Full wwPDB EM Validation Report ⓘ

Jul 11, 2023 – 02:12 pm BST

PDB ID	:	8PKP
EMDB ID	:	EMD-17751
Title	:	Cryo-EM structure of the apo Anaphase-promoting complex/cyclosome (APC/C) at 3.2 Angstrom resolution
Authors	:	Hoefler, A.; Yu, J.; Chang, L.; Zhang, Z.; Yang, J.; Boland, A.; Barford, D.
Deposited on	:	2023-06-27
Resolution	:	3.20 Å(reported)
Based on initial model	:	5G05

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:

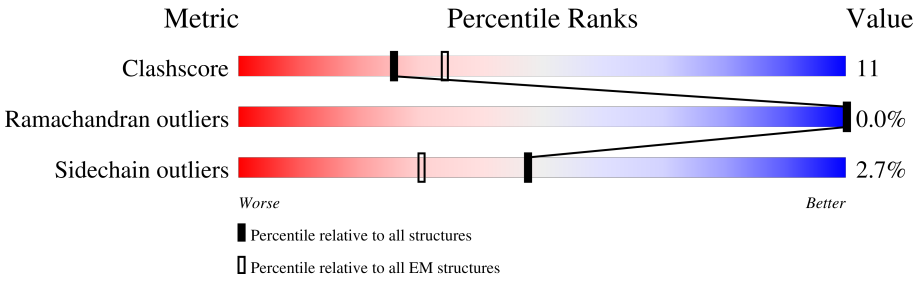
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1944	60% 21% • 19%
2	D	121	40% 7% 54%
3	G	85	22% 9% 68%
3	W	85	25% 5% 71%
4	H	110	39% 12% • 48%
5	J	824	42% 16% 42%
5	P	824	41% 17% • 41%
6	K	620	65% 17% • 17%

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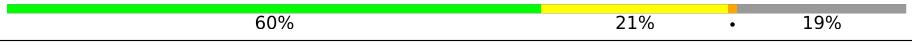
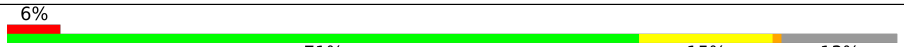
Mol	Chain	Length	Quality of chain
6	Q	620	
7	L	185	
8	M	74	
9	O	755	
10	U	597	
10	V	597	
11	Y	565	
11	Z	565	
12	I	814	
13	N	822	
14	C	84	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 64691 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1580	12311	7891	2074	2260	86	0	0

- Molecule 2 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	56	458	291	77	89	1	0	0

- Molecule 3 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	27	226	142	42	41	1	0	0
			Total	C	N	O	S		
3	W	25	217	136	41	39	1	0	0

- Molecule 4 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	57	459	296	75	86	2	0	0

- Molecule 5 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	476	3601	2300	615	662	24	1	0
			Total	C	N	O	S		
5	P	484	3883	2497	653	707	26	0	0

- Molecule 6 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	512	Total	C	N	O	S	0	0
			4134	2657	697	755	25		
6	Q	504	Total	C	N	O	S	0	0
			4049	2603	681	741	24		

- Molecule 7 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	179	Total	C	N	O	S	0	0
			1446	906	263	270	7		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	58	Total	C	N	O	S	0	0
			478	301	78	97	2		

- Molecule 9 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	683	Total	C	N	O	S	0	0
			5404	3444	941	993	26		

- Molecule 10 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	521	Total	C	N	O	S	0	0
			4221	2715	708	773	25		
10	V	534	Total	C	N	O	S	0	0
			4393	2826	740	802	25		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	499	Total	C	N	O	S	1	0
			3907	2471	681	728	27		
11	Z	486	Total	C	N	O	S	1	0
			3807	2413	664	705	25		

- Molecule 12 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	718	Total	C	N	O	S	0	0
			5722	3664	950	1074	34		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	809	GLU	-	expression tag	UNP Q9UJX5
I	810	ASN	-	expression tag	UNP Q9UJX5
I	811	LEU	-	expression tag	UNP Q9UJX5
I	812	TYR	-	expression tag	UNP Q9UJX5
I	813	PHE	-	expression tag	UNP Q9UJX5
I	814	GLN	-	expression tag	UNP Q9UJX5

- Molecule 13 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	652	Total	C	N	O	S	0	0
			5294	3362	933	972	27		

- Molecule 14 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	84	Total	C	N	O	S	0	0
			680	431	123	110	16		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

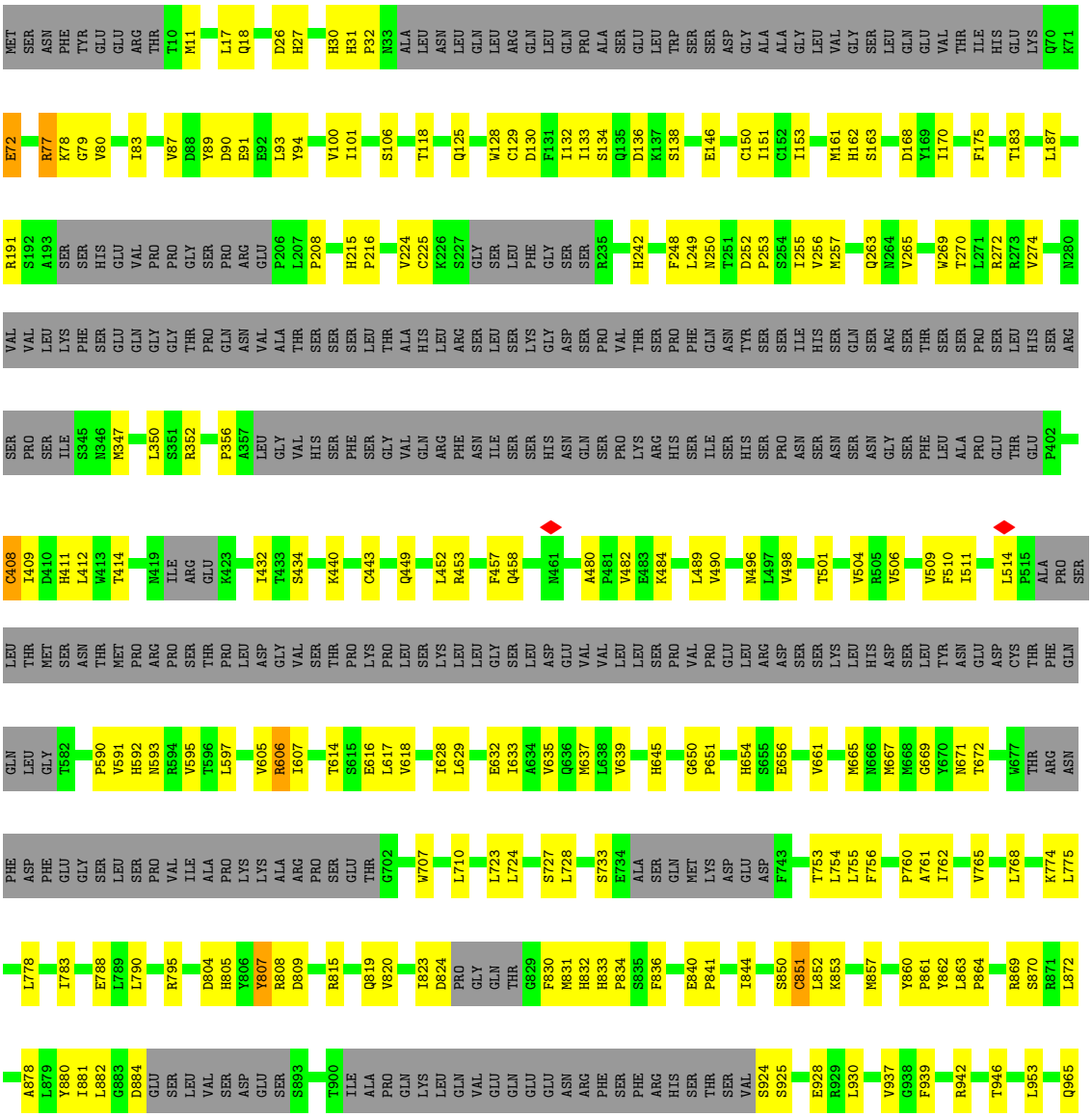
Mol	Chain	Residues	Atoms		AltConf
15	N	1	Total	Zn	0
			1	1	

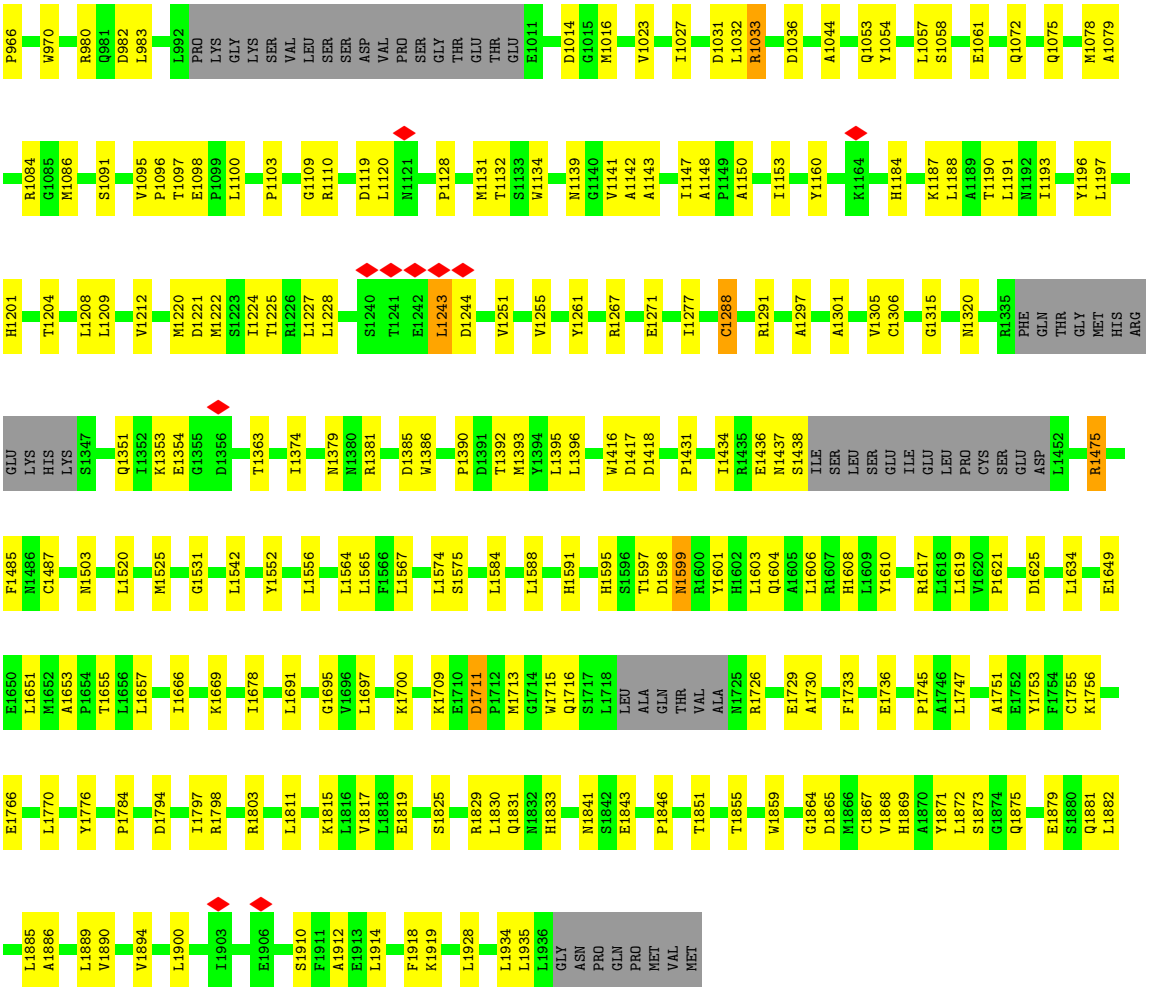
3 Residue-property plots (i)

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

- Molecule 1: Anaphase-promoting complex subunit 1

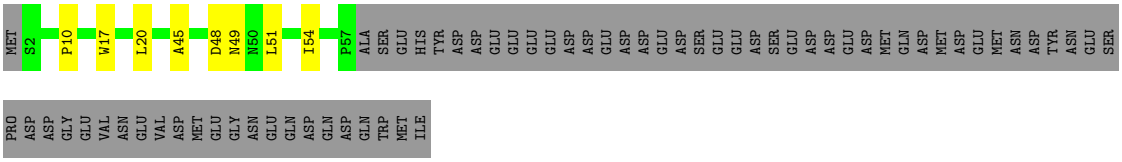
Chain A:





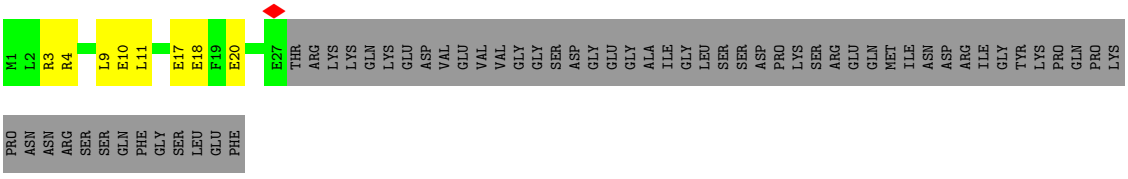
• Molecule 2: Anaphase-promoting complex subunit 15

Chain D:



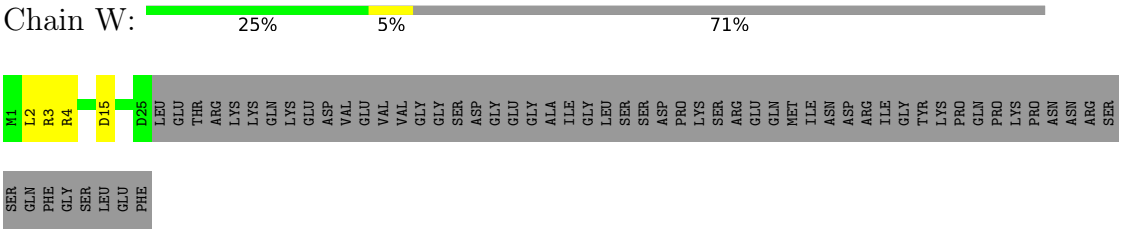
• Molecule 3: Anaphase-promoting complex subunit CDC26

Chain G:



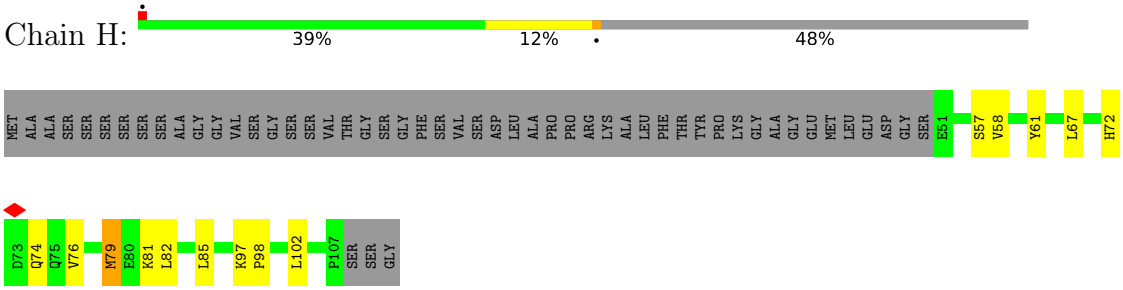
• Molecule 3: Anaphase-promoting complex subunit CDC26

Chain W:



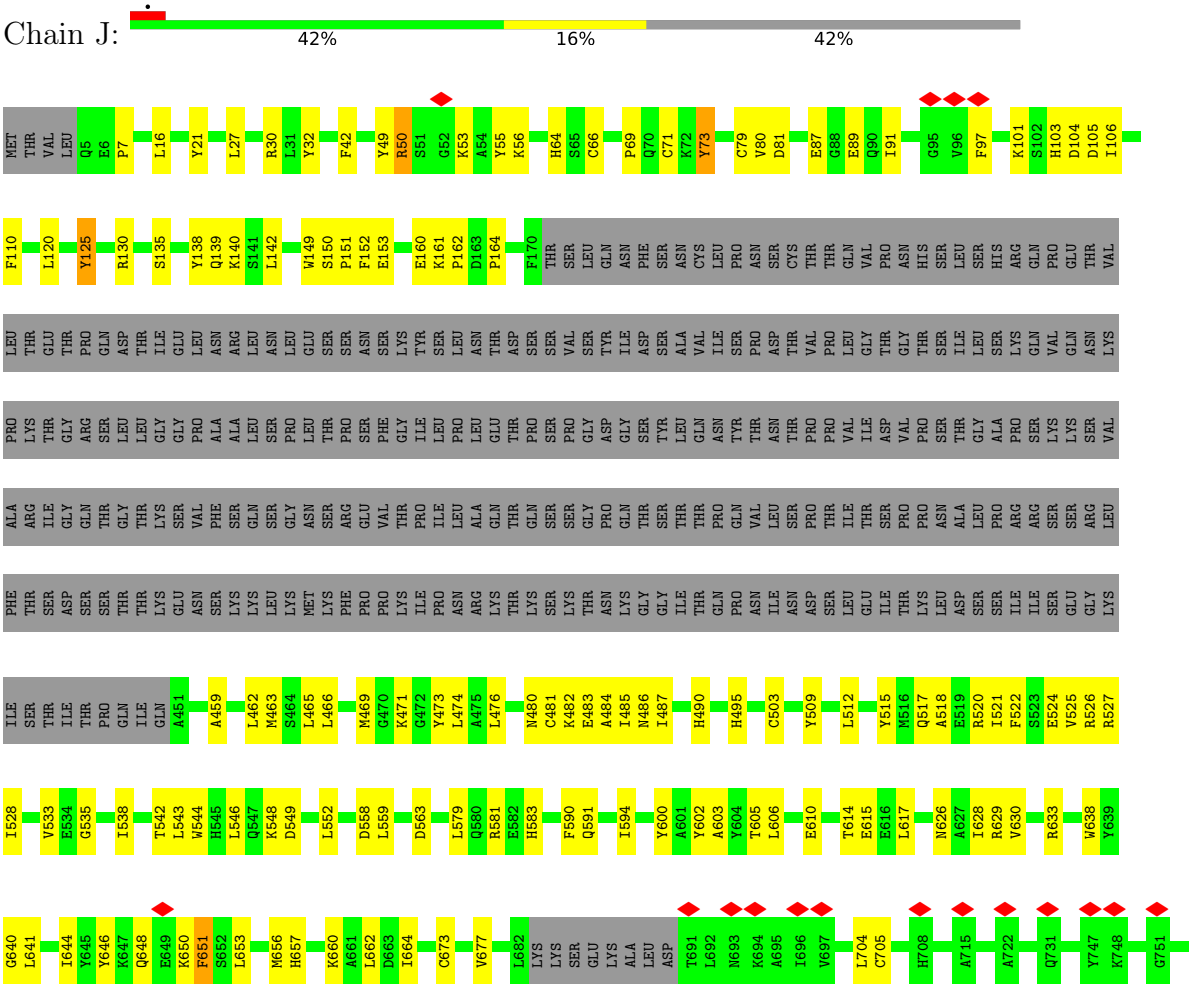
• Molecule 4: Anaphase-promoting complex subunit 16

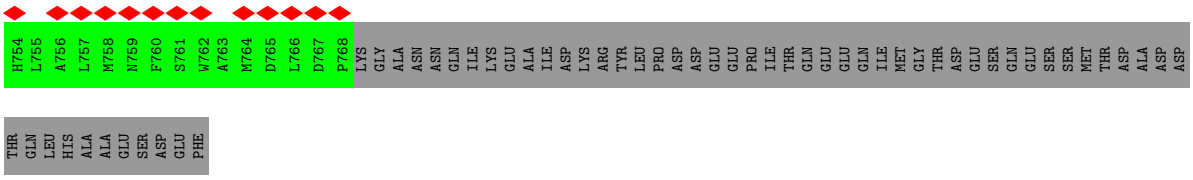
Chain H:



• Molecule 5: Cell division cycle protein 27 homolog

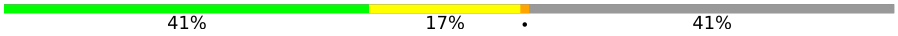
Chain J:

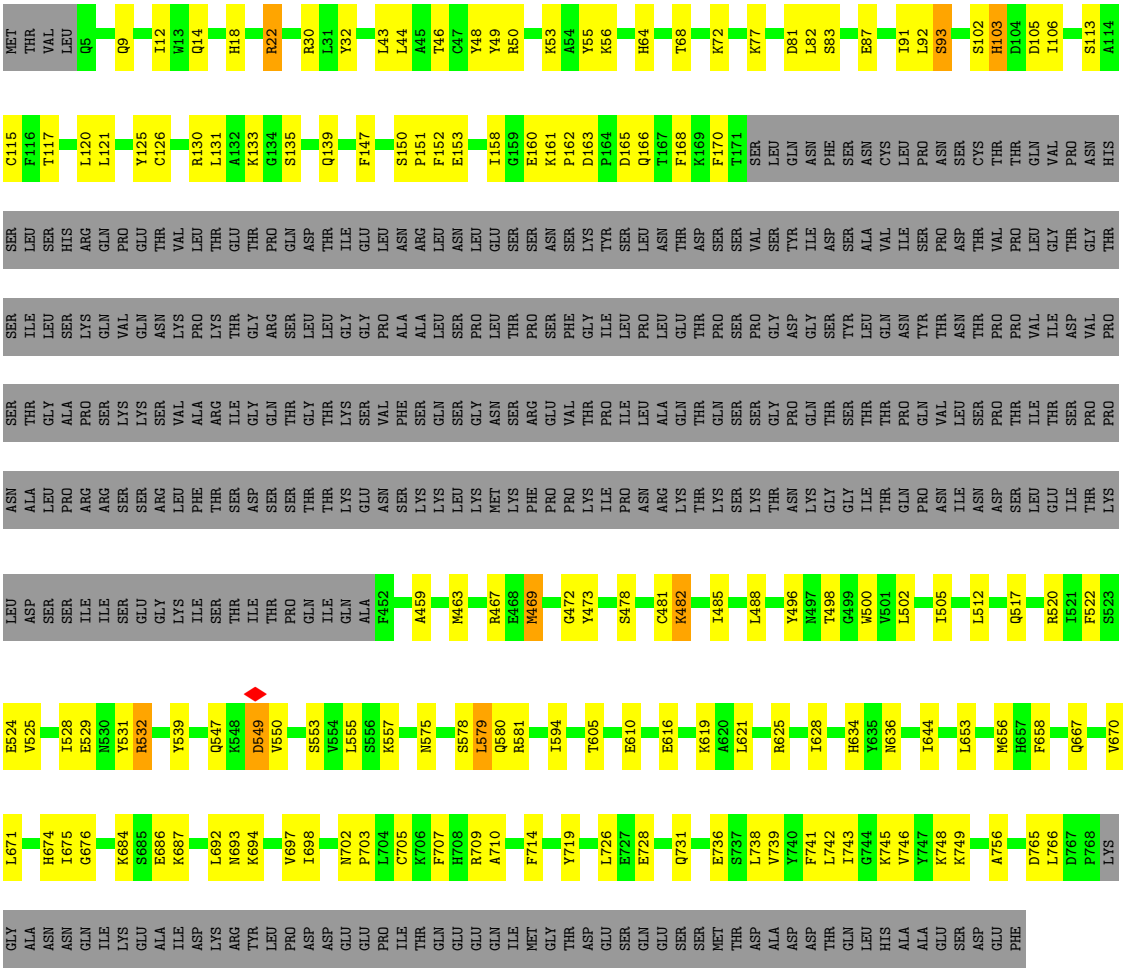




• Molecule 5: Cell division cycle protein 27 homolog

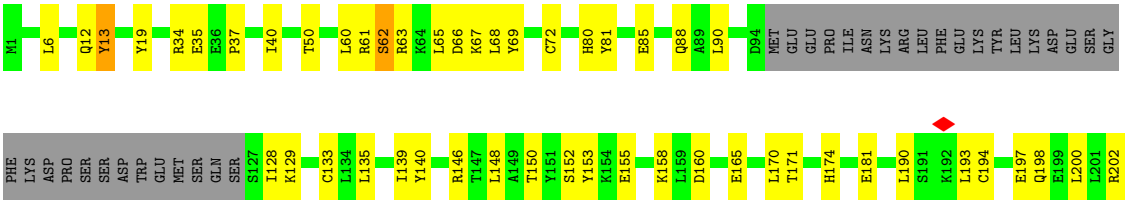
Chain P:

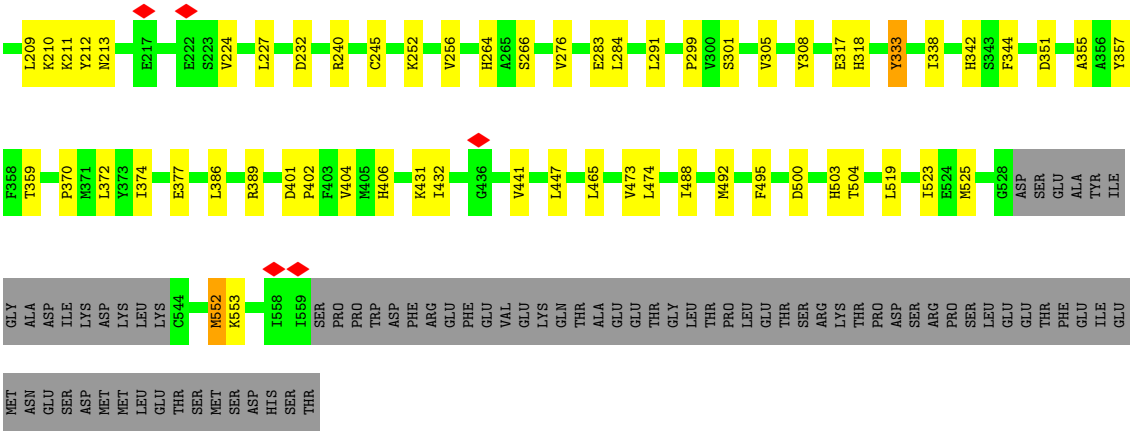




• Molecule 6: Cell division cycle protein 16 homolog

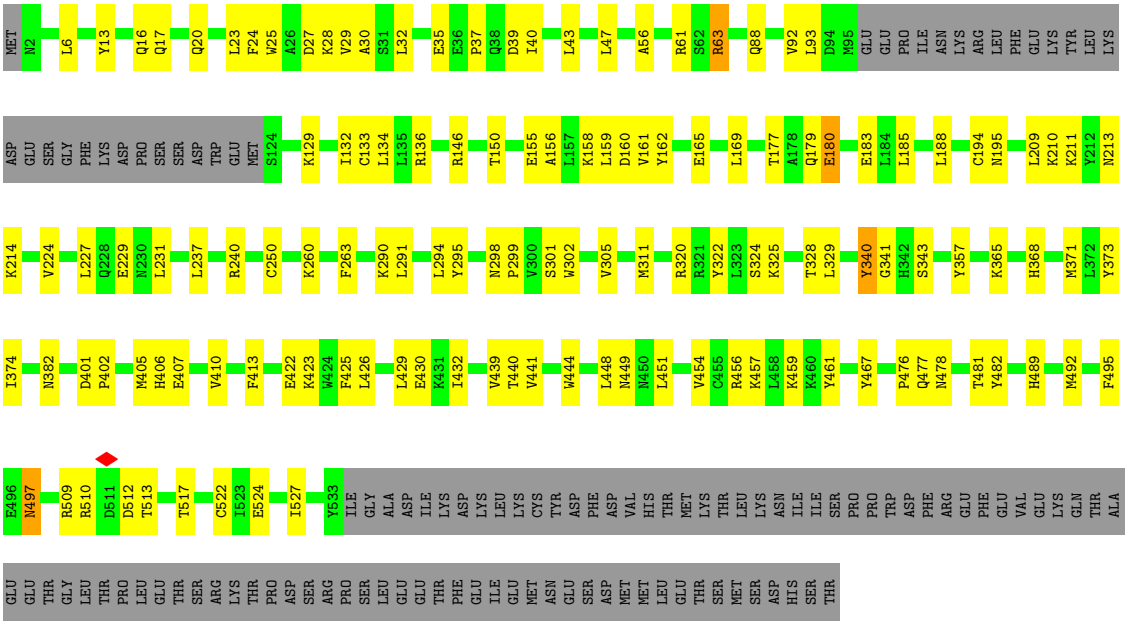
Chain K:





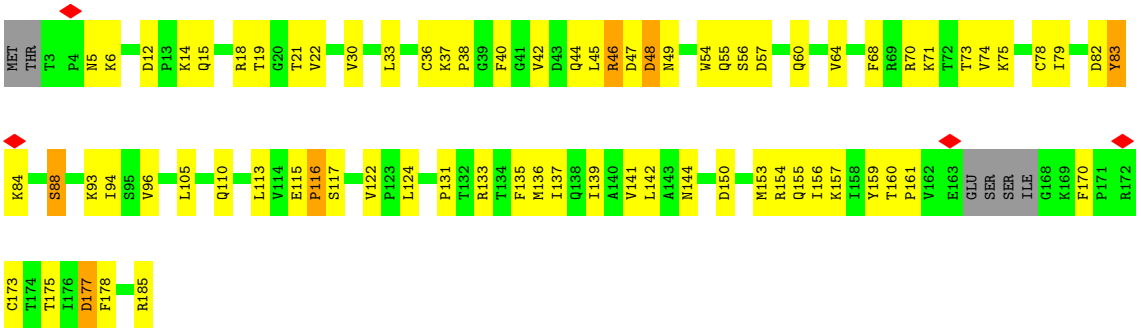
• Molecule 6: Cell division cycle protein 16 homolog

Chain Q:



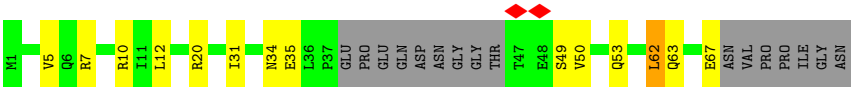
• Molecule 7: Anaphase-promoting complex subunit 10

Chain L:



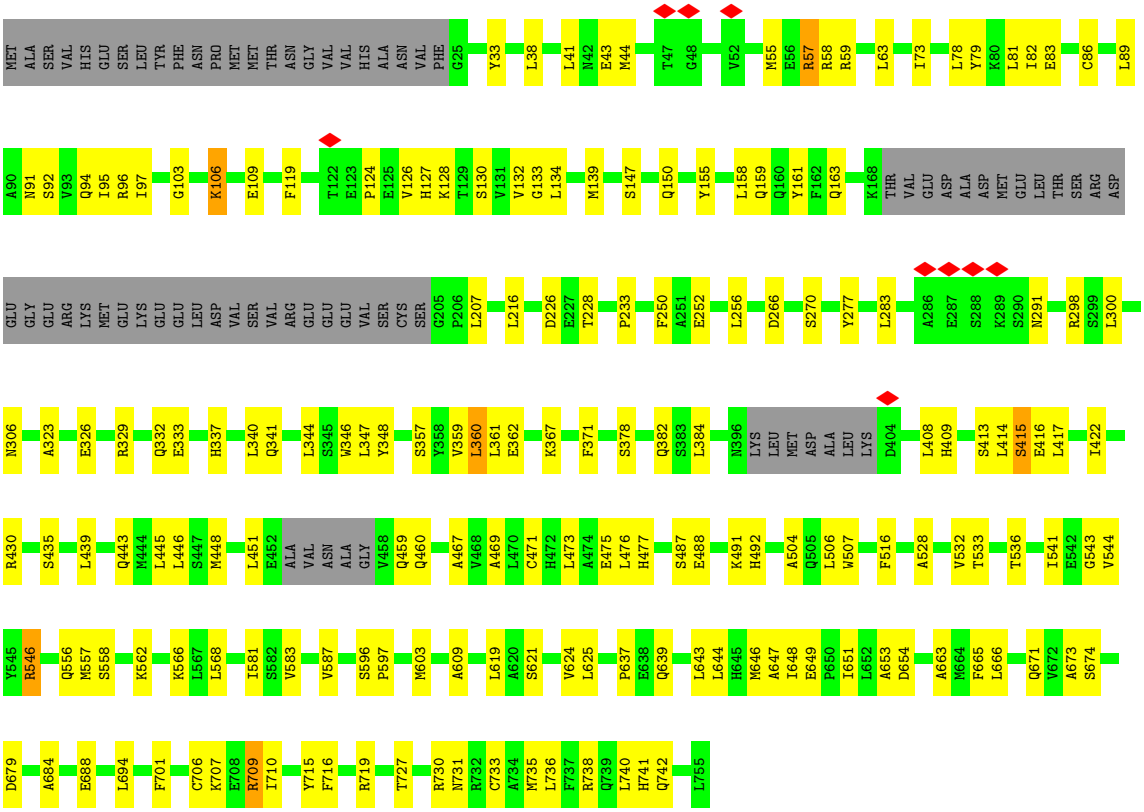
• Molecule 8: Anaphase-promoting complex subunit 13

Chain M:



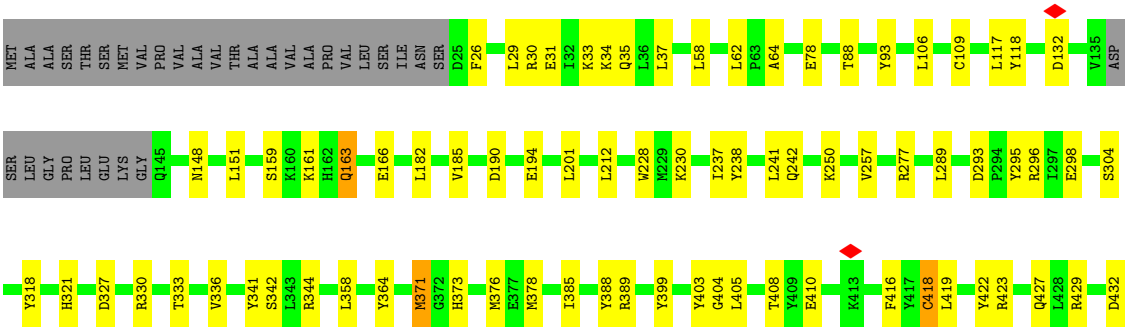
• Molecule 9: Anaphase-promoting complex subunit 5

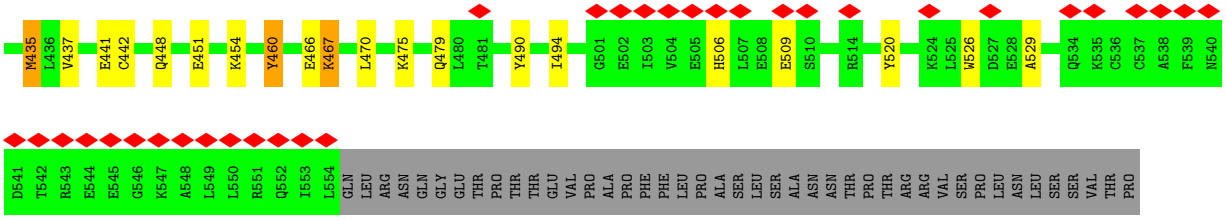
Chain O:



• Molecule 10: Cell division cycle protein 23 homolog

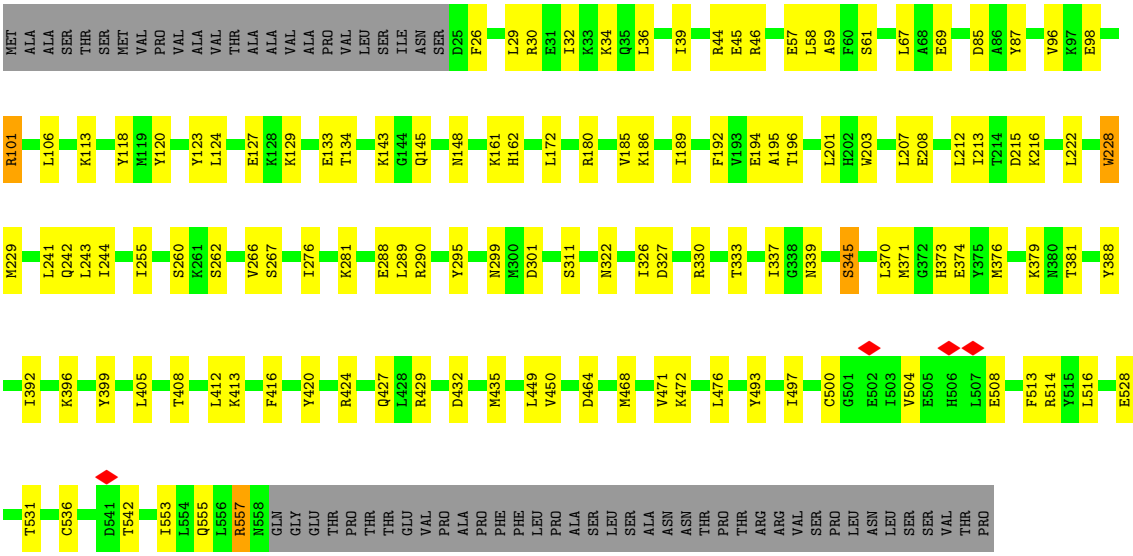
Chain U:





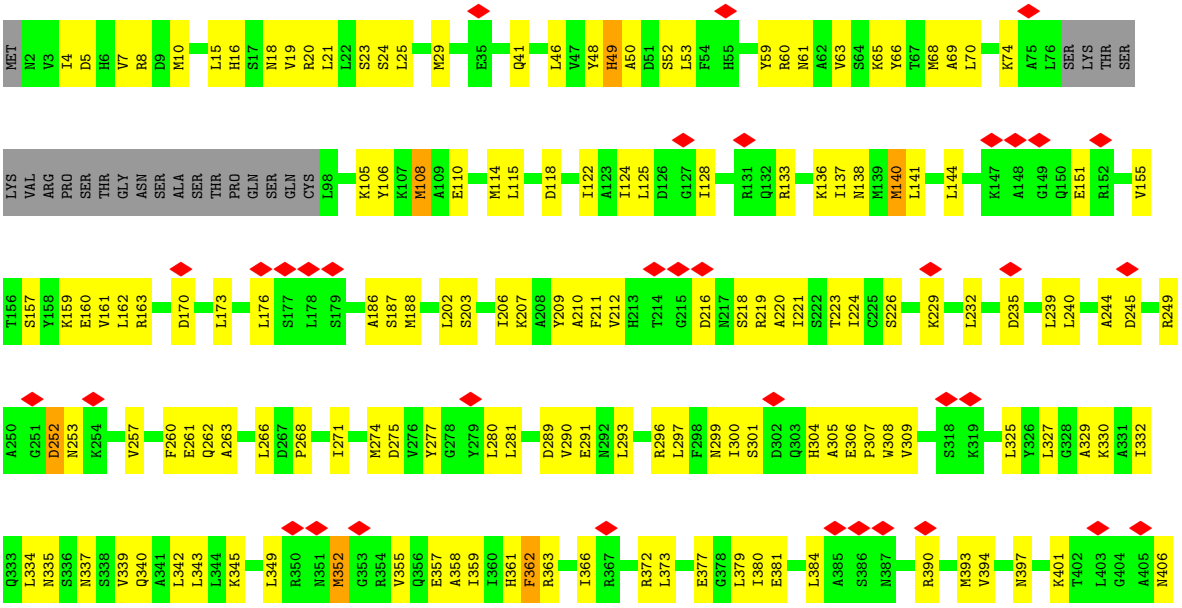
• Molecule 10: Cell division cycle protein 23 homolog

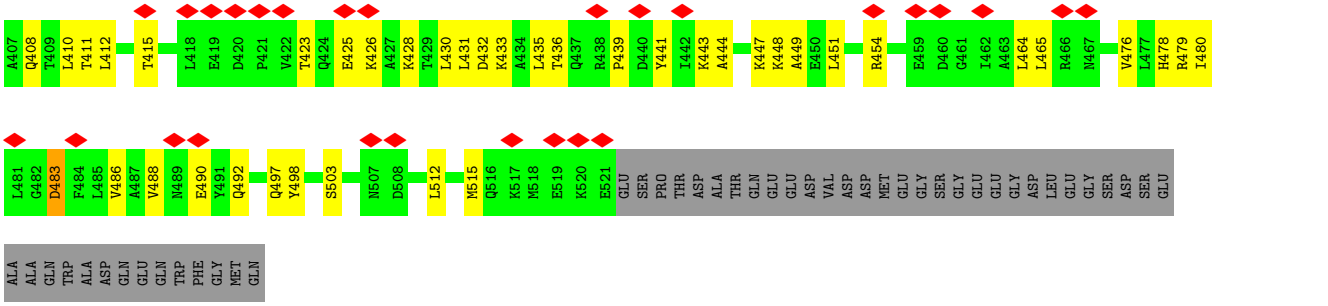
Chain V:



• Molecule 11: Anaphase-promoting complex subunit 7

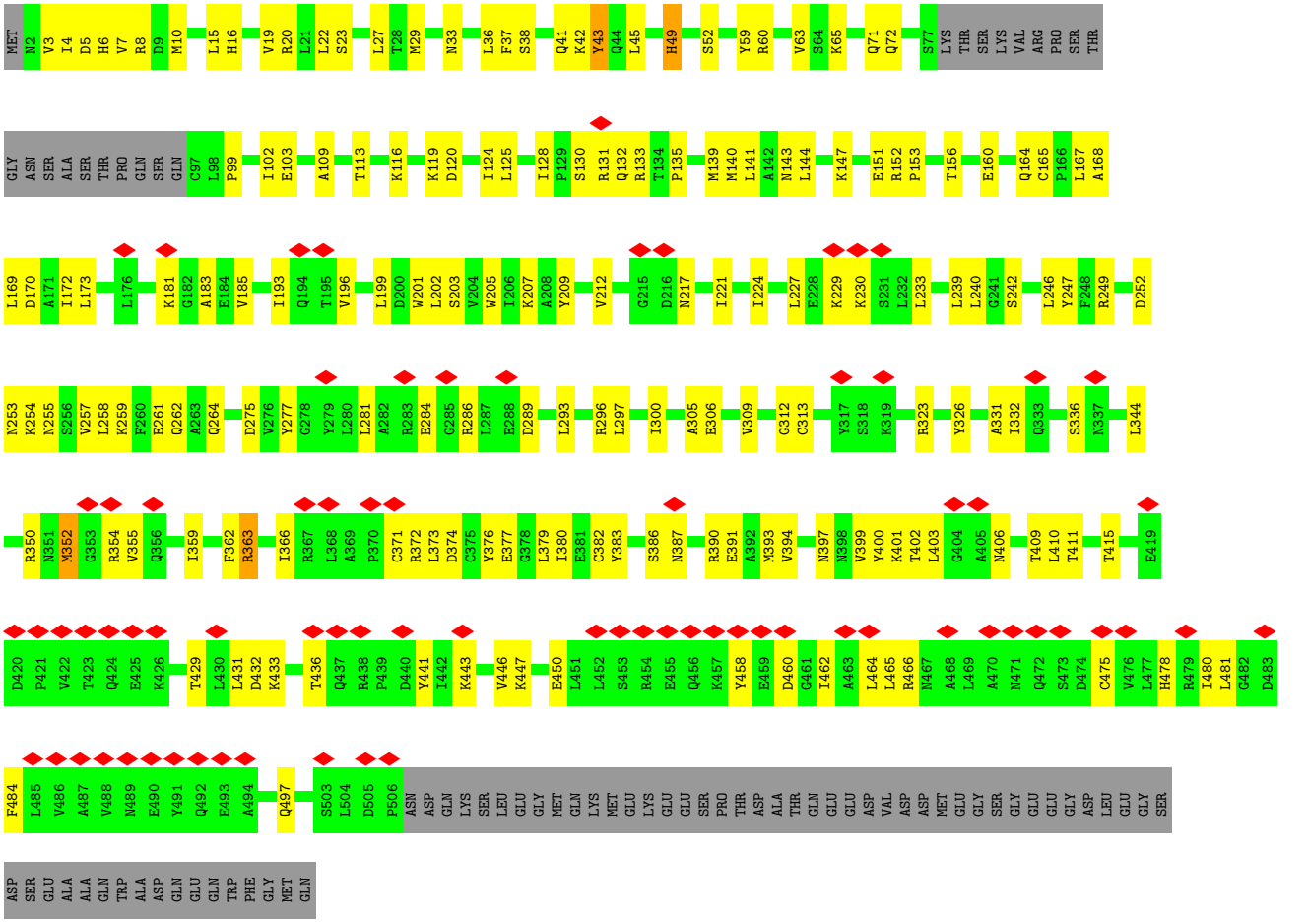
Chain Y:





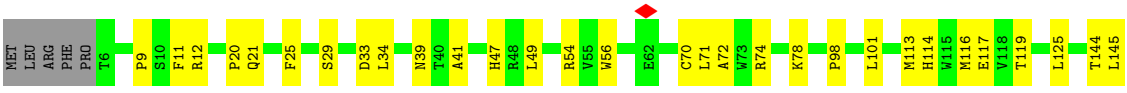
• Molecule 11: Anaphase-promoting complex subunit 7

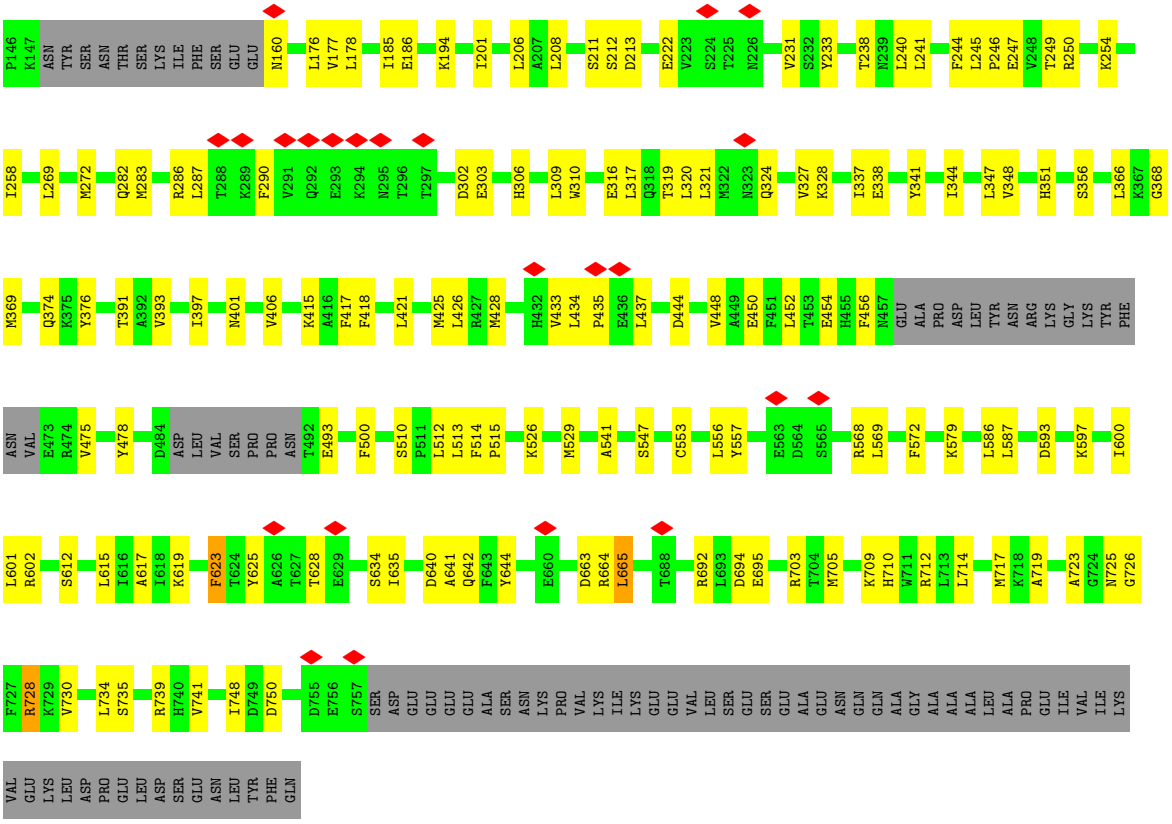
Chain Z:



• Molecule 12: Anaphase-promoting complex subunit 4

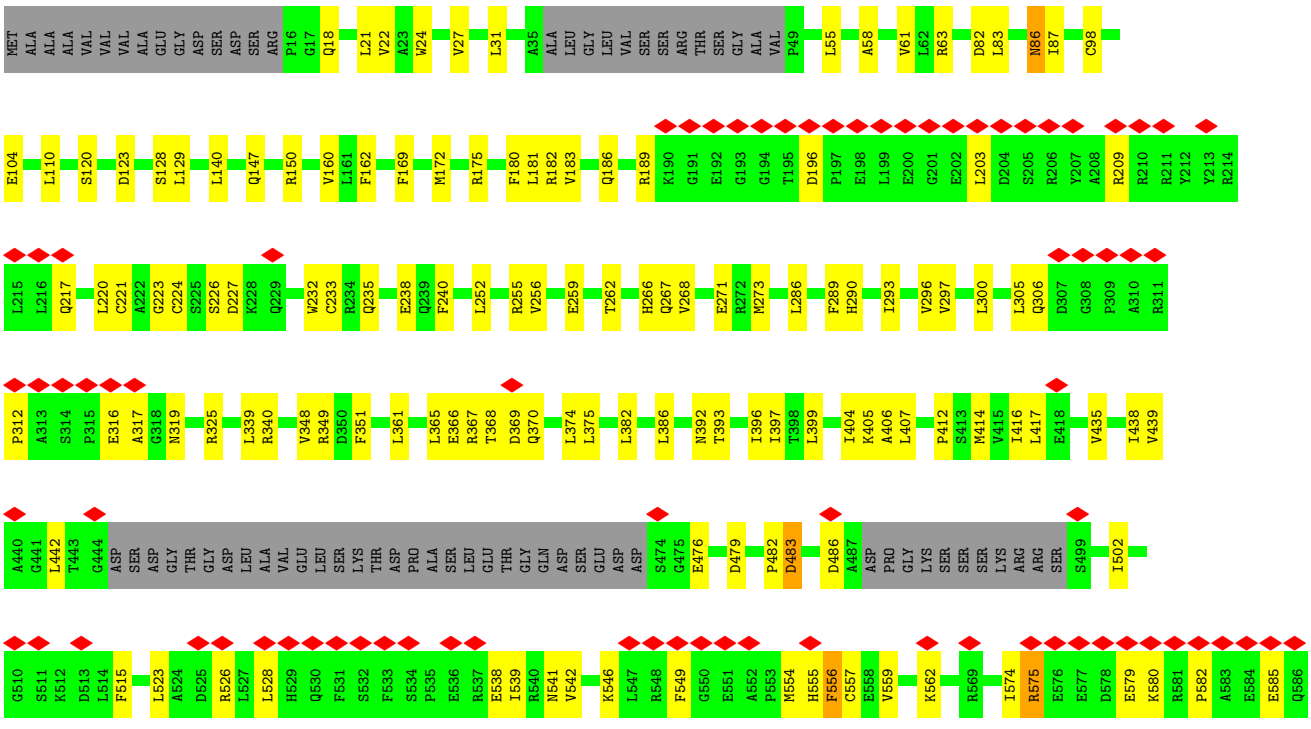
Chain I:

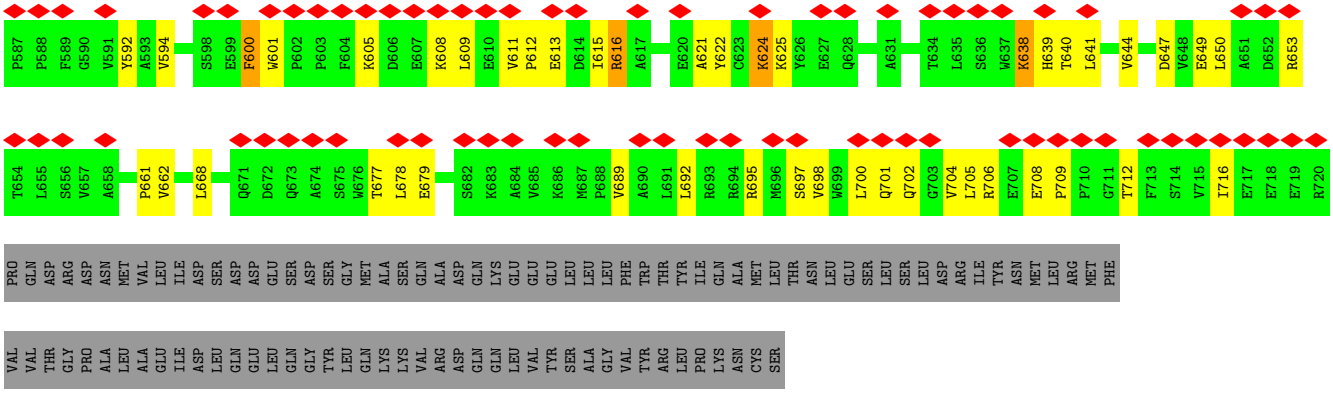




• Molecule 13: Anaphase-promoting complex subunit 2

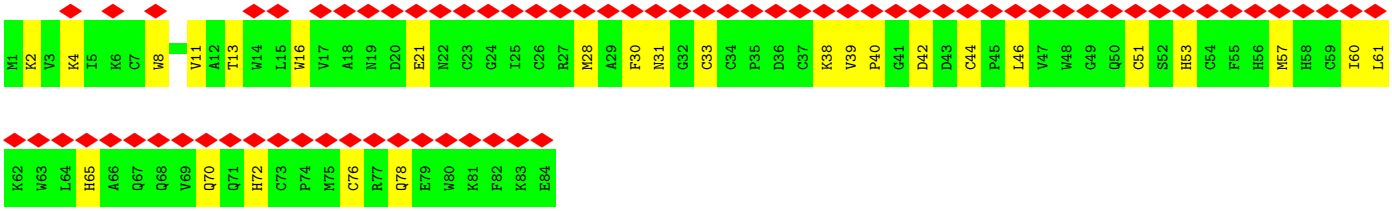
Chain N:





• Molecule 14: Anaphase-promoting complex subunit 11

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174356	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.975	Depositor
Minimum map value	-0.749	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.37	0/12594	0.53	0/17122
2	D	0.35	0/470	0.47	0/643
3	G	0.27	0/227	0.60	0/302
3	W	0.33	0/218	0.60	0/288
4	H	0.30	0/468	0.45	0/631
5	J	0.31	0/3686	0.50	0/5000
5	P	0.34	0/3975	0.48	0/5371
6	K	0.32	0/4233	0.47	0/5730
6	Q	0.34	0/4148	0.50	0/5620
7	L	0.32	0/1480	0.55	0/2005
8	M	0.29	0/486	0.52	0/658
9	O	0.36	0/5504	0.49	0/7435
10	U	0.32	0/4318	0.49	0/5839
10	V	0.37	0/4493	0.49	0/6065
11	Y	0.28	0/3970	0.55	0/5365
11	Z	0.28	0/3870	0.53	0/5233
12	I	0.31	0/5841	0.52	0/7909
13	N	0.28	0/5405	0.53	0/7315
14	C	0.23	0/703	0.42	0/951
All	All	0.33	0/66089	0.51	0/89482

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12311	0	12224	277	0
2	D	458	0	434	9	0
3	G	226	0	233	10	0
3	W	217	0	231	3	0
4	H	459	0	449	12	0
5	J	3601	0	3314	100	0
5	P	3883	0	3834	115	0
6	K	4134	0	4060	75	0
6	Q	4049	0	3948	100	0
7	L	1446	0	1423	53	0
8	M	478	0	454	11	0
9	O	5404	0	5452	137	0
10	U	4221	0	4106	65	0
10	V	4393	0	4362	94	0
11	Y	3907	0	3975	165	0
11	Z	3807	0	3885	136	0
12	I	5722	0	5680	118	0
13	N	5294	0	5294	116	0
14	C	680	0	649	24	0
15	N	1	0	0	0	0
All	All	64691	0	64007	1461	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 11.

All (1461) 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)
9:O:443:GLN:HE22	12:I:514:PHE:H	1.22	0.86
5:P:12:ILE:HG21	5:P:43:LEU:HD21	1.57	0.86
11:Y:105:LYS:HA	11:Y:108:MET:HE3	1.57	0.85
1:A:1193:ILE:HG23	1:A:1208:LEU:HD21	1.62	0.80
5:J:160:GLU:HG3	5:J:161:LYS:HG2	1.63	0.80
11:Z:411:THR:HG21	11:Z:441:TYR:HE2	1.49	0.77
6:Q:325:LYS:HE2	6:Q:329:LEU:HD21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:224:VAL:HG11	6:Q:227:LEU:HB2	1.65	0.77
9:O:430:ARG:HD3	9:O:476:LEU:HD11	1.67	0.76
1:A:1100:LEU:HD13	1:A:1147:ILE:HD11	1.66	0.76
13:N:609:LEU:HD12	13:N:639:HIS:HB2	1.67	0.76
9:O:671:GLN:HE22	12:I:374:GLN:HE22	1.34	0.76
11:Y:70:LEU:HD11	11:Y:108:MET:HE1	1.66	0.76
6:Q:23:LEU:HD11	6:Q:47:LEU:HD12	1.68	0.75
13:N:641:LEU:HB3	14:C:11:VAL:HB	1.69	0.75
9:O:443:GLN:HE22	12:I:514:PHE:N	1.85	0.74
6:K:473:VAL:HG21	5:P:130:ARG:HH22	1.52	0.74
5:P:726:LEU:HD23	5:P:739:VAL:HG13	1.70	0.74
4:H:57:SER:OG	11:Z:323:ARG:NH2	2.21	0.74
11:Z:193:ILE:HG22	11:Z:199:LEU:HB2	1.71	0.73
12:I:719:ALA:HA	12:I:735:SER:HA	1.71	0.73
13:N:613:GLU:HA	13:N:616:ARG:HG3	1.70	0.73
9:O:742:GLN:OE1	9:O:742:GLN:N	2.19	0.72
11:Z:102:ILE:HG13	11:Z:103:GLU:N	2.04	0.72
1:A:1096:PRO:HG2	9:O:347:LEU:HD21	1.71	0.72
1:A:272:ARG:NH1	1:A:408:CYS:SG	2.63	0.72
7:L:83:TYR:HD2	7:L:115:GLU:HG3	1.55	0.71
11:Y:515:MET:SD	11:Y:515:MET:N	2.63	0.71
11:Y:297:LEU:HB3	11:Y:307:PRO:HB3	1.72	0.71
13:N:438:ILE:HG21	13:N:515:PHE:HZ	1.54	0.71
12:I:556:LEU:HD21	12:I:586:LEU:HD21	1.73	0.71
11:Y:271:ILE:HG22	11:Y:306:GLU:HG3	1.71	0.71
5:J:27:LEU:HD21	5:P:147:PHE:HB3	1.73	0.71
9:O:448:MET:SD	12:I:401:ASN:ND2	2.63	0.71
9:O:649:GLU:HG2	12:I:369:MET:HG2	1.74	0.70
11:Z:257:VAL:HG11	11:Z:286:ARG:HH22	1.57	0.70
10:U:159:SER:O	10:U:163:GLN:NE2	2.24	0.70
10:U:242:GLN:HE22	10:U:429:ARG:HE	1.39	0.70
5:J:162:PRO:HB2	5:J:474:LEU:HD21	1.74	0.70
6:Q:368:HIS:NE2	6:Q:401:ASP:OD2	2.24	0.70
11:Z:130:SER:HA	11:Z:133:ARG:HE	1.55	0.70
1:A:1390:PRO:HB2	1:A:1396:LEU:HD23	1.75	0.69
11:Y:512:LEU:HA	11:Y:515:MET:HG2	1.73	0.69
1:A:191:ARG:NH2	1:A:208:PRO:O	2.25	0.69
1:A:352:ARG:NH1	10:V:339:ASN:OD1	2.24	0.69
6:Q:432:ILE:HD11	6:Q:444:TRP:CG	2.28	0.69
11:Y:50:ALA:HB1	11:Y:66:TYR:CE1	2.28	0.69
11:Y:268:PRO:O	11:Y:296:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:765:ASP:OD2	11:Z:363:ARG:NH1	2.26	0.69
12:I:692:ARG:HE	12:I:694:ASP:HB3	1.57	0.69
12:I:714:LEU:HB3	12:I:717:MET:HB2	1.75	0.69
9:O:291:ASN:O	9:O:298:ARG:NH2	2.26	0.69
10:U:298:GLU:OE2	10:V:101:ARG:NH1	2.26	0.68
5:J:80:VAL:HG11	5:J:120:LEU:HD11	1.74	0.68
5:J:463:MET:HA	5:J:466:LEU:HD12	1.76	0.68
5:P:714:PHE:HD2	5:P:746:VAL:HG22	1.58	0.68
9:O:459:GLN:NE2	12:I:493:GLU:O	2.26	0.68
11:Y:137:ILE:HD12	11:Y:138:ASN:N	2.09	0.68
5:P:707:PHE:CE2	5:P:738:LEU:HB3	2.29	0.68
10:U:26:PHE:HB2	10:U:257:VAL:HG21	1.76	0.68
11:Y:479:ARG:NH1	11:Y:483:ASP:OD2	2.26	0.68
3:G:10:GLU:N	3:G:10:GLU:OE1	2.26	0.67
1:A:1531:GLY:HA2	1:A:1565:LEU:HG	1.75	0.67
9:O:435:SER:H	9:O:654:ASP:HB3	1.59	0.67
5:P:549:ASP:OD1	5:P:550:VAL:N	2.27	0.67
11:Z:23:SER:HB3	11:Z:49:HIS:HB2	1.75	0.67
11:Z:169:LEU:HA	11:Z:172:ILE:HD12	1.76	0.67
11:Z:281:LEU:HD21	11:Z:289:ASP:HB3	1.76	0.67
1:A:1912:ALA:HB3	13:N:21:LEU:HD12	1.75	0.67
13:N:611:VAL:HG23	13:N:616:ARG:HG2	1.75	0.67
1:A:1109:GLY:C	1:A:1110:ARG:HD2	2.15	0.67
9:O:329:ARG:NH2	10:V:413:LYS:O	2.27	0.67
12:I:586:LEU:HD23	12:I:601:LEU:HD23	1.77	0.67
11:Z:240:LEU:HD11	11:Z:262:GLN:HE22	1.60	0.67
11:Y:53:LEU:HD21	11:Y:61:ASN:HB3	1.77	0.67
11:Z:37:PHE:HB3	11:Z:41:GLN:HG3	1.77	0.67
5:J:656:MET:HG3	11:Y:492:GLN:HB2	1.77	0.67
6:Q:61:ARG:HH12	6:Q:92:VAL:HG22	1.58	0.67
10:U:429:ARG:HB2	10:U:435:MET:HE1	1.77	0.67
7:L:70:ARG:HG2	7:L:71:LYS:H	1.60	0.66
13:N:647:ASP:HB3	14:C:4:LYS:HB3	1.76	0.66
11:Y:335:ASN:OD1	11:Y:337:ASN:ND2	2.27	0.66
11:Y:448:LYS:HD3	11:Y:464:LEU:HD21	1.78	0.66
5:J:103:HIS:HB3	5:J:140:LYS:HE2	1.76	0.66
8:M:35:GLU:OE2	8:M:35:GLU:N	2.21	0.66
9:O:443:GLN:NE2	12:I:514:PHE:H	1.92	0.66
10:U:161:LYS:HE3	10:U:166:GLU:HB2	1.76	0.66
5:P:748:LYS:HG2	5:P:756:ALA:HB1	1.77	0.66
9:O:648:ILE:HD12	9:O:663:ALA:HB1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:509:ARG:HD3	6:Q:512:ASP:HB2	1.78	0.66
7:L:40:PHE:HA	7:L:44:GLN:HG3	1.77	0.66
11:Z:411:THR:HG21	11:Z:441:TYR:CE2	2.30	0.66
12:I:29:SER:O	12:I:725:ASN:ND2	2.29	0.66
11:Y:232:LEU:HB3	11:Z:29:MET:SD	2.35	0.65
11:Y:435:LEU:HD12	11:Y:448:LYS:HE2	1.78	0.65
9:O:736:LEU:O	9:O:740:LEU:HD12	1.97	0.65
13:N:404:ILE:HD13	13:N:417:LEU:HD21	1.78	0.65
10:V:36:LEU:HD21	10:V:58:LEU:HB3	1.78	0.65
12:I:185:ILE:HD11	12:I:201:ILE:HG13	1.79	0.65
5:P:488:LEU:HD23	5:P:505:ILE:HG13	1.79	0.65
10:V:497:ILE:HB	10:V:504:VAL:HG21	1.79	0.65
11:Y:50:ALA:HB1	11:Y:66:TYR:HE1	1.61	0.65
13:N:98:CYS:HA	13:N:110:LEU:HD23	1.79	0.65
1:A:1031:ASP:HB2	13:N:482:PRO:HB2	1.79	0.64
5:J:591:GLN:HA	5:J:594:ILE:HD12	1.79	0.64
5:P:522:PHE:HB3	5:P:539:TYR:CD2	2.33	0.64
11:Y:342:LEU:HA	11:Y:345:LYS:HD2	1.79	0.64
11:Y:23:SER:HB2	11:Y:49:HIS:HD2	1.62	0.64
11:Y:444:ALA:O	11:Y:448:LYS:HG3	1.98	0.64
5:P:693:ASN:OD1	5:P:709:ARG:NH1	2.31	0.64
1:A:443:CYS:HB3	1:A:452:LEU:HD21	1.80	0.64
10:V:536:CYS:SG	10:V:542:THR:OG1	2.55	0.64
1:A:1191:LEU:HD11	1:A:1196:TYR:HE2	1.62	0.64
5:P:684:LYS:HG3	5:P:687:LYS:HB2	1.80	0.64
13:N:407:LEU:HB2	13:N:417:LEU:HD13	1.78	0.64
4:H:72:HIS:O	4:H:76:VAL:HG23	1.98	0.64
11:Y:277:TYR:HD2	11:Y:293:LEU:HD22	1.62	0.64
1:A:1058:SER:HB2	1:A:1061:GLU:HB3	1.79	0.63
1:A:1574:LEU:O	1:A:1617:ARG:NH2	2.31	0.63
9:O:415:SER:HB2	9:O:451:LEU:HD12	1.80	0.63
6:Q:524:GLU:HG2	10:U:416:PHE:CZ	2.33	0.63
5:P:728:GLU:HA	11:Z:152:ARG:HH22	1.62	0.63
6:Q:478:ASN:HB3	6:Q:481:THR:HG22	1.80	0.63
11:Y:170:ASP:HA	11:Y:173:LEU:HD23	1.80	0.63
11:Y:226:SER:HA	11:Y:229:LYS:HE3	1.80	0.63
12:I:287:LEU:HD21	12:I:456:PHE:CZ	2.33	0.63
6:K:401:ASP:HB3	6:K:404:VAL:HG12	1.81	0.63
10:U:88:THR:HG23	10:V:44:ARG:HH22	1.63	0.63
11:Y:449:ALA:HB1	11:Y:480:ILE:HG21	1.78	0.63
9:O:57:ARG:HH21	12:I:306:HIS:HE1	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:181:LYS:HE2	11:Z:183:ALA:HB3	1.81	0.63
11:Z:193:ILE:HA	11:Z:199:LEU:HD13	1.80	0.63
6:Q:6:LEU:HG	6:Q:29:VAL:HG22	1.79	0.63
11:Z:350:ARG:NE	11:Z:382:CYS:SG	2.71	0.63
12:I:327:VAL:HG22	12:I:425:MET:HB3	1.79	0.63
10:V:185:VAL:HG13	10:V:212:LEU:HD12	1.80	0.63
2:D:20:LEU:HD21	9:O:252:GLU:HG2	1.79	0.62
1:A:274:VAL:HG22	1:A:408:CYS:HB3	1.79	0.62
13:N:368:THR:HG22	13:N:370:GLN:HG2	1.81	0.62
13:N:612:PRO:HG3	13:N:668:LEU:HG	1.80	0.62
13:N:709:PRO:HD2	13:N:712:THR:HB	1.82	0.62
1:A:1150:ALA:HB1	1:A:1187:LYS:HE2	1.81	0.62
5:J:482:LYS:HD3	5:J:512:LEU:HD11	1.82	0.62
11:Y:260:PHE:HB3	11:Y:277:TYR:CD1	2.35	0.62
5:P:158:ILE:HG22	5:P:160:GLU:H	1.64	0.62
1:A:1711:ASP:OD1	1:A:1716:GLN:NE2	2.33	0.62
11:Y:357:GLU:O	11:Y:361:HIS:ND1	2.31	0.62
11:Z:432:ASP:O	11:Z:436:THR:HG23	1.99	0.62
1:A:869:ARG:NH2	1:A:946:THR:OG1	2.33	0.62
12:I:269:LEU:HD23	12:I:526:LYS:HD3	1.81	0.62
1:A:1381:ARG:NH2	1:A:1418:ASP:OD2	2.33	0.62
13:N:554:MET:SD	13:N:557:CYS:HB2	2.39	0.62
12:I:640:ASP:OD1	12:I:641:ALA:N	2.33	0.61
6:K:523:ILE:HG21	5:P:653:LEU:HD22	1.82	0.61
13:N:692:LEU:HD23	13:N:695:ARG:HH12	1.65	0.61
5:J:543:LEU:HB2	5:J:552:LEU:HD13	1.81	0.61
11:Z:172:ILE:HG23	11:Z:185:VAL:HG11	1.82	0.61
1:A:1770:LEU:HD22	1:A:1794:ASP:OD2	2.00	0.61
1:A:89:TYR:HA	9:O:533:THR:HG23	1.82	0.61
7:L:173:CYS:HB3	7:L:178:PHE:HB3	1.82	0.61
6:K:85:GLU:OE2	6:K:88:GLN:NE2	2.33	0.61
7:L:60:GLN:NE2	7:L:142:LEU:O	2.33	0.61
6:Q:371:MET:HA	6:Q:374:ILE:HD12	1.83	0.61
11:Y:274:MET:HG3	11:Y:297:LEU:HD21	1.82	0.61
6:K:81:TYR:HD2	6:K:139:ILE:HG12	1.64	0.61
9:O:443:GLN:OE1	12:I:513:LEU:HA	2.00	0.61
6:Q:429:LEU:O	6:Q:432:ILE:HG22	2.01	0.61
10:V:471:VAL:HG11	10:V:508:GLU:HG3	1.81	0.61
6:Q:441:VAL:HG21	6:Q:444:TRP:HD1	1.66	0.61
7:L:48:ASP:OD1	7:L:157:LYS:NZ	2.34	0.60
5:P:14:GLN:HG2	5:P:18:HIS:HD2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:163:ASP:HB3	5:P:166:GLN:HB2	1.83	0.60
11:Y:24:SER:HB3	11:Y:49:HIS:HE2	1.66	0.60
13:N:414:MET:HE3	13:N:417:LEU:HB3	1.83	0.60
7:L:154:ARG:O	7:L:155:GLN:NE2	2.34	0.60
11:Z:383:TYR:OH	11:Z:391:GLU:HB3	2.01	0.60
1:A:506:VAL:HG22	1:A:639:VAL:HG22	1.82	0.60
1:A:1267:ARG:NH1	1:A:1315:GLY:O	2.34	0.60
9:O:207:LEU:HB3	10:V:145:GLN:HE22	1.66	0.60
11:Z:261:GLU:O	11:Z:264:GLN:NE2	2.34	0.60
6:K:190:LEU:O	6:K:198:GLN:NE2	2.23	0.60
11:Y:300:ILE:HA	11:Z:60:ARG:HG3	1.83	0.60
1:A:590:PRO:HB3	1:A:595:VAL:HG22	1.83	0.60
1:A:774:LYS:NZ	1:A:809:ASP:OD2	2.34	0.60
1:A:982:ASP:OD1	1:A:983:LEU:N	2.34	0.60
6:Q:177:THR:HG22	6:Q:180:GLU:HB2	1.82	0.60
11:Y:5:ASP:OD1	11:Y:8:ARG:NH2	2.34	0.60
1:A:953:LEU:HD22	1:A:1817:VAL:HG22	1.84	0.60
6:K:523:ILE:HD12	5:P:656:MET:HE3	1.84	0.60
7:L:68:PHE:HE2	7:L:137:ILE:HD12	1.65	0.60
10:U:33:LYS:NZ	10:V:85:ASP:OD2	2.23	0.60
10:V:244:ILE:HG21	10:V:276:ILE:HB	1.81	0.60
6:Q:425:PHE:HB3	6:Q:451:LEU:HG	1.84	0.60
13:N:679:GLU:OE1	13:N:679:GLU:N	2.28	0.60
1:A:434:SER:HB2	1:A:440:LYS:HD3	1.83	0.60
7:L:94:ILE:HG12	7:L:141:VAL:HG12	1.84	0.60
9:O:130:SER:OG	12:I:309:LEU:O	2.20	0.60
5:J:617:LEU:HD23	5:J:648:GLN:HE21	1.67	0.59
10:V:30:ARG:O	10:V:34:LYS:HG3	2.02	0.59
10:V:290:ARG:NH2	10:V:322:ASN:OD1	2.33	0.59
12:I:119:THR:HG1	12:I:212:SER:HG	1.49	0.59
13:N:653:ARG:NH2	13:N:702:GLN:O	2.35	0.59
4:H:102:LEU:HD23	5:P:594:ILE:HG22	1.83	0.59
11:Y:59:TYR:HB2	11:Y:115:LEU:HD21	1.84	0.59
11:Y:162:LEU:HD23	11:Y:188:MET:HG2	1.84	0.59
7:L:37:LYS:HG3	7:L:38:PRO:HD2	1.85	0.59
7:L:96:VAL:HG21	7:L:122:VAL:HG11	1.85	0.59
9:O:694:LEU:HD11	9:O:716:PHE:HD2	1.67	0.59
11:Z:466[A]:ARG:HE	11:Z:481:LEU:HD11	1.66	0.59
14:C:2:LYS:HE3	14:C:4:LYS:HB2	1.83	0.59
1:A:928:GLU:HG3	1:A:970:TRP:HZ2	1.68	0.59
6:Q:325:LYS:O	6:Q:329:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:439:VAL:HG21	6:Q:448:LEU:HD21	1.82	0.59
11:Y:373:LEU:HD11	11:Y:412:LEU:HD22	1.84	0.59
13:N:129:LEU:HD11	13:N:150:ARG:HA	1.84	0.59
1:A:1599:ASN:HD22	1:A:1603:LEU:HD12	1.67	0.59
10:V:255:ILE:HD13	10:V:260:SER:HA	1.84	0.59
11:Y:70:LEU:HD11	11:Y:108:MET:CE	2.32	0.59
14:C:57:MET:SD	14:C:57:MET:N	2.75	0.59
9:O:79:TYR:O	9:O:83:GLU:HG2	2.03	0.59
11:Y:349:LEU:HD13	11:Y:357:GLU:HB2	1.84	0.59
1:A:411:HIS:NE2	1:A:414:THR:OG1	2.33	0.59
1:A:850:SER:OG	1:A:857:MET:SD	2.57	0.59
5:J:30:ARG:HH22	5:P:498:THR:HG21	1.67	0.59
7:L:73:THR:O	7:L:160:THR:HG22	2.03	0.59
10:U:33:LYS:HE2	10:U:64:ALA:HA	1.84	0.59
10:U:35:GLN:HB3	10:U:201:LEU:HD21	1.84	0.59
11:Y:359:ILE:O	11:Y:363:ARG:HG3	2.02	0.59
1:A:504:VAL:HG21	1:A:635:VAL:HG11	1.84	0.59
10:V:216:LYS:HD3	10:V:243:LEU:HD11	1.84	0.59
1:A:1525:MET:SD	1:A:1588:LEU:HD13	2.43	0.59
5:J:662:LEU:HD12	5:J:704:LEU:HD13	1.85	0.59
6:K:200:LEU:HD12	6:K:224:VAL:HG11	1.84	0.59
11:Y:4:ILE:HG21	11:Y:41:GLN:HG2	1.85	0.59
11:Y:218:SER:HA	11:Y:221:ILE:HD12	1.85	0.59
1:A:768:LEU:HD21	1:A:861:PRO:HB2	1.83	0.59
1:A:1221:ASP:HB3	1:A:1224:ILE:HG22	1.83	0.59
5:P:517:GLN:OE1	5:P:520:ARG:NH1	2.36	0.59
5:P:731:GLN:HG2	11:Z:151:GLU:HB2	1.85	0.59
11:Z:259:LYS:HA	11:Z:262:GLN:HE21	1.67	0.59
11:Y:65:LYS:HA	11:Y:68:MET:HG3	1.85	0.58
12:I:125:LEU:HD21	12:I:249:THR:HG21	1.85	0.58
13:N:556:PHE:O	13:N:559:VAL:HG22	2.03	0.58
1:A:87:VAL:HB	9:O:544:VAL:HG12	1.86	0.58
10:V:180:ARG:NH2	10:V:208:GLU:OE2	2.36	0.58
12:I:417:PHE:HA	12:I:448:VAL:HG22	1.84	0.58
9:O:103:GLY:O	9:O:155:TYR:OH	2.22	0.58
13:N:203:LEU:HD12	13:N:209:ARG:HG2	1.86	0.58
1:A:756:PHE:HE2	1:A:830:PHE:HB2	1.68	0.58
11:Z:139:MET:HE2	11:Z:139:MET:HA	1.86	0.58
11:Z:203:SER:O	11:Z:207:LYS:HG2	2.03	0.58
5:P:702:ASN:ND2	5:P:705:CYS:HB2	2.18	0.58
13:N:574:ILE:HG12	13:N:625:LYS:HZ3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:MET:HE2	1:A:1715:TRP:HE1	1.69	0.58
11:Y:23:SER:HB2	11:Y:49:HIS:CD2	2.37	0.58
11:Y:349:LEU:HB2	11:Y:358:ALA:HB2	1.86	0.58
12:I:356:SER:HB3	12:I:397:ILE:HG12	1.86	0.58
13:N:262:THR:O	13:N:266:HIS:ND1	2.36	0.58
1:A:733:SER:OG	9:O:719:ARG:NH1	2.36	0.58
12:I:338:GLU:OE1	12:I:415:LYS:NZ	2.36	0.58
1:A:760:PRO:HB2	1:A:834:PRO:HD3	1.86	0.58
1:A:1753:TYR:O	9:O:639:GLN:NE2	2.30	0.58
6:Q:133:CYS:HB3	6:Q:156:ALA:HB2	1.84	0.58
11:Z:284:GLU:OE1	11:Z:286:ARG:NH2	2.35	0.58
13:N:220:LEU:HA	13:N:227:ASP:HA	1.86	0.58
1:A:1843:GLU:HA	1:A:1846:PRO:HG2	1.86	0.58
11:Y:394:VAL:HA	11:Y:397:ASN:HD21	1.69	0.58
11:Y:441:TYR:HD2	11:Y:444:ALA:H	1.51	0.58
12:I:393:VAL:O	12:I:397:ILE:HG13	2.04	0.58
2:D:48:ASP:N	2:D:48:ASP:OD1	2.37	0.57
5:J:465:LEU:HG	5:J:469:MET:CE	2.33	0.57
10:V:388:TYR:O	10:V:392:ILE:HD12	2.04	0.57
11:Y:476:VAL:O	11:Y:480:ILE:HG13	2.04	0.57
13:N:83:LEU:HA	13:N:87:ILE:HB	1.86	0.57
13:N:162:PHE:O	13:N:255:ARG:NH2	2.36	0.57
1:A:1306:CYS:HB2	1:A:1374:ILE:HG12	1.86	0.57
11:Y:478:HIS:ND1	11:Y:497:GLN:OE1	2.31	0.57
6:Q:161:VAL:HG23	6:Q:188:LEU:HD23	1.86	0.57
6:Q:451:LEU:HB3	6:Q:467:TYR:HD2	1.69	0.57
11:Y:425:GLU:HA	11:Y:428:LYS:HD2	1.85	0.57
5:J:538:ILE:O	5:J:542:THR:HG23	2.05	0.57
7:L:175:THR:HG23	7:L:178:PHE:H	1.68	0.57
13:N:82:ASP:OD1	13:N:86:ASN:ND2	2.38	0.57
5:J:42:PHE:HB2	5:J:71:CYS:SG	2.44	0.57
10:V:127:GLU:OE1	10:V:148:ASN:ND2	2.35	0.57
12:I:11:PHE:O	12:I:712:ARG:NH1	2.37	0.57
1:A:628:ILE:HD11	1:A:836:PHE:CZ	2.39	0.57
5:J:673:CYS:O	5:J:677:VAL:HG23	2.05	0.57
5:P:547:GLN:HA	5:P:579:LEU:HD11	1.86	0.57
11:Y:106:TYR:CE1	11:Y:136:LYS:HD2	2.40	0.57
13:N:232:TRP:HB2	13:N:235:GLN:HE21	1.70	0.57
9:O:147:SER:OG	9:O:150:GLN:OE1	2.23	0.57
1:A:168:ASP:OD1	1:A:168:ASP:N	2.36	0.57
5:J:605:THR:HG23	5:J:606:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:93:SER:HB2	5:P:106:ILE:HD11	1.86	0.57
11:Y:260:PHE:HB3	11:Y:277:TYR:HD1	1.68	0.57
12:I:231:VAL:HG12	12:I:556:LEU:HD13	1.87	0.57
1:A:150:CYS:HA	1:A:163:SER:HA	1.87	0.57
6:Q:231:LEU:HD21	6:Q:260:LYS:HB2	1.86	0.57
9:O:684:ALA:O	9:O:688:GLU:HG3	2.05	0.57
5:P:32:TYR:OH	5:P:64:HIS:NE2	2.36	0.57
12:I:448:VAL:O	12:I:452:LEU:HD22	2.05	0.57
13:N:706:ARG:HB2	13:N:716:ILE:HD11	1.87	0.57
1:A:629:LEU:HD23	1:A:762:ILE:HD11	1.85	0.56
6:K:19:TYR:HB3	6:K:50:THR:HG22	1.85	0.56
1:A:1354:GLU:HB3	7:L:30:VAL:HG13	1.87	0.56
5:J:69:PRO:HB3	5:J:110:PHE:HA	1.87	0.56
9:O:41:LEU:HD13	9:O:132:VAL:HG13	1.86	0.56
5:P:667:GLN:HG3	5:P:698:ILE:HD12	1.87	0.56
6:Q:524:GLU:HG2	10:U:416:PHE:CE2	2.40	0.56
10:U:475:LYS:O	10:U:479:GLN:NE2	2.38	0.56
10:V:345:SER:O	10:V:345:SER:OG	2.22	0.56
11:Y:253:ASN:HB3	11:Y:280:LEU:HD11	1.87	0.56
13:N:267:GLN:O	13:N:271:GLU:HG2	2.05	0.56
1:A:1255:VAL:HG21	1:A:1606:LEU:HD11	1.86	0.56
9:O:643:LEU:HA	9:O:646:MET:HE3	1.86	0.56
13:N:286:LEU:O	13:N:290:HIS:ND1	2.39	0.56
6:K:386:LEU:HD22	6:K:389:ARG:HH21	1.70	0.56
9:O:344:LEU:HD22	9:O:359:VAL:HG21	1.87	0.56
11:Z:41:GLN:O	11:Z:45:LEU:HG	2.06	0.56
13:N:181:LEU:HD23	13:N:268:VAL:HG21	1.86	0.56
5:J:164:PRO:HB2	5:J:471:LYS:HG3	1.87	0.56
9:O:207:LEU:O	10:V:145:GLN:NE2	2.39	0.56
1:A:449:GLN:OE1	1:A:453:ARG:NH2	2.39	0.56
1:A:723:LEU:HB3	1:A:724:LEU:HD12	1.86	0.56
5:J:462:LEU:O	5:J:466:LEU:HG	2.05	0.56
9:O:446:LEU:O	9:O:460:GLN:NE2	2.39	0.56
2:D:54:ILE:HG12	6:Q:510:ARG:HH22	1.70	0.56
4:H:58:VAL:HA	11:Z:323:ARG:HH12	1.70	0.56
1:A:823:ILE:HG22	1:A:824:ASP:H	1.71	0.56
3:G:11:LEU:HD21	6:Q:456:ARG:HH12	1.70	0.56
6:Q:324:SER:O	6:Q:328:THR:HG23	2.06	0.56
11:Y:136:LYS:HG3	11:Y:137:ILE:N	2.20	0.56
12:I:25:PHE:HD2	12:I:71:LEU:HB2	1.70	0.56
1:A:1736:GLU:HG3	1:A:1756:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:35:GLU:OE2	6:Q:63:ARG:NH1	2.35	0.55
11:Z:140:MET:HA	11:Z:143:ASN:HD21	1.71	0.55
13:N:528:LEU:HD11	13:N:641:LEU:HD21	1.87	0.55
14:C:61:LEU:HD22	14:C:65:HIS:HE1	1.71	0.55
5:P:46:THR:O	5:P:50:ARG:HG2	2.06	0.55
10:U:106:LEU:HB2	10:U:118:TYR:HB2	1.88	0.55
10:U:190:ASP:O	10:U:194:GLU:HG3	2.06	0.55
11:Z:49:HIS:O	11:Z:49:HIS:ND1	2.39	0.55
12:I:206:LEU:HD11	12:I:222:GLU:HB2	1.88	0.55
5:J:617:LEU:HG	5:J:644:ILE:HG13	1.87	0.55
7:L:47:ASP:HB3	7:L:49:ASN:OD1	2.05	0.55
5:P:130:ARG:HD2	5:P:133:LYS:HD2	1.87	0.55
10:V:370:LEU:O	10:V:374:GLU:HG2	2.06	0.55
11:Z:399:VAL:HG22	11:Z:409:THR:HG22	1.88	0.55
1:A:1431:PRO:HG2	1:A:1434:ILE:HG13	1.88	0.55
1:A:1914:LEU:HD21	1:A:1935:LEU:HB3	1.89	0.55
1:A:1859:TRP:HE1	1:A:1881:GLN:HG2	1.72	0.55
10:V:528:GLU:HA	10:V:531:THR:HG22	1.89	0.55
6:K:35:GLU:HG3	6:K:40:ILE:HD11	1.89	0.55
6:K:174:HIS:NE2	6:K:211:LYS:HD2	2.21	0.55
6:Q:161:VAL:HG13	6:Q:162:TYR:HD1	1.72	0.55
10:V:267:SER:OG	10:V:299:ASN:OD1	2.23	0.55
14:C:70:GLN:HB2	14:C:72:HIS:HD2	1.71	0.55
5:J:138:TYR:HD1	5:J:151:PRO:HB3	1.72	0.55
5:P:739:VAL:O	5:P:743:ILE:HG13	2.07	0.55
5:J:73:TYR:HE2	5:P:18:HIS:HD1	1.53	0.55
6:K:357:TYR:HB3	6:K:374:ILE:HG13	1.89	0.55
7:L:170:PHE:HB3	5:P:738:LEU:HD21	1.87	0.55
5:P:621:LEU:HD13	5:P:644:ILE:HG21	1.89	0.55
5:P:736:GLU:OE1	5:P:736:GLU:N	2.39	0.55
10:V:96:VAL:HG23	10:V:98:GLU:HG3	1.89	0.55
10:V:381:THR:HG21	10:V:412:LEU:HD11	1.87	0.55
11:Z:201:TRP:O	11:Z:205:TRP:HB2	2.07	0.55
12:I:557:TYR:HA	12:I:694:ASP:HB2	1.88	0.55
13:N:104:GLU:OE2	13:N:175:ARG:NH2	2.40	0.55
1:A:249:LEU:HG	1:A:256:VAL:HG22	1.89	0.55
10:U:490:TYR:O	10:U:494:ILE:HG12	2.06	0.55
10:V:34:LYS:NZ	10:V:69:GLU:O	2.29	0.55
11:Y:46:LEU:HD22	11:Y:69:ALA:HB2	1.89	0.55
11:Y:257:VAL:HA	11:Y:260:PHE:HD2	1.72	0.55
9:O:97:ILE:HD11	9:O:158:LEU:HD11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:87:GLU:O	5:P:91:ILE:HG22	2.07	0.54
5:P:605:THR:HG21	5:P:636:ASN:HB3	1.89	0.54
11:Y:359:ILE:HG22	11:Y:363:ARG:HE	1.72	0.54
11:Z:36:LEU:HG	11:Z:37:PHE:CD1	2.42	0.54
1:A:618:VAL:HG21	1:A:656:GLU:HG2	1.90	0.54
12:I:664:ARG:NH1	12:I:719:ALA:O	2.39	0.54
7:L:12:ASP:HB3	7:L:15:GLN:HG2	1.87	0.54
5:P:92:LEU:HD11	5:P:117:THR:HB	1.90	0.54
5:P:93:SER:O	5:P:93:SER:OG	2.24	0.54
13:N:83:LEU:HB3	13:N:160:VAL:HG11	1.90	0.54
13:N:412:PRO:HB2	13:N:486:ASP:HB2	1.88	0.54
5:J:135:SER:HB2	5:J:161:LYS:HE3	1.89	0.54
11:Z:429:THR:O	11:Z:433:LYS:HD2	2.07	0.54
12:I:426:LEU:HB3	12:I:433:VAL:HG22	1.89	0.54
1:A:480:ALA:HB1	1:A:590:PRO:HG3	1.90	0.54
1:A:482:VAL:HG23	1:A:593:ASN:HA	1.88	0.54
5:P:710:ALA:HB1	5:P:726:LEU:HD11	1.90	0.54
6:Q:320:ARG:NH1	6:Q:343:SER:OG	2.41	0.54
10:U:358:LEU:HD22	10:U:371:MET:HE1	1.89	0.54
1:A:1825:SER:OG	1:A:1829:ARG:NH2	2.35	0.54
11:Y:50:ALA:HA	11:Y:65:LYS:HE3	1.90	0.54
11:Y:411:THR:O	11:Y:415:THR:HG23	2.07	0.54
12:I:211:SER:OG	12:I:213:ASP:OD1	2.25	0.54
13:N:594:VAL:HB	14:C:11:VAL:HG22	1.89	0.54
11:Y:19:VAL:HG23	11:Y:52:SER:HB3	1.88	0.54
12:I:21:GLN:HG2	12:I:41:ALA:HB2	1.89	0.54
7:L:18:ARG:NH2	5:P:580:GLN:OE1	2.41	0.54
11:Y:137:ILE:HA	11:Y:140:MET:SD	2.47	0.54
1:A:1564:LEU:HD23	1:A:1567:LEU:HD13	1.90	0.54
5:J:626:ASN:O	5:J:630:VAL:HG22	2.08	0.54
9:O:226:ASP:OD1	9:O:228:THR:OG1	2.25	0.54
10:V:215:ASP:OD1	10:V:215:ASP:N	2.39	0.54
11:Y:25:LEU:O	11:Y:29:MET:HG2	2.08	0.54
13:N:180:PHE:HB2	13:N:240:PHE:CE2	2.43	0.54
1:A:592:HIS:CG	1:A:592:HIS:O	2.60	0.53
1:A:1803:ARG:HH12	1:A:1859:TRP:HD1	1.56	0.53
5:J:628:ILE:HD13	5:J:638:TRP:CZ3	2.42	0.53
5:P:482:LYS:HE2	5:P:667:GLN:HE22	1.71	0.53
6:K:473:VAL:HG23	5:P:130:ARG:HH12	1.73	0.53
9:O:216:LEU:HD22	9:O:256:LEU:HD22	1.89	0.53
5:P:93:SER:HB3	5:P:121:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:179:GLN:NE2	6:Q:183:GLU:OE2	2.41	0.53
10:U:106:LEU:HD11	10:U:117:LEU:HD23	1.91	0.53
12:I:117:GLU:O	12:I:579:LYS:NZ	2.37	0.53
1:A:880:TYR:HB2	1:A:930:LEU:HD22	1.90	0.53
2:D:45:ALA:HA	10:U:378:MET:CE	2.38	0.53
3:G:4:ARG:N	6:Q:373:TYR:OH	2.34	0.53
9:O:82:ILE:O	9:O:86:CYS:N	2.34	0.53
5:P:529:GLU:HG2	5:P:532:ARG:HB2	1.89	0.53
11:Y:252:ASP:OD1	11:Y:252:ASP:N	2.38	0.53
11:Y:362:PHE:HB2	11:Y:379:LEU:HD13	1.88	0.53
12:I:734:LEU:HD12	12:I:741:VAL:HG12	1.90	0.53
5:J:522:PHE:HA	5:J:525:VAL:HG12	1.90	0.53
6:K:165:GLU:HG2	6:Q:20:GLN:HB3	1.90	0.53
11:Z:255:ASN:O	11:Z:258:LEU:HG	2.09	0.53
11:Z:411:THR:O	11:Z:415:THR:OG1	2.25	0.53
14:C:57:MET:HA	14:C:60:ILE:HG12	1.90	0.53
6:K:88:GLN:N	6:K:88:GLN:OE1	2.42	0.53
11:Y:118:ASP:OD1	11:Y:118:ASP:N	2.40	0.53
11:Y:274:MET:HB3	11:Y:297:LEU:HD11	1.91	0.53
12:I:244:PHE:HB3	12:I:247:GLU:HB2	1.89	0.53
13:N:375:LEU:HD21	13:N:416:ILE:HG13	1.89	0.53
1:A:614:THR:O	9:O:556:GLN:NE2	2.42	0.53
13:N:592:TYR:N	14:C:8:TRP:O	2.37	0.53
1:A:151:ILE:O	1:A:161:MET:HA	2.08	0.53
7:L:78:CYS:SG	7:L:157:LYS:HB2	2.48	0.53
11:Z:156:THR:O	11:Z:160:GLU:HG3	2.09	0.53
12:I:692:ARG:NH1	12:I:695:GLU:OE1	2.42	0.53
7:L:12:ASP:OD2	7:L:14:LYS:HE3	2.09	0.53
13:N:698:VAL:O	13:N:701:GLN:NE2	2.37	0.53
1:A:1103:PRO:HD2	1:A:1143:ALA:HB2	1.90	0.53
5:J:651:PHE:HE1	5:J:705:CYS:HB3	1.73	0.53
9:O:106:LYS:O	10:U:344:ARG:NH2	2.37	0.53
10:V:266:VAL:HG11	10:V:288:GLU:OE2	2.08	0.53
13:N:374:LEU:HD22	13:N:416:ILE:HD11	1.90	0.53
5:P:694:LYS:O	5:P:697:VAL:HG12	2.08	0.53
11:Z:376:TYR:O	11:Z:380:ILE:HG12	2.08	0.53
6:K:227:LEU:HG	6:Q:32:LEU:HD13	1.91	0.52
6:Q:35:GLU:HG3	6:Q:40:ILE:HD11	1.91	0.52
10:U:385:ILE:O	10:U:389:ARG:HG3	2.10	0.52
11:Y:393:MET:O	11:Y:397:ASN:ND2	2.42	0.52
11:Z:227:LEU:HA	11:Z:230:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:MET:SD	1:A:1084:ARG:HG3	2.49	0.52
8:M:31:ILE:HD13	6:Q:302:TRP:HZ3	1.74	0.52
11:Y:7:VAL:HG12	11:Y:48:TYR:HD2	1.74	0.52
6:K:351:ASP:OD1	10:V:557:ARG:NH2	2.38	0.52
8:M:63:GLN:HA	8:M:67:GLU:HA	1.91	0.52
10:V:493:TYR:O	10:V:497:ILE:HG23	2.08	0.52
13:N:574:ILE:HD13	13:N:622:TYR:HE1	1.74	0.52
1:A:484:LYS:HB2	1:A:592:HIS:HD1	1.74	0.52
1:A:807:TYR:OH	1:A:1885:LEU:HD23	2.08	0.52
5:J:600:TYR:HD2	5:J:603:ALA:HB2	1.74	0.52
7:L:22:VAL:HB	7:L:159:TYR:HB3	1.90	0.52
9:O:727:THR:HG22	9:O:731:ASN:HD21	1.73	0.52
11:Z:59:TYR:O	11:Z:63:VAL:HG23	2.10	0.52
11:Z:131:ARG:HG3	11:Z:132:GLN:OE1	2.09	0.52
1:A:1095:VAL:HG23	1:A:1098:GLU:HB2	1.90	0.52
13:N:650:LEU:HD22	13:N:704:VAL:HG12	1.91	0.52
5:P:126:CYS:SG	5:P:158:ILE:HD11	2.49	0.52
10:V:34:LYS:NZ	10:V:69:GLU:OE2	2.40	0.52
11:Y:406:ASN:OD1	11:Y:408:GLN:HG2	2.10	0.52
5:P:726:LEU:HD21	5:P:742:LEU:HD23	1.90	0.52
10:V:464:ASP:OD1	10:V:464:ASP:N	2.36	0.52
11:Z:394:VAL:HA	11:Z:397:ASN:HD21	1.75	0.52
5:J:79:CYS:SG	5:J:87:GLU:HB2	2.49	0.52
11:Z:3:VAL:O	11:Z:7:VAL:HG23	2.10	0.52
12:I:254:LYS:O	12:I:258:ILE:HG12	2.08	0.52
9:O:467:ALA:HB1	9:O:506:LEU:HD11	1.91	0.52
11:Y:275:ASP:HB2	11:Y:306:GLU:OE1	2.09	0.52
1:A:1208:LEU:O	1:A:1212:VAL:HG12	2.10	0.52
5:P:92:LEU:HD22	5:P:120:LEU:HD23	1.92	0.52
6:Q:229:GLU:OE2	6:Q:229:GLU:N	2.35	0.52
11:Y:406:ASN:O	11:Y:410:LEU:HG	2.10	0.52
11:Z:217:ASN:O	11:Z:221:ILE:HG23	2.10	0.52
11:Z:275:ASP:HB2	11:Z:306:GLU:HG3	1.92	0.52
11:Z:400:TYR:HA	11:Z:409:THR:HB	1.90	0.52
11:Z:441:TYR:CE2	11:Z:443:LYS:HB3	2.45	0.52
12:I:303:GLU:HB3	12:I:317:LEU:HD12	1.92	0.52
10:V:333:THR:O	10:V:337:ILE:HG12	2.10	0.51
1:A:133:ILE:HG22	1:A:146:GLU:HA	1.91	0.51
1:A:1160:TYR:OH	1:A:1190:THR:OG1	2.27	0.51
5:J:465:LEU:HD21	5:J:495:HIS:CE1	2.44	0.51
5:J:549:ASP:OD1	5:J:549:ASP:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:284:LEU:HD22	6:K:308:TYR:HB2	1.93	0.51
11:Y:363:ARG:HA	11:Y:366:ILE:HD12	1.93	0.51
11:Z:38:SER:O	11:Z:42:LYS:HG3	2.10	0.51
13:N:523:LEU:O	13:N:526:ARG:HG2	2.10	0.51
1:A:632:GLU:HG2	1:A:633:ILE:N	2.25	0.51
1:A:1023:VAL:O	1:A:1027:ILE:HG13	2.11	0.51
7:L:83:TYR:CD2	7:L:115:GLU:HG3	2.42	0.51
5:P:472:GLY:HA3	5:P:488:LEU:HD13	1.91	0.51
6:Q:341:GLY:HA3	6:Q:357:TYR:CE1	2.44	0.51
6:Q:441:VAL:HG21	6:Q:444:TRP:CD1	2.44	0.51
11:Z:109:ALA:O	11:Z:113:THR:HG23	2.11	0.51
1:A:1815:LYS:O	1:A:1819:GLU:HG3	2.10	0.51
10:V:192:PHE:O	10:V:196:THR:HG23	2.11	0.51
11:Z:458:TYR:HD1	11:Z:484:PHE:HD1	1.58	0.51
13:N:647:ASP:N	14:C:4:LYS:O	2.42	0.51
10:U:373:HIS:ND1	10:U:388:TYR:OH	2.38	0.51
10:V:123:TYR:HD2	10:V:124:LEU:HD22	1.75	0.51
11:Z:227:LEU:HB3	11:Z:233:LEU:HD23	1.91	0.51
13:N:221:CYS:N	13:N:226:SER:O	2.33	0.51
13:N:351:PHE:HB2	13:N:406:ALA:HB2	1.91	0.51
1:A:252:ASP:HB2	1:A:253:PRO:HD3	1.92	0.51
1:A:1871:TYR:CZ	1:A:1889:LEU:HD21	2.45	0.51
7:L:19:THR:HG23	7:L:21:THR:HG22	1.92	0.51
6:Q:213:ASN:OD1	6:Q:214:LYS:N	2.44	0.51
11:Y:157:SER:O	11:Y:161:VAL:HG23	2.11	0.51
11:Y:159:LYS:O	11:Y:163:ARG:HG3	2.10	0.51
11:Y:340:GLN:HE21	11:Y:372:ARG:HH12	1.59	0.51
11:Z:373:LEU:O	11:Z:377:GLU:HG3	2.11	0.51
11:Z:458:TYR:O	11:Z:462:ILE:HG12	2.10	0.51
13:N:539:ILE:HA	13:N:542:VAL:HG22	1.92	0.51
1:A:151:ILE:HG22	1:A:162:HIS:O	2.10	0.51
9:O:625:LEU:HD22	9:O:666:LEU:HD23	1.92	0.51
6:Q:413:PHE:CD2	6:Q:454:VAL:HG12	2.45	0.51
10:U:506:HIS:HB2	10:U:509:GLU:HB2	1.93	0.51
12:I:597:LYS:HE3	12:I:617:ALA:HB1	1.92	0.51
1:A:1128:PRO:HG2	1:A:1131:MET:HB2	1.92	0.51
1:A:1197:LEU:HD12	1:A:1227:LEU:HD11	1.92	0.51
10:U:318:TYR:HA	10:U:321:HIS:CD2	2.46	0.51
13:N:297:VAL:HG21	13:N:325:ARG:HB2	1.92	0.51
6:K:135:LEU:O	6:K:139:ILE:HG13	2.10	0.51
5:J:480:ASN:O	5:J:480:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:13:TYR:OH	6:Q:160:ASP:OD2	2.22	0.51
13:N:442:LEU:HD11	13:N:502:ILE:HD11	1.94	0.51
13:N:575:ARG:O	13:N:579:GLU:HG3	2.11	0.51
1:A:591:VAL:HG22	1:A:606:ARG:HH22	1.76	0.50
5:J:465:LEU:HG	5:J:469:MET:HE3	1.94	0.50
9:O:562:LYS:O	9:O:566:LYS:HG3	2.11	0.50
6:Q:25:TRP:O	6:Q:29:VAL:HG23	2.11	0.50
10:U:388:TYR:HB3	10:U:405:LEU:HG	1.93	0.50
12:I:406:VAL:HG21	12:I:478:TYR:HE2	1.76	0.50
1:A:89:TYR:HB3	9:O:536:THR:HG23	1.93	0.50
5:J:610:GLU:O	5:J:614:THR:HG22	2.11	0.50
10:V:288:GLU:OE2	10:V:289:LEU:N	2.44	0.50
11:Y:133:ARG:HB3	11:Y:137:ILE:HD11	1.91	0.50
12:I:290:PHE:CZ	12:I:320:LEU:HD13	2.46	0.50
12:I:717:MET:HG3	12:I:719:ALA:HB2	1.91	0.50
13:N:638:LYS:HZ2	14:C:13:THR:HG23	1.76	0.50
1:A:1747:LEU:HD11	1:A:1784:PRO:HB3	1.93	0.50
5:P:742:LEU:O	5:P:746:VAL:HG23	2.12	0.50
6:Q:476:PRO:HG2	10:U:182:LEU:HD22	1.93	0.50
11:Z:199:LEU:HB3	11:Z:202:LEU:HB3	1.93	0.50
11:Z:362:PHE:HB2	11:Z:379:LEU:HD13	1.93	0.50
11:Z:478:HIS:ND1	11:Z:497:GLN:OE1	2.43	0.50
1:A:1595:HIS:CE1	1:A:1598:ASP:HB2	2.46	0.50
6:K:465:LEU:HG	6:K:488:ILE:HD13	1.94	0.50
7:L:88:SER:O	7:L:88:SER:OG	2.28	0.50
9:O:439:LEU:HD11	12:I:512:LEU:HD13	1.93	0.50
11:Y:160:GLU:HG3	11:Y:163:ARG:NH2	2.26	0.50
1:A:862:TYR:CZ	1:A:864:PRO:HA	2.47	0.50
1:A:1014:ASP:HB3	1:A:1044:ALA:HB3	1.94	0.50
1:A:1086:MET:HG3	1:A:1610:TYR:CZ	2.47	0.50
6:K:338:ILE:HD11	6:K:370:PRO:HG3	1.93	0.50
11:Y:390:ARG:O	11:Y:394:VAL:HG13	2.11	0.50
1:A:1119:ASP:OD1	1:A:1120:LEU:N	2.45	0.50
6:K:146:ARG:O	6:K:150:THR:HG23	2.11	0.50
5:P:616:GLU:HG2	5:P:619:LYS:HD3	1.94	0.50
1:A:253:PRO:HB2	1:A:255:ILE:HG23	1.94	0.50
9:O:109:GLU:HB2	10:U:344:ARG:NH2	2.25	0.50
10:U:451:GLU:HA	10:U:454:LYS:HE3	1.94	0.50
10:V:133:GLU:N	10:V:133:GLU:OE1	2.45	0.50
11:Z:15:LEU:HD23	11:Z:15:LEU:H	1.76	0.50
11:Z:355:VAL:O	11:Z:359:ILE:HG13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:365:LEU:HD11	13:N:374:LEU:HD13	1.93	0.50
1:A:1872:LEU:HD23	1:A:1900:LEU:HD11	1.94	0.50
9:O:91:ASN:O	9:O:95:ILE:HG23	2.12	0.50
9:O:653:ALA:HB2	12:I:368:GLY:HA3	1.93	0.50
10:U:93:TYR:OH	10:V:57:GLU:OE2	2.27	0.50
10:V:449:LEU:HD12	10:V:476:LEU:HD11	1.93	0.50
10:V:468:MET:O	10:V:472:LYS:HG3	2.12	0.50
11:Z:43:TYR:OH	11:Z:99:PRO:O	2.25	0.50
11:Z:242:SER:O	11:Z:246:LEU:HG	2.12	0.50
1:A:1277:ILE:HG22	1:A:1363:THR:HG23	1.94	0.50
5:J:104:ASP:OD1	5:J:105:ASP:N	2.45	0.50
6:K:264:HIS:CE1	6:K:266:SER:HB3	2.47	0.50
5:P:463:MET:O	5:P:467:ARG:HG3	2.12	0.50
10:U:185:VAL:HG13	10:U:212:LEU:HD22	1.93	0.50
10:U:410:GLU:HB2	10:U:418:CYS:SG	2.52	0.50
12:I:406:VAL:HG12	12:I:475:VAL:HG22	1.94	0.50
1:A:77:ARG:HE	1:A:91:GLU:CD	2.15	0.49
5:J:49:TYR:OH	5:J:81:ASP:OD2	2.24	0.49
6:K:232:ASP:OD2	6:Q:28:LYS:NZ	2.45	0.49
7:L:78:CYS:HG	7:L:159:TYR:HE2	1.59	0.49
7:L:82:ASP:HA	7:L:117:SER:HA	1.93	0.49
11:Z:16:HIS:HA	11:Z:19:VAL:HG12	1.94	0.49
11:Z:312:GLY:HA3	11:Z:344:LEU:HD21	1.92	0.49
1:A:1619:LEU:HD21	1:A:1697:LEU:HD22	1.95	0.49
6:K:160:ASP:OD2	6:Q:13:TYR:OH	2.24	0.49
7:L:47:ASP:C	7:L:49:ASN:H	2.16	0.49
10:U:520:TYR:HB3	10:U:529:ALA:HB2	1.94	0.49
11:Y:289:ASP:OD1	11:Y:289:ASP:N	2.39	0.49
11:Z:362:PHE:O	11:Z:366:ILE:HG23	2.12	0.49
11:Z:372:ARG:HH21	11:Z:374:ASP:HB2	1.77	0.49
12:I:391:THR:HB	12:I:515:PRO:HD3	1.94	0.49
5:J:97:PHE:CD2	11:Y:252:ASP:HB3	2.47	0.49
5:J:459:ALA:O	5:J:463:MET:HG3	2.12	0.49
6:Q:88:GLN:O	6:Q:92:VAL:HG23	2.12	0.49
11:Z:147:LYS:HE2	11:Z:336:SER:HB3	1.94	0.49
12:I:328:LYS:NZ	14:C:21:GLU:OE1	2.43	0.49
12:I:601:LEU:HB2	12:I:615:LEU:HD13	1.94	0.49
1:A:1864:GLY:O	1:A:1868:VAL:HG12	2.11	0.49
1:A:1865:ASP:HB3	1:A:1934:LEU:HD21	1.93	0.49
6:Q:155:GLU:OE1	6:Q:159:LEU:HG	2.13	0.49
11:Y:274:MET:HA	11:Y:277:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:431:LEU:HD13	11:Y:451:LEU:HD21	1.94	0.49
13:N:538:GLU:HA	13:N:541:ASN:HD21	1.77	0.49
9:O:477:HIS:NE2	12:I:510:SER:OG	2.38	0.49
11:Z:257:VAL:HG13	11:Z:277:TYR:HE1	1.78	0.49
13:N:612:PRO:HG2	13:N:615:ILE:HG12	1.94	0.49
6:K:66:ASP:HA	6:K:72:CYS:HB3	1.93	0.49
6:K:519:LEU:O	6:K:523:ILE:HG12	2.12	0.49
11:Z:352:MET:SD	11:Z:354:ARG:NH2	2.86	0.49
12:I:286:ARG:O	12:I:324:GLN:NE2	2.46	0.49
1:A:161:MET:SD	1:A:216:PRO:HG3	2.53	0.49
1:A:1910:SER:HB2	13:N:21:LEU:HD11	1.94	0.49
5:J:525:VAL:HA	5:J:528:ILE:HG22	1.95	0.49
9:O:568:LEU:HB2	9:O:583:VAL:HG11	1.93	0.49
9:O:596:SER:O	9:O:596:SER:OG	2.29	0.49
6:Q:324:SER:HB3	6:Q:340:TYR:OH	2.12	0.49
10:U:358:LEU:CD2	10:U:371:MET:HE1	2.42	0.49
1:A:637:MET:HG3	1:A:667:MET:HE1	1.95	0.49
2:D:45:ALA:HA	10:U:378:MET:HE3	1.94	0.49
4:H:74:GLN:NE2	11:Y:291:GLU:OE1	2.46	0.49
5:J:139:GLN:NE2	5:J:161:LYS:HB3	2.27	0.49
5:J:651:PHE:CE1	5:J:705:CYS:HB3	2.47	0.49
9:O:329:ARG:O	9:O:333:GLU:HG2	2.13	0.49
6:Q:451:LEU:HB3	6:Q:467:TYR:CD2	2.47	0.49
11:Y:431:LEU:HD21	11:Y:448:LYS:HG2	1.95	0.49
1:A:1653:ALA:O	1:A:1655:THR:N	2.39	0.49
7:L:36:CYS:HA	7:L:56:SER:HA	1.93	0.49
9:O:38:LEU:HD11	9:O:139:MET:HB3	1.94	0.49
9:O:78:LEU:O	9:O:82:ILE:HG12	2.12	0.49
11:Z:7:VAL:HG22	11:Z:22:LEU:HD21	1.95	0.49
11:Z:139:MET:O	11:Z:143:ASN:ND2	2.46	0.49
11:Z:224:ILE:HD11	11:Z:239:LEU:HD21	1.95	0.49
12:I:421:LEU:O	12:I:425:MET:HG2	2.12	0.49
1:A:728:LEU:HA	9:O:673:ALA:HB2	1.94	0.49
1:A:850:SER:HA	1:A:853:LYS:HE2	1.95	0.49
1:A:884:ASP:OD1	1:A:884:ASP:N	2.45	0.49
10:V:26:PHE:HE1	10:V:228:TRP:HE3	1.59	0.49
11:Z:399:VAL:HG23	11:Z:403:LEU:HD13	1.94	0.49
12:I:12:ARG:HH21	12:I:748:ILE:HD12	1.76	0.49
12:I:194:LYS:HD2	12:I:541:ALA:HB1	1.94	0.49
4:H:79:MET:SD	5:P:580:GLN:NE2	2.86	0.48
9:O:126:VAL:HG23	12:I:310:TRP:HE3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:15:LEU:HB3	11:Y:18:ASN:HB2	1.95	0.48
11:Z:306:GLU:HA	11:Z:309:VAL:HG22	1.94	0.48
11:Z:431:LEU:HD11	11:Z:447:LYS:HG3	1.95	0.48
1:A:942:ARG:NH1	9:O:603:MET:SD	2.86	0.48
3:G:18:GLU:OE1	6:Q:457:LYS:NZ	2.39	0.48
9:O:378:SER:HB3	9:O:409:HIS:CE1	2.48	0.48
5:P:102:SER:N	5:P:105:ASP:OD2	2.46	0.48
11:Y:10:MET:HB3	11:Y:19:VAL:HG12	1.95	0.48
12:I:145:LEU:HD23	12:I:351:HIS:CD2	2.48	0.48
13:N:31:LEU:O	13:N:128:SER:OG	2.21	0.48
1:A:250:ASN:ND2	1:A:432:ILE:HD12	2.29	0.48
2:D:17:TRP:O	9:O:277:TYR:OH	2.21	0.48
11:Y:498:TYR:HB3	11:Y:515:MET:SD	2.52	0.48
11:Z:43:TYR:HB2	11:Z:72:GLN:HG2	1.94	0.48
11:Z:296:ARG:O	11:Z:300:ILE:HG12	2.13	0.48
1:A:1766:GLU:HG3	1:A:1798:ARG:HH22	1.79	0.48
5:J:7:PRO:HG2	5:P:459:ALA:HB2	1.95	0.48
7:L:74:VAL:HG11	7:L:137:ILE:HD11	1.94	0.48
7:L:93:LYS:HB3	7:L:142:LEU:HB2	1.96	0.48
9:O:57:ARG:HE	12:I:306:HIS:CE1	2.31	0.48
11:Y:106:TYR:CD2	11:Y:136:LYS:HE3	2.48	0.48
1:A:1713:MET:HB2	1:A:1715:TRP:CD1	2.48	0.48
1:A:1726:ARG:HA	1:A:1729:GLU:OE2	2.14	0.48
9:O:706:CYS:O	9:O:710:ILE:HG13	2.13	0.48
5:P:55:TYR:HA	5:P:82:LEU:HD21	1.95	0.48
10:V:203:TRP:CD1	10:V:207:LEU:HD12	2.49	0.48
11:Y:301:SER:HB2	11:Y:304:HIS:ND1	2.29	0.48
11:Y:394:VAL:HA	11:Y:397:ASN:ND2	2.29	0.48
12:I:20:PRO:HA	12:I:739:ARG:HH21	1.78	0.48
13:N:640:THR:HA	13:N:662:VAL:HG23	1.95	0.48
1:A:17:LEU:HD11	1:A:511:ILE:HG23	1.95	0.48
1:A:1110:ARG:HD2	1:A:1110:ARG:N	2.28	0.48
6:Q:24:PHE:CE1	6:Q:28:LYS:HE2	2.49	0.48
6:Q:401:ASP:O	6:Q:405:MET:HB3	2.13	0.48
11:Y:349:LEU:HD23	11:Y:352:MET:HE1	1.95	0.48
11:Z:20:ARG:HB2	11:Z:52:SER:HB2	1.95	0.48
12:I:587:LEU:HD22	12:I:600:ILE:HG22	1.96	0.48
3:G:3:ARG:HG3	3:G:3:ARG:HH11	1.79	0.48
11:Y:232:LEU:HD21	11:Z:33:ASN:HB3	1.96	0.48
11:Y:355:VAL:O	11:Y:359:ILE:HG13	2.13	0.48
1:A:819:GLN:NE2	1:A:820:VAL:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:73:THR:HG23	7:L:133:ARG:HG2	1.95	0.48
9:O:73:ILE:O	9:O:161:TYR:OH	2.22	0.48
10:V:123:TYR:CD2	10:V:124:LEU:HD22	2.49	0.48
11:Z:252:ASP:OD1	11:Z:252:ASP:N	2.39	0.48
1:A:100:VAL:HG21	1:A:153:ILE:HG12	1.95	0.48
5:J:87:GLU:O	5:J:91:ILE:HD12	2.12	0.48
5:J:142:LEU:HD21	5:J:151:PRO:HB2	1.96	0.48
5:P:522:PHE:HB3	5:P:539:TYR:CE2	2.49	0.48
11:Y:240:LEU:HG	11:Y:263:ALA:HB2	1.95	0.48
12:I:634:SER:OG	12:I:635:ILE:N	2.47	0.48
1:A:1109:GLY:O	1:A:1110:ARG:HD2	2.13	0.47
1:A:1267:ARG:NE	1:A:1271:GLU:OE2	2.43	0.47
5:J:485:ILE:HD13	5:J:509:TYR:CE1	2.49	0.47
6:K:401:ASP:OD2	3:W:3:ARG:NH1	2.47	0.47
9:O:337:HIS:O	9:O:341:GLN:HG2	2.13	0.47
9:O:416:GLU:HG2	9:O:417:LEU:N	2.29	0.47
9:O:644:LEU:HD22	9:O:648:ILE:HD11	1.96	0.47
9:O:644:LEU:HD11	9:O:666:LEU:HG	1.96	0.47
5:P:44:LEU:O	5:P:48:TYR:HD1	1.96	0.47
6:Q:185:LEU:HD22	6:Q:209:LEU:HD11	1.94	0.47
11:Y:479:ARG:HH21	11:Y:480:ILE:HG12	1.78	0.47
11:Z:125:LEU:HD13	11:Z:128:ILE:HD12	1.96	0.47
12:I:9:PRO:HG2	12:I:750:ASP:HB3	1.96	0.47
4:H:61:TYR:HD1	11:Z:326:TYR:CG	2.31	0.47
6:K:500:ASP:O	6:K:504:THR:HG23	2.14	0.47
7:L:64:VAL:HB	7:L:139:ILE:HB	1.96	0.47
9:O:348:TYR:CZ	9:O:361:LEU:HD11	2.49	0.47
13:N:169:PHE:O	13:N:172:MET:HG3	2.15	0.47
1:A:852:LEU:HB3	1:A:881:ILE:HD13	1.95	0.47
11:Y:349:LEU:HA	11:Y:352:MET:CE	2.44	0.47
11:Z:38:SER:O	11:Z:41:GLN:HG2	2.15	0.47
11:Z:253:ASN:O	11:Z:257:VAL:HG23	2.15	0.47
11:Z:446:VAL:O	11:Z:450:GLU:HG2	2.14	0.47
12:I:434:LEU:HD12	12:I:435:PRO:HD2	1.97	0.47
1:A:1209:LEU:HD22	1:A:1228:LEU:HD23	1.96	0.47
5:J:476:LEU:HG	5:J:484:ALA:HB1	1.96	0.47
10:U:460:TYR:HE2	10:U:470:LEU:HD21	1.79	0.47
13:N:351:PHE:CE2	13:N:405:LYS:HB3	2.49	0.47
13:N:538:GLU:HA	13:N:541:ASN:ND2	2.30	0.47
13:N:689:VAL:HA	13:N:692:LEU:HG	1.96	0.47
1:A:118:THR:OG1	9:O:266:ASP:OD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:ASP:HB3	1:A:1224:ILE:CG2	2.44	0.47
6:K:62:SER:O	6:K:63:ARG:HG2	2.14	0.47
5:P:14:GLN:HG2	5:P:18:HIS:CD2	2.48	0.47
11:Y:16:HIS:HA	11:Y:19:VAL:HG22	1.96	0.47
11:Z:23:SER:CB	11:Z:49:HIS:HB2	2.43	0.47
5:J:533:VAL:HG23	5:J:559:LEU:HD22	1.96	0.47
6:K:181:GLU:HG3	6:K:209:LEU:HG	1.96	0.47
6:Q:27:ASP:HA	6:Q:43:LEU:HD22	1.96	0.47
6:Q:440:THR:O	6:Q:440:THR:OG1	2.32	0.47
6:Q:495:PHE:HB3	6:Q:522:CYS:SG	2.54	0.47
10:U:26:PHE:CE1	10:U:228:TRP:HB2	2.50	0.47
10:V:180:ARG:HD3	10:V:212:LEU:HD21	1.96	0.47
12:I:125:LEU:HD23	12:I:125:LEU:HA	1.74	0.47
13:N:316:GLU:OE1	13:N:319:ASN:ND2	2.41	0.47
1:A:1520:LEU:HD22	1:A:1542:LEU:HD12	1.96	0.47
1:A:1651:LEU:HD22	6:K:553:LYS:HB2	1.96	0.47
4:H:97:LYS:HG2	4:H:98:PRO:HD2	1.95	0.47
5:J:515:TYR:HB3	5:J:546:LEU:HD11	1.96	0.47
6:K:90:LEU:HD21	6:K:140:TYR:CE1	2.50	0.47
6:K:128:ILE:HG23	6:K:129:LYS:HD2	1.97	0.47
10:U:242:GLN:NE2	10:U:429:ARG:HE	2.10	0.47
10:U:466:GLU:O	10:U:467:LYS:HG3	2.15	0.47
11:Y:59:TYR:CD1	11:Y:114:MET:HG2	2.50	0.47
11:Y:235:ASP:HB3	11:Y:266:LEU:HD21	1.96	0.47
11:Y:373:LEU:O	11:Y:377:GLU:HG2	2.15	0.47
11:Z:36:LEU:HG	11:Z:37:PHE:CE1	2.50	0.47
13:N:393:THR:HA	13:N:396:ILE:HB	1.95	0.47
1:A:263:GLN:HB2	1:A:265:VAL:HG22	1.97	0.47
1:A:1797:ILE:HD13	1:A:1851:THR:HG21	1.97	0.47
10:V:106:LEU:HB3	10:V:118:TYR:HB2	1.97	0.47
11:Y:151:GLU:O	11:Y:155:VAL:HG13	2.15	0.47
14:C:40:PRO:HA	14:C:44:CYS:HB3	1.97	0.47
9:O:44:MET:HG3	9:O:89:LEU:HD21	1.97	0.47
10:V:134:THR:HG23	10:V:143:LYS:HG3	1.97	0.47
12:I:144:THR:HG1	12:I:160:ASN:N	2.13	0.47
1:A:31:HIS:CD2	1:A:32:PRO:HD2	2.50	0.47
1:A:250:ASN:HD22	1:A:432:ILE:HD12	1.79	0.47
1:A:965:GLN:HB2	1:A:1833:HIS:NE2	2.30	0.47
5:J:482:LYS:HD2	5:J:482:LYS:HA	1.69	0.47
7:L:45:LEU:HD11	7:L:156:ILE:HG13	1.96	0.47
5:P:671:LEU:O	5:P:675:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:432:ILE:HD11	6:Q:444:TRP:CD2	2.50	0.47
10:V:58:LEU:O	10:V:61:SER:OG	2.33	0.47
11:Y:29:MET:HE2	11:Z:233:LEU:HD13	1.97	0.47
11:Z:481:LEU:HD22	11:Z:497:GLN:HG3	1.97	0.47
1:A:80:VAL:HG12	1:A:91:GLU:OE2	2.15	0.46
1:A:90:ASP:OD1	1:A:106:SER:HB3	2.14	0.46
1:A:775:LEU:HD11	1:A:844:ILE:HD13	1.97	0.46
5:J:653:LEU:O	5:J:657:HIS:ND1	2.46	0.46
11:Y:274:MET:SD	11:Y:296:ARG:NH2	2.88	0.46
11:Z:5:ASP:OD1	11:Z:8:ARG:NH2	2.47	0.46
12:I:282:GLN:HB2	12:I:337:ILE:HD11	1.96	0.46
12:I:625:TYR:HB2	12:I:628:THR:HG23	1.98	0.46
13:N:189:ARG:HG3	13:N:196:ASP:HB2	1.97	0.46
1:A:778:LEU:HB3	9:O:557:MET:HB3	1.97	0.46
5:J:162:PRO:CB	5:J:474:LEU:HD21	2.44	0.46
7:L:75:LYS:HE3	7:L:161:PRO:HB3	1.97	0.46
6:Q:357:TYR:CE2	6:Q:373:TYR:HB3	2.50	0.46
11:Z:196:VAL:HG12	11:Z:199:LEU:HD11	1.97	0.46
11:Z:397:ASN:OD1	11:Z:401:LYS:NZ	2.45	0.46
12:I:72:ALA:HB2	12:I:113:MET:HG2	1.97	0.46
1:A:27:HIS:HB3	1:A:101:ILE:HD13	1.95	0.46
1:A:872:LEU:HD11	1:A:937:VAL:HG11	1.96	0.46
1:A:1098:GLU:HG3	9:O:367:LYS:HZ2	1.79	0.46
6:K:210:LYS:HB2	6:K:240:ARG:HH22	1.81	0.46
5:P:692:LEU:HD12	5:P:705:CYS:O	2.16	0.46
11:Y:339:VAL:O	11:Y:343:LEU:HG	2.15	0.46
11:Z:43:TYR:HE1	11:Z:99:PRO:HD2	1.80	0.46
11:Z:120:ASP:O	11:Z:124:ILE:HG22	2.16	0.46
11:Z:390:ARG:O	11:Z:394:VAL:HG13	2.16	0.46
11:Z:465:LEU:HD21	11:Z:480:ILE:HB	1.97	0.46
1:A:1621:PRO:HG3	1:A:1653:ALA:HB3	1.98	0.46
1:A:1918:PHE:HB2	1:A:1928:LEU:HD11	1.98	0.46
7:L:177:ASP:OD2	11:Z:119:LYS:NZ	2.37	0.46
9:O:378:SER:HB3	9:O:409:HIS:HE1	1.80	0.46
12:I:663:ASP:OD1	12:I:663:ASP:N	2.36	0.46
13:N:63:ARG:HH12	13:N:140:LEU:HA	1.80	0.46
1:A:707:TRP:CE3	9:O:730:ARG:HD3	2.50	0.46
1:A:1148:ALA:HB3	1:A:1153:ILE:HD13	1.98	0.46
1:A:1288:CYS:SG	1:A:1351:GLN:NE2	2.88	0.46
6:K:61:ARG:NH1	6:K:80:HIS:HE1	2.13	0.46
9:O:583:VAL:O	9:O:587:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:578:SER:OG	5:P:610:GLU:OE1	2.25	0.46
11:Y:29:MET:HE3	11:Z:201:TRP:CD2	2.50	0.46
11:Y:431:LEU:HD11	11:Y:448:LYS:HG2	1.97	0.46
11:Y:465:LEU:HD21	11:Y:480:ILE:HB	1.97	0.46
13:N:638:LYS:HZ3	14:C:11:VAL:HG12	1.81	0.46
1:A:661:VAL:O	1:A:665:MET:HG3	2.15	0.46
1:A:1201:HIS:HB3	1:A:1204:THR:HB	1.98	0.46
5:J:641:LEU:HA	5:J:644:ILE:HG22	1.98	0.46
9:O:621:SER:HB3	9:O:651:ILE:HG13	1.96	0.46
5:P:707:PHE:HE2	5:P:738:LEU:HB3	1.74	0.46
10:V:301:ASP:OD1	10:V:301:ASP:N	2.46	0.46
12:I:33:ASP:HB3	12:I:728:ARG:HD3	1.97	0.46
1:A:1160:TYR:CD1	1:A:1188:LEU:HD13	2.50	0.46
5:J:21:TYR:HE1	5:J:50:ARG:HB3	1.81	0.46
5:J:53:LYS:NZ	5:J:55:TYR:OH	2.49	0.46
5:J:517:GLN:HG2	5:J:520:ARG:HE	1.81	0.46
5:J:590:PHE:O	5:J:594:ILE:HD12	2.16	0.46
6:K:171:THR:O	6:K:171:THR:OG1	2.28	0.46
5:P:496:TYR:CE1	11:Z:71:GLN:HG3	2.51	0.46
5:P:502:LEU:HD23	5:P:502:LEU:HA	1.67	0.46
6:Q:461:TYR:HD2	6:Q:492:MET:HG2	1.80	0.46
10:U:404:GLY:O	10:U:408:THR:HG22	2.16	0.46
11:Y:176:LEU:HD12	11:Y:210:ALA:HA	1.96	0.46
11:Y:306:GLU:H	11:Y:306:GLU:HG2	1.55	0.46
11:Z:249:ARG:NH2	11:Z:371:CYS:O	2.45	0.46
1:A:669:GLY:HA2	1:A:753:THR:HG21	1.98	0.46
1:A:1244:ASP:OD1	1:A:1244:ASP:N	2.38	0.46
5:J:56:LYS:NZ	5:P:531:TYR:O	2.47	0.46
6:K:495:PHE:CZ	6:K:525:MET:HG3	2.51	0.46
9:O:79:TYR:OH	9:O:94:GLN:HA	2.15	0.46
10:V:129:LYS:HA	10:V:129:LYS:HD3	1.68	0.46
10:V:186:LYS:O	10:V:189:ILE:HG22	2.15	0.46
11:Y:257:VAL:O	11:Y:261:GLU:HG3	2.16	0.46
11:Y:330:LYS:O	11:Y:334:LEU:HG	2.15	0.46
11:Z:399:VAL:HA	11:Z:402:THR:HG22	1.97	0.46
13:N:273:MET:SD	13:N:339:LEU:HD22	2.56	0.46
1:A:170:ILE:HG21	10:V:427:GLN:HB2	1.98	0.46
9:O:445:LEU:HD23	9:O:469:ALA:HB2	1.97	0.46
6:Q:6:LEU:HD12	6:Q:6:LEU:O	2.16	0.46
6:Q:30:ALA:HA	6:Q:39:ASP:HB3	1.97	0.46
6:Q:134:LEU:HD21	6:Q:165:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:423:THR:HB	11:Y:426:LYS:HE2	1.98	0.46
12:I:642:GLN:OE1	12:I:723:ALA:HA	2.15	0.46
13:N:366:GLU:HB2	13:N:367:ARG:HH11	1.81	0.46
13:N:649:GLU:HG3	14:C:2:LYS:HE2	1.97	0.46
1:A:1097:THR:HG23	9:O:340:LEU:HD22	1.97	0.46
5:J:524:GLU:O	5:J:527:ARG:HG3	2.16	0.46
5:J:660:LYS:O	5:J:664:ILE:HD12	2.16	0.46
6:K:402:PRO:HG3	6:K:431:LYS:HB3	1.98	0.46
5:P:53:LYS:HG2	5:P:56:LYS:HD2	1.98	0.46
5:P:125:TYR:HE1	5:P:130:ARG:HH21	1.63	0.46
11:Y:15:LEU:HD11	11:Z:135:PRO:HB2	1.98	0.46
11:Y:186:ALA:HB2	11:Y:206:ILE:HG21	1.97	0.46
11:Y:224:ILE:HD11	11:Y:239:LEU:HD11	1.97	0.46
11:Y:240:LEU:HD21	11:Y:262:GLN:HB3	1.97	0.46
11:Z:6:HIS:O	11:Z:10:MET:HG2	2.16	0.46
11:Z:305:ALA:HB1	11:Z:331:ALA:HB1	1.98	0.46
13:N:435:VAL:O	13:N:439:VAL:HG13	2.16	0.46
1:A:224:VAL:HG23	1:A:408:CYS:HB2	1.98	0.45
5:J:139:GLN:HG3	5:J:161:LYS:NZ	2.31	0.45
6:K:301:SER:O	6:K:305:VAL:HG23	2.16	0.45
6:K:406:HIS:HD2	6:K:447:LEU:HD13	1.81	0.45
5:P:53:LYS:HG3	5:P:55:TYR:CE1	2.51	0.45
10:U:304:SER:HB3	10:U:336:VAL:HG22	1.97	0.45
11:Y:401:LYS:HA	11:Y:401:LYS:HD3	1.77	0.45
13:N:542:VAL:O	13:N:546:LYS:HG2	2.15	0.45
4:H:82:LEU:O	4:H:85:LEU:HG	2.15	0.45
5:J:473:TYR:HA	5:J:476:LEU:HD12	1.98	0.45
5:J:517:GLN:O	5:J:521:ILE:HG22	2.17	0.45
7:L:113:LEU:HB3	7:L:116:PRO:HG3	1.97	0.45
8:M:50:VAL:HA	8:M:53:GLN:HG2	1.98	0.45
9:O:492:HIS:HB2	12:I:500:PHE:CZ	2.52	0.45
5:P:49:TYR:OH	5:P:81:ASP:OD2	2.26	0.45
10:U:78:GLU:OE1	10:V:67:LEU:HD11	2.16	0.45
10:V:213:ILE:HD11	10:V:222:LEU:HD12	1.98	0.45
11:Y:106:TYR:CE2	11:Y:136:LYS:HE3	2.50	0.45
11:Z:140:MET:HA	11:Z:143:ASN:ND2	2.31	0.45
1:A:79:GLY:N	1:A:90:ASP:HA	2.32	0.45
1:A:761:ALA:O	1:A:765:VAL:HG22	2.16	0.45
6:Q:194:CYS:SG	6:Q:195:ASN:N	2.89	0.45
11:Z:165:CYS:SG	11:Z:168:ALA:HB2	2.56	0.45
13:N:392:ASN:OD1	13:N:392:ASN:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ARG:NH2	1:A:1894:VAL:O	2.38	0.45
1:A:1054:TYR:HB2	1:A:1057:LEU:HB2	1.98	0.45
7:L:71:LYS:HD2	7:L:135:PHE:CE2	2.51	0.45
11:Z:125:LEU:HB3	11:Z:141:LEU:HD13	1.99	0.45
1:A:765:VAL:HG12	1:A:863:LEU:HD21	1.97	0.45
1:A:1251:VAL:HG23	1:A:1297:ALA:HB2	1.98	0.45
6:K:245:CYS:SG	6:K:402:PRO:HD2	2.56	0.45
6:K:503:HIS:O	5:P:625:ARG:HD3	2.17	0.45
9:O:532:VAL:HG22	9:O:546:ARG:HB3	1.98	0.45
6:Q:29:VAL:HG12	6:Q:39:ASP:OD2	2.15	0.45
10:V:330:ARG:HB2	10:V:333:THR:HG23	1.98	0.45
11:Y:106:TYR:CD1	11:Y:140:MET:HE1	2.52	0.45
11:Z:27:LEU:HD12	11:Z:49:HIS:HD2	1.81	0.45
11:Z:152:ARG:O	11:Z:156:THR:OG1	2.28	0.45
13:N:435:VAL:HG12	13:N:515:PHE:HE1	1.80	0.45
13:N:638:LYS:HE2	13:N:638:LYS:HB2	1.65	0.45
1:A:1666:ILE:HG23	1:A:1678:ILE:HB	1.97	0.45
1:A:1716:GLN:OE1	13:N:369:ASP:HB3	2.16	0.45
1:A:1733:PHE:CD2	1:A:1776:TYR:HB2	2.52	0.45
6:K:194:CYS:N	6:K:197:GLU:OE2	2.47	0.45
7:L:105:LEU:HD21	7:L:136:MET:HG2	1.98	0.45
9:O:55:MET:O	9:O:59:ARG:HG2	2.15	0.45
9:O:266:ASP:O	9:O:270:SER:OG	2.22	0.45
10:V:36:LEU:HB3	10:V:59:ALA:HB2	1.99	0.45
10:V:553:ILE:O	10:V:557:ARG:N	2.47	0.45
11:Y:277:TYR:CD2	11:Y:293:LEU:HD22	2.48	0.45
12:I:178:LEU:HB2	12:I:186:GLU:HB2	1.99	0.45
13:N:305:LEU:HB3	13:N:312:PRO:HG3	1.98	0.45
1:A:352:ARG:HH21	10:V:373:HIS:HD2	1.64	0.45
1:A:1031:ASP:OD1	1:A:1033:ARG:NH2	2.39	0.45
1:A:1091:SER:O	1:A:1091:SER:OG	2.30	0.45
1:A:1097:THR:O	9:O:332:GLN:NE2	2.50	0.45
1:A:1745:PRO:HB2	9:O:609:ALA:HB1	1.99	0.45
3:G:17:GLU:HA	3:G:20:GLU:CD	2.37	0.45
6:K:276:VAL:HG21	3:W:2:LEU:HD11	1.99	0.45
5:P:676:GLY:HA3	5:P:692:LEU:CD2	2.47	0.45
5:P:684:LYS:HZ1	5:P:686:GLU:CD	2.19	0.45
5:P:741:PHE:CE2	5:P:745:LYS:HE3	2.51	0.45
6:Q:477:GLN:OE1	10:U:148:ASN:ND2	2.49	0.45
9:O:504:ALA:HA	9:O:507:TRP:CD1	2.52	0.45
11:Y:202:LEU:HD12	11:Y:202:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:289:PHE:O	13:N:293:ILE:HG12	2.17	0.45
13:N:608:LYS:O	13:N:609:LEU:HD23	2.17	0.45
1:A:1617:ARG:NH1	1:A:1657:LEU:O	2.43	0.45
5:P:102:SER:OG	5:P:103:HIS:N	2.49	0.45
10:U:293:ASP:OD2	10:U:296:ARG:HB2	2.17	0.45
10:U:423:ARG:O	10:U:427:GLN:HG3	2.17	0.45
12:I:238:THR:HB	12:I:241:LEU:HD13	1.98	0.45
12:I:600:ILE:O	12:I:600:ILE:HG13	2.17	0.45
5:J:483:GLU:O	5:J:487:ILE:HG22	2.17	0.45
7:L:82:ASP:N	7:L:82:ASP:OD1	2.50	0.45
9:O:58:ARG:HG3	12:I:302:ASP:OD1	2.17	0.45
9:O:430:ARG:CD	9:O:476:LEU:HD11	2.43	0.45
10:V:186:LYS:HB3	10:V:186:LYS:HE2	1.89	0.45
11:Y:483:ASP:O	11:Y:486:VAL:HG12	2.17	0.45
13:N:120:SER:HA	13:N:123:ASP:OD2	2.17	0.45
5:J:650:LYS:HE2	5:J:653:LEU:HD12	1.99	0.44
9:O:541:ILE:HD13	9:O:541:ILE:HA	1.61	0.44
9:O:624:VAL:HG11	9:O:647:ALA:HB3	1.98	0.44
6:Q:407:GLU:HA	6:Q:410:VAL:HG12	1.98	0.44
6:Q:527:ILE:HD12	6:Q:527:ILE:HA	1.86	0.44
11:Y:209:TYR:O	11:Y:212:VAL:HG12	2.17	0.44
1:A:440:LYS:HB3	1:A:457:PHE:CE1	2.53	0.44
1:A:1078:MET:HE3	1:A:1132:THR:HG22	2.00	0.44
1:A:1830:LEU:C	1:A:1831:GLN:HG2	2.37	0.44
6:K:90:LEU:HD21	6:K:140:TYR:HE1	1.83	0.44
9:O:422:ILE:HG21	9:O:445:LEU:HB2	1.99	0.44
6:Q:298:ASN:OD1	6:Q:299:PRO:HD2	2.17	0.44
11:Y:18:ASN:OD1	11:Z:170:ASP:N	2.45	0.44
11:Y:122:ILE:HG23	11:Y:144:LEU:HD23	1.99	0.44
11:Z:140:MET:SD	11:Z:144:LEU:HD23	2.57	0.44
12:I:177:VAL:HG12	12:I:208:LEU:HD13	1.98	0.44
12:I:321:LEU:HD23	12:I:428:MET:HE1	1.99	0.44
13:N:183:VAL:HG13	13:N:233:CYS:HB3	2.00	0.44
14:C:57:MET:O	14:C:61:LEU:HG	2.17	0.44
1:A:727:SER:O	1:A:728:LEU:HG	2.17	0.44
1:A:790:LEU:HA	1:A:790:LEU:HD23	1.76	0.44
1:A:860:TYR:HE2	1:A:870:SER:HG	1.65	0.44
5:J:552:LEU:HD12	5:J:552:LEU:HA	1.82	0.44
9:O:733:CYS:HA	9:O:736:LEU:HD12	1.99	0.44
5:P:9:GLN:OE1	5:P:9:GLN:N	2.31	0.44
10:U:29:LEU:HB2	10:U:30:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:31:GLU:HA	10:U:34:LYS:HG2	1.99	0.44
12:I:222:GLU:HB2	12:I:231:VAL:HG22	1.99	0.44
1:A:591:VAL:HG22	1:A:606:ARG:NH2	2.33	0.44
2:D:10:PRO:HG2	9:O:346:TRP:CE2	2.52	0.44
7:L:46:ARG:C	7:L:48:ASP:H	2.21	0.44
6:Q:294:LEU:HB3	6:Q:295:TYR:HD1	1.82	0.44
13:N:186:GLN:HG3	13:N:223:GLY:HA3	2.00	0.44
1:A:851:CYS:SG	1:A:882:LEU:HD11	2.58	0.44
1:A:1301:ALA:O	1:A:1305:VAL:HG23	2.18	0.44
1:A:1709:LYS:HE3	1:A:1709:LYS:HB2	1.85	0.44
3:G:11:LEU:HD23	3:G:11:LEU:HA	1.85	0.44
5:J:89:GLU:CD	5:J:130:ARG:HH12	2.21	0.44
5:J:486:ASN:OD1	5:J:490:HIS:NE2	2.50	0.44
6:K:317:GLU:HG2	6:K:318:HIS:N	2.33	0.44
5:P:130:ARG:HG3	5:P:130:ARG:HH11	1.81	0.44
10:U:29:LEU:HD12	10:U:62:LEU:HD21	2.00	0.44
10:V:420:TYR:OH	10:V:424:ARG:NH1	2.50	0.44
12:I:246:PRO:O	12:I:250:ARG:HG3	2.18	0.44
13:N:340:ARG:HB3	13:N:361:LEU:HD22	2.00	0.44
1:A:1584:LEU:HD22	1:A:1588:LEU:HD11	1.99	0.44
5:P:113:SER:O	5:P:117:THR:HG23	2.18	0.44
5:P:469:MET:HE3	5:P:469:MET:HB3	1.89	0.44
12:I:450:GLU:O	12:I:454:GLU:HB2	2.17	0.44
1:A:132:ILE:HG22	1:A:134:SER:H	1.83	0.44
1:A:270:THR:HB	1:A:412:LEU:HD11	1.98	0.44
1:A:597:LEU:HD11	1:A:607:ILE:HD13	1.99	0.44
1:A:966:PRO:HG3	1:A:980:ARG:HH12	1.83	0.44
1:A:1184:HIS:O	1:A:1188:LEU:HG	2.18	0.44
5:P:68:THR:O	5:P:72:LYS:HG3	2.18	0.44
6:Q:263:PHE:HZ	6:Q:290:LYS:HB3	1.83	0.44
12:I:444:ASP:O	12:I:448:VAL:HG23	2.16	0.44
1:A:1222:MET:SD	10:V:514:ARG:NE	2.91	0.44
1:A:1243:LEU:HD23	1:A:1243:LEU:H	1.83	0.44
5:J:164:PRO:CG	5:J:474:LEU:HD22	2.48	0.44
9:O:159:GLN:O	9:O:163:GLN:HG2	2.17	0.44
5:P:131:LEU:HD11	5:P:158:ILE:HG23	1.99	0.44
11:Z:173:LEU:HD11	11:Z:205:TRP:CH2	2.53	0.44
13:N:58:ALA:O	13:N:61:VAL:HG12	2.17	0.44
1:A:133:ILE:O	10:V:450:VAL:HG11	2.18	0.44
1:A:1841:ASN:ND2	13:N:147:GLN:OE1	2.51	0.44
5:J:628:ILE:HG21	5:J:638:TRP:CH2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:361:LEU:HB3	9:O:384:LEU:HG	2.00	0.44
10:V:39:ILE:HG12	10:V:201:LEU:O	2.18	0.44
11:Y:451:LEU:O	11:Y:454:ARG:HG2	2.17	0.44
1:A:724:LEU:HD21	9:O:597:PRO:HG2	2.00	0.43
1:A:1095:VAL:CG2	1:A:1098:GLU:HB2	2.48	0.43
5:J:149:TRP:NE1	5:J:153:GLU:OE1	2.49	0.43
7:L:79:ILE:HD11	7:L:153:MET:SD	2.58	0.43
6:Q:158:LYS:HB2	6:Q:158:LYS:HE2	1.79	0.43
6:Q:451:LEU:HD22	6:Q:467:TYR:HE2	1.83	0.43
1:A:490:VAL:HG13	1:A:498:VAL:HG23	2.00	0.43
1:A:1584:LEU:HB3	1:A:1588:LEU:HD12	2.00	0.43
5:J:97:PHE:CG	11:Y:252:ASP:HB3	2.53	0.43
6:K:299:PRO:HB2	6:K:333:TYR:CD2	2.53	0.43
7:L:96:VAL:HG11	7:L:124:LEU:HD22	1.99	0.43
7:L:185:ARG:HE	5:P:575:ASN:HD21	1.65	0.43
5:P:539:TYR:CD1	5:P:555:LEU:HD22	2.52	0.43
11:Y:373:LEU:HD22	11:Y:408:GLN:NE2	2.34	0.43
11:Y:430:LEU:HA	11:Y:433:LYS:HD3	1.99	0.43
1:A:77:ARG:HD2	1:A:128:TRP:CZ3	2.54	0.43
1:A:248:PHE:HB3	1:A:257:MET:HB3	2.00	0.43
1:A:1392:THR:OG1	1:A:1395:LEU:HD12	2.18	0.43
1:A:1711:ASP:OD2	1:A:1715:TRP:N	2.52	0.43
5:J:53:LYS:HZ1	5:J:56:LYS:HD2	1.83	0.43
6:K:155:GLU:O	6:K:158:LYS:HG2	2.18	0.43
6:K:377:GLU:OE2	3:W:4:ARG:NH2	2.46	0.43
5:P:165:ASP:HA	5:P:467:ARG:HE	1.84	0.43
6:Q:489:HIS:ND1	6:Q:497:ASN:HB2	2.32	0.43
10:V:45:GLU:O	10:V:87:TYR:OH	2.35	0.43
12:I:9:PRO:O	12:I:750:ASP:N	2.45	0.43
12:I:113:MET:HG3	12:I:176:LEU:HD11	1.98	0.43
12:I:145:LEU:HD23	12:I:351:HIS:HD2	1.82	0.43
1:A:11:MET:SD	1:A:510:PHE:HB2	2.59	0.43
1:A:774:LYS:HG2	1:A:783:ILE:HD11	1.99	0.43
1:A:1134:TRP:CD1	1:A:1597:THR:HA	2.53	0.43
3:G:11:LEU:HD21	6:Q:456:ARG:NH1	2.33	0.43
4:H:67:LEU:HD22	11:Y:308:TRP:CH2	2.53	0.43
9:O:536:THR:HB	9:O:543:GLY:HA3	1.99	0.43
5:P:684:LYS:NZ	5:P:686:GLU:OE1	2.45	0.43
6:Q:16:GLN:O	6:Q:17:GLN:HG2	2.19	0.43
10:V:58:LEU:HD23	10:V:58:LEU:HA	1.80	0.43
10:V:281:LYS:HD2	10:V:281:LYS:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:125:LEU:HD13	11:Y:141:LEU:HB3	2.01	0.43
11:Y:203:SER:O	11:Y:207:LYS:HG3	2.18	0.43
11:Y:332:ILE:HD12	11:Y:332:ILE:HA	1.83	0.43
12:I:602:ARG:NH2	12:I:612:SER:O	2.36	0.43
13:N:55:LEU:HD23	13:N:55:LEU:HA	1.83	0.43
1:A:350:LEU:HD11	10:V:399:TYR:HE2	1.83	0.43
1:A:966:PRO:HG3	1:A:980:ARG:NH1	2.33	0.43
1:A:1103:PRO:O	1:A:1139:ASN:ND2	2.52	0.43
1:A:1730:ALA:HA	1:A:1776:TYR:CD2	2.54	0.43
1:A:1867:CYS:HB3	1:A:1885:LEU:HD13	1.99	0.43
5:J:73:TYR:HE2	5:P:18:HIS:ND1	2.16	0.43
5:J:629:ARG:HH21	11:Y:503:SER:HB2	1.84	0.43
6:K:372:LEU:HD11	6:K:404:VAL:HA	2.00	0.43
9:O:706:CYS:SG	9:O:709:ARG:HD3	2.59	0.43
6:Q:93:LEU:HD22	6:Q:132:ILE:HG23	2.00	0.43
6:Q:357:TYR:HB3	6:Q:374:ILE:HG13	2.01	0.43
10:U:403:TYR:CD1	10:U:422:TYR:HE1	2.36	0.43
10:U:448:GLN:OE1	10:U:451:GLU:HG3	2.18	0.43
10:V:120:TYR:O	10:V:124:LEU:HD23	2.18	0.43
11:Z:293:LEU:O	11:Z:297:LEU:HG	2.18	0.43
1:A:352:ARG:HH21	10:V:373:HIS:CD2	2.37	0.43
1:A:633:ILE:HG23	1:A:754:LEU:HD21	2.00	0.43
7:L:33:LEU:HD22	7:L:54:TRP:CE2	2.54	0.43
7:L:73:THR:HG22	7:L:131:PRO:HB2	2.00	0.43
6:Q:301:SER:O	6:Q:305:VAL:HG23	2.18	0.43
10:U:289:LEU:HD11	10:U:296:ARG:HD3	1.99	0.43
12:I:56:TRP:CE3	12:I:98:PRO:HB3	2.54	0.43
12:I:240:LEU:HD22	12:I:547:SER:HB2	2.00	0.43
13:N:555:HIS:CE1	14:C:38:LYS:HG3	2.54	0.43
1:A:93:LEU:HD11	1:A:151:ILE:HD11	2.01	0.43
1:A:1141:VAL:HG11	1:A:1608:HIS:CG	2.53	0.43
1:A:1351:GLN:H	1:A:1351:GLN:HG2	1.59	0.43
2:D:49:ASN:OD1	2:D:49:ASN:N	2.51	0.43
8:M:35:GLU:C	6:Q:325:LYS:HZ2	2.18	0.43
6:Q:47:LEU:HB3	6:Q:56:ALA:HB2	2.01	0.43
6:Q:291:LEU:HB3	6:Q:301:SER:HB2	1.98	0.43
10:U:327:ASP:O	10:U:333:THR:HG21	2.19	0.43
11:Y:329:ALA:O	11:Y:332:ILE:HG22	2.18	0.43
11:Z:169:LEU:HD11	11:Z:205:TRP:CZ3	2.54	0.43
12:I:21:GLN:HB3	12:I:39:ASN:HB2	2.01	0.43
1:A:72:GLU:HB2	1:A:94:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:HD11	9:O:715:TYR:CD1	2.54	0.43
1:A:710:LEU:HD11	9:O:715:TYR:CE1	2.54	0.43
1:A:1251:VAL:HG23	1:A:1297:ALA:CB	2.49	0.43
5:J:546:LEU:HD23	5:J:548:LYS:HE3	2.00	0.43
5:J:640:GLY:O	5:J:644:ILE:HG22	2.18	0.43
6:K:153:TYR:HB2	6:K:170:LEU:HD21	2.01	0.43
5:P:621:LEU:O	5:P:625:ARG:HG3	2.19	0.43
5:P:707:PHE:CD1	5:P:707:PHE:C	2.92	0.43
6:Q:426:LEU:O	6:Q:430:GLU:HG2	2.19	0.43
10:U:330:ARG:HB2	10:U:333:THR:HG22	2.01	0.43
11:Y:377:GLU:O	11:Y:381:GLU:HG2	2.19	0.43
11:Y:432:ASP:O	11:Y:436:THR:HG23	2.18	0.43
1:A:183:THR:HG22	1:A:249:LEU:HD21	2.00	0.43
1:A:501:THR:O	1:A:501:THR:OG1	2.35	0.43
1:A:795:ARG:NH2	1:A:815:ARG:O	2.52	0.43
5:J:101:LYS:HE3	5:J:106:ILE:HD11	2.01	0.43
9:O:326:GLU:OE2	10:V:416:PHE:N	2.43	0.43
5:P:719:TYR:HE2	5:P:749:LYS:HB3	1.83	0.43
6:Q:129:LYS:HB3	6:Q:159:LEU:HD13	2.01	0.43
13:N:306:GLN:HE22	13:N:317:ALA:HA	1.84	0.43
1:A:1599:ASN:N	1:A:1599:ASN:OD1	2.52	0.43
1:A:1669:LYS:HB2	1:A:1669:LYS:HE3	1.73	0.43
7:L:144:ASN:ND2	7:L:150:ASP:O	2.52	0.43
5:P:55:TYR:CE2	5:P:56:LYS:HG3	2.53	0.43
6:Q:422:GLU:O	6:Q:426:LEU:HD12	2.19	0.43
11:Y:108:MET:SD	11:Y:124:ILE:HG13	2.58	0.43
11:Y:281:LEU:HG	11:Y:290:VAL:HG23	2.01	0.43
11:Z:397:ASN:C	11:Z:401:LYS:HZ2	2.21	0.43
11:Z:447:LYS:HD3	11:Z:447:LYS:HA	1.75	0.43
1:A:1053:GLN:HG3	1:A:1057:LEU:HD23	2.00	0.42
1:A:1134:TRP:HD1	1:A:1597:THR:HA	1.84	0.42
6:K:552:MET:HB3	6:K:552:MET:HE3	1.83	0.42
9:O:33:TYR:CE2	9:O:73:ILE:HG12	2.54	0.42
9:O:119:PHE:HD2	9:O:128:LYS:HG2	1.84	0.42
6:Q:231:LEU:HD11	6:Q:260:LYS:HD2	2.00	0.42
11:Y:106:TYR:O	11:Y:110:GLU:HG2	2.19	0.42
11:Y:340:GLN:H	11:Y:340:GLN:CD	2.21	0.42
11:Z:65:LYS:HE2	11:Z:65:LYS:HB2	1.88	0.42
12:I:434:LEU:HG	12:I:437:LEU:H	1.84	0.42
12:I:692:ARG:HG2	12:I:694:ASP:H	1.84	0.42
1:A:878:ALA:HA	1:A:882:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1879:GLU:O	1:A:1882:LEU:HG	2.18	0.42
5:J:465:LEU:HD21	5:J:495:HIS:ND1	2.34	0.42
6:K:283:GLU:OE1	6:K:283:GLU:N	2.49	0.42
6:K:432:ILE:HA	6:K:432:ILE:HD13	1.77	0.42
9:O:63:LEU:HD11	9:O:81:LEU:HB3	2.01	0.42
9:O:435:SER:HB3	9:O:654:ASP:HB3	2.01	0.42
5:P:161:LYS:HE2	5:P:478:SER:HB3	2.01	0.42
6:Q:146:ARG:O	6:Q:150:THR:HG23	2.19	0.42
10:V:295:TYR:HA	10:V:326:ILE:HD13	2.02	0.42
10:V:381:THR:HG21	10:V:412:LEU:HD21	2.01	0.42
11:Y:21:LEU:HG	11:Z:169:LEU:HD23	2.01	0.42
11:Z:399:VAL:O	11:Z:403:LEU:HB2	2.19	0.42
11:Z:406:ASN:O	11:Z:410:LEU:HG	2.19	0.42
11:Z:464:LEU:HD12	11:Z:464:LEU:HA	1.88	0.42
1:A:26:ASP:OD1	1:A:26:ASP:N	2.46	0.42
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.71	0.42
1:A:1131:MET:HG2	1:A:1132:THR:HG23	2.01	0.42
1:A:1886:ALA:O	1:A:1890:VAL:HG12	2.19	0.42
5:J:660:LYS:HE2	11:Y:492:GLN:NE2	2.34	0.42
10:V:32:ILE:HG23	10:V:228:TRP:CH2	2.55	0.42
10:V:396:LYS:HD3	10:V:396:LYS:HA	1.84	0.42
11:Y:8:ARG:HA	11:Y:48:TYR:CE2	2.55	0.42
11:Y:219:ARG:O	11:Y:223:THR:HG22	2.19	0.42
13:N:476:GLU:N	13:N:479:ASP:OD2	2.52	0.42
1:A:805:HIS:CD2	1:A:841:PRO:HB2	2.54	0.42
1:A:1729:GLU:OE2	1:A:1729:GLU:N	2.41	0.42
1:A:1875:GLN:N	1:A:1875:GLN:OE1	2.52	0.42
5:J:641:LEU:HB3	5:J:657:HIS:CD2	2.54	0.42
6:K:66:ASP:OD1	6:K:67:LYS:N	2.53	0.42
6:K:81:TYR:CD2	6:K:139:ILE:HG12	2.50	0.42
6:K:291:LEU:HB3	6:K:301:SER:HB2	2.01	0.42
10:U:151:LEU:HD23	10:U:151:LEU:HA	1.90	0.42
10:U:526:TRP:HA	10:U:529:ALA:HB3	2.01	0.42
10:V:161:LYS:HE3	10:V:161:LYS:HB3	1.90	0.42
11:Y:439:PRO:C	11:Y:441:TYR:H	2.22	0.42
12:I:245:LEU:HB3	12:I:246:PRO:HD3	2.00	0.42
1:A:1379:ASN:ND2	1:A:1417:ASP:OD2	2.52	0.42
1:A:1851:THR:O	1:A:1855:THR:HG22	2.19	0.42
5:J:473:TYR:HA	5:J:476:LEU:HB2	2.00	0.42
6:Q:459:LYS:HA	6:Q:461:TYR:CE1	2.54	0.42
10:U:58:LEU:HD23	10:U:58:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:249:ARG:HA	11:Y:249:ARG:NH1	2.35	0.42
12:I:644:TYR:O	12:I:726:GLY:HA2	2.20	0.42
13:N:232:TRP:HE3	13:N:235:GLN:HE22	1.67	0.42
13:N:697:SER:HA	13:N:700:LEU:HB2	2.02	0.42
14:C:42:ASP:N	14:C:42:ASP:OD1	2.51	0.42
1:A:175:PHE:HB2	1:A:191:ARG:HD3	2.01	0.42
1:A:347:MET:HG2	10:V:376:MET:HE1	2.02	0.42
1:A:671:ASN:O	1:A:672:THR:HG22	2.20	0.42
5:J:503:CYS:SG	5:J:535:GLY:HA3	2.58	0.42
6:K:133:CYS:O	6:K:152:SER:OG	2.37	0.42
9:O:516:PHE:CE2	9:O:528:ALA:HB1	2.54	0.42
6:Q:365:LYS:HE2	6:Q:365:LYS:HB2	1.70	0.42
6:Q:402:PRO:O	6:Q:406:HIS:HB3	2.19	0.42
11:Y:144:LEU:HD12	11:Y:144:LEU:HA	1.83	0.42
12:I:47:HIS:ND1	12:I:54:ARG:HA	2.34	0.42
12:I:344:ILE:O	12:I:348:VAL:HG23	2.20	0.42
12:I:568:ARG:HD2	12:I:569:LEU:N	2.35	0.42
1:A:129:CYS:HB3	1:A:187:LEU:HD21	2.01	0.42
1:A:628:ILE:HD11	1:A:836:PHE:HZ	1.83	0.42
1:A:1649:GLU:HG2	1:A:1651:LEU:HD21	2.01	0.42
5:J:139:GLN:HG3	5:J:161:LYS:HZ2	1.85	0.42
6:K:232:ASP:OD1	6:K:264:HIS:NE2	2.51	0.42
9:O:417:LEU:HD23	9:O:417:LEU:HA	1.92	0.42
9:O:735:MET:HA	9:O:738:ARG:HG2	2.01	0.42
11:Y:60:ARG:HE	11:Z:300:ILE:HG22	1.85	0.42
12:I:272:MET:CE	12:I:347:LEU:HB3	2.50	0.42
12:I:366:LEU:HD23	12:I:366:LEU:HA	1.84	0.42
12:I:417:PHE:HD1	12:I:448:VAL:HG13	1.85	0.42
13:N:252:LEU:O	13:N:256:VAL:HG12	2.20	0.42
14:C:30:PHE:HB3	14:C:46:LEU:HD11	2.01	0.42
1:A:628:ILE:HD12	1:A:765:VAL:HG13	2.02	0.42
5:J:509:TYR:HB3	5:J:518:ALA:HB2	2.01	0.42
9:O:644:LEU:O	9:O:648:ILE:HG12	2.19	0.42
5:P:48:TYR:CD2	5:P:56:LYS:HD3	2.55	0.42
6:Q:263:PHE:HE2	6:Q:294:LEU:HD13	1.85	0.42
10:U:419:LEU:HD13	10:U:442:CYS:HB3	2.02	0.42
10:U:437:VAL:HG12	10:U:441:GLU:OE2	2.20	0.42
10:V:172:LEU:HB3	10:V:195:ALA:HB2	2.02	0.42
10:V:379:LYS:HA	10:V:379:LYS:HD3	1.69	0.42
11:Y:157:SER:HA	11:Y:160:GLU:OE1	2.20	0.42
11:Y:244:ALA:HB1	11:Y:260:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:332:ILE:HD12	11:Z:336:SER:HA	2.01	0.42
13:N:621:ALA:O	13:N:624:LYS:HG3	2.20	0.42
1:A:650:GLY:N	1:A:651:PRO:HD3	2.34	0.42
1:A:1869:HIS:O	1:A:1873:SER:OG	2.36	0.42
4:H:81:LYS:HD2	5:P:557:LYS:HZ1	1.85	0.42
5:J:150:SER:HB3	5:P:22:ARG:HD2	2.02	0.42
9:O:323:ALA:HB2	10:V:416:PHE:CE2	2.55	0.42
11:Y:10:MET:HB3	11:Y:19:VAL:CG1	2.50	0.42
1:A:489:LEU:HD21	1:A:509:VAL:HG21	2.01	0.42
1:A:514:LEU:HD21	1:A:605:VAL:HG11	2.02	0.42
1:A:924:SER:OG	1:A:925:SER:N	2.52	0.42
2:D:51:LEU:HD23	2:D:51:LEU:HA	1.82	0.42
5:J:641:LEU:HA	5:J:644:ILE:CG2	2.50	0.42
6:K:190:LEU:HD12	6:K:202:ARG:HE	1.85	0.42
7:L:139:ILE:HD13	7:L:139:ILE:HA	1.88	0.42
8:M:31:ILE:HD13	6:Q:302:TRP:CZ3	2.54	0.42
9:O:360:LEU:HD23	9:O:360:LEU:HA	1.78	0.42
9:O:488:GLU:O	9:O:491:LYS:HG2	2.19	0.42
10:U:277:ARG:NH1	10:U:432:ASP:OD1	2.53	0.42
11:Y:377:GLU:O	11:Y:380:ILE:HG12	2.20	0.42
11:Z:173:LEU:HD11	11:Z:205:TRP:HH2	1.84	0.42
12:I:101:LEU:HD23	12:I:101:LEU:HA	1.89	0.42
12:I:421:LEU:HD12	12:I:421:LEU:HA	1.84	0.42
12:I:426:LEU:HD23	12:I:426:LEU:HA	1.86	0.42
12:I:709:LYS:HG3	12:I:710:HIS:ND1	2.35	0.42
13:N:562:LYS:HE3	14:C:39:VAL:HG21	2.02	0.42
14:C:16:TRP:HE1	14:C:31:ASN:HA	1.84	0.42
1:A:215:HIS:CG	1:A:216:PRO:HD2	2.55	0.41
1:A:1552:TYR:OH	1:A:1604:GLN:NE2	2.53	0.41
1:A:1691:LEU:HA	1:A:1695:GLY:HA2	2.01	0.41
5:J:526:ARG:NH2	5:J:558:ASP:OD2	2.53	0.41
5:J:653:LEU:HD23	5:J:653:LEU:HA	1.83	0.41
7:L:40:PHE:CD2	7:L:55:GLN:HB3	2.54	0.41
9:O:581:ILE:HB	9:O:619:LEU:HD13	2.01	0.41
5:P:135:SER:O	5:P:139:GLN:HG3	2.19	0.41
10:U:238:TYR:CE2	10:U:250:LYS:HE2	2.55	0.41
11:Y:377:GLU:HA	11:Y:380:ILE:HG12	2.01	0.41
11:Z:406:ASN:OD1	11:Z:409:THR:HG23	2.19	0.41
12:I:703:ARG:HH11	12:I:705:MET:HG2	1.85	0.41
1:A:1032:LEU:HD12	13:N:483:ASP:HB2	2.00	0.41
6:K:6:LEU:HD23	6:K:6:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:252:LYS:O	6:K:256:VAL:HG13	2.20	0.41
9:O:727:THR:HG22	9:O:731:ASN:ND2	2.34	0.41
5:P:93:SER:OG	5:P:121:LEU:HD11	2.20	0.41
5:P:473:TYR:CD2	5:P:500:TRP:HZ2	2.39	0.41
5:P:749:LYS:HB2	5:P:749:LYS:HE2	1.75	0.41
10:U:237:ILE:O	10:U:241:LEU:N	2.48	0.41
11:Y:128:ILE:HD12	11:Y:128:ILE:H	1.84	0.41
11:Y:488:VAL:HG12	11:Y:490:GLU:HG2	2.02	0.41
13:N:348:VAL:HG23	13:N:406:ALA:HB3	2.02	0.41
13:N:706:ARG:HB3	13:N:708:GLU:OE1	2.19	0.41
14:C:76:CYS:SG	14:C:78:GLN:HB2	2.60	0.41
1:A:645:HIS:NE2	1:A:656:GLU:OE1	2.53	0.41
1:A:1220:MET:HG2	1:A:1261:TYR:CE1	2.55	0.41
1:A:1485:PHE:CG	6:K:552:MET:HE1	2.55	0.41
5:J:641:LEU:HA	5:J:641:LEU:HD23	1.83	0.41
8:M:20:ARG:NH1	10:U:132:ASP:O	2.53	0.41
10:V:162:HIS:NE2	10:V:194:GLU:OE1	2.53	0.41
11:Z:152:ARG:HB3	11:Z:153:PRO:HD3	2.02	0.41
12:I:417:PHE:CZ	12:I:421:LEU:HD22	2.55	0.41
13:N:259:GLU:O	13:N:262:THR:OG1	2.29	0.41
1:A:756:PHE:CE2	1:A:830:PHE:HB2	2.53	0.41
5:J:581:ARG:HA	5:J:583:HIS:CE1	2.55	0.41
6:K:441:VAL:HB	6:K:474:LEU:HD22	2.02	0.41
9:O:127:HIS:O	9:O:133:GLY:HA3	2.21	0.41
9:O:439:LEU:HG	9:O:476:LEU:HD22	2.03	0.41
5:P:482:LYS:HE2	5:P:667:GLN:NE2	2.34	0.41
13:N:182:ARG:HB3	13:N:223:GLY:HA2	2.02	0.41
13:N:296:VAL:O	13:N:300:LEU:HG	2.20	0.41
1:A:269:TRP:HB3	1:A:409:ILE:HB	2.02	0.41
1:A:728:LEU:HD13	9:O:716:PHE:HE1	1.86	0.41
1:A:1811:LEU:HD12	1:A:1811:LEU:HA	1.83	0.41
13:N:18:GLN:O	13:N:22:VAL:HG12	2.20	0.41
3:G:9:LEU:H	6:Q:449:ASN:ND2	2.19	0.41
5:J:32:TYR:HH	5:J:64:HIS:CE1	2.38	0.41
5:J:517:GLN:O	5:J:520:ARG:HG2	2.20	0.41
7:L:46:ARG:HH12	7:L:157:LYS:HA	1.85	0.41
9:O:637:PRO:HB2	9:O:674:SER:HB3	2.01	0.41
5:P:150:SER:N	5:P:151:PRO:HD2	2.34	0.41
5:P:469:MET:HE2	5:P:500:TRP:HZ3	1.85	0.41
5:P:658:PHE:HB3	5:P:675:ILE:HG12	2.01	0.41
6:Q:510:ARG:O	6:Q:510:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:325:LEU:HD21	11:Y:352:MET:HE1	2.02	0.41
11:Y:381:GLU:HA	11:Y:384:LEU:HG	2.03	0.41
13:N:397:ILE:HD13	13:N:397:ILE:HA	1.89	0.41
1:A:17:LEU:O	1:A:18:GLN:NE2	2.53	0.41
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.89	0.41
1:A:1075:GLN:H	1:A:1075:GLN:HG2	1.67	0.41
1:A:1436:GLU:OE2	1:A:1437:ASN:N	2.54	0.41
1:A:1794:ASP:O	1:A:1797:ILE:HG13	2.18	0.41
7:L:5:ASN:OD1	7:L:5:ASN:N	2.54	0.41
9:O:439:LEU:HD23	9:O:473:LEU:HD12	2.02	0.41
6:Q:61:ARG:NH1	6:Q:61:ARG:HG2	2.36	0.41
10:V:405:LEU:HA	10:V:408:THR:HG22	2.01	0.41
11:Y:410:LEU:HD13	11:Y:433:LYS:HB2	2.03	0.41
11:Z:116:LYS:HE2	11:Z:116:LYS:HB2	1.82	0.41
13:N:180:PHE:HB2	13:N:240:PHE:CZ	2.56	0.41
13:N:349:ARG:HE	13:N:399:LEU:HD12	1.85	0.41
13:N:382:LEU:HD13	13:N:386:LEU:HD23	2.02	0.41
1:A:77:ARG:HD3	1:A:91:GLU:HB2	2.02	0.41
1:A:833:HIS:HA	1:A:834:PRO:HD3	1.85	0.41
1:A:1871:TYR:CE2	1:A:1889:LEU:HD21	2.55	0.41
5:J:16:LEU:HD23	5:J:16:LEU:HA	1.80	0.41
5:J:125:TYR:HD1	5:J:130:ARG:HE	1.68	0.41
6:K:68:LEU:HB2	6:K:69:TYR:CD1	2.55	0.41
9:O:362:GLU:HG3	9:O:384:LEU:HD11	2.03	0.41
5:P:168:PHE:HB2	5:P:467:ARG:HG2	2.02	0.41
5:P:670:VAL:HG12	5:P:674:HIS:CD2	2.56	0.41
11:Y:308:TRP:HE3	11:Y:327:LEU:HD13	1.86	0.41
11:Z:393:MET:O	11:Z:397:ASN:ND2	2.54	0.41
12:I:114:HIS:NE2	12:I:116:MET:HB3	2.35	0.41
1:A:616:GLU:OE2	9:O:558:SER:OG	2.34	0.41
1:A:805:HIS:HD2	1:A:841:PRO:HB2	1.86	0.41
1:A:1353:LYS:HB3	7:L:42:VAL:HG11	2.02	0.41
1:A:1416:TRP:CH2	1:A:1475:ARG:HA	2.56	0.41
1:A:1591:HIS:HD2	1:A:1601:TYR:CG	2.39	0.41
8:M:5:VAL:O	8:M:7:ARG:HD2	2.21	0.41
9:O:43:GLU:OE2	9:O:92:SER:OG	2.34	0.41
9:O:119:PHE:O	9:O:124:PRO:HB3	2.20	0.41
9:O:671:GLN:HE22	12:I:374:GLN:NE2	2.11	0.41
9:O:701:PHE:CD2	9:O:709:ARG:HB3	2.56	0.41
5:P:150:SER:HA	5:P:153:GLU:HG2	2.02	0.41
5:P:524:GLU:OE1	5:P:525:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:766:LEU:HD23	5:P:766:LEU:HA	1.93	0.41
6:Q:169:LEU:HD23	6:Q:169:LEU:HA	1.81	0.41
10:U:106:LEU:HA	10:U:109:CYS:SG	2.61	0.41
10:V:29:LEU:HD23	10:V:29:LEU:HA	1.86	0.41
10:V:516:LEU:HD23	10:V:516:LEU:HA	1.83	0.41
11:Y:20:ARG:O	11:Y:49:HIS:NE2	2.54	0.41
11:Y:232:LEU:HD11	11:Z:33:ASN:HB2	2.02	0.41
11:Y:443:LYS:HB3	11:Y:447:LYS:HZ1	1.85	0.41
11:Z:160:GLU:O	11:Z:164:GLN:HG2	2.21	0.41
11:Z:209:TYR:HA	11:Z:212:VAL:HG23	2.02	0.41
12:I:316:GLU:O	12:I:319:THR:OG1	2.30	0.41
12:I:623:PHE:CD2	12:I:665:LEU:HD22	2.56	0.41
13:N:24:TRP:HA	13:N:27:VAL:HG12	2.03	0.41
13:N:644:VAL:HG23	13:N:661:PRO:HG3	2.03	0.41
1:A:831:MET:O	1:A:833:HIS:N	2.54	0.41
3:G:9:LEU:HD23	3:G:9:LEU:HA	1.79	0.41
4:H:79:MET:HE2	4:H:79:MET:HB2	1.94	0.41
5:J:544:TRP:CD1	5:J:579:LEU:HD13	2.56	0.41
6:K:60:LEU:HD22	6:K:72:CYS:SG	2.60	0.41
9:O:378:SER:O	9:O:382:GLN:HG2	2.20	0.41
5:P:605:THR:HG1	5:P:634:HIS:CD2	2.39	0.41
12:I:74:ARG:HH21	12:I:78:LYS:NZ	2.19	0.41
13:N:638:LYS:NZ	14:C:13:THR:HG23	2.36	0.41
13:N:704:VAL:HG23	13:N:705:LEU:HD23	2.02	0.41
1:A:30:HIS:O	9:O:233:PRO:HG2	2.22	0.40
1:A:136:ASP:N	1:A:136:ASP:OD1	2.54	0.40
6:K:355:ALA:O	6:K:359:THR:HG22	2.21	0.40
8:M:34:ASN:O	8:M:50:VAL:HG22	2.21	0.40
9:O:300:LEU:HD23	9:O:300:LEU:HA	1.83	0.40
9:O:344:LEU:HD23	9:O:344:LEU:HA	1.88	0.40
5:P:152:PHE:CE1	5:P:162:PRO:HG2	2.56	0.40
5:P:512:LEU:HD12	5:P:512:LEU:HA	1.84	0.40
10:V:46:ARG:HG2	10:V:46:ARG:HH11	1.86	0.40
10:V:201:LEU:H	10:V:229:MET:HG3	1.86	0.40
11:Z:362:PHE:HE2	11:Z:382:CYS:SG	2.44	0.40
12:I:49:LEU:HD13	12:I:730:VAL:HG11	2.03	0.40
13:N:677:THR:OG1	13:N:678:LEU:N	2.54	0.40
14:C:51:CYS:HB3	14:C:53:HIS:CE1	2.55	0.40
1:A:356:PRO:O	10:V:242:GLN:NE2	2.51	0.40
1:A:1079:ALA:HB1	1:A:1556:LEU:HA	2.02	0.40
1:A:1084:ARG:HH21	1:A:1142:ALA:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:THR:HB	10:V:514:ARG:NH2	2.36	0.40
5:J:615:GLU:HA	5:J:615:GLU:OE1	2.21	0.40
5:J:617:LEU:HD23	5:J:648:GLN:NE2	2.33	0.40
8:M:31:ILE:HD12	6:Q:322:TYR:CE1	2.57	0.40
9:O:95:ILE:HG13	9:O:96:ARG:N	2.35	0.40
9:O:134:LEU:HD23	9:O:134:LEU:HA	1.91	0.40
9:O:471:CYS:O	9:O:475:GLU:HG3	2.21	0.40
5:P:628:ILE:HD13	5:P:628:ILE:HA	1.81	0.40
6:Q:210:LYS:HB3	6:Q:210:LYS:HE3	1.89	0.40
6:Q:513:THR:O	6:Q:517:THR:HG23	2.21	0.40
10:U:37:LEU:HD23	10:U:37:LEU:HA	1.90	0.40
10:V:45:GLU:HG3	10:V:113:LYS:HE3	2.03	0.40
10:V:180:ARG:NE	10:V:208:GLU:OE1	2.55	0.40
10:V:241:LEU:HA	10:V:241:LEU:HD23	1.83	0.40
11:Y:244:ALA:HB1	11:Y:260:PHE:CD1	2.56	0.40
11:Y:305:ALA:O	11:Y:309:VAL:HG23	2.21	0.40
11:Z:4:ILE:HD12	11:Z:45:LEU:HD21	2.02	0.40
11:Z:255:ASN:HA	11:Z:258:LEU:CD2	2.52	0.40
13:N:235:GLN:O	13:N:238:GLU:HG3	2.20	0.40
13:N:600:PHE:CD1	13:N:600:PHE:N	2.88	0.40
1:A:1751:ALA:HA	1:A:1755:CYS:SG	2.61	0.40
5:J:524:GLU:OE2	5:J:527:ARG:NH2	2.47	0.40
6:K:37:PRO:HA	6:K:65:LEU:HD21	2.03	0.40
6:K:193:LEU:O	6:K:198:GLN:NE2	2.55	0.40
8:M:62:LEU:H	8:M:62:LEU:HD12	1.87	0.40
6:Q:237:LEU:HD23	6:Q:240:ARG:HH11	1.86	0.40
11:Z:386:SER:O	11:Z:387:ASN:ND2	2.55	0.40
12:I:233:TYR:CD2	12:I:586:LEU:HD22	2.56	0.40
1:A:482:VAL:CG2	1:A:593:ASN:HA	2.52	0.40
1:A:788:GLU:H	1:A:788:GLU:HG2	1.72	0.40
1:A:1634:LEU:HD13	1:A:1666:ILE:HD11	2.04	0.40
6:K:148:LEU:HD12	6:K:148:LEU:H	1.87	0.40
6:K:232:ASP:OD1	6:K:232:ASP:N	2.53	0.40
6:K:473:VAL:CG2	5:P:130:ARG:HH12	2.33	0.40
7:L:37:LYS:NZ	7:L:57:ASP:HB3	2.37	0.40
9:O:283:LEU:HA	9:O:283:LEU:HD12	1.83	0.40
9:O:413:SER:O	9:O:413:SER:OG	2.33	0.40
5:P:481:CYS:O	5:P:485:ILE:HG12	2.22	0.40
10:V:228:TRP:H	10:V:228:TRP:HD1	1.68	0.40
10:V:327:ASP:O	10:V:333:THR:HG21	2.22	0.40
11:Y:59:TYR:O	11:Y:63:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:211:PHE:HB2	11:Y:220:ALA:HB2	2.03	0.40
11:Y:211:PHE:N	11:Y:211:PHE:CD1	2.89	0.40
11:Y:349:LEU:HA	11:Y:352:MET:HE2	2.03	0.40
13:N:582:PRO:HG2	13:N:585:GLU:HB2	2.04	0.40
1:A:853:LYS:HE2	1:A:853:LYS:HB2	1.88	0.40
1:A:1625:ASP:OD2	1:A:1700:LYS:NZ	2.44	0.40
1:A:1715:TRP:CD1	13:N:367:ARG:HG2	2.57	0.40
7:L:6:LYS:HB3	7:L:115:GLU:OE1	2.21	0.40
9:O:414:LEU:H	9:O:414:LEU:HD23	1.86	0.40
9:O:541:ILE:HG23	9:O:541:ILE:HD12	1.59	0.40
5:P:524:GLU:O	5:P:528:ILE:HG23	2.20	0.40
6:Q:93:LEU:HD13	6:Q:136:ARG:HG2	2.04	0.40
6:Q:382:ASN:O	6:Q:382:ASN:ND2	2.55	0.40
10:U:230:LYS:HB3	10:U:230:LYS:HE3	1.77	0.40
10:U:295:TYR:HB2	10:V:101:ARG:HG3	2.02	0.40
10:V:429:ARG:HG2	10:V:432:ASP:HB2	2.04	0.40
12:I:369:MET:HE3	12:I:369:MET:HB3	1.98	0.40
12:I:369:MET:HE3	12:I:376:TYR:CE2	2.57	0.40
12:I:597:LYS:HZ1	12:I:619:LYS:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1546/1944 (80%)	1491 (96%)	53 (3%)	2 (0%)	51 83
2	D	54/121 (45%)	53 (98%)	1 (2%)	0	100 100
3	G	25/85 (29%)	25 (100%)	0	0	100 100
3	W	23/85 (27%)	23 (100%)	0	0	100 100
4	H	55/110 (50%)	55 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	471/824 (57%)	458 (97%)	13 (3%)	0	100	100
5	P	480/824 (58%)	468 (98%)	11 (2%)	1 (0%)	47	79
6	K	506/620 (82%)	492 (97%)	14 (3%)	0	100	100
6	Q	500/620 (81%)	488 (98%)	12 (2%)	0	100	100
7	L	175/185 (95%)	163 (93%)	11 (6%)	1 (1%)	25	64
8	M	54/74 (73%)	51 (94%)	3 (6%)	0	100	100
9	O	675/755 (89%)	664 (98%)	11 (2%)	0	100	100
10	U	517/597 (87%)	506 (98%)	11 (2%)	0	100	100
10	V	532/597 (89%)	523 (98%)	9 (2%)	0	100	100
11	Y	496/565 (88%)	482 (97%)	14 (3%)	0	100	100
11	Z	483/565 (86%)	472 (98%)	11 (2%)	0	100	100
12	I	710/814 (87%)	692 (98%)	18 (2%)	0	100	100
13	N	644/822 (78%)	624 (97%)	20 (3%)	0	100	100
14	C	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	8028/10291 (78%)	7808 (97%)	216 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1393	MET
7	L	48	ASP
5	P	703	PRO
1	A	832	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1357/1720 (79%)	1320 (97%)	37 (3%)	44	75
2	D	52/115 (45%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	24/77 (31%)	24 (100%)	0	100	100
3	W	24/77 (31%)	23 (96%)	1 (4%)	30	65
4	H	49/89 (55%)	48 (98%)	1 (2%)	55	80
5	J	343/727 (47%)	331 (96%)	12 (4%)	36	69
5	P	414/727 (57%)	399 (96%)	15 (4%)	35	69
6	K	439/548 (80%)	428 (98%)	11 (2%)	47	77
6	Q	425/548 (78%)	415 (98%)	10 (2%)	49	77
7	L	163/170 (96%)	156 (96%)	7 (4%)	29	64
8	M	52/67 (78%)	48 (92%)	4 (8%)	13	44
9	O	582/650 (90%)	566 (97%)	16 (3%)	44	75
10	U	434/520 (84%)	423 (98%)	11 (2%)	47	77
10	V	464/520 (89%)	453 (98%)	11 (2%)	49	77
11	Y	423/484 (87%)	411 (97%)	12 (3%)	43	74
11	Z	412/484 (85%)	401 (97%)	11 (3%)	44	75
12	I	638/736 (87%)	626 (98%)	12 (2%)	57	81
13	N	578/724 (80%)	564 (98%)	14 (2%)	49	77
14	C	75/75 (100%)	73 (97%)	2 (3%)	44	75
All	All	6948/9058 (77%)	6761 (97%)	187 (3%)	48	75

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	77	ARG
1	A	78	LYS
1	A	83	ILE
1	A	125	GLN
1	A	130	ASP
1	A	138	SER
1	A	225	CYS
1	A	242	HIS
1	A	408	CYS
1	A	458	GLN
1	A	496	ASN
1	A	606	ARG
1	A	617	LEU

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Mol	Chain	Res	Type
1	A	654	HIS
1	A	804	ASP
1	A	807	TYR
1	A	840	GLU
1	A	851	CYS
1	A	939	PHE
1	A	1033	ARG
1	A	1036	ASP
1	A	1072	GLN
1	A	1243	LEU
1	A	1288	CYS
1	A	1291	ARG
1	A	1320	ASN
1	A	1385	ASP
1	A	1386	TRP
1	A	1438	SER
1	A	1475	ARG
1	A	1487	CYS
1	A	1503	ASN
1	A	1575	SER
1	A	1599	ASN
1	A	1711	ASP
1	A	1919	LYS
4	H	79	MET
5	J	50	ARG
5	J	66	CYS
5	J	73	TYR
5	J	125	TYR
5	J	152	PHE
5	J	481	CYS
5	J	563	ASP
5	J	602	TYR
5	J	633[A]	ARG
5	J	633[B]	ARG
5	J	646	TYR
5	J	651	PHE
6	K	12	GLN
6	K	13	TYR
6	K	34	ARG
6	K	62	SER
6	K	212	TYR
6	K	213	ASN

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Mol	Chain	Res	Type
6	K	333	TYR
6	K	342	HIS
6	K	344	PHE
6	K	492	MET
6	K	552	MET
7	L	46	ARG
7	L	83	TYR
7	L	84	LYS
7	L	88	SER
7	L	110	GLN
7	L	116	PRO
7	L	177	ASP
8	M	10	ARG
8	M	12	LEU
8	M	49	SER
8	M	62	LEU
9	O	57	ARG
9	O	106	LYS
9	O	250	PHE
9	O	306	ASN
9	O	357	SER
9	O	360	LEU
9	O	371	PHE
9	O	408	LEU
9	O	415	SER
9	O	487	SER
9	O	546	ARG
9	O	665	PHE
9	O	679	ASP
9	O	707	LYS
9	O	709	ARG
9	O	741	HIS
5	P	22	ARG
5	P	30	ARG
5	P	77	LYS
5	P	83	SER
5	P	93	SER
5	P	103	HIS
5	P	115	CYS
5	P	170	PHE
5	P	469	MET
5	P	482	LYS

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Mol	Chain	Res	Type
5	P	532	ARG
5	P	549	ASP
5	P	553	SER
5	P	579	LEU
5	P	581	ARG
6	Q	37	PRO
6	Q	63	ARG
6	Q	180	GLU
6	Q	211	LYS
6	Q	250	CYS
6	Q	311	MET
6	Q	340	TYR
6	Q	423	LYS
6	Q	482	TYR
6	Q	497	ASN
10	U	163	GLN
10	U	341	TYR
10	U	342	SER
10	U	364	TYR
10	U	371	MET
10	U	376	MET
10	U	399	TYR
10	U	418	CYS
10	U	435	MET
10	U	460	TYR
10	U	467	LYS
10	V	101	ARG
10	V	228	TRP
10	V	262	SER
10	V	311	SER
10	V	345	SER
10	V	371	MET
10	V	435	MET
10	V	500	CYS
10	V	513	PHE
10	V	555	GLN
10	V	557	ARG
3	W	15	ASP
11	Y	49	HIS
11	Y	74	LYS
11	Y	108	MET
11	Y	140	MET

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Mol	Chain	Res	Type
11	Y	187	SER
11	Y	216	ASP
11	Y	245	ASP
11	Y	252	ASP
11	Y	299	ASN
11	Y	352	MET
11	Y	362	PHE
11	Y	483	ASP
11	Z	43	TYR
11	Z	49	HIS
11	Z	167	LEU
11	Z	229	LYS
11	Z	247	TYR
11	Z	254	LYS
11	Z	313	CYS
11	Z	352	MET
11	Z	363	ARG
11	Z	460	ASP
11	Z	475	CYS
12	I	34	LEU
12	I	70	CYS
12	I	283	MET
12	I	341	TYR
12	I	418	PHE
12	I	529	MET
12	I	553	CYS
12	I	572	PHE
12	I	593	ASP
12	I	623	PHE
12	I	665	LEU
12	I	728	ARG
13	N	86	ASN
13	N	217	GLN
13	N	224	CYS
13	N	483	ASP
13	N	549	PHE
13	N	556	PHE
13	N	575	ARG
13	N	580	LYS
13	N	600	PHE
13	N	601	TRP
13	N	605	LYS

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Mol	Chain	Res	Type
13	N	616	ARG
13	N	624	LYS
13	N	638	LYS
14	C	28	MET
14	C	33	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	266	HIS
1	A	1201	HIS
1	A	1351	GLN
1	A	1591	HIS
1	A	1604	GLN
1	A	1627	ASN
1	A	1763	GLN
1	A	1832	ASN
5	J	139	GLN
5	J	480	ASN
5	J	495	HIS
5	J	583	HIS
5	J	634	HIS
5	J	648	GLN
6	K	80	HIS
6	K	352	GLN
6	K	415	ASN
7	L	60	GLN
7	L	145	HIS
7	L	146	GLN
9	O	261	ASN
9	O	306	ASN
9	O	332	GLN
9	O	443	GLN
9	O	671	GLN
9	O	731	ASN
5	P	575	ASN
5	P	599	ASN
5	P	667	GLN
5	P	674	HIS
6	Q	12	GLN
6	Q	20	GLN

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Mol	Chain	Res	Type
6	Q	45	GLN
6	Q	88	GLN
6	Q	179	GLN
6	Q	449	ASN
6	Q	468	HIS
10	U	107	HIS
10	U	347	HIS
10	U	534	GLN
10	V	145	GLN
10	V	373	HIS
11	Y	31	ASN
11	Y	213	HIS
11	Y	335	ASN
11	Y	337	ASN
11	Y	397	ASN
11	Y	408	GLN
11	Z	143	ASN
11	Z	213	HIS
11	Z	262	GLN
11	Z	387	ASN
12	I	301	GLN
12	I	584	HIS
13	N	235	GLN
13	N	586	GLN
13	N	663	GLN
14	C	58	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

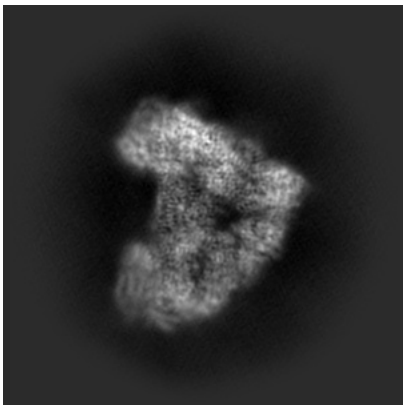
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17751. These allow visual inspection of the internal detail of the map and identification of artifacts.

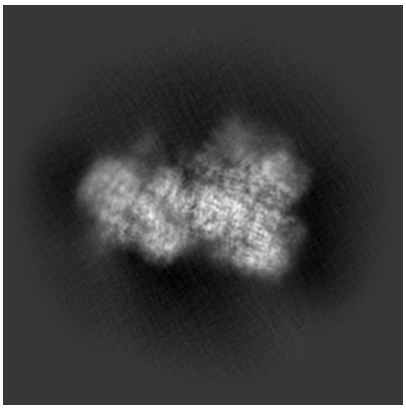
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

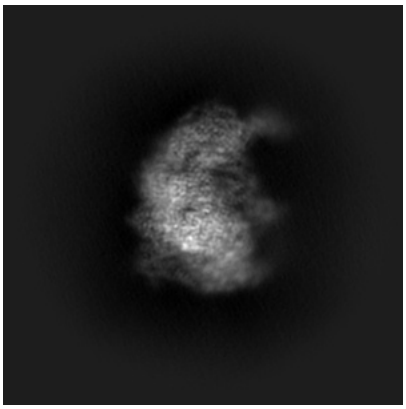
6.1.1 Primary map



X

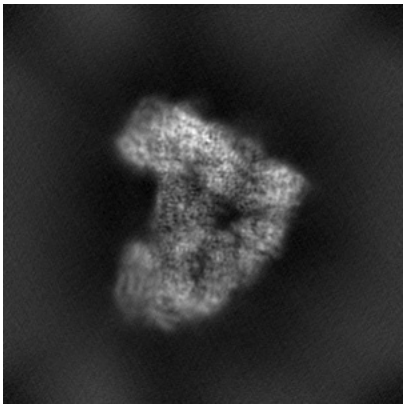


Y

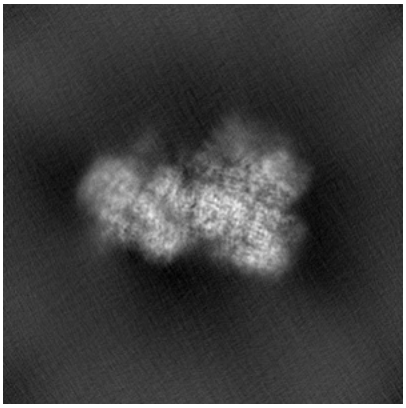


Z

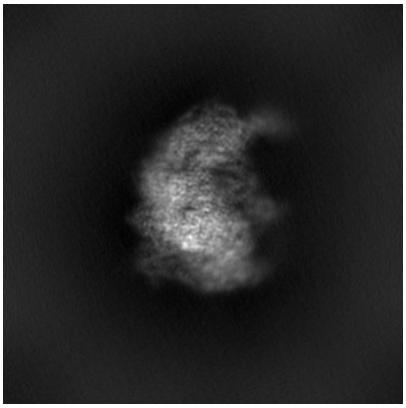
6.1.2 Raw map



X



Y

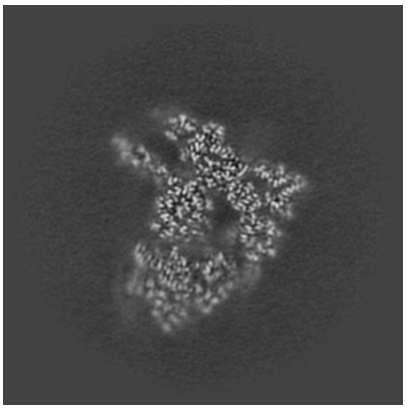


Z

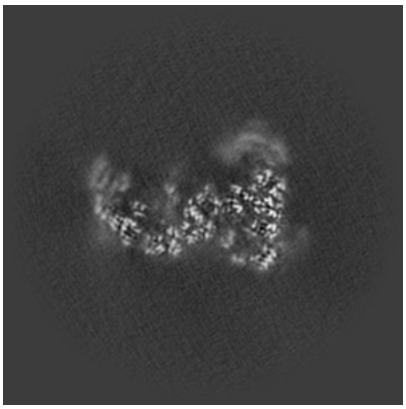
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

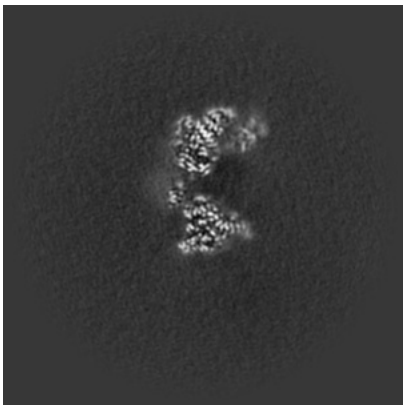
6.2.1 Primary map



X Index: 180

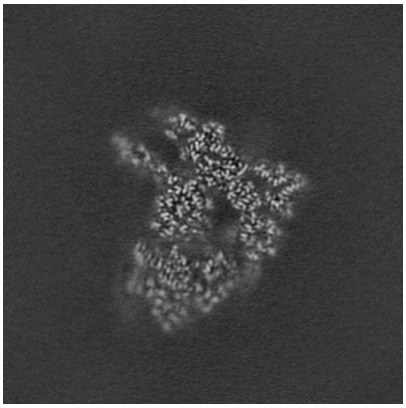


Y Index: 180

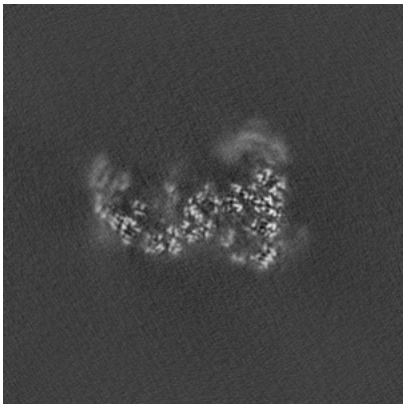


Z Index: 180

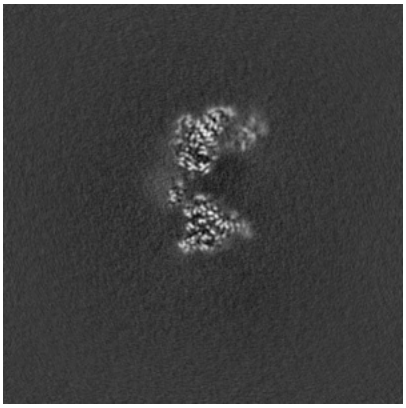
6.2.2 Raw map



X Index: 180



Y Index: 180

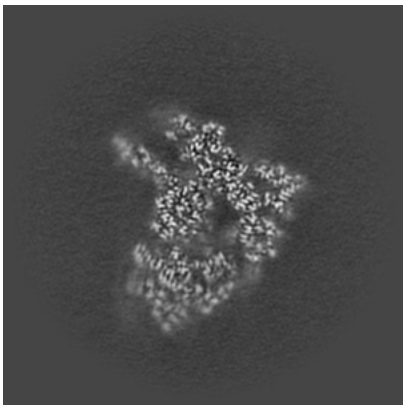


Z Index: 180

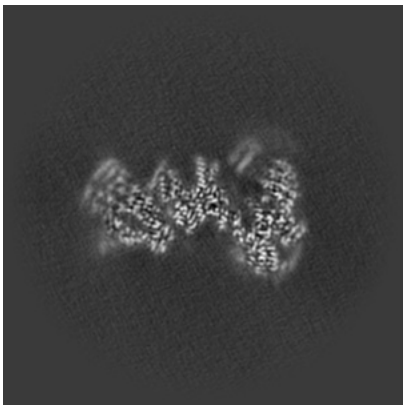
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

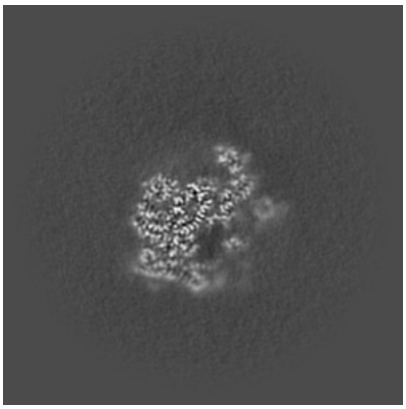
6.3.1 Primary map



X Index: 179

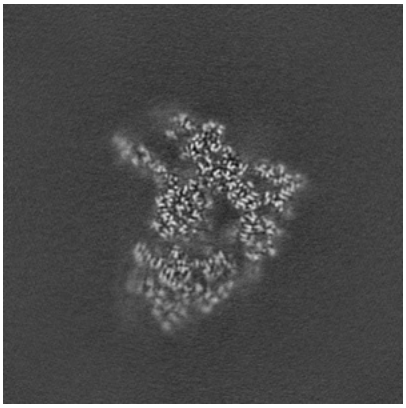


Y Index: 160

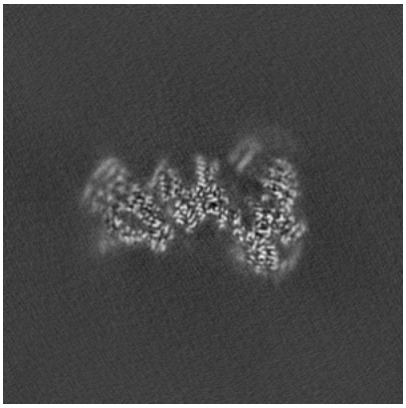


Z Index: 232

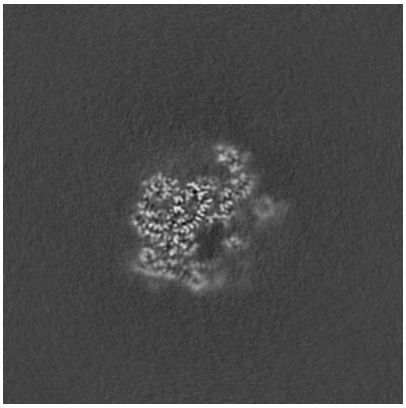
6.3.2 Raw map



X Index: 179



Y Index: 160

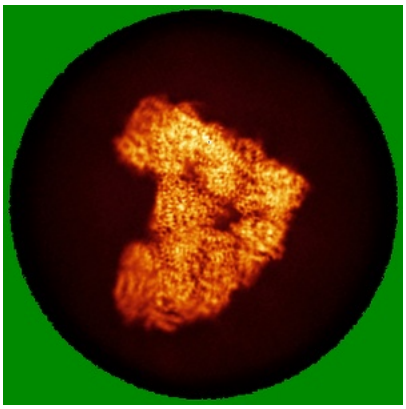


Z Index: 232

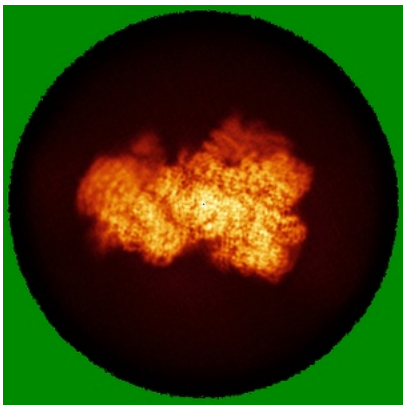
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

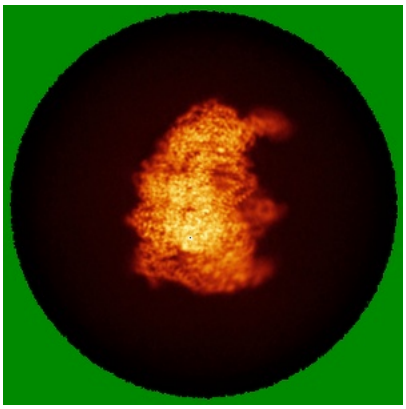
6.4.1 Primary map



X

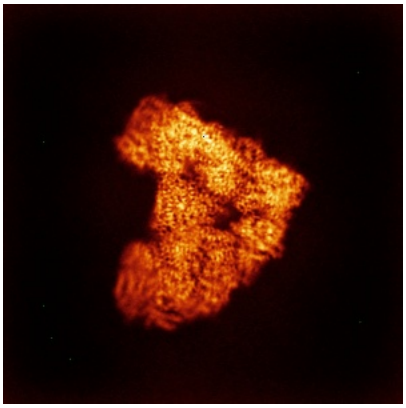


Y

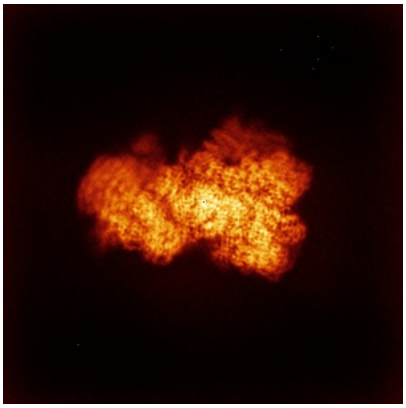


Z

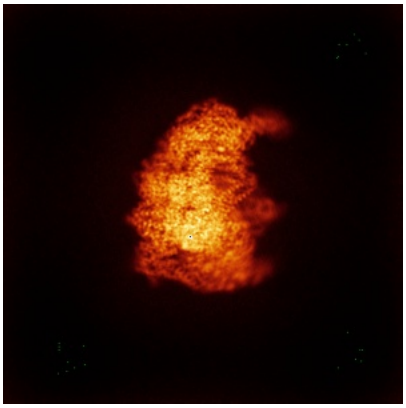
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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

X Y Z

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.

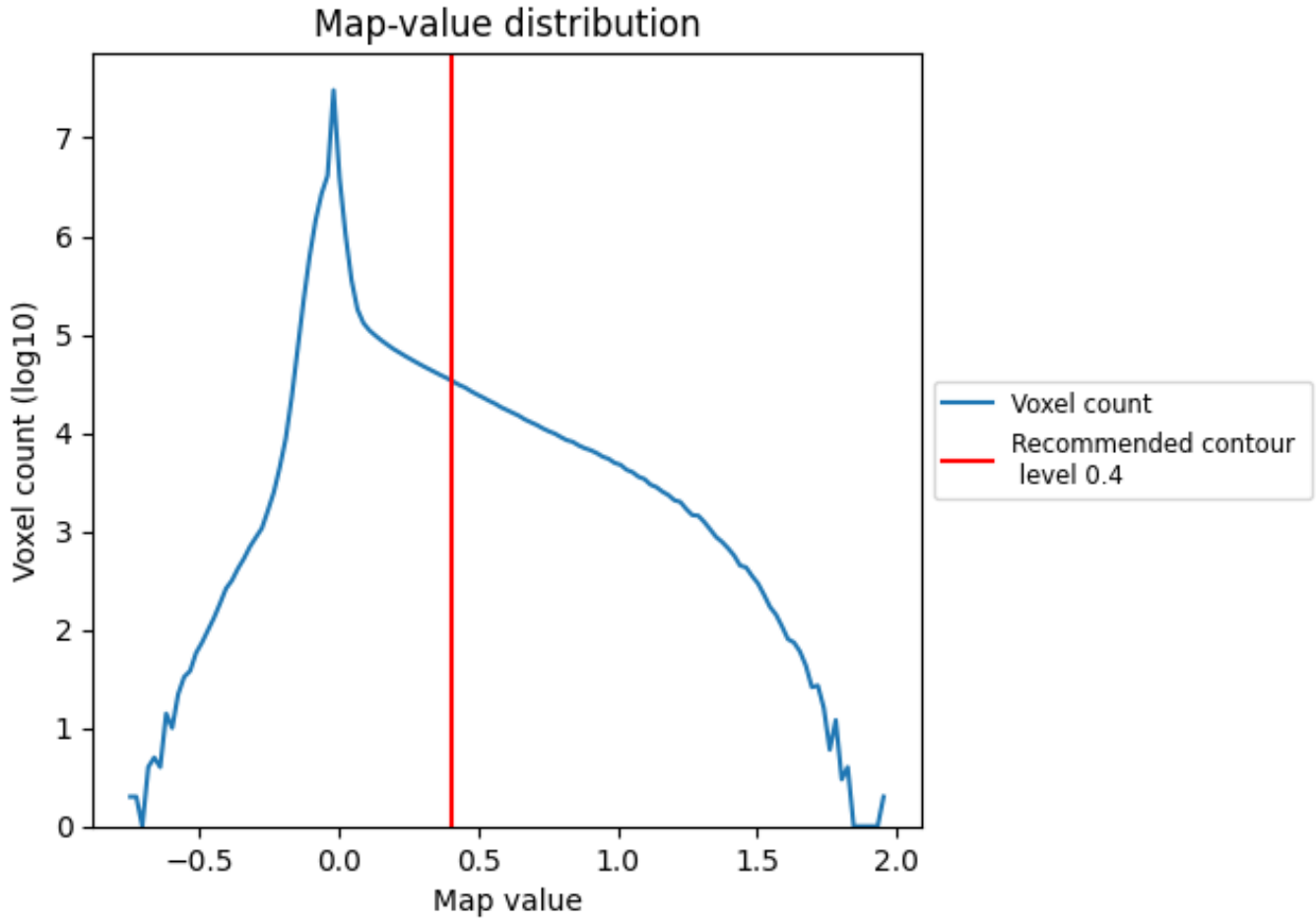
6.6 Mask visualisation (i)

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

7 Map analysis

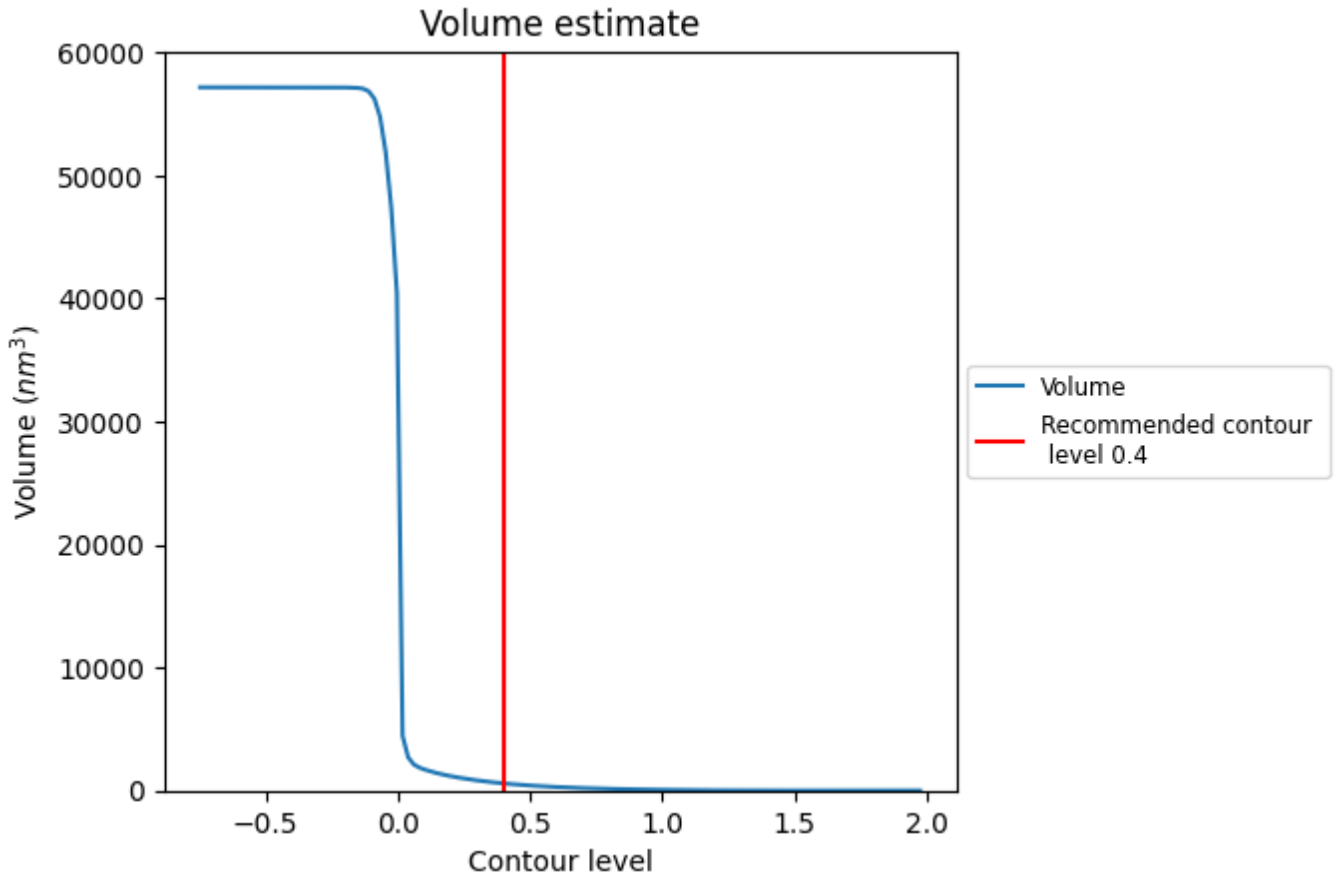
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

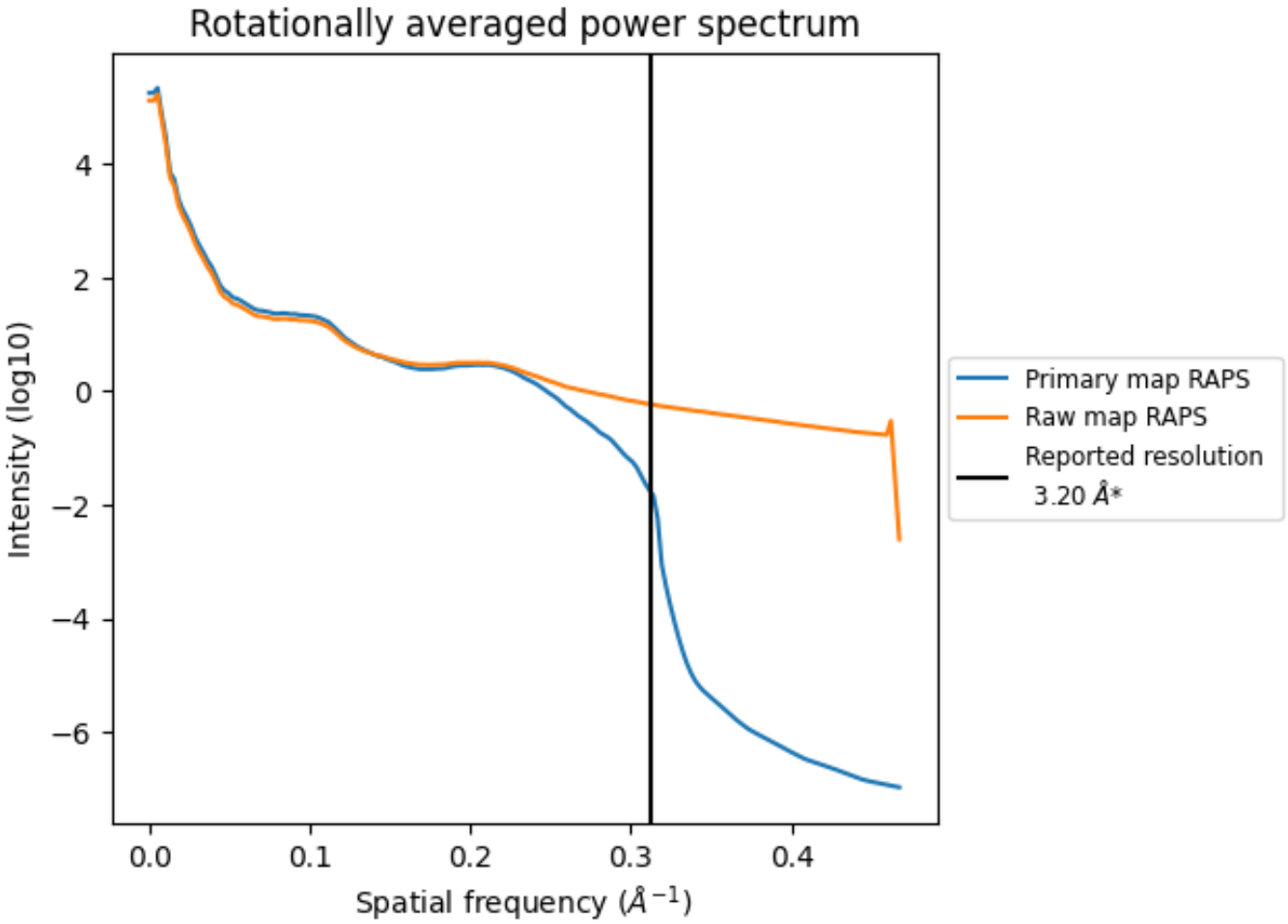
7.2 Volume estimate



The volume at the recommended contour level is 582 nm^3; this corresponds to an approximate mass of 526 kDa.

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

7.3 Rotationally averaged power spectrum (i)

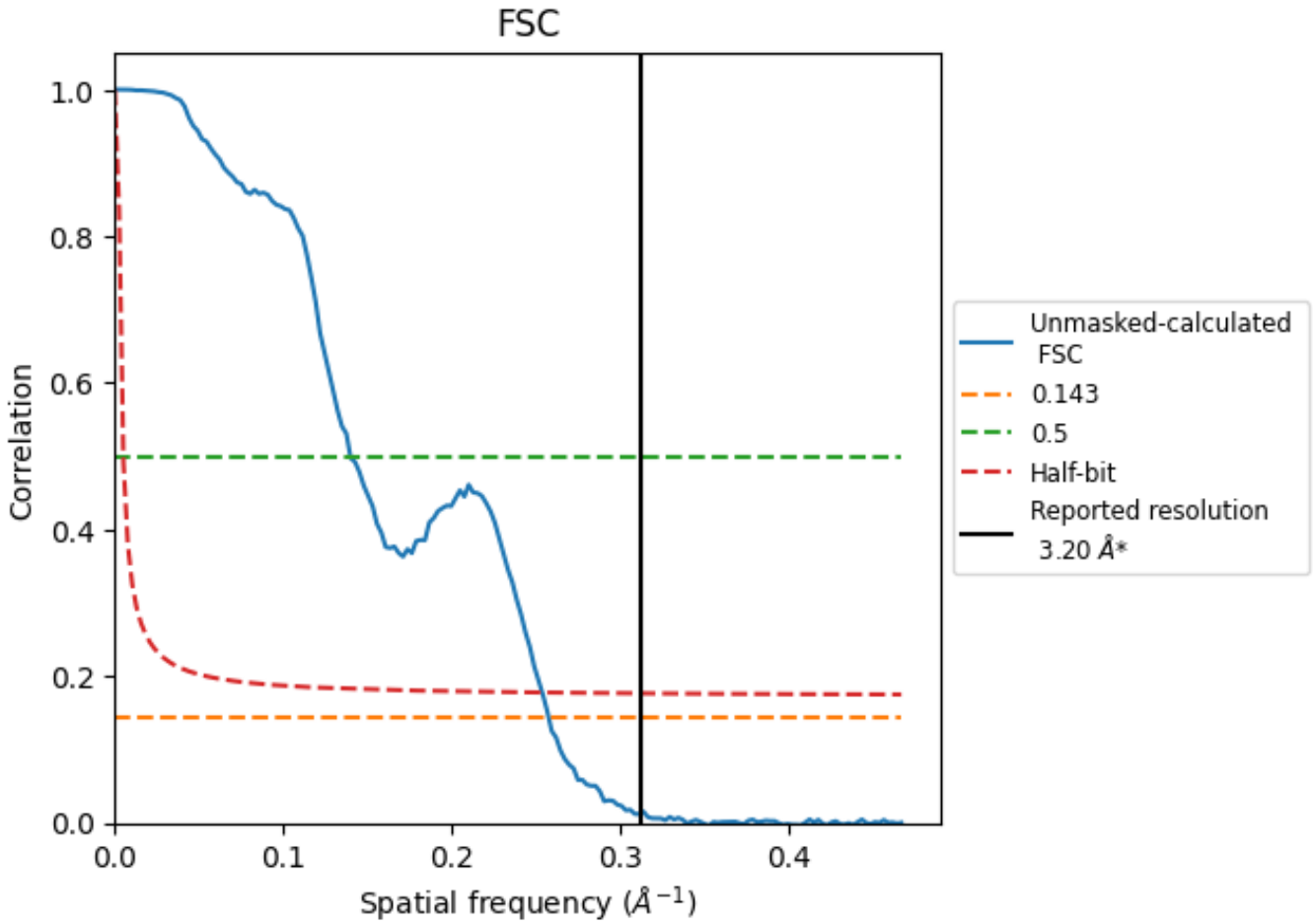


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

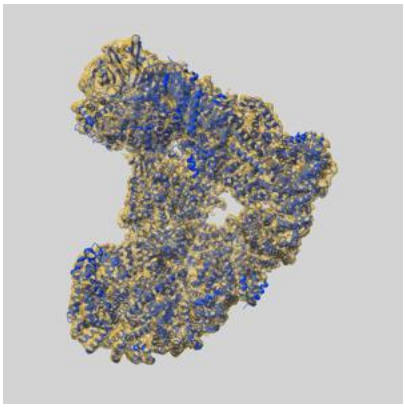
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	7.14	3.94

*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 3.88 differs from the reported value 3.2 by more than 10 %

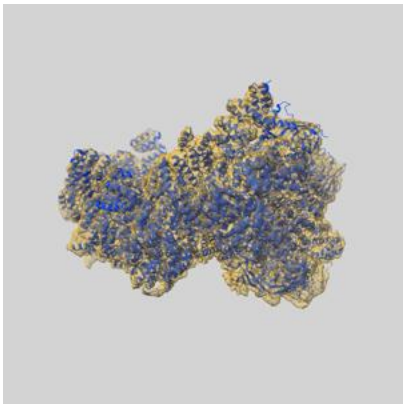
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17751 and PDB model 8PKP. Per-residue inclusion information can be found in section 3 on page 7.

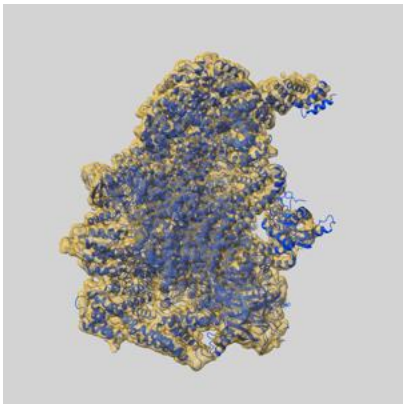
9.1 Map-model overlay



X



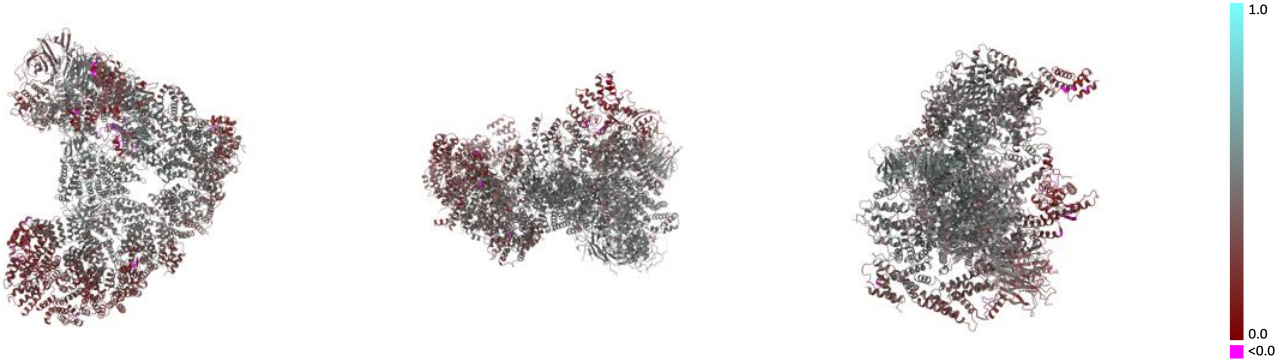
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

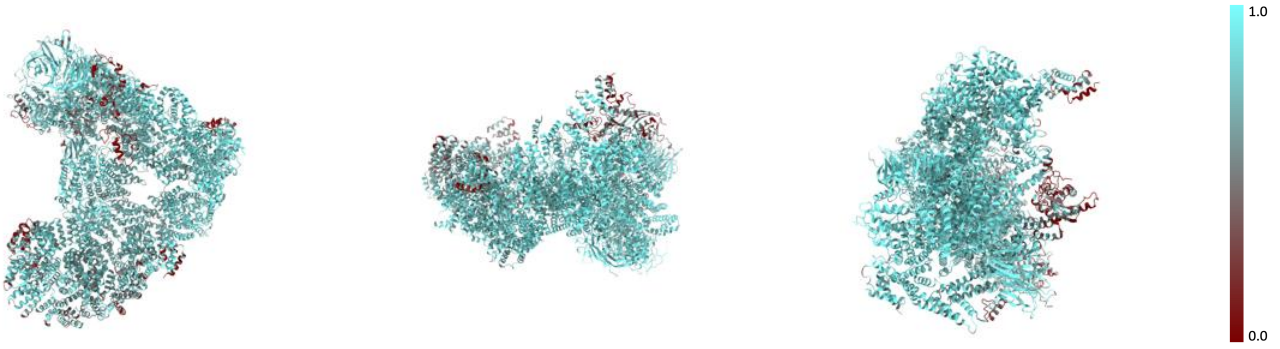
9.2 Q-score mapped to coordinate model



X Y Z

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

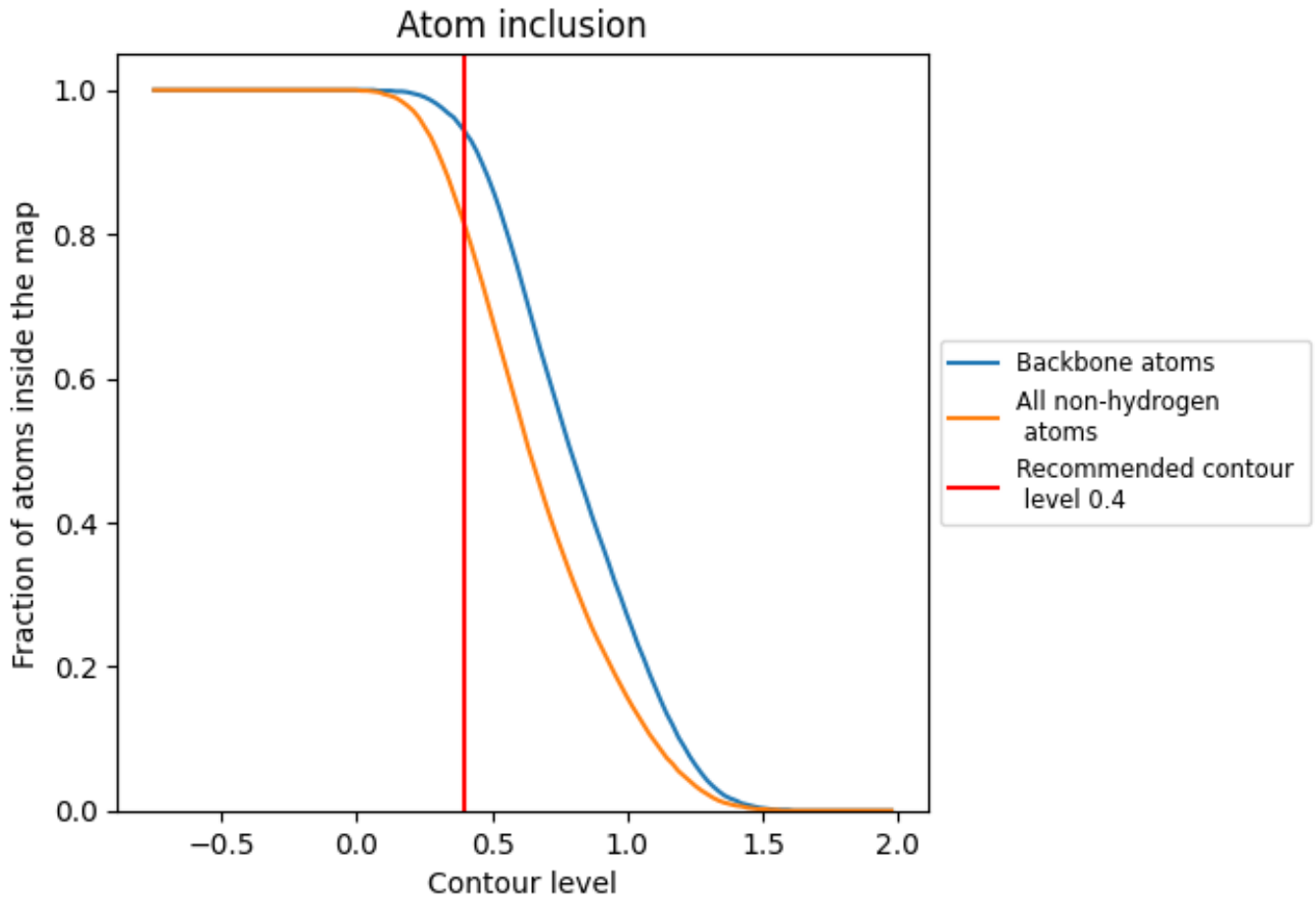
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8100	0.4090
A	0.8920	0.4780
C	0.1070	0.1150
D	0.7850	0.4620
G	0.7840	0.4230
H	0.7700	0.3860
I	0.8390	0.4210
J	0.7830	0.3820
K	0.8580	0.4400
L	0.8310	0.4350
M	0.7420	0.4490
N	0.6350	0.3290
O	0.8860	0.4750
P	0.8590	0.4300
Q	0.8640	0.4160
U	0.8280	0.4020
V	0.8800	0.4700
W	0.7800	0.4880
Y	0.6700	0.2650
Z	0.6850	0.2580