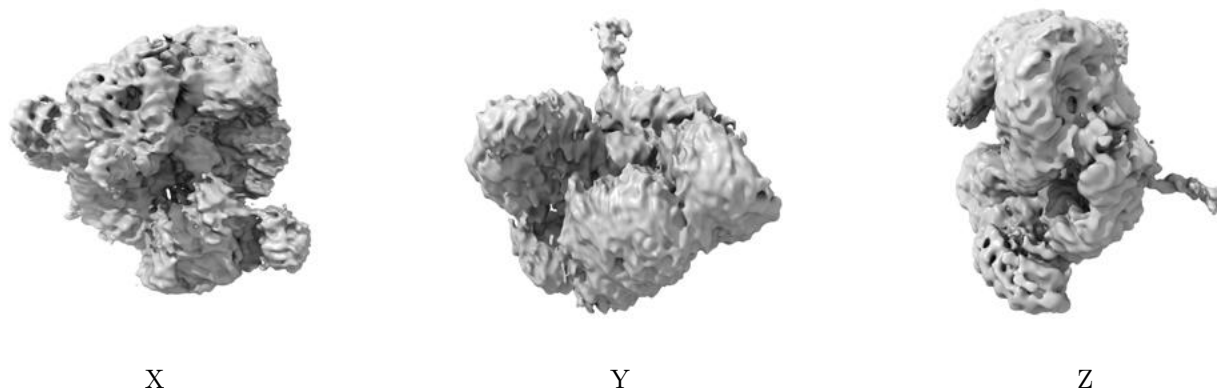


Z

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.

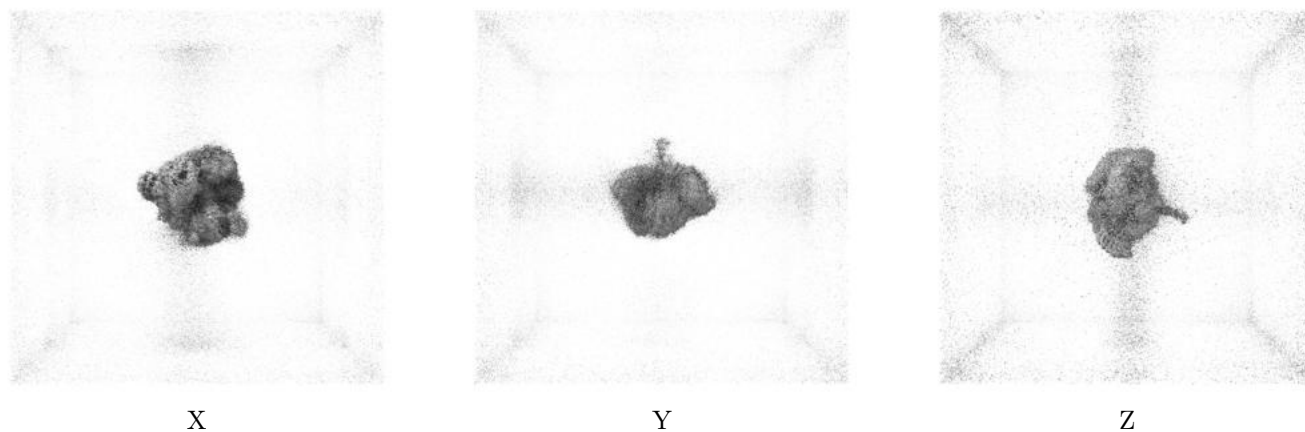
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

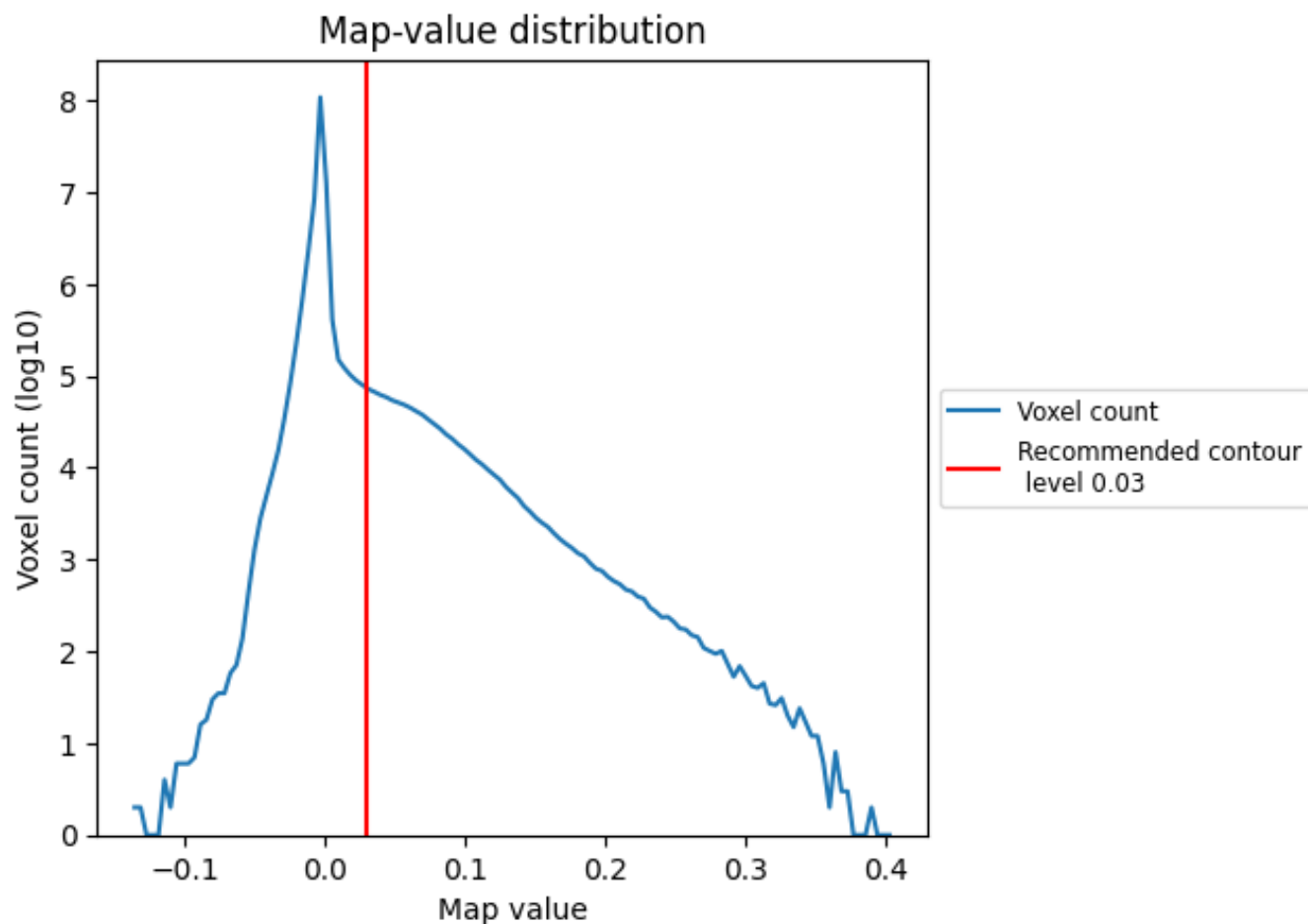
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

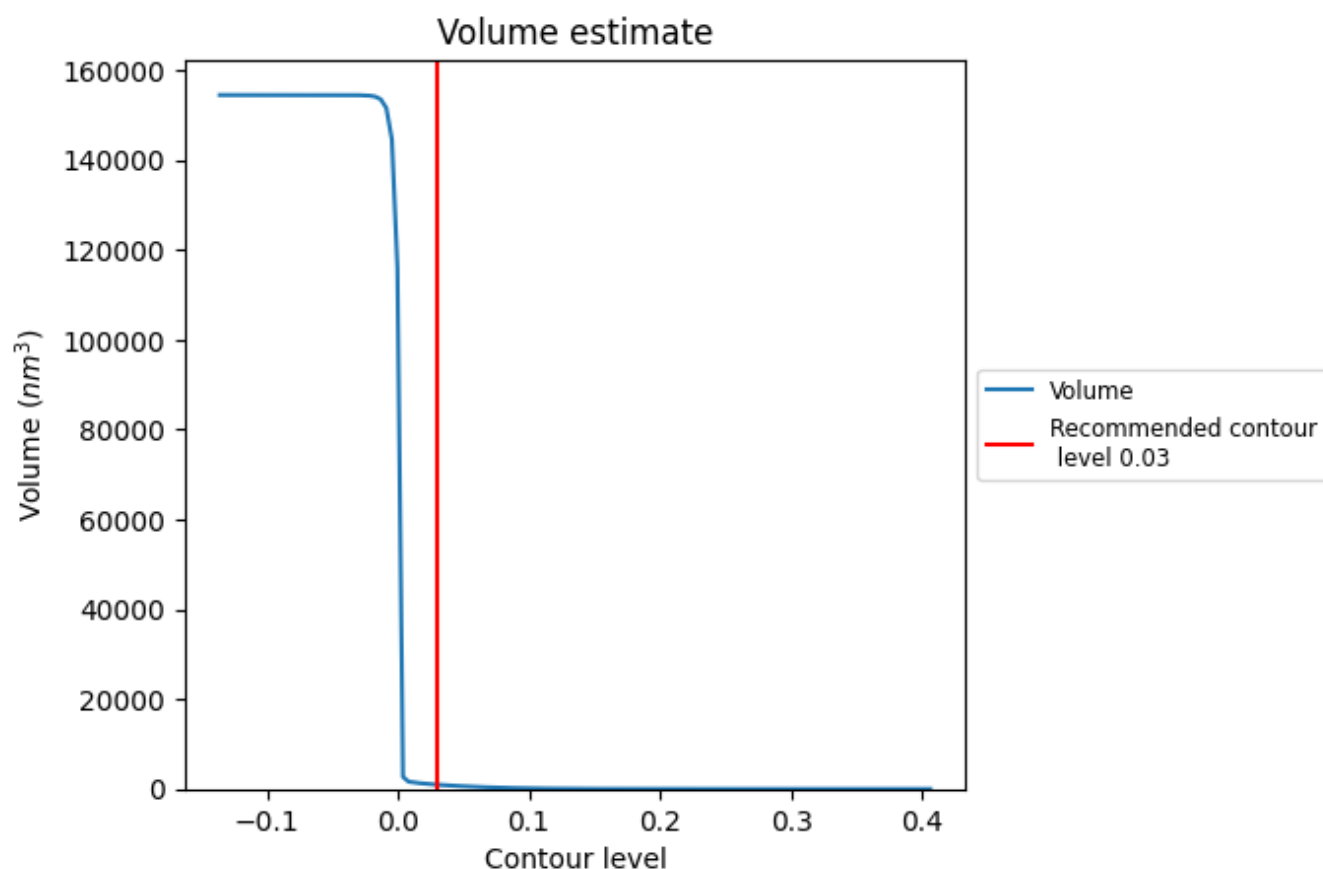
This section contains the results of statistical analysis of the map.

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.

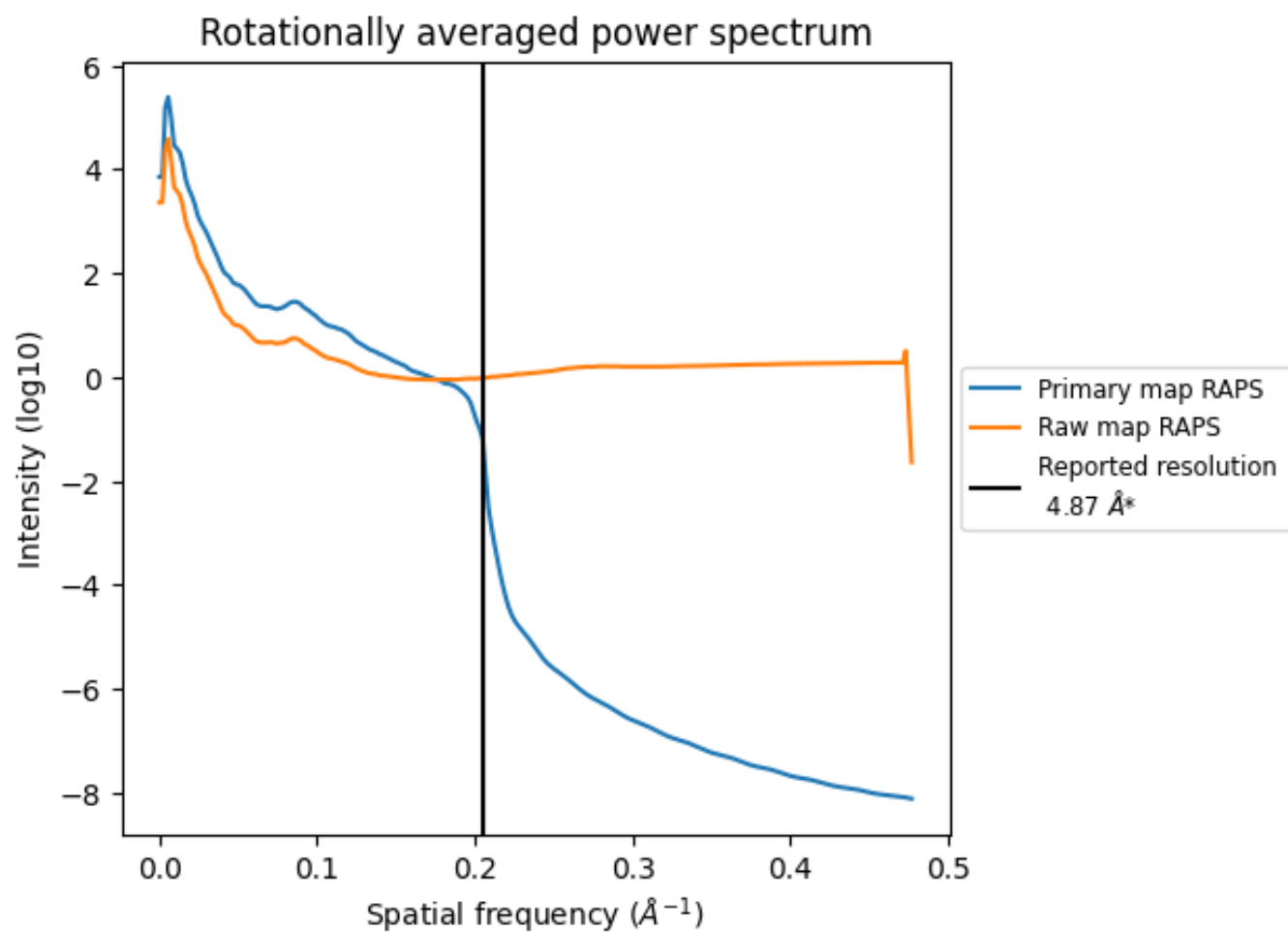
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 952 nm^3 ; this corresponds to an approximate mass of 860 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 ⓘ

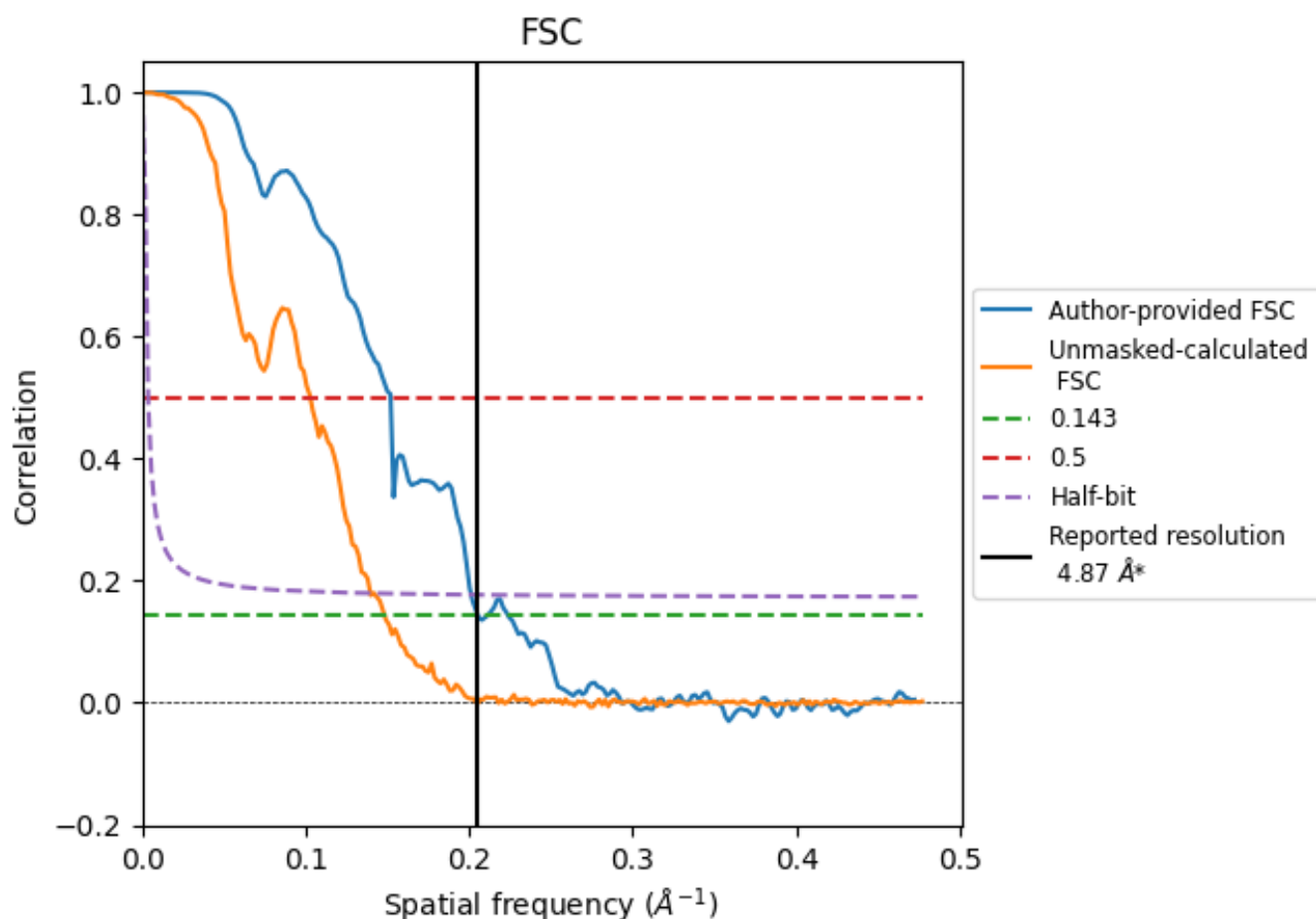


*Reported resolution corresponds to spatial frequency of 0.205 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.205 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

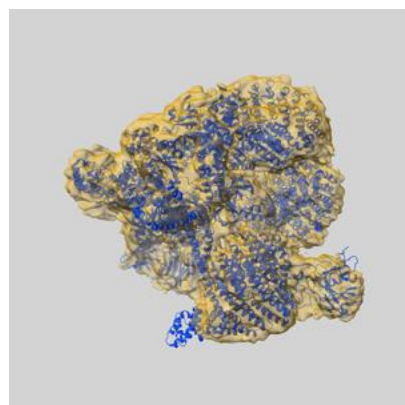
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.87	-	-
Author-provided FSC curve	4.87	6.58	4.97
Unmasked-calculated*	6.74	9.73	7.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.74 differs from the reported value 4.87 by more than 10 %

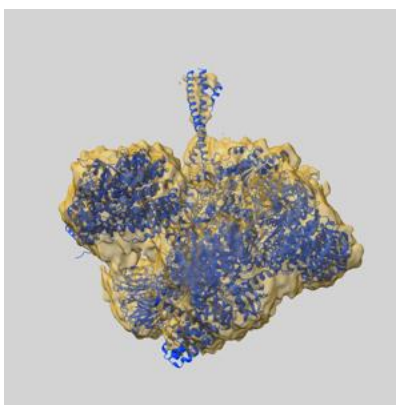
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77338 and PDB model 36AX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

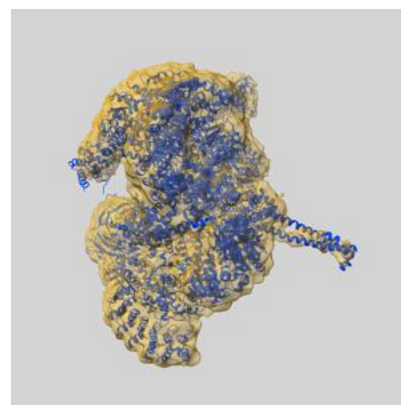
9.1 Map-model overlay [i](#)



X



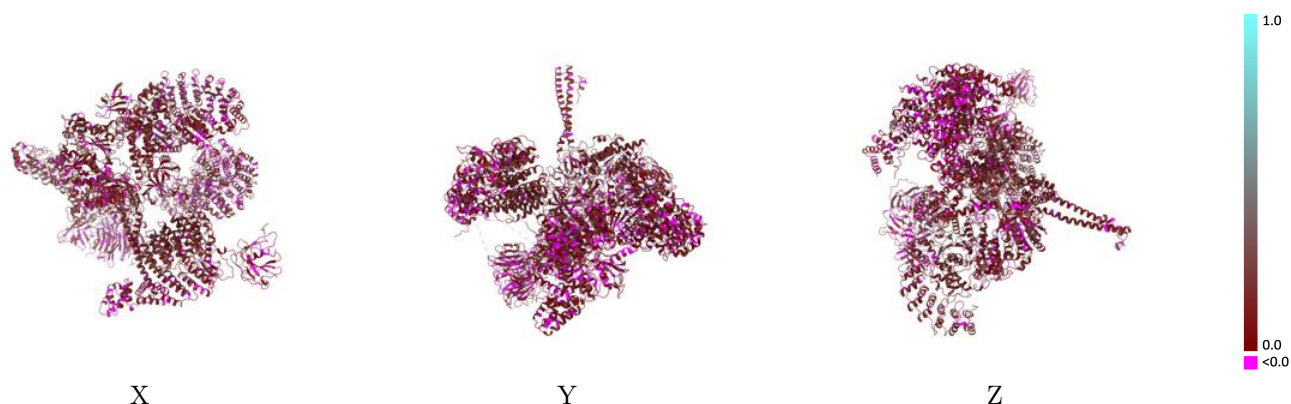
Y



Z

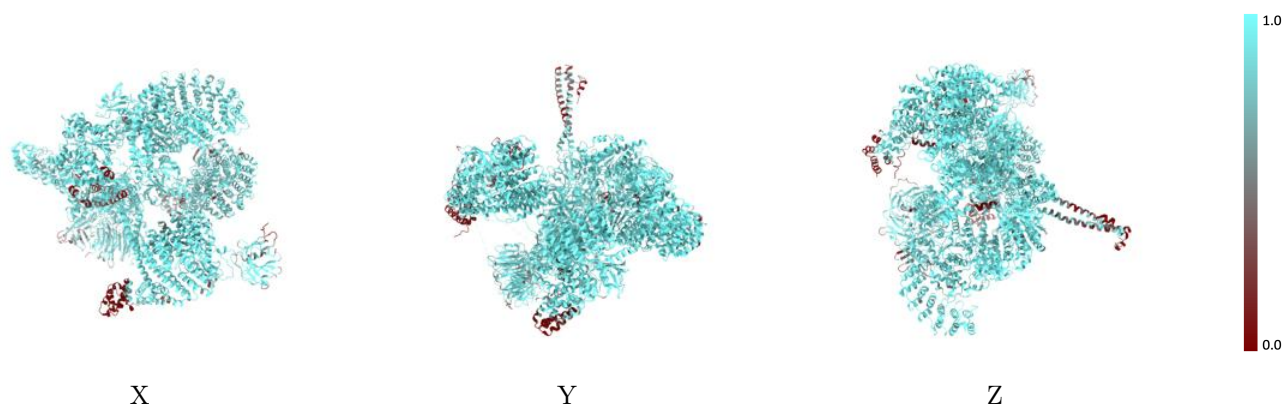
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



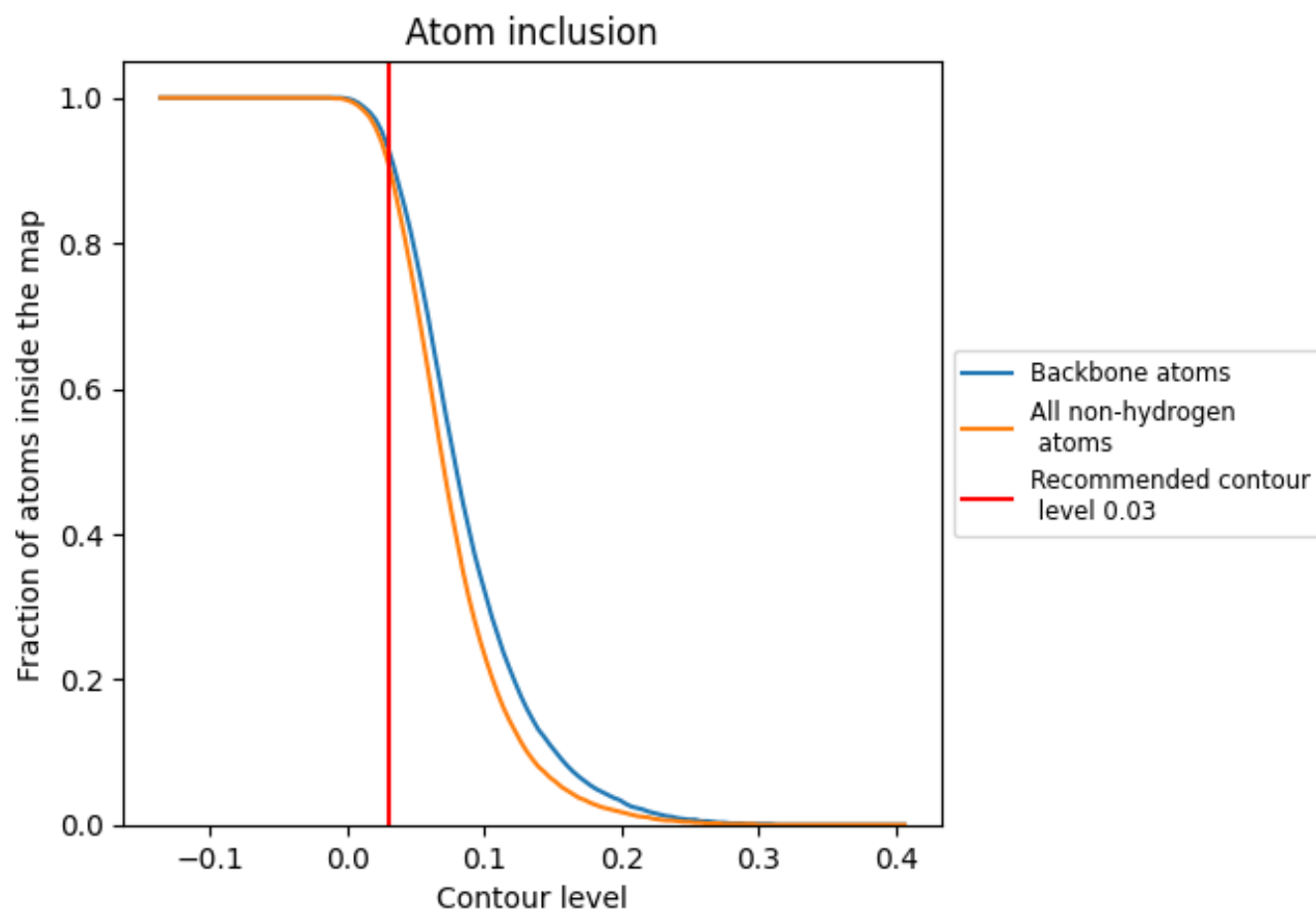
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.1220
A	 0.9230	 0.1100
B	 0.9320	 0.1030
C	 0.8980	 0.0750
D	 0.9750	 0.1060
I	 0.9720	 0.1390
J	 0.9510	 0.1810
K	 0.9250	 0.1410
L	 0.7540	 0.1130
M	 0.8550	 0.0590
N	 0.9540	 0.1670
P	 0.8660	 0.1490
R	 0.9670	 0.1550
Z	 0.8660	 0.1470

