



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:13 PM UTC

PDB ID : 8PKP / pdb_00008pkp
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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

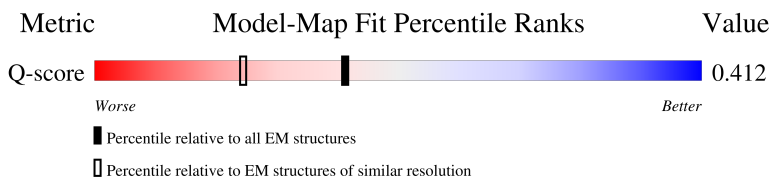
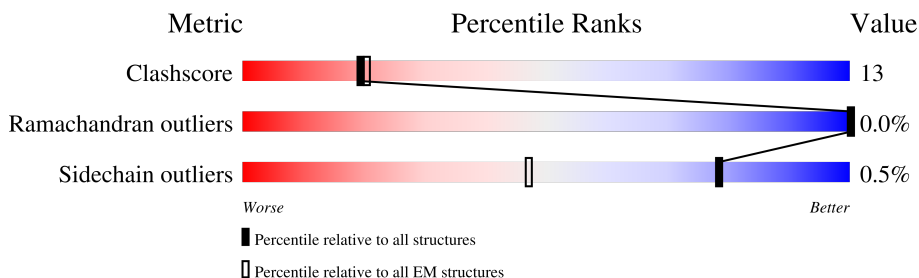
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

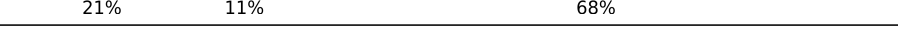
The reported resolution of this entry is 3.20 Å.

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.



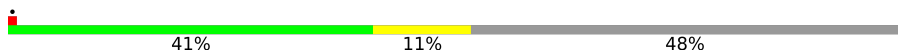
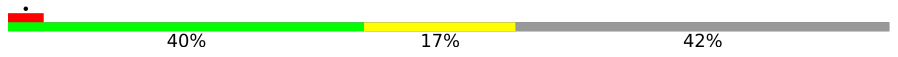
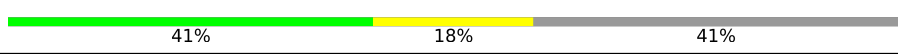
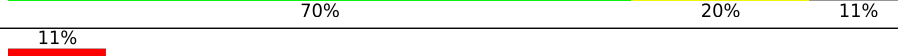
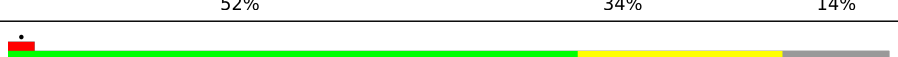
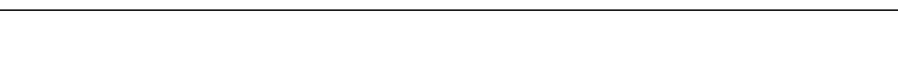
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	1944	
2	D	121	
3	G	85	
3	W	85	

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Mol	Chain	Length	Quality of chain
4	H	110	
5	J	824	
5	P	824	
6	K	620	
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 63749 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
1	A	1580	Total	C	N	O	S	0	0
			12284	7873	2074	2251	86		

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

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

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

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

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

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

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

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

- 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	503	Total	C	N	O	S	0	0
			4121	2655	690	751	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
			5705	3656	945	1070	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	612	Total	C	N	O	S	0	0
			4601	2913	805	858	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	83	Total	C	N	O	S	0	0
			572	365	102	93	12		

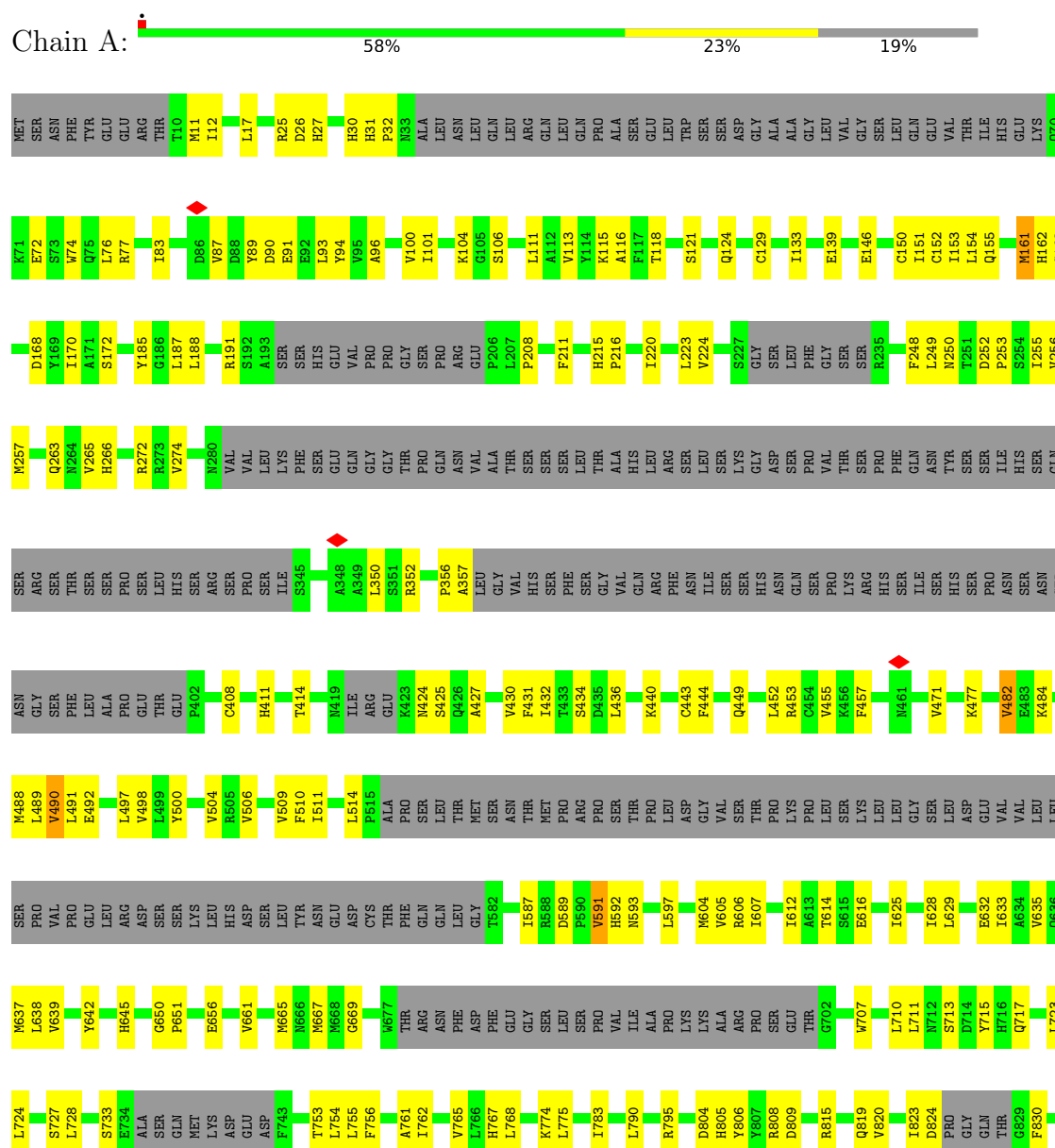
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

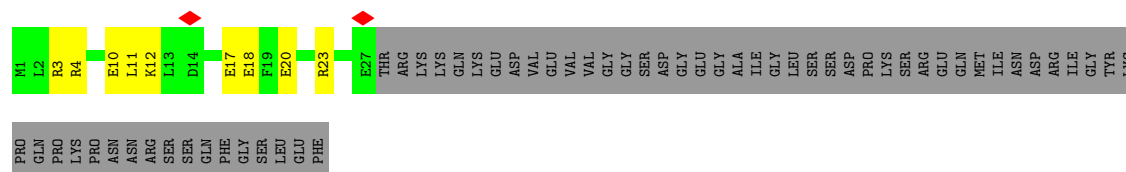
Mol	Chain	Residues	Atoms		AltConf
15	N	1	Total	Zn	0
			1	1	
15	C	3	Total	Zn	0
			3	3	

3 Residue-property plots

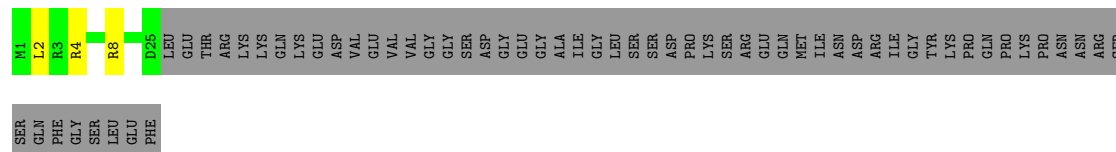
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Anaphase-promoting complex subunit 1

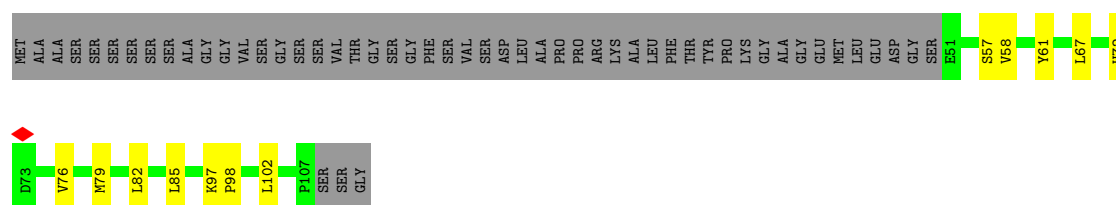




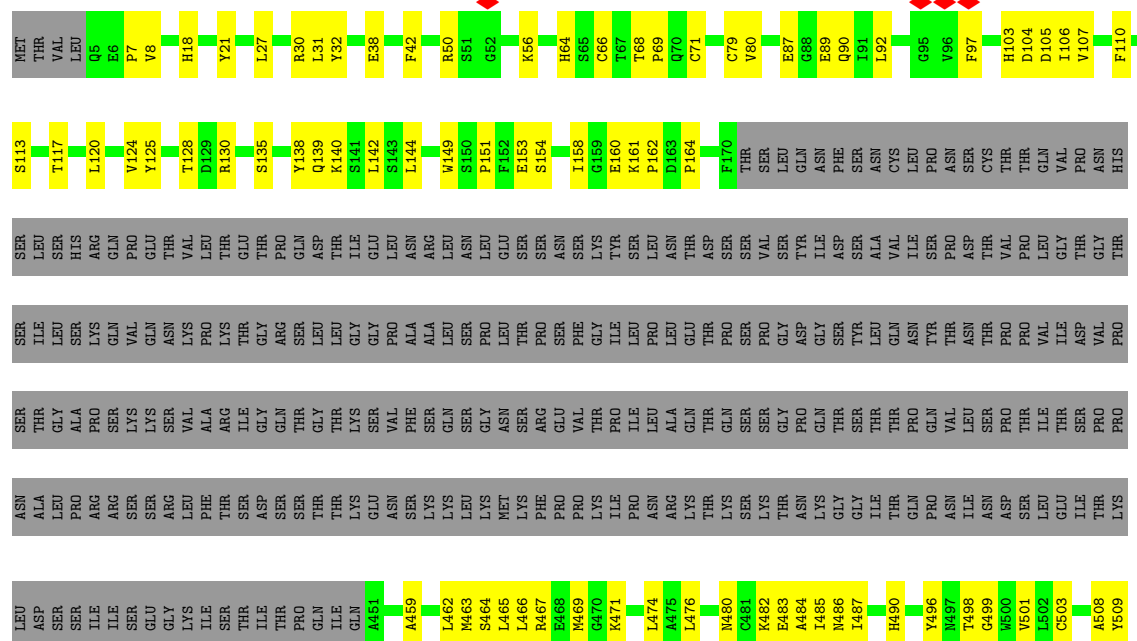
• Molecule 3: Anaphase-promoting complex subunit CDC26

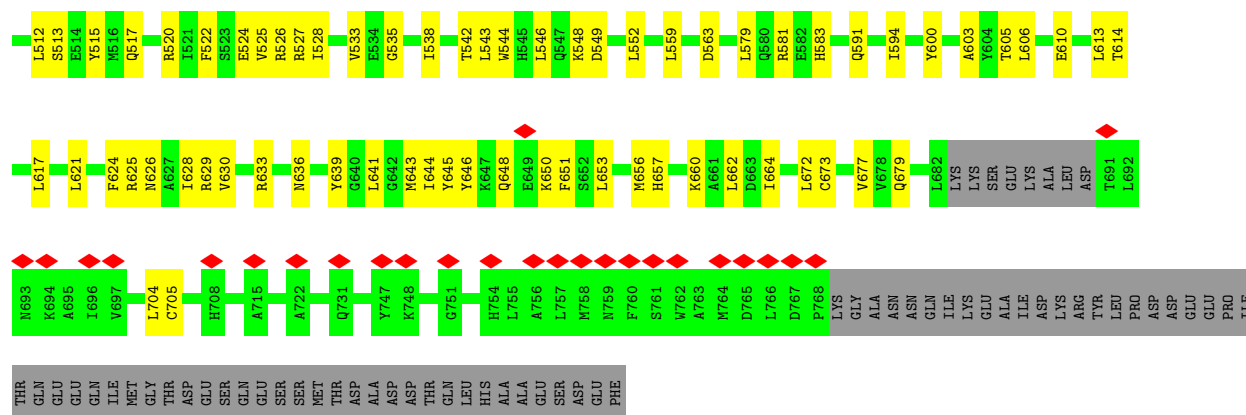


• Molecule 4: Anaphase-promoting complex subunit 16



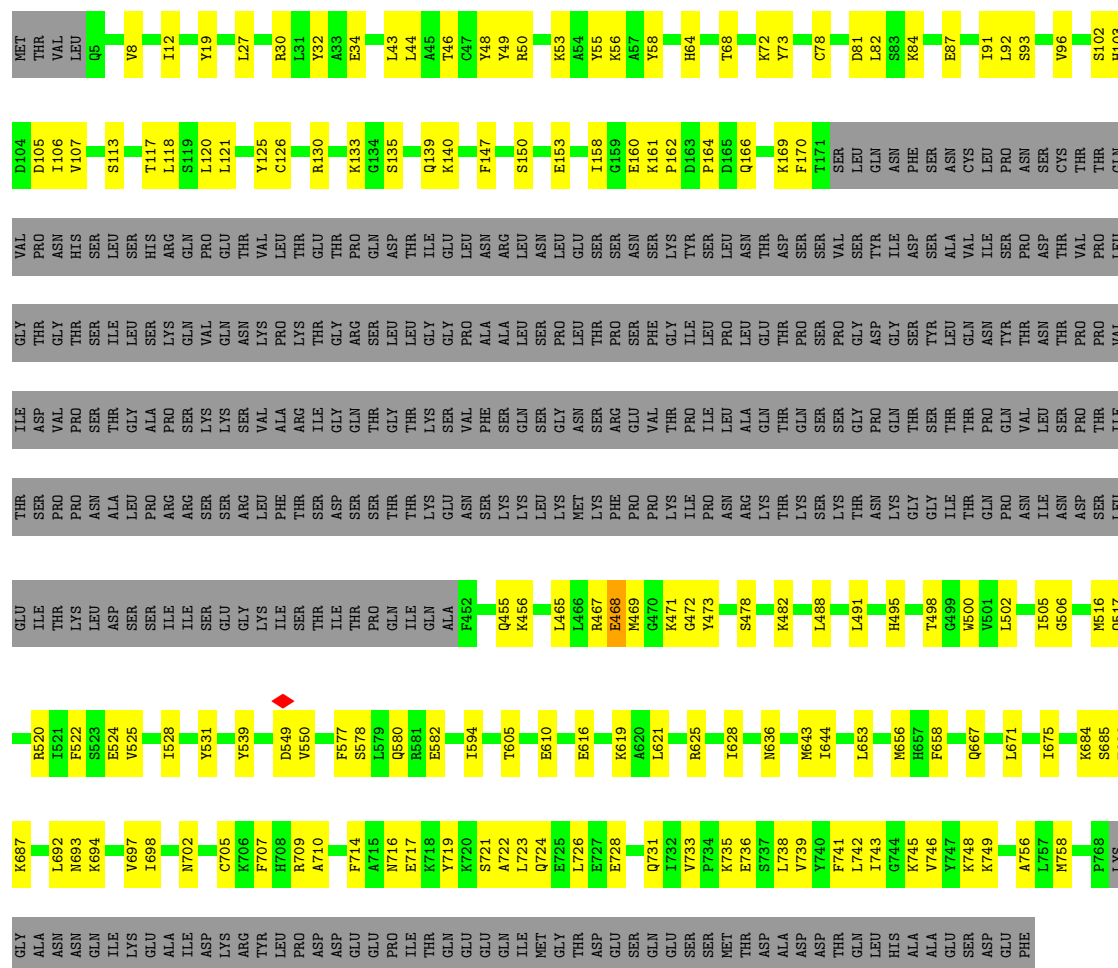
• Molecule 5: Cell division cycle protein 27 homolog





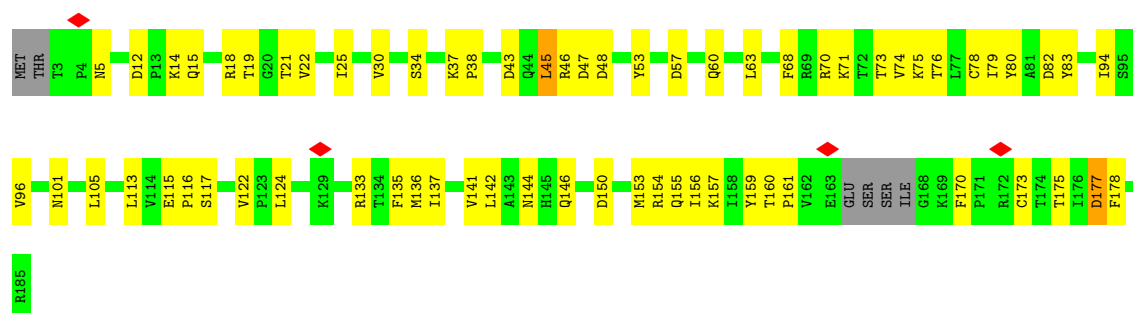
• Molecule 5: Cell division cycle protein 27 homolog

Chain P: 41% 18% 41%

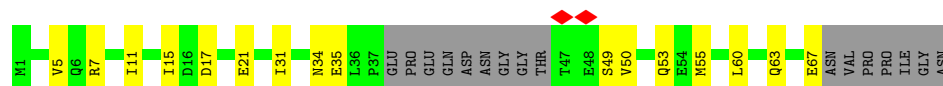


• Molecule 6: Cell division cycle protein 16 homolog

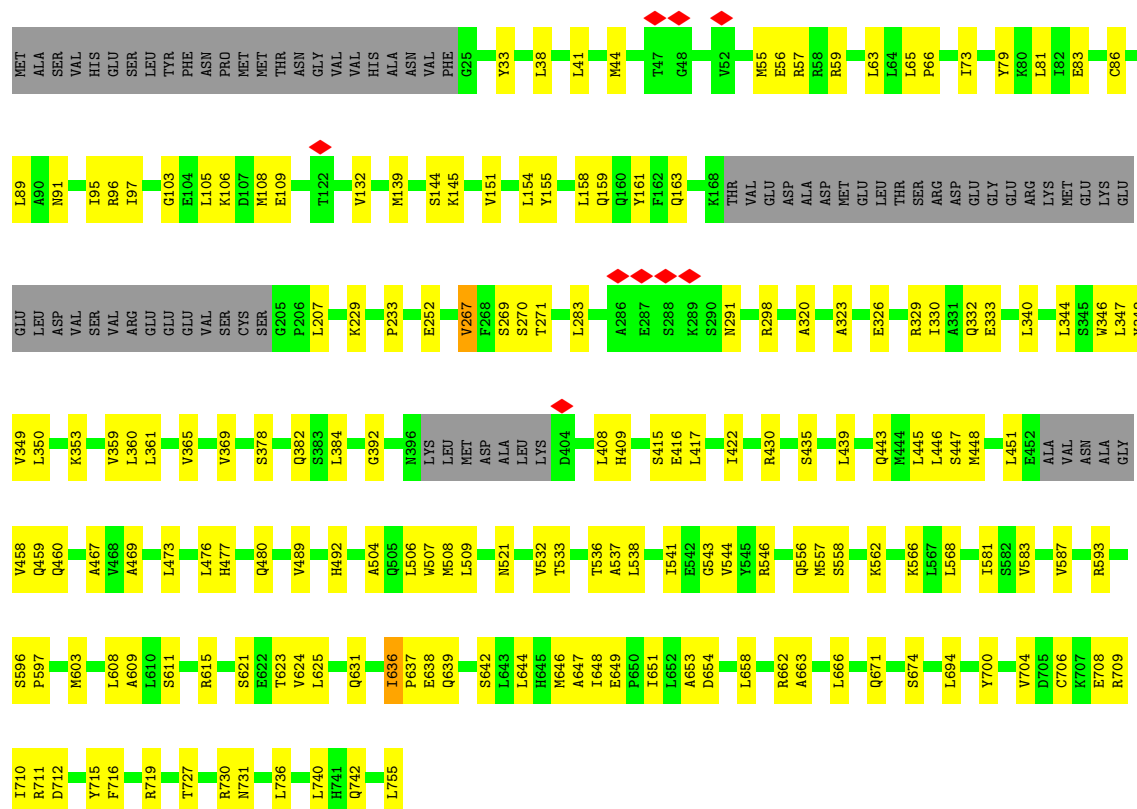
Chain K: 64% 18% 17%



• Molecule 8: Anaphase-promoting complex subunit 13

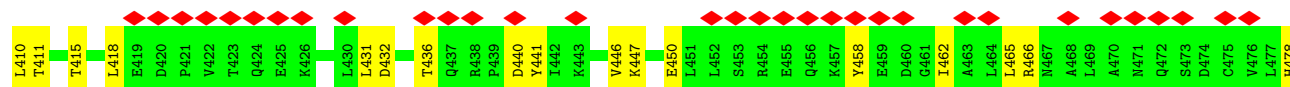


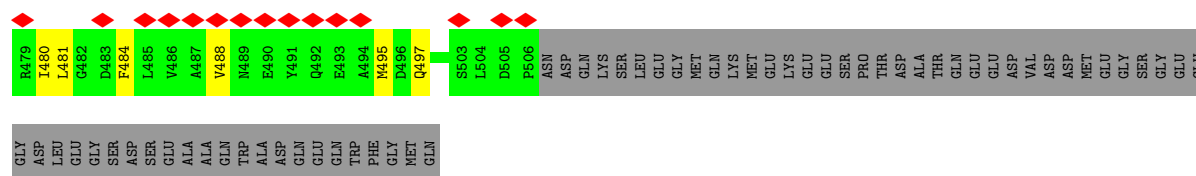
• Molecule 9: Anaphase-promoting complex subunit 5



• Molecule 10: Cell division cycle protein 23 homolog

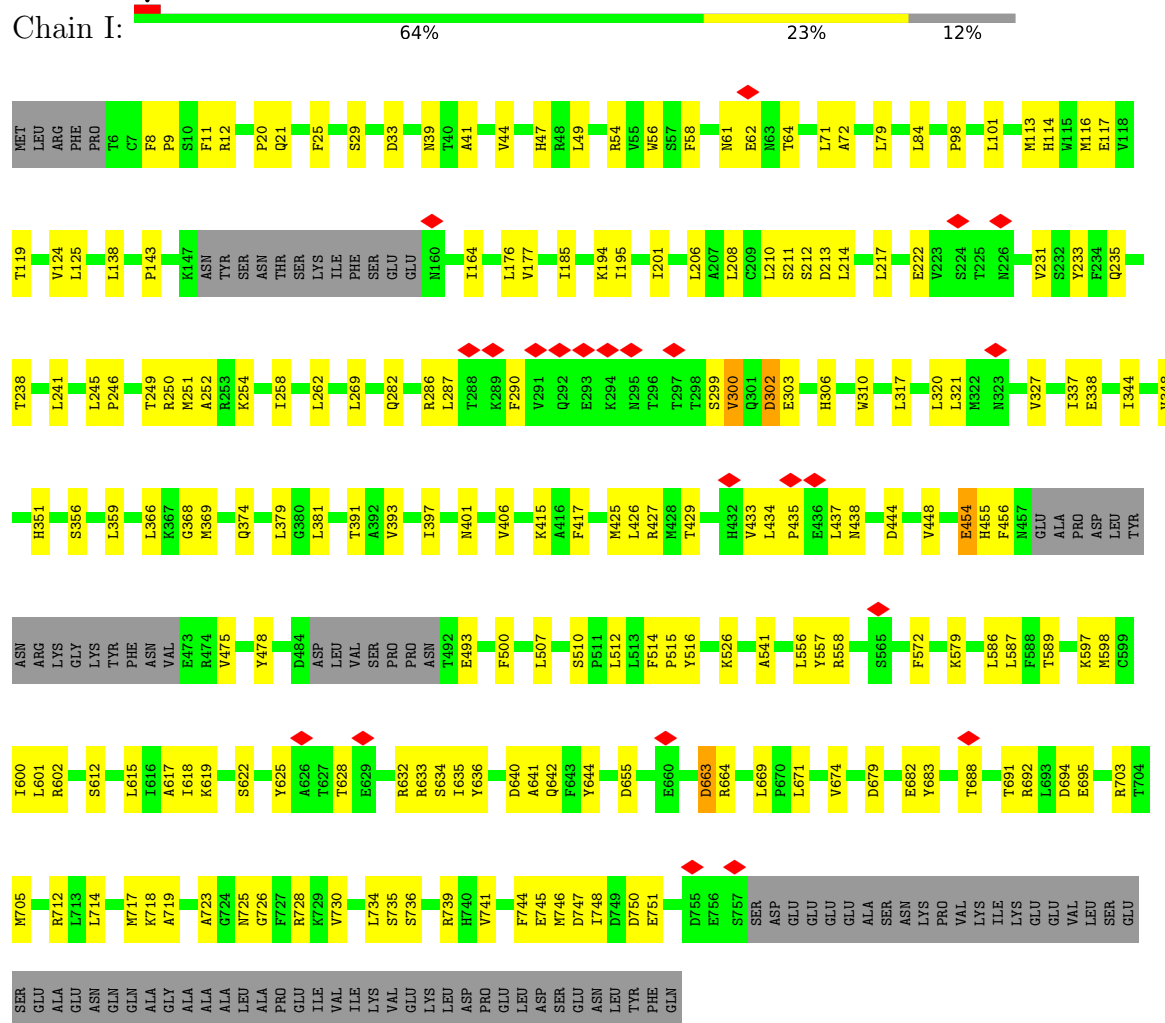






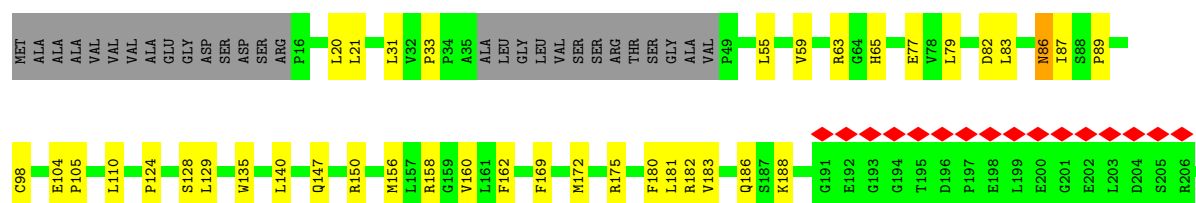
• Molecule 12: Anaphase-promoting complex subunit 4

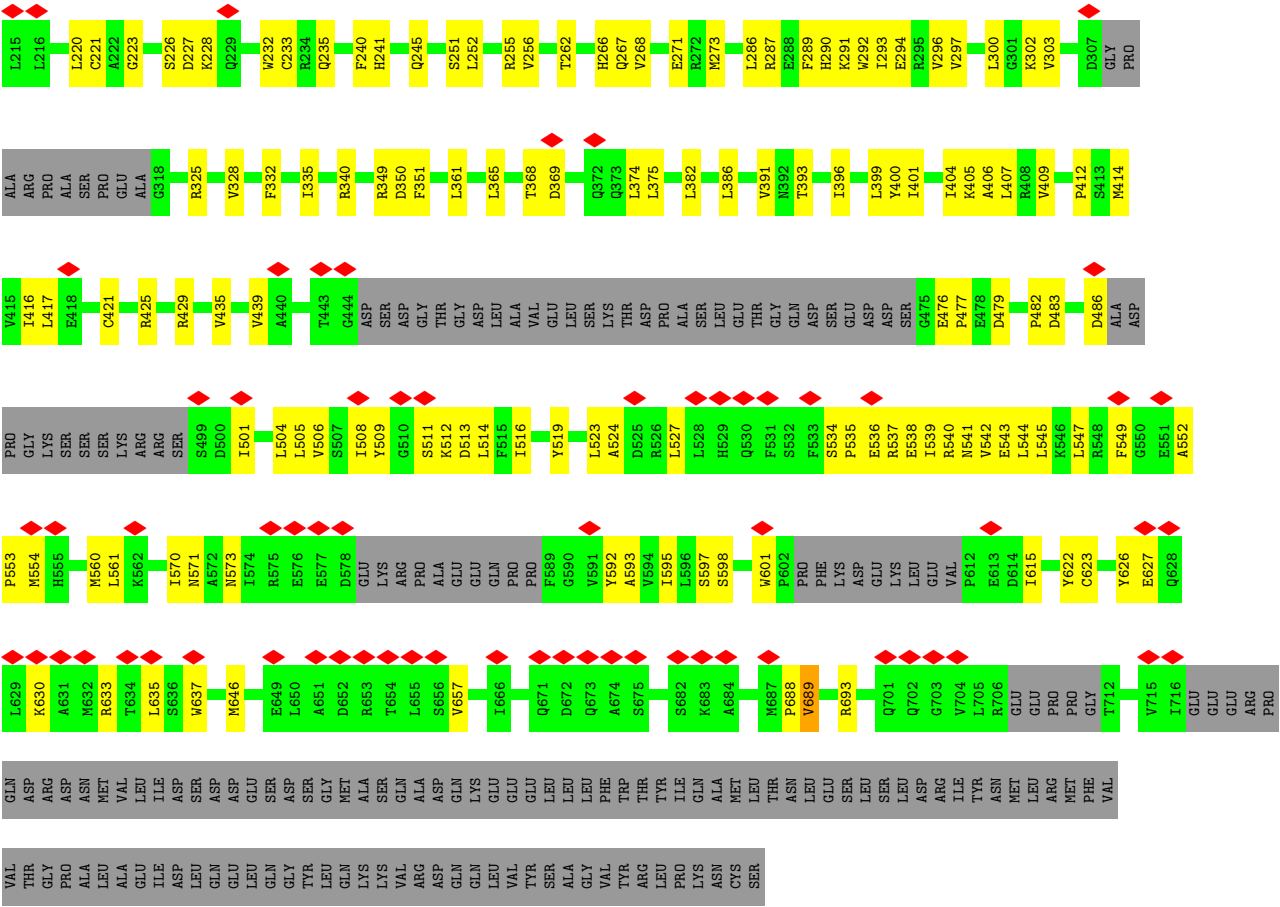
Chain I:



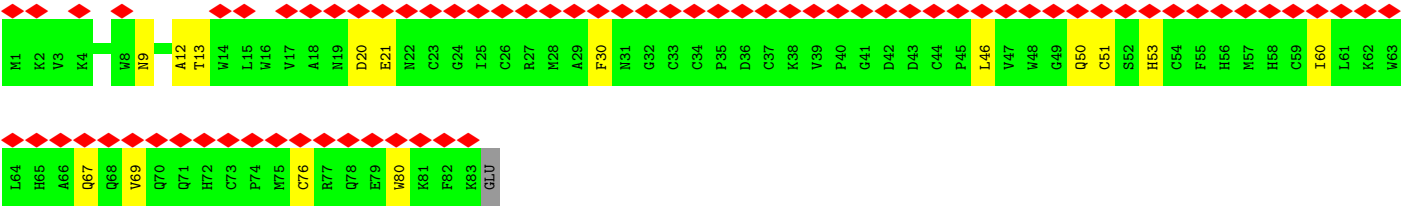
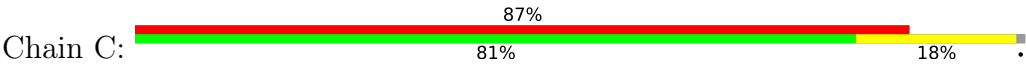
• Molecule 13: Anaphase-promoting complex subunit 2

Chain N: 10% 53% 21% 26%





● Molecule 14: Anaphase-promoting complex subunit 11



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.20	0/12566	0.37	0/17085
2	D	0.14	0/470	0.26	0/643
3	G	0.12	0/227	0.29	0/302
3	W	0.15	0/218	0.31	0/288
4	H	0.15	0/468	0.30	0/631
5	J	0.17	0/3686	0.37	0/5000
5	P	0.20	0/3975	0.35	0/5371
6	K	0.16	0/4233	0.33	0/5730
6	Q	0.17	0/4148	0.36	0/5620
7	L	0.16	0/1480	0.37	0/2005
8	M	0.16	0/486	0.35	0/658
9	O	0.28	0/5504	0.42	2/7435 (0.0%)
10	U	0.16	0/4218	0.33	0/5701
10	V	0.22	0/4493	0.35	0/6065
11	Y	0.19	0/3970	0.41	0/5365
11	Z	0.14	0/3870	0.36	0/5233
12	I	0.22	0/5824	0.38	0/7888
13	N	0.20	0/4683	0.41	0/6369
14	C	0.31	0/592	0.47	1/819 (0.1%)
All	All	0.20	0/65111	0.37	3/88208 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	271	THR	N-CA-C	-5.36	106.87	113.41
9	O	270	SER	N-CA-C	-5.16	107.02	113.72
14	C	50	GLN	N-CA-C	-5.04	107.08	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12284	0	12181	328	0
2	D	458	0	434	13	0
3	G	226	0	233	10	0
3	W	217	0	231	3	0
4	H	459	0	449	11	0
5	J	3601	0	3314	106	0
5	P	3883	0	3834	123	0
6	K	4134	0	4060	88	0
6	Q	4049	0	3948	114	0
7	L	1446	0	1423	46	0
8	M	478	0	454	17	0
9	O	5404	0	5452	138	0
10	U	4121	0	4046	81	0
10	V	4393	0	4362	92	0
11	Y	3907	0	3975	172	0
11	Z	3807	0	3885	151	0
12	I	5705	0	5655	136	0
13	N	4601	0	4327	126	0
14	C	572	0	452	9	0
15	C	3	0	0	0	0
15	N	1	0	0	0	0
All	All	63749	0	62715	1599	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 13.

All (1599) 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)
5:P:12:ILE:HG21	5:P:43:LEU:HD21	1.56	0.86
12:I:719:ALA:HA	12:I:735:SER:HA	1.58	0.83
1:A:83:ILE:HD11	9:O:541:ILE:HD13	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:161:VAL:HG23	6:Q:188:LEU:HD12	1.62	0.81
11:Y:112:TYR:HB3	11:Y:117:GLN:HB2	1.60	0.81
13:N:400:TYR:HE2	13:N:508:ILE:HG21	1.45	0.80
9:O:448:MET:SD	12:I:401:ASN:ND2	2.57	0.77
9:O:430:ARG:HD3	9:O:476:LEU:HD11	1.67	0.77
6:K:473:VAL:HG21	5:P:130:ARG:HH22	1.50	0.77
6:Q:157:LEU:HG	6:Q:188:LEU:HD11	1.66	0.77
7:L:83:TYR:HD2	7:L:115:GLU:HG3	1.50	0.77
1:A:121:SER:HB2	1:A:155:GLN:HE21	1.50	0.75
9:O:671:GLN:HE22	12:I:374:GLN:HE22	1.34	0.75
7:L:34:SER:HB3	7:L:63:LEU:HB2	1.68	0.75
10:V:536:CYS:SG	10:V:542:THR:OG1	2.45	0.75
1:A:1354:GLU:HB3	7:L:30:VAL:HG13	1.69	0.74
6:Q:23:LEU:HD11	6:Q:47:LEU:HD12	1.70	0.74
11:Z:332:ILE:HD12	11:Z:336:SER:HA	1.69	0.74
4:H:102:LEU:HD23	5:P:594:ILE:HG22	1.70	0.74
7:L:48:ASP:OD1	7:L:157:LYS:NZ	2.20	0.73
11:Y:50:ALA:HB1	11:Y:66:TYR:CE1	2.23	0.73
12:I:692:ARG:HE	12:I:694:ASP:HB3	1.54	0.73
11:Z:193:ILE:HG22	11:Z:199:LEU:HB2	1.70	0.73
11:Y:271:ILE:HG22	11:Y:306:GLU:HG3	1.69	0.73
6:Q:432:ILE:HD11	6:Q:444:TRP:CG	2.23	0.73
11:Z:139:MET:HE1	11:Z:171:ALA:HB2	1.70	0.73
6:K:474:LEU:HD21	5:P:96:VAL:HG21	1.69	0.72
1:A:1193:ILE:HG23	1:A:1208:LEU:HD21	1.71	0.72
9:O:329:ARG:NH2	10:V:413:LYS:O	2.23	0.72
4:H:57:SER:OG	11:Z:323:ARG:NH2	2.23	0.72
10:V:36:LEU:HD21	10:V:58:LEU:HB3	1.71	0.72
12:I:556:LEU:HD21	12:I:586:LEU:HD21	1.71	0.71
1:A:869:ARG:NH2	1:A:946:THR:OG1	2.23	0.71
11:Z:193:ILE:HA	11:Z:199:LEU:HD13	1.71	0.71
5:J:160:GLU:HG3	5:J:161:LYS:HG2	1.71	0.71
13:N:539:ILE:HG22	13:N:561:LEU:HD23	1.71	0.71
12:I:714:LEU:HB3	12:I:717:MET:HB2	1.73	0.71
1:A:1910:SER:HB2	13:N:21:LEU:HD11	1.71	0.71
11:Y:297:LEU:HB3	11:Y:307:PRO:HB3	1.72	0.71
1:A:191:ARG:NH2	1:A:208:PRO:O	2.23	0.71
1:A:1133:SER:HB2	1:A:1203:MET:HE1	1.73	0.70
10:U:159:SER:O	10:U:163:GLN:NE2	2.24	0.70
11:Y:137:ILE:HA	11:Y:140:MET:SD	2.31	0.70
5:P:684:LYS:HG3	5:P:687:LYS:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:478:ASN:HB3	6:Q:481:THR:HG22	1.73	0.70
10:U:298:GLU:OE2	10:V:101:ARG:NH1	2.24	0.70
1:A:1221:ASP:HB3	1:A:1224:ILE:HG22	1.74	0.70
5:J:80:VAL:HG11	5:J:120:LEU:HD11	1.74	0.70
11:Y:342:LEU:HA	11:Y:345:LYS:HD2	1.74	0.70
9:O:291:ASN:O	9:O:298:ARG:NH2	2.25	0.69
11:Y:268:PRO:O	11:Y:296:ARG:NH1	2.23	0.69
1:A:272:ARG:NH1	1:A:408:CYS:SG	2.66	0.69
1:A:1096:PRO:HG2	9:O:347:LEU:HD21	1.74	0.69
5:P:726:LEU:HD23	5:P:739:VAL:HG13	1.74	0.69
6:Q:368:HIS:NE2	6:Q:401:ASP:OD2	2.25	0.69
11:Z:130:SER:HA	11:Z:133:ARG:HE	1.56	0.69
13:N:286:LEU:O	13:N:290:HIS:ND1	2.26	0.69
6:K:232:ASP:OD2	6:Q:28:LYS:NZ	2.26	0.69
5:P:549:ASP:OD1	5:P:550:VAL:N	2.26	0.69
13:N:241:HIS:O	13:N:245:GLN:HG3	1.92	0.69
5:J:591:GLN:HA	5:J:594:ILE:HD12	1.75	0.69
11:Z:169:LEU:HA	11:Z:172:ILE:HD12	1.74	0.69
5:J:651:PHE:HE1	5:J:705:CYS:HB3	1.58	0.68
11:Y:335:ASN:OD1	11:Y:337:ASN:ND2	2.26	0.68
13:N:414:MET:HE1	13:N:417:LEU:HD23	1.75	0.68
1:A:356:PRO:O	10:V:242:GLN:NE2	2.26	0.68
11:Y:448:LYS:HD3	11:Y:464:LEU:HD21	1.73	0.68
5:P:707:PHE:CE2	5:P:738:LEU:HB3	2.29	0.68
6:Q:509:ARG:HD3	6:Q:512:ASP:HB2	1.74	0.68
10:U:161:LYS:HE3	10:U:166:GLU:HB2	1.74	0.68
12:I:177:VAL:HG12	12:I:208:LEU:HD13	1.76	0.68
9:O:459:GLN:NE2	12:I:493:GLU:O	2.26	0.67
1:A:1713:MET:HB2	1:A:1715:TRP:CD1	2.29	0.67
7:L:60:GLN:NE2	7:L:142:LEU:O	2.27	0.67
6:Q:518:MET:HE3	6:Q:518:MET:O	1.95	0.67
10:U:242:GLN:HE22	10:U:429:ARG:HE	1.41	0.67
1:A:1031:ASP:HB2	13:N:482:PRO:HB2	1.77	0.67
1:A:1150:ALA:HB1	1:A:1187:LYS:HE2	1.76	0.67
3:G:11:LEU:HD21	6:Q:456:ARG:HH12	1.60	0.67
1:A:443:CYS:HB3	1:A:452:LEU:HD21	1.75	0.67
10:V:237:ILE:O	10:V:241:LEU:HB2	1.95	0.67
9:O:521:ASN:HD21	9:O:658:LEU:HD22	1.60	0.67
2:D:20:LEU:HD21	9:O:252:GLU:HG2	1.75	0.67
11:Y:444:ALA:O	11:Y:448:LYS:HG3	1.95	0.67
1:A:352:ARG:NH1	10:V:339:ASN:OD1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:88:THR:HG23	10:V:44:ARG:HH22	1.58	0.67
11:Z:37:PHE:HB3	11:Z:41:GLN:HG3	1.77	0.67
1:A:1531:GLY:HA2	1:A:1565:LEU:HG	1.77	0.66
11:Y:476:VAL:O	11:Y:480:ILE:HG13	1.95	0.66
5:P:169:LYS:HB3	5:P:467:ARG:HH21	1.61	0.66
1:A:629:LEU:HD23	1:A:762:ILE:HD11	1.77	0.66
5:J:103:HIS:HB3	5:J:140:LYS:HE2	1.77	0.66
1:A:504:VAL:HG21	1:A:635:VAL:HG11	1.78	0.66
1:A:1574:LEU:O	1:A:1617:ARG:NH2	2.29	0.66
2:D:45:ALA:HA	10:U:378:MET:HE3	1.76	0.66
11:Y:232:LEU:HD21	11:Z:33:ASN:HB3	1.78	0.66
1:A:1753:TYR:O	9:O:639:GLN:NE2	2.27	0.66
8:M:35:GLU:OE2	8:M:35:GLU:N	2.21	0.66
9:O:105:LEU:HD11	9:O:151:VAL:HG12	1.77	0.66
11:Z:198:ASN:O	11:Z:201:TRP:NE1	2.28	0.66
9:O:649:GLU:HG2	12:I:369:MET:HG2	1.77	0.65
10:U:29:LEU:HB2	10:U:30:ARG:NH2	2.11	0.65
1:A:1897:PRO:HA	1:A:1900:LEU:HD12	1.77	0.65
7:L:96:VAL:HG21	7:L:122:VAL:HG11	1.77	0.65
11:Y:300:ILE:HA	11:Z:60:ARG:HG3	1.78	0.65
11:Y:515:MET:SD	11:Y:515:MET:N	2.70	0.65
11:Z:399:VAL:HG22	11:Z:409:THR:HG22	1.79	0.65
11:Z:257:VAL:HG11	11:Z:286:ARG:HH22	1.61	0.65
13:N:232:TRP:HB2	13:N:235:GLN:HE21	1.60	0.65
11:Y:53:LEU:HD21	11:Y:61:ASN:HB3	1.79	0.65
9:O:736:LEU:O	9:O:740:LEU:HD12	1.97	0.65
9:O:415:SER:HB2	9:O:451:LEU:HD12	1.79	0.65
5:P:488:LEU:HD23	5:P:505:ILE:HG13	1.78	0.65
11:Z:399:VAL:HG23	11:Z:403:LEU:HD13	1.78	0.65
11:Y:232:LEU:HB3	11:Z:29:MET:HE1	1.78	0.65
11:Y:162:LEU:HD23	11:Y:188:MET:HG2	1.78	0.64
5:J:486:ASN:OD1	5:J:490:HIS:NE2	2.30	0.64
9:O:694:LEU:HD11	9:O:716:PHE:HD2	1.62	0.64
6:Q:439:VAL:HG21	6:Q:448:LEU:HD21	1.78	0.64
1:A:733:SER:OG	9:O:719:ARG:NH1	2.30	0.64
7:L:12:ASP:HB3	7:L:15:GLN:HG2	1.79	0.64
1:A:506:VAL:HG22	1:A:639:VAL:HG22	1.79	0.64
11:Z:411:THR:HG21	11:Z:441:TYR:HE2	1.61	0.64
11:Y:435:LEU:HD12	11:Y:448:LYS:HE2	1.79	0.64
11:Y:449:ALA:HB1	11:Y:480:ILE:HG21	1.78	0.64
11:Z:23:SER:HB3	11:Z:49:HIS:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:ASP:OD1	1:A:983:LEU:N	2.30	0.64
9:O:106:LYS:O	10:U:344:ARG:NH2	2.30	0.64
1:A:928:GLU:HG3	1:A:970:TRP:HZ2	1.63	0.64
5:J:465:LEU:HG	5:J:469:MET:HE2	1.80	0.64
6:K:523:ILE:HG21	5:P:653:LEU:HD22	1.80	0.64
7:L:96:VAL:HG11	7:L:124:LEU:HD22	1.80	0.64
10:U:35:GLN:HB3	10:U:201:LEU:HD21	1.80	0.64
11:Y:23:SER:HB2	11:Y:49:HIS:HD2	1.63	0.64
11:Z:172:ILE:HG23	11:Z:185:VAL:HG11	1.80	0.63
9:O:79:TYR:O	9:O:83:GLU:HG2	1.99	0.63
11:Z:432:ASP:O	11:Z:436:THR:HG23	1.98	0.63
13:N:537:ARG:HH12	13:N:541:ASN:HB2	1.64	0.63
5:J:69:PRO:HB3	5:J:110:PHE:HA	1.80	0.63
5:J:543:LEU:HB2	5:J:552:LEU:HD13	1.78	0.63
6:Q:35:GLU:OE2	6:Q:63:ARG:NH1	2.28	0.63
12:I:269:LEU:HD23	12:I:526:LYS:HD3	1.80	0.63
1:A:774:LYS:NZ	1:A:809:ASP:OD2	2.30	0.63
5:P:465:LEU:HD11	5:P:469:MET:HE3	1.81	0.63
6:Q:476:PRO:HG2	10:U:182:LEU:HD22	1.81	0.63
11:Z:59:TYR:O	11:Z:63:VAL:HG23	1.99	0.63
11:Y:66:TYR:CD2	11:Y:108:MET:HB3	2.34	0.63
12:I:64:THR:HG22	12:I:84:LEU:HD11	1.80	0.63
13:N:374:LEU:HD22	13:N:416:ILE:HD11	1.79	0.63
1:A:1277:ILE:HG22	1:A:1363:THR:HG23	1.80	0.63
6:K:401:ASP:HB3	6:K:404:VAL:HG12	1.81	0.63
7:L:22:VAL:HB	7:L:159:TYR:HB3	1.81	0.62
1:A:249:LEU:HG	1:A:256:VAL:HG22	1.82	0.62
5:J:30:ARG:HH22	5:P:498:THR:HG21	1.64	0.62
11:Y:373:LEU:HD11	11:Y:412:LEU:HD22	1.80	0.62
1:A:1761:MET:HE3	9:O:638:GLU:HB2	1.80	0.62
6:Q:371:MET:HA	6:Q:374:ILE:HD12	1.81	0.62
11:Z:200:ASP:OD2	11:Z:201:TRP:N	2.33	0.62
6:Q:451:LEU:HB3	6:Q:467:TYR:HD2	1.65	0.62
13:N:349:ARG:HE	13:N:399:LEU:HD12	1.63	0.62
1:A:482:VAL:HG23	1:A:593:ASN:HA	1.82	0.62
3:G:4:ARG:N	6:Q:373:TYR:OH	2.32	0.62
6:K:35:GLU:HG3	6:K:40:ILE:HD11	1.82	0.62
10:U:106:LEU:HD11	10:U:117:LEU:HD23	1.82	0.62
1:A:1220:MET:HE2	1:A:1264:THR:HB	1.82	0.62
9:O:207:LEU:HB3	10:V:145:GLN:HE22	1.64	0.62
11:Z:458:TYR:O	11:Z:462:ILE:HG12	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:58:VAL:HA	11:Z:323:ARG:HH12	1.64	0.62
5:P:693:ASN:OD1	5:P:709:ARG:NH1	2.32	0.62
6:Q:179:GLN:NE2	6:Q:183:GLU:OE2	2.33	0.62
12:I:356:SER:HB3	12:I:397:ILE:HG12	1.82	0.62
9:O:648:ILE:HD12	9:O:663:ALA:HB1	1.82	0.61
12:I:231:VAL:HG12	12:I:556:LEU:HD13	1.82	0.61
10:U:475:LYS:O	10:U:479:GLN:NE2	2.33	0.61
1:A:1912:ALA:HB3	13:N:21:LEU:HD12	1.81	0.61
10:V:127:GLU:OE1	10:V:148:ASN:ND2	2.32	0.61
11:Y:5:ASP:OD1	11:Y:8:ARG:NH2	2.33	0.61
11:Y:257:VAL:O	11:Y:261:GLU:HG3	2.00	0.61
13:N:407:LEU:HB2	13:N:417:LEU:HD13	1.82	0.61
5:P:32:TYR:OH	5:P:64:HIS:NE2	2.32	0.61
13:N:129:LEU:HD11	13:N:150:ARG:HA	1.81	0.61
6:K:81:TYR:HD2	6:K:139:ILE:HG12	1.65	0.61
7:L:68:PHE:HE2	7:L:137:ILE:HD12	1.66	0.61
1:A:1306:CYS:HB2	1:A:1374:ILE:HG12	1.83	0.61
12:I:327:VAL:HG22	12:I:425:MET:HB3	1.82	0.61
7:L:70:ARG:HG2	7:L:71:LYS:H	1.66	0.61
7:L:173:CYS:HB3	7:L:178:PHE:HB3	1.81	0.61
11:Z:284:GLU:OE1	11:Z:286:ARG:NH2	2.34	0.61
12:I:29:SER:O	12:I:725:ASN:ND2	2.33	0.61
12:I:251:MET:HE2	12:I:381:LEU:HG	1.81	0.61
6:K:85:GLU:OE2	6:K:88:GLN:NE2	2.34	0.61
6:Q:401:ASP:O	6:Q:405:MET:HB3	2.01	0.61
11:Z:281:LEU:HD21	11:Z:289:ASP:HB3	1.83	0.61
12:I:338:GLU:OE1	12:I:415:LYS:NZ	2.34	0.61
11:Y:46:LEU:HD22	11:Y:69:ALA:HB2	1.82	0.61
5:J:162:PRO:HB2	5:J:474:LEU:HD21	1.82	0.60
5:P:714:PHE:HD2	5:P:746:VAL:HG22	1.65	0.60
13:N:623:CYS:SG	13:N:637:TRP:NE1	2.68	0.60
5:P:517:GLN:OE1	5:P:520:ARG:NH1	2.34	0.60
11:Y:253:ASN:HB3	11:Y:280:LEU:HD11	1.83	0.60
12:I:11:PHE:O	12:I:712:ARG:NH1	2.34	0.60
1:A:808:ARG:NH2	1:A:1894:VAL:O	2.28	0.60
5:J:466:LEU:HA	5:J:469:MET:HE3	1.82	0.60
11:Y:29:MET:SD	11:Z:232:LEU:HB3	2.41	0.60
13:N:571:ASN:ND2	13:N:593:ALA:O	2.26	0.60
8:M:17:ASP:O	8:M:21:GLU:HG3	2.01	0.60
11:Z:181:LYS:HE2	11:Z:183:ALA:HB3	1.84	0.60
9:O:103:GLY:O	9:O:155:TYR:OH	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:497:ILE:HB	10:V:504:VAL:HG21	1.84	0.60
12:I:206:LEU:HD11	12:I:222:GLU:HB2	1.82	0.60
13:N:386:LEU:HD22	13:N:399:LEU:HD22	1.83	0.60
6:Q:254:THR:O	6:Q:258:MET:HG2	2.02	0.60
10:V:30:ARG:O	10:V:34:LYS:HG3	2.01	0.60
11:Y:137:ILE:HD12	11:Y:138:ASN:N	2.16	0.60
13:N:429:ARG:N	13:N:509:TYR:OH	2.35	0.60
7:L:154:ARG:O	7:L:155:GLN:NE2	2.35	0.59
9:O:207:LEU:O	10:V:145:GLN:NE2	2.35	0.59
1:A:591:VAL:HG22	1:A:606:ARG:NH2	2.17	0.59
5:J:107:VAL:HG22	5:J:144:LEU:HD21	1.83	0.59
10:V:255:ILE:HD13	10:V:260:SER:HA	1.84	0.59
11:Y:349:LEU:HD13	11:Y:357:GLU:HB2	1.84	0.59
5:J:641:LEU:HA	5:J:644:ILE:HG22	1.84	0.59
5:P:748:LYS:HG2	5:P:756:ALA:HB1	1.83	0.59
12:I:303:GLU:HB3	12:I:317:LEU:HD12	1.84	0.59
7:L:43:ASP:O	7:L:47:ASP:HB2	2.02	0.59
1:A:1267:ARG:NH1	1:A:1315:GLY:O	2.36	0.59
1:A:1431:PRO:HG2	1:A:1434:ILE:HG13	1.83	0.59
10:V:388:TYR:O	10:V:392:ILE:HD12	2.02	0.59
11:Y:393:MET:HA	11:Y:393:MET:HE3	1.85	0.59
1:A:274:VAL:HG22	1:A:408:CYS:HB3	1.85	0.59
1:A:1381:ARG:NH2	1:A:1418:ASP:OD2	2.36	0.59
13:N:297:VAL:HG21	13:N:325:ARG:HB2	1.85	0.59
1:A:411:HIS:NE2	1:A:414:THR:OG1	2.31	0.59
6:K:354:MET:HE3	6:K:354:MET:HA	1.83	0.59
5:P:53:LYS:HG2	5:P:56:LYS:HD2	1.85	0.59
11:Y:359:ILE:O	11:Y:363:ARG:HG3	2.02	0.59
11:Z:49:HIS:O	11:Z:49:HIS:ND1	2.35	0.59
5:P:46:THR:O	5:P:50:ARG:HG2	2.03	0.59
5:P:465:LEU:O	5:P:469:MET:HG2	2.03	0.59
5:P:702:ASN:ND2	5:P:705:CYS:SG	2.75	0.59
11:Z:383:TYR:OH	11:Z:391:GLU:HB3	2.02	0.59
1:A:1016:MET:SD	1:A:1084:ARG:HG3	2.43	0.59
1:A:1599:ASN:HD22	1:A:1603:LEU:HD12	1.68	0.59
6:Q:477:GLN:OE1	10:U:148:ASN:ND2	2.36	0.59
13:N:512:LYS:O	13:N:516:ILE:HG12	2.02	0.59
5:J:610:GLU:O	5:J:614:THR:HG22	2.02	0.58
6:Q:6:LEU:HG	6:Q:29:VAL:HG22	1.84	0.58
12:I:664:ARG:NH1	12:I:719:ALA:O	2.36	0.58
13:N:393:THR:HA	13:N:396:ILE:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:175:THR:HG23	7:L:178:PHE:H	1.68	0.58
1:A:1864:GLY:O	1:A:1868:VAL:HG12	2.03	0.58
5:P:728:GLU:HA	11:Z:152:ARG:HH22	1.68	0.58
10:U:423:ARG:HG3	10:U:423:ARG:HH11	1.67	0.58
1:A:1736:GLU:HG3	1:A:1756:LYS:HE2	1.84	0.58
6:Q:429:LEU:O	6:Q:432:ILE:HG22	2.04	0.58
10:V:180:ARG:NH2	10:V:208:GLU:OE2	2.35	0.58
11:Y:109:ALA:O	11:Y:113:THR:HG23	2.04	0.58
11:Y:465:LEU:HD21	11:Y:480:ILE:HB	1.83	0.58
11:Z:240:LEU:HD11	11:Z:262:GLN:HE22	1.67	0.58
12:I:321:LEU:HG	12:I:425:MET:HE1	1.84	0.58
5:P:684:LYS:NZ	5:P:686:GLU:OE1	2.30	0.58
6:Q:325:LYS:HE2	6:Q:329:LEU:HD21	1.85	0.58
12:I:9:PRO:HG2	12:I:750:ASP:HB3	1.84	0.58
13:N:375:LEU:HD21	13:N:416:ILE:HG13	1.86	0.58
1:A:497:LEU:HD11	1:A:587:ILE:HD11	1.85	0.58
1:A:761:ALA:O	1:A:765:VAL:HG22	2.03	0.58
10:V:96:VAL:HG23	10:V:98:GLU:HG3	1.85	0.58
1:A:880:TYR:HB2	1:A:930:LEU:HD22	1.86	0.58
1:A:1016:MET:HE3	1:A:1038:ARG:HA	1.86	0.58
9:O:41:LEU:HD13	9:O:132:VAL:HG13	1.86	0.58
1:A:1023:VAL:O	1:A:1027:ILE:HG13	2.04	0.58
9:O:435:SER:HB3	9:O:654:ASP:HB3	1.84	0.58
13:N:98:CYS:HA	13:N:110:LEU:HD23	1.86	0.58
9:O:97:ILE:HD11	9:O:158:LEU:HD11	1.84	0.58
11:Y:357:GLU:O	11:Y:361:HIS:ND1	2.36	0.58
12:I:117:GLU:O	12:I:579:LYS:NZ	2.34	0.58
1:A:76:LEU:HD12	1:A:589:ASP:HB3	1.84	0.58
1:A:1635:GLU:HB2	1:A:1669:LYS:HD2	1.86	0.58
9:O:344:LEU:HD22	9:O:359:VAL:HG21	1.85	0.58
5:P:522:PHE:HB3	5:P:539:TYR:CD2	2.39	0.58
12:I:393:VAL:O	12:I:397:ILE:HG13	2.04	0.58
5:J:42:PHE:HB2	5:J:71:CYS:SG	2.44	0.57
11:Z:203:SER:O	11:Z:207:LYS:HG2	2.04	0.57
11:Z:350:ARG:NE	11:Z:382:CYS:SG	2.76	0.57
11:Z:355:VAL:O	11:Z:359:ILE:HG13	2.04	0.57
12:I:25:PHE:HD2	12:I:71:LEU:HB2	1.69	0.57
6:K:174:HIS:NE2	6:K:211:LYS:HD2	2.20	0.57
11:Y:394:VAL:HA	11:Y:397:ASN:HD21	1.69	0.57
5:J:538:ILE:O	5:J:542:THR:HG23	2.05	0.57
7:L:73:THR:O	7:L:160:THR:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:207:ASN:HD21	6:Q:233:VAL:HG13	1.69	0.57
10:V:370:LEU:O	10:V:374:GLU:HG2	2.05	0.57
11:Z:431:LEU:HD11	11:Z:447:LYS:HG3	1.87	0.57
13:N:220:LEU:HA	13:N:227:ASP:HA	1.85	0.57
5:P:130:ARG:HD2	5:P:133:LYS:HD2	1.85	0.57
11:Y:108:MET:HE3	11:Y:112:TYR:CE2	2.39	0.57
1:A:1095:VAL:HG23	1:A:1098:GLU:HB2	1.86	0.57
2:D:48:ASP:N	2:D:48:ASP:OD1	2.36	0.57
10:V:322:ASN:O	10:V:326:ILE:HG13	2.05	0.57
11:Y:4:ILE:HG21	11:Y:41:GLN:HG2	1.87	0.57
11:Y:377:GLU:O	11:Y:381:GLU:HG2	2.04	0.57
11:Y:431:LEU:HD21	11:Y:448:LYS:HG2	1.87	0.57
13:N:221:CYS:N	13:N:226:SER:O	2.35	0.57
11:Y:425:GLU:HA	11:Y:428:LYS:HD2	1.86	0.57
9:O:435:SER:H	9:O:654:ASP:HB3	1.69	0.57
11:Y:218:SER:HA	11:Y:221:ILE:HD12	1.87	0.57
11:Y:235:ASP:HB3	11:Y:266:LEU:HD21	1.86	0.57
11:Z:217:ASN:O	11:Z:221:ILE:HG23	2.05	0.57
7:L:82:ASP:HA	7:L:117:SER:HA	1.86	0.57
10:U:33:LYS:HE2	10:U:64:ALA:HA	1.87	0.57
1:A:612:ILE:HD13	1:A:642:TYR:HD1	1.69	0.57
5:J:149:TRP:NE1	5:J:153:GLU:OE1	2.35	0.57
11:Y:24:SER:HB3	11:Y:49:HIS:HE2	1.69	0.57
11:Z:466[A]:ARG:HE	11:Z:481:LEU:HD11	1.70	0.57
1:A:1032:LEU:HD12	13:N:483:ASP:HB2	1.86	0.56
10:V:34:LYS:NZ	10:V:69:GLU:O	2.27	0.56
10:V:449:LEU:HD12	10:V:476:LEU:HD11	1.86	0.56
11:Y:441:TYR:HD2	11:Y:444:ALA:H	1.53	0.56
9:O:446:LEU:O	9:O:460:GLN:NE2	2.38	0.56
6:Q:451:LEU:HB3	6:Q:467:TYR:CD2	2.39	0.56
11:Y:260:PHE:HB3	11:Y:277:TYR:CD1	2.41	0.56
11:Z:102:ILE:HG13	11:Z:103:GLU:N	2.19	0.56
12:I:185:ILE:HD11	12:I:201:ILE:HG13	1.86	0.56
1:A:1255:VAL:HG21	1:A:1606:LEU:HD11	1.86	0.56
1:A:1634:LEU:O	1:A:1650:GLU:HA	2.05	0.56
5:P:126:CYS:SG	5:P:158:ILE:HD11	2.44	0.56
6:Q:146:ARG:O	6:Q:150:THR:HG23	2.06	0.56
6:Q:177:THR:HG22	6:Q:180:GLU:HB2	1.86	0.56
11:Z:400:TYR:HA	11:Z:409:THR:HB	1.86	0.56
12:I:61:ASN:CG	12:I:62:GLU:H	2.13	0.56
13:N:267:GLN:O	13:N:271:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:LEU:HD11	1:A:937:VAL:HG11	1.88	0.56
5:J:522:PHE:HA	5:J:525:VAL:HG12	1.87	0.56
7:L:37:LYS:HG3	7:L:38:PRO:HD2	1.88	0.56
10:V:34:LYS:NZ	10:V:69:GLU:OE2	2.36	0.56
10:V:133:GLU:N	10:V:133:GLU:OE1	2.39	0.56
10:V:213:ILE:HD11	10:V:222:LEU:HD12	1.87	0.56
11:Z:100:SER:O	11:Z:104:VAL:HG23	2.05	0.56
4:H:72:HIS:O	4:H:76:VAL:HG23	2.06	0.56
11:Z:352:MET:SD	11:Z:354:ARG:NH2	2.78	0.56
13:N:104:GLU:OE2	13:N:175:ARG:NH2	2.37	0.56
1:A:1564:LEU:HD23	1:A:1567:LEU:HD13	1.87	0.56
5:P:736:GLU:OE1	5:P:736:GLU:N	2.38	0.56
6:Q:441:VAL:HG21	6:Q:444:TRP:HD1	1.70	0.56
10:U:185:VAL:HG13	10:U:212:LEU:HD22	1.86	0.56
11:Y:274:MET:HB3	11:Y:297:LEU:HD11	1.88	0.56
12:I:717:MET:HG3	12:I:719:ALA:HB2	1.86	0.56
13:N:181:LEU:HD23	13:N:268:VAL:HG21	1.86	0.56
5:J:38:GLU:HG3	5:J:66:CYS:HB2	1.87	0.56
5:P:158:ILE:HG22	5:P:160:GLU:H	1.70	0.56
6:Q:161:VAL:HG13	6:Q:162:TYR:HD2	1.71	0.56
11:Y:339:VAL:O	11:Y:343:LEU:HG	2.05	0.56
13:N:386:LEU:HD12	13:N:391:VAL:HG11	1.88	0.56
1:A:985:LYS:O	1:A:989:GLU:HG2	2.06	0.56
5:J:138:TYR:HD1	5:J:151:PRO:HB3	1.71	0.56
10:U:520:TYR:HB3	10:U:529:ALA:HB2	1.88	0.56
11:Z:38:SER:O	11:Z:42:LYS:HG3	2.05	0.56
9:O:644:LEU:HD11	9:O:666:LEU:HG	1.88	0.56
13:N:162:PHE:O	13:N:255:ARG:NH2	2.37	0.56
1:A:851:CYS:SG	1:A:882:LEU:HD11	2.46	0.55
9:O:44:MET:HG3	9:O:89:LEU:HD21	1.88	0.55
11:Y:274:MET:HG3	11:Y:297:LEU:HD21	1.88	0.55
7:L:45:LEU:HD21	7:L:153:MET:HG2	1.88	0.55
5:P:605:THR:HG21	5:P:636:ASN:HB3	1.89	0.55
11:Y:118:ASP:OD1	11:Y:118:ASP:N	2.39	0.55
12:I:125:LEU:HD21	12:I:249:THR:HG21	1.87	0.55
11:Z:259:LYS:HA	11:Z:262:GLN:HE21	1.72	0.55
1:A:1525:MET:SD	1:A:1588:LEU:HD13	2.47	0.55
1:A:1540:ARG:HG3	1:A:1540:ARG:HH11	1.72	0.55
1:A:1625:ASP:OD2	1:A:1700:LYS:NZ	2.40	0.55
6:Q:341:GLY:HA3	6:Q:357:TYR:CE1	2.41	0.55
10:V:244:ILE:HG21	10:V:276:ILE:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:5:ASP:OD1	11:Z:8:ARG:NH2	2.39	0.55
5:P:707:PHE:HE2	5:P:738:LEU:HB3	1.70	0.55
11:Z:161:VAL:O	11:Z:165:CYS:HB3	2.07	0.55
12:I:734:LEU:HD12	12:I:741:VAL:HG12	1.89	0.55
7:L:78:CYS:SG	7:L:157:LYS:HB2	2.47	0.55
11:Y:27:LEU:O	11:Y:31:ASN:ND2	2.40	0.55
11:Y:359:ILE:HG22	11:Y:363:ARG:HE	1.72	0.55
11:Z:140:MET:HA	11:Z:143:ASN:HD21	1.72	0.55
13:N:262:THR:O	13:N:266:HIS:ND1	2.39	0.55
10:V:26:PHE:HE1	10:V:228:TRP:HE3	1.55	0.55
11:Y:469:LEU:HD12	11:Y:473:SER:HA	1.88	0.55
9:O:536:THR:HB	9:O:543:GLY:HA3	1.88	0.55
11:Y:65:LYS:HA	11:Y:68:MET:HG3	1.89	0.55
1:A:430:VAL:HG13	1:A:444:PHE:HB3	1.89	0.55
1:A:953:LEU:HD22	1:A:1817:VAL:HG22	1.89	0.55
5:J:605:THR:HG23	5:J:606:LEU:HD22	1.89	0.55
6:K:212:TYR:OH	6:K:368:HIS:ND1	2.40	0.55
9:O:727:THR:HG22	9:O:731:ASN:HD21	1.71	0.55
10:V:301:ASP:OD1	10:V:301:ASP:N	2.38	0.55
1:A:1100:LEU:HD13	1:A:1147:ILE:HD11	1.89	0.54
6:K:338:ILE:HD11	6:K:370:PRO:HG3	1.89	0.54
6:Q:461:TYR:HD2	6:Q:492:MET:HG2	1.72	0.54
11:Z:296:ARG:O	11:Z:300:ILE:HG12	2.07	0.54
11:Z:373:LEU:O	11:Z:377:GLU:HG3	2.07	0.54
6:K:212:TYR:HH	6:K:368:HIS:HD1	1.55	0.54
12:I:598:MET:HE1	12:I:669:LEU:HD21	1.89	0.54
13:N:504:LEU:O	13:N:508:ILE:HG23	2.07	0.54
6:K:165:GLU:HG2	6:Q:20:GLN:HB3	1.89	0.54
10:V:290:ARG:NH2	10:V:322:ASN:OD1	2.34	0.54
13:N:83:LEU:HA	13:N:87:ILE:HB	1.89	0.54
13:N:351:PHE:CE1	13:N:409:VAL:HG11	2.42	0.54
1:A:1875:GLN:N	1:A:1875:GLN:OE1	2.40	0.54
10:U:467:LYS:NZ	10:U:506:HIS:HB3	2.23	0.54
13:N:626:TYR:CE2	13:N:635:LEU:HG	2.41	0.54
1:A:170:ILE:HG21	10:V:427:GLN:HB2	1.90	0.54
11:Y:105:LYS:HA	11:Y:108:MET:CG	2.38	0.54
11:Y:305:ALA:O	11:Y:309:VAL:HG23	2.08	0.54
12:I:601:LEU:HB2	12:I:615:LEU:HD13	1.89	0.54
12:I:692:ARG:NH1	12:I:695:GLU:OE1	2.41	0.54
10:V:471:VAL:HG11	10:V:508:GLU:HG3	1.90	0.54
13:N:537:ARG:NH1	13:N:541:ASN:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1595:HIS:CE1	1:A:1598:ASP:HB2	2.43	0.54
5:J:97:PHE:CD2	11:Y:252:ASP:HB3	2.42	0.54
5:J:626:ASN:O	5:J:630:VAL:HG13	2.08	0.54
6:K:368:HIS:HA	6:K:371:MET:HE3	1.88	0.54
10:U:410:GLU:HB2	10:U:418:CYS:SG	2.47	0.54
10:V:216:LYS:HD3	10:V:243:LEU:HD11	1.89	0.54
11:Z:372:ARG:HH21	11:Z:374:ASP:HB2	1.73	0.54
13:N:31:LEU:O	13:N:128:SER:OG	2.22	0.54
1:A:252:ASP:HB2	1:A:253:PRO:HD3	1.90	0.54
12:I:282:GLN:HB2	12:I:337:ILE:HD11	1.90	0.54
12:I:640:ASP:OD1	12:I:641:ALA:N	2.40	0.54
13:N:535:PRO:O	13:N:539:ILE:HG23	2.08	0.54
1:A:768:LEU:HD21	1:A:861:PRO:HB2	1.90	0.54
9:O:57:ARG:HH21	12:I:306:HIS:HE1	1.53	0.54
10:V:58:LEU:O	10:V:61:SER:OG	2.26	0.54
5:J:617:LEU:HG	5:J:644:ILE:HG13	1.90	0.54
11:Y:19:VAL:HG23	11:Y:52:SER:HB3	1.90	0.54
11:Z:465:LEU:HD21	11:Z:480:ILE:HB	1.90	0.54
12:I:254:LYS:O	12:I:258:ILE:HG12	2.08	0.54
1:A:1672:ARG:NH1	1:A:1706:LEU:O	2.41	0.53
5:P:53:LYS:HB3	5:P:56:LYS:HB2	1.89	0.53
11:Z:41:GLN:O	11:Z:45:LEU:HG	2.08	0.53
13:N:83:LEU:HB3	13:N:160:VAL:HG11	1.91	0.53
1:A:862:TYR:CZ	1:A:864:PRO:HA	2.43	0.53
1:A:1131:MET:HG2	1:A:1132:THR:HG23	1.90	0.53
5:J:645:TYR:HE2	11:Y:495:MET:HE1	1.73	0.53
6:K:19:TYR:HB3	6:K:50:THR:HG22	1.90	0.53
5:P:758:MET:HE1	11:Z:398:ASN:HB2	1.91	0.53
10:U:29:LEU:HB2	10:U:30:ARG:HH21	1.70	0.53
10:V:381:THR:HG21	10:V:412:LEU:HD11	1.90	0.53
11:Y:479:ARG:HD2	11:Y:510:LYS:HB3	1.90	0.53
11:Z:3:VAL:O	11:Z:7:VAL:HG23	2.08	0.53
11:Z:156:THR:O	11:Z:160:GLU:HG3	2.08	0.53
5:J:515:TYR:HB3	5:J:546:LEU:HD11	1.91	0.53
7:L:170:PHE:HB3	5:P:738:LEU:HD21	1.90	0.53
6:Q:276:VAL:HA	6:Q:311:MET:HE2	1.90	0.53
11:Z:257:VAL:HG13	11:Z:277:TYR:HE1	1.73	0.53
1:A:728:LEU:HD13	9:O:716:PHE:HE1	1.73	0.53
1:A:765:VAL:HG12	1:A:863:LEU:HD21	1.90	0.53
11:Z:227:LEU:HA	11:Z:230:LYS:HE3	1.89	0.53
12:I:683:TYR:CE2	12:I:703:ARG:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:GLN:HB2	1:A:1833:HIS:NE2	2.24	0.53
13:N:400:TYR:HE1	13:N:421:CYS:HG	1.55	0.53
6:K:90:LEU:HD21	6:K:140:TYR:CE1	2.44	0.53
9:O:44:MET:HE2	12:I:310:TRP:HZ2	1.74	0.53
11:Y:257:VAL:HA	11:Y:260:PHE:HD1	1.73	0.53
10:V:493:TYR:O	10:V:497:ILE:HG23	2.08	0.53
12:I:425:MET:O	12:I:429:THR:HG22	2.09	0.53
1:A:489:LEU:HD21	1:A:509:VAL:HG21	1.90	0.53
4:H:61:TYR:HD1	11:Z:326:TYR:CG	2.26	0.53
7:L:105:LEU:HD21	7:L:136:MET:HG2	1.89	0.53
5:P:92:LEU:HD22	5:P:120:LEU:HD23	1.91	0.53
10:U:190:ASP:O	10:U:194:GLU:HG3	2.09	0.53
1:A:77:ARG:NE	1:A:91:GLU:OE2	2.32	0.53
6:K:519:LEU:O	6:K:523:ILE:HG12	2.09	0.53
11:Y:362:PHE:HB2	11:Y:379:LEU:HD13	1.90	0.53
1:A:100:VAL:HG21	1:A:153:ILE:HG12	1.91	0.53
9:O:378:SER:HB3	9:O:409:HIS:CE1	2.43	0.53
5:P:93:SER:HB2	5:P:106:ILE:HD11	1.91	0.53
10:U:327:ASP:O	10:U:333:THR:HG21	2.09	0.53
10:V:429:ARG:HG2	10:V:432:ASP:HB2	1.91	0.53
11:Z:7:VAL:HG22	11:Z:22:LEU:HD21	1.90	0.53
11:Z:306:GLU:HA	11:Z:309:VAL:HG22	1.90	0.53
1:A:449:GLN:OE1	1:A:453:ARG:NH2	2.42	0.52
1:A:1527:MET:HE2	1:A:1532:ASN:HD22	1.73	0.52
7:L:113:LEU:HB3	7:L:116:PRO:HG3	1.91	0.52
10:U:253:ASN:O	10:U:257:VAL:HG13	2.09	0.52
1:A:632:GLU:HG2	1:A:633:ILE:N	2.24	0.52
5:J:79:CYS:SG	5:J:87:GLU:HB2	2.48	0.52
5:J:125:TYR:HD1	5:J:130:ARG:HE	1.57	0.52
6:K:264:HIS:CE1	6:K:266:SER:HB3	2.44	0.52
7:L:21:THR:HG23	7:L:22:VAL:HG13	1.89	0.52
12:I:750:ASP:OD2	12:I:751:GLU:N	2.41	0.52
1:A:27:HIS:HB3	1:A:101:ILE:HD13	1.91	0.52
7:L:177:ASP:OD2	11:Z:119:LYS:NZ	2.34	0.52
9:O:489:VAL:HG23	12:I:507:LEU:HD11	1.90	0.52
9:O:562:LYS:O	9:O:566:LYS:HG3	2.10	0.52
11:Y:176:LEU:HD21	11:Y:185:VAL:HG21	1.89	0.52
12:I:557:TYR:HA	12:I:694:ASP:HB2	1.91	0.52
1:A:1267:ARG:NE	1:A:1271:GLU:OE2	2.39	0.52
5:J:113:SER:O	5:J:117:THR:HG23	2.09	0.52
5:J:549:ASP:OD1	5:J:549:ASP:N	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:37:PRO:HA	6:K:65:LEU:HD21	1.92	0.52
9:O:504:ALA:HA	9:O:507:TRP:CD1	2.45	0.52
5:P:55:TYR:HA	5:P:82:LEU:HD21	1.91	0.52
6:Q:263:PHE:HE2	6:Q:294:LEU:HD13	1.74	0.52
11:Y:18:ASN:OD1	11:Z:170:ASP:N	2.37	0.52
13:N:626:TYR:OH	13:N:633:ARG:HB3	2.10	0.52
1:A:614:THR:O	9:O:556:GLN:NE2	2.43	0.52
1:A:884:ASP:OD1	1:A:884:ASP:N	2.42	0.52
1:A:1197:LEU:HD12	1:A:1227:LEU:HD11	1.91	0.52
1:A:1552:TYR:OH	1:A:1604:GLN:NE2	2.42	0.52
5:J:662:LEU:HD12	5:J:704:LEU:HD13	1.90	0.52
6:K:402:PRO:HG3	6:K:431:LYS:HB3	1.90	0.52
5:P:472:GLY:HA3	5:P:488:LEU:HD13	1.92	0.52
12:I:214:LEU:O	12:I:238:THR:OG1	2.27	0.52
5:J:164:PRO:HB2	5:J:471:LYS:HG3	1.92	0.52
9:O:73:ILE:O	9:O:161:TYR:OH	2.21	0.52
9:O:378:SER:HB3	9:O:409:HIS:HE1	1.75	0.52
12:I:417:PHE:HA	12:I:448:VAL:HG22	1.91	0.52
9:O:109:GLU:HB2	10:U:344:ARG:NH2	2.25	0.52
5:P:482:LYS:HE2	5:P:667:GLN:HE22	1.75	0.52
10:U:385:ILE:O	10:U:389:ARG:HG3	2.10	0.52
12:I:586:LEU:HD23	12:I:601:LEU:HD23	1.92	0.52
1:A:1201:HIS:HB3	1:A:1204:THR:HB	1.91	0.52
5:J:624:PHE:O	5:J:628:ILE:HG13	2.10	0.52
9:O:625:LEU:HD22	9:O:666:LEU:HD23	1.91	0.52
5:P:721:SER:O	5:P:724:GLN:HG2	2.10	0.52
10:V:295:TYR:HA	10:V:326:ILE:HD13	1.92	0.52
11:Y:7:VAL:HG12	11:Y:48:TYR:HD2	1.75	0.52
11:Z:261:GLU:O	11:Z:264:GLN:NE2	2.43	0.52
11:Z:458:TYR:HD1	11:Z:484:PHE:HD1	1.58	0.52
1:A:116:ALA:O	9:O:267:VAL:HG23	2.10	0.52
1:A:250:ASN:HD22	1:A:432:ILE:HD12	1.75	0.52
6:K:357:TYR:HB3	6:K:374:ILE:HG13	1.91	0.52
11:Z:15:LEU:HD23	11:Z:15:LEU:H	1.74	0.52
1:A:111:LEU:H	9:O:508:MET:HE2	1.75	0.52
5:J:533:VAL:HG23	5:J:559:LEU:HD22	1.91	0.52
11:Y:277:TYR:HD2	11:Y:293:LEU:HD22	1.75	0.52
13:N:412:PRO:HB2	13:N:486:ASP:HB2	1.92	0.52
13:N:560:MET:HE3	13:N:601:TRP:CE2	2.44	0.52
13:N:598:SER:HB3	14:C:13:THR:HB	1.91	0.52
3:G:17:GLU:HA	3:G:20:GLU:CD	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:153:TYR:HB2	6:K:170:LEU:HD21	1.92	0.51
6:K:167:PHE:CZ	6:K:209:LEU:HD13	2.46	0.51
5:P:49:TYR:OH	5:P:81:ASP:OD2	2.23	0.51
6:Q:354:MET:HE3	6:Q:377:GLU:HB3	1.92	0.51
11:Y:406:ASN:O	11:Y:410:LEU:HG	2.10	0.51
13:N:365:LEU:HD11	13:N:374:LEU:HD13	1.91	0.51
13:N:435:VAL:O	13:N:439:VAL:HG13	2.11	0.51
1:A:1914:LEU:HD21	1:A:1935:LEU:HB3	1.93	0.51
5:J:656:MET:HG3	11:Y:492:GLN:HB2	1.92	0.51
6:K:90:LEU:HD21	6:K:140:TYR:HE1	1.75	0.51
6:K:500:ASP:O	6:K:504:THR:HG23	2.10	0.51
10:U:373:HIS:ND1	10:U:388:TYR:OH	2.38	0.51
1:A:514:LEU:HD21	1:A:605:VAL:HG11	1.93	0.51
6:K:171:THR:HG21	6:K:209:LEU:HD11	1.92	0.51
10:U:38:LEU:HB3	10:U:71:GLN:HE22	1.76	0.51
1:A:1797:ILE:HD13	1:A:1851:THR:HG21	1.93	0.51
5:J:600:TYR:HD2	5:J:603:ALA:HB2	1.75	0.51
8:M:31:ILE:HD13	6:Q:302:TRP:HZ3	1.75	0.51
9:O:653:ALA:HB2	12:I:368:GLY:HA3	1.90	0.51
10:V:333:THR:O	10:V:337:ILE:HG12	2.10	0.51
13:N:570:ILE:HA	13:N:573:ASN:HD21	1.76	0.51
13:N:595:ILE:HD12	14:C:12:ALA:HB3	1.93	0.51
1:A:819:GLN:NE2	1:A:820:VAL:O	2.44	0.51
10:U:471:VAL:HG21	10:U:508:GLU:HG3	1.90	0.51
11:Z:242:SER:O	11:Z:246:LEU:HG	2.11	0.51
11:Z:411:THR:HG21	11:Z:441:TYR:CE2	2.44	0.51
1:A:1086:MET:HG3	1:A:1610:TYR:CZ	2.46	0.51
1:A:1815:LYS:O	1:A:1819:GLU:HG3	2.10	0.51
12:I:434:LEU:HD12	12:I:435:PRO:HD2	1.92	0.51
13:N:534:SER:HB2	13:N:537:ARG:HB3	1.92	0.51
1:A:1865:ASP:HB3	1:A:1934:LEU:HD21	1.93	0.51
5:J:613:LEU:HD12	5:J:679:GLN:HG2	1.93	0.51
5:J:653:LEU:HA	5:J:656:MET:HE3	1.92	0.51
6:Q:133:CYS:HB3	6:Q:156:ALA:HB2	1.92	0.51
11:Y:465:LEU:HD11	11:Y:477:LEU:HD22	1.93	0.51
11:Z:362:PHE:O	11:Z:366:ILE:HG23	2.10	0.51
1:A:1485:PHE:CG	6:K:552:MET:HE1	2.45	0.51
5:J:673:CYS:O	5:J:677:VAL:HG23	2.10	0.51
8:M:35:GLU:C	6:Q:325:LYS:HZ2	2.19	0.51
6:Q:320:ARG:NH1	6:Q:343:SER:OG	2.44	0.51
1:A:1871:TYR:CZ	1:A:1889:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:93:SER:O	5:P:93:SER:OG	2.26	0.51
11:Z:275:ASP:HB2	11:Z:306:GLU:HG3	1.93	0.51
1:A:1930:ARG:HH22	13:N:77:GLU:CD	2.17	0.51
4:H:82:LEU:O	4:H:85:LEU:HG	2.10	0.51
6:K:473:VAL:HG23	5:P:130:ARG:HH12	1.75	0.51
10:U:289:LEU:HD11	10:U:296:ARG:HD3	1.92	0.51
10:V:106:LEU:HB3	10:V:118:TYR:HB2	1.92	0.51
11:Z:394:VAL:HA	11:Z:397:ASN:HD21	1.76	0.51
12:I:21:GLN:HG2	12:I:41:ALA:HB2	1.92	0.51
13:N:540:ARG:O	13:N:543:GLU:HG3	2.11	0.51
1:A:121:SER:HB2	1:A:155:GLN:NE2	2.23	0.50
1:A:133:ILE:HG22	1:A:146:GLU:HA	1.92	0.50
6:K:372:LEU:HD13	6:K:404:VAL:HG23	1.92	0.50
10:V:464:ASP:OD1	10:V:464:ASP:N	2.38	0.50
10:V:528:GLU:HA	10:V:531:THR:HG22	1.93	0.50
11:Y:133:ARG:HB3	11:Y:137:ILE:HD11	1.93	0.50
11:Z:43:TYR:HB2	11:Z:72:GLN:HG2	1.92	0.50
1:A:434:SER:HB2	1:A:440:LYS:HD3	1.91	0.50
1:A:942:ARG:NH1	9:O:603:MET:SD	2.85	0.50
9:O:91:ASN:O	9:O:95:ILE:HG23	2.12	0.50
9:O:467:ALA:HB1	9:O:506:LEU:HD11	1.93	0.50
6:Q:213:ASN:OD1	6:Q:214:LYS:N	2.45	0.50
10:U:432:ASP:HB2	10:U:435:MET:HE1	1.93	0.50
13:N:180:PHE:HB2	13:N:240:PHE:CE2	2.47	0.50
1:A:188:LEU:HD11	1:A:223:LEU:HD13	1.93	0.50
1:A:490:VAL:HG13	1:A:498:VAL:HG23	1.92	0.50
1:A:625:ILE:HG12	1:A:762:ILE:HD12	1.92	0.50
1:A:1119:ASP:OD1	1:A:1120:LEU:N	2.45	0.50
5:P:742:LEU:O	5:P:746:VAL:HG23	2.11	0.50
11:Y:301:SER:HB2	11:Y:304:HIS:ND1	2.26	0.50
11:Z:328:GLY:O	11:Z:332:ILE:HG22	2.12	0.50
12:I:211:SER:OG	12:I:213:ASP:OD1	2.24	0.50
12:I:674:VAL:HA	12:I:703:ARG:HD3	1.93	0.50
1:A:1209:LEU:HD22	1:A:1228:LEU:HD23	1.93	0.50
1:A:1713:MET:HB2	1:A:1715:TRP:HD1	1.77	0.50
6:K:523:ILE:HD12	5:P:656:MET:HE3	1.93	0.50
9:O:329:ARG:O	9:O:333:GLU:HG2	2.11	0.50
11:Z:173:LEU:HD11	11:Z:205:TRP:CH2	2.46	0.50
1:A:31:HIS:CD2	1:A:32:PRO:HD2	2.47	0.50
1:A:455:VAL:HB	1:A:471:VAL:HG22	1.94	0.50
5:J:650:LYS:HE2	5:J:653:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:135:LEU:O	6:K:139:ILE:HG13	2.11	0.50
11:Z:362:PHE:HB2	11:Z:379:LEU:HD13	1.94	0.50
1:A:484:LYS:HB2	1:A:592:HIS:HD1	1.77	0.50
1:A:484:LYS:HG3	1:A:592:HIS:CE1	2.46	0.50
1:A:592:HIS:CG	1:A:592:HIS:O	2.65	0.50
1:A:727:SER:O	1:A:728:LEU:HG	2.11	0.50
1:A:805:HIS:NE2	1:A:843:SER:HB2	2.26	0.50
11:Y:478:HIS:ND1	11:Y:497:GLN:OE1	2.38	0.50
11:Z:411:THR:O	11:Z:415:THR:OG1	2.30	0.50
12:I:597:LYS:HZ1	12:I:619:LYS:HB2	1.77	0.50
9:O:624:VAL:HG11	9:O:647:ALA:HB3	1.94	0.50
5:P:731:GLN:HG2	11:Z:151:GLU:HB2	1.93	0.50
11:Y:483:ASP:O	11:Y:486:VAL:HG12	2.12	0.50
11:Y:485:LEU:HB3	11:Y:490:GLU:HG3	1.93	0.50
11:Z:199:LEU:HB3	11:Z:202:LEU:HB3	1.94	0.50
1:A:616:GLU:OE2	9:O:558:SER:OG	2.25	0.50
1:A:1097:THR:HG23	9:O:340:LEU:HD22	1.93	0.50
3:G:10:GLU:OE2	3:G:10:GLU:N	2.45	0.50
9:O:38:LEU:HD11	9:O:139:MET:HB3	1.93	0.50
9:O:439:LEU:HD23	9:O:473:LEU:HD12	1.93	0.50
5:P:93:SER:HB3	5:P:121:LEU:HD21	1.94	0.50
5:P:166:GLN:O	5:P:169:LYS:NZ	2.33	0.50
1:A:637:MET:HG3	1:A:667:MET:HE1	1.94	0.50
1:A:645:HIS:NE2	1:A:656:GLU:OE1	2.44	0.50
11:Z:139:MET:O	11:Z:143:ASN:ND2	2.45	0.50
13:N:186:GLN:HG3	13:N:223:GLY:HA3	1.94	0.50
1:A:250:ASN:ND2	1:A:432:ILE:HD12	2.27	0.49
1:A:1770:LEU:HD22	1:A:1794:ASP:OD2	2.11	0.49
2:D:45:ALA:HA	10:U:378:MET:CE	2.42	0.49
5:J:139:GLN:NE2	5:J:161:LYS:HB3	2.27	0.49
10:U:388:TYR:HB3	10:U:405:LEU:HG	1.94	0.49
12:I:747:ASP:OD1	12:I:747:ASP:N	2.45	0.49
13:N:646:MET:HG3	13:N:657:VAL:HG22	1.94	0.49
1:A:724:LEU:HD21	9:O:597:PRO:HG2	1.95	0.49
1:A:1729:GLU:H	1:A:1729:GLU:CD	2.19	0.49
6:K:194:CYS:O	6:K:198:GLN:HB2	2.12	0.49
5:P:719:TYR:HE2	5:P:749:LYS:HB3	1.77	0.49
10:U:330:ARG:HB2	10:U:333:THR:HG22	1.94	0.49
1:A:17:LEU:HD11	1:A:511:ILE:HG23	1.94	0.49
1:A:1148:ALA:HB3	1:A:1153:ILE:HD13	1.94	0.49
7:L:83:TYR:OH	7:L:146:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:284:LEU:O	6:Q:288:SER:OG	2.24	0.49
6:Q:432:ILE:HD11	6:Q:444:TRP:CD2	2.47	0.49
1:A:151:ILE:HG22	1:A:162:HIS:O	2.12	0.49
6:K:3:LEU:O	6:K:7:ARG:HG3	2.13	0.49
6:Q:413:PHE:CD2	6:Q:454:VAL:HG12	2.47	0.49
11:Y:110:GLU:CD	11:Y:140:MET:HE2	2.37	0.49
11:Y:349:LEU:HB2	11:Y:358:ALA:HB2	1.93	0.49
11:Y:393:MET:O	11:Y:397:ASN:ND2	2.45	0.49
11:Z:406:ASN:O	11:Z:410:LEU:HG	2.13	0.49
12:I:72:ALA:HB2	12:I:113:MET:HG2	1.94	0.49
12:I:406:VAL:HG12	12:I:475:VAL:HG22	1.94	0.49
1:A:118:THR:HG22	9:O:269:SER:HB3	1.93	0.49
1:A:151:ILE:O	1:A:161:MET:HA	2.12	0.49
1:A:1666:ILE:HG23	1:A:1678:ILE:HB	1.94	0.49
5:J:464:SER:HA	5:J:467:ARG:HE	1.77	0.49
6:K:146:ARG:O	6:K:150:THR:HG23	2.11	0.49
6:Q:324:SER:HB3	6:Q:340:TYR:OH	2.13	0.49
6:Q:342:HIS:O	6:Q:346:VAL:HG13	2.12	0.49
6:Q:510:ARG:O	6:Q:510:ARG:HD3	2.12	0.49
11:Z:397:ASN:OD1	11:Z:401:LYS:NZ	2.42	0.49
4:H:97:LYS:HG2	4:H:98:PRO:HD2	1.94	0.49
9:O:568:LEU:HB2	9:O:583:VAL:HG11	1.94	0.49
11:Y:203:SER:O	11:Y:207:LYS:HG3	2.12	0.49
11:Z:390:ARG:O	11:Z:394:VAL:HG13	2.13	0.49
12:I:746:MET:HE2	12:I:746:MET:N	2.28	0.49
1:A:966:PRO:HG3	1:A:980:ARG:HH12	1.78	0.49
6:K:386:LEU:HA	6:K:389:ARG:HG2	1.95	0.49
10:U:423:ARG:O	10:U:427:GLN:HG3	2.13	0.49
11:Z:495:MET:HA	11:Z:495:MET:HE3	1.95	0.49
12:I:195:ILE:O	12:I:541:ALA:HA	2.12	0.49
12:I:300:VAL:HG13	12:I:456:PHE:HB3	1.95	0.49
13:N:252:LEU:O	13:N:256:VAL:HG12	2.12	0.49
1:A:25:ARG:NH2	1:A:72:GLU:OE2	2.39	0.49
5:P:578:SER:OG	5:P:610:GLU:OE1	2.27	0.49
6:Q:146:ARG:HG2	6:Q:175:MET:HE1	1.94	0.49
6:Q:231:LEU:HA	6:Q:234:VAL:HG22	1.95	0.49
10:U:403:TYR:CD2	10:U:422:TYR:HE1	2.31	0.49
13:N:511:SER:HB3	13:N:514:LEU:HD22	1.95	0.49
1:A:1019:MET:SD	1:A:1024:MET:HE1	2.53	0.49
7:L:144:ASN:ND2	7:L:150:ASP:O	2.45	0.49
8:M:35:GLU:H	8:M:35:GLU:CD	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:324:SER:O	6:Q:328:THR:HG23	2.12	0.49
10:V:468:MET:O	10:V:472:LYS:HG3	2.12	0.49
11:Z:134:THR:HG23	11:Z:137:ILE:HD12	1.94	0.49
13:N:476:GLU:N	13:N:479:ASP:OD2	2.46	0.49
14:C:51:CYS:SG	14:C:53:HIS:HB2	2.52	0.49
1:A:1137:PHE:CD1	1:A:1203:MET:HG2	2.48	0.49
1:A:1621:PRO:HG3	1:A:1653:ALA:HB3	1.95	0.49
1:A:1634:LEU:HD13	1:A:1666:ILE:HD11	1.94	0.49
5:J:459:ALA:O	5:J:463:MET:HG3	2.12	0.49
9:O:583:VAL:O	9:O:587:VAL:HG23	2.12	0.49
12:I:194:LYS:HD2	12:I:541:ALA:HB1	1.94	0.49
1:A:1109:GLY:C	1:A:1110:ARG:HD2	2.38	0.48
1:A:1843:GLU:HA	1:A:1846:PRO:HG2	1.95	0.48
1:A:1859:TRP:HE1	1:A:1881:GLN:HG2	1.77	0.48
5:J:651:PHE:CE1	5:J:705:CYS:HB3	2.43	0.48
6:K:194:CYS:N	6:K:197:GLU:OE2	2.39	0.48
6:K:401:ASP:O	6:K:404:VAL:HG12	2.13	0.48
9:O:56:GLU:HB2	9:O:86:CYS:SG	2.53	0.48
9:O:439:LEU:HG	9:O:476:LEU:HD22	1.94	0.48
6:Q:440:THR:O	6:Q:440:THR:OG1	2.31	0.48
11:Z:6:HIS:O	11:Z:10:MET:HG2	2.13	0.48
1:A:253:PRO:HB2	1:A:255:ILE:HG23	1.94	0.48
1:A:1727:ASN:HB3	1:A:1843:GLU:OE1	2.14	0.48
1:A:1825:SER:OG	1:A:1829:ARG:NH2	2.41	0.48
5:J:135:SER:HB2	5:J:161:LYS:HE3	1.94	0.48
6:K:338:ILE:HG12	6:K:364:MET:HE1	1.95	0.48
9:O:621:SER:HB3	9:O:651:ILE:HG13	1.95	0.48
5:P:84:LYS:HB3	5:P:87:GLU:HG3	1.95	0.48
5:P:621:LEU:O	5:P:625:ARG:HG3	2.13	0.48
5:P:739:VAL:O	5:P:743:ILE:HG13	2.13	0.48
11:Y:389:ILE:O	11:Y:393:MET:HG2	2.13	0.48
12:I:600:ILE:O	12:I:600:ILE:HG13	2.13	0.48
13:N:20:LEU:HD13	13:N:65:HIS:CD2	2.49	0.48
5:J:154:SER:O	5:J:158:ILE:HG12	2.13	0.48
11:Y:232:LEU:HB3	11:Z:29:MET:CE	2.44	0.48
1:A:104:LYS:O	9:O:537:ALA:HB1	2.14	0.48
1:A:633:ILE:HG23	1:A:754:LEU:HD21	1.95	0.48
1:A:1521:LEU:HD22	1:A:1588:LEU:HD22	1.95	0.48
9:O:55:MET:O	9:O:59:ARG:HG2	2.12	0.48
9:O:439:LEU:HD11	12:I:512:LEU:HD13	1.96	0.48
11:Y:15:LEU:HD11	11:Z:135:PRO:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:151:GLU:O	11:Y:155:VAL:HG12	2.13	0.48
11:Z:343:LEU:HD11	11:Z:375:CYS:HA	1.96	0.48
13:N:300:LEU:HA	13:N:303:VAL:HG12	1.96	0.48
1:A:482:VAL:CG2	1:A:593:ASN:HA	2.44	0.48
1:A:1074:CYS:O	1:A:1078:MET:HG3	2.13	0.48
1:A:1527:MET:HE2	1:A:1532:ASN:ND2	2.28	0.48
1:A:1830:LEU:C	1:A:1831:GLN:HG2	2.38	0.48
1:A:1886:ALA:O	1:A:1890:VAL:HG12	2.13	0.48
5:P:685:SER:HB3	5:P:716:ASN:HD21	1.77	0.48
6:Q:35:GLU:HG3	6:Q:40:ILE:HD11	1.96	0.48
11:Y:308:TRP:HE3	11:Y:327:LEU:HD13	1.78	0.48
11:Z:264:GLN:HE22	11:Z:265:MET:HE2	1.78	0.48
13:N:129:LEU:HD21	13:N:150:ARG:HB2	1.95	0.48
13:N:523:LEU:O	13:N:527:LEU:HG	2.13	0.48
13:N:688:PRO:O	13:N:689:VAL:C	2.56	0.48
1:A:774:LYS:HG2	1:A:783:ILE:HD11	1.96	0.48
6:K:88:GLN:N	6:K:88:GLN:OE1	2.44	0.48
5:P:68:THR:O	5:P:72:LYS:HG3	2.13	0.48
6:Q:61:ARG:HH22	6:Q:88:GLN:NE2	2.11	0.48
10:U:106:LEU:HB2	10:U:118:TYR:HB2	1.95	0.48
10:V:228:TRP:H	10:V:228:TRP:CD1	2.32	0.48
11:Y:20:ARG:O	11:Y:49:HIS:NE2	2.46	0.48
11:Y:281:LEU:HD21	11:Y:289:ASP:CG	2.38	0.48
11:Y:390:ARG:O	11:Y:394:VAL:HG13	2.13	0.48
11:Y:431:LEU:HD13	11:Y:451:LEU:HD21	1.96	0.48
11:Z:376:TYR:O	11:Z:380:ILE:HG12	2.13	0.48
12:I:56:TRP:CE3	12:I:98:PRO:HB3	2.49	0.48
12:I:246:PRO:O	12:I:250:ARG:HG3	2.14	0.48
12:I:587:LEU:HD22	12:I:600:ILE:HG22	1.95	0.48
1:A:850:SER:OG	1:A:857:MET:SD	2.58	0.48
1:A:1658:PRO:HG2	1:A:1663:LEU:HD13	1.95	0.48
1:A:1830:LEU:O	1:A:1831:GLN:HG2	2.14	0.48
1:A:1866:MET:HE2	1:A:1866:MET:N	2.29	0.48
7:L:94:ILE:HG12	7:L:141:VAL:HG12	1.95	0.48
5:P:726:LEU:HD22	5:P:743:ILE:HG13	1.94	0.48
10:U:451:GLU:HA	10:U:454:LYS:HE3	1.96	0.48
11:Y:136:LYS:HG3	11:Y:137:ILE:N	2.29	0.48
11:Y:224:ILE:HD11	11:Y:239:LEU:HD11	1.95	0.48
12:I:625:TYR:HB2	12:I:628:THR:HG23	1.96	0.48
1:A:352:ARG:HH21	10:V:373:HIS:HD2	1.60	0.48
5:J:643:MET:HA	5:J:646:TYR:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:25:ILE:N	7:L:25:ILE:HD12	2.28	0.48
9:O:706:CYS:O	9:O:710:ILE:HG13	2.14	0.48
6:Q:25:TRP:O	6:Q:29:VAL:HG23	2.13	0.48
10:U:238:TYR:CD1	10:U:243:LEU:HD12	2.49	0.48
11:Z:208:ALA:O	11:Z:212:VAL:HG23	2.14	0.48
12:I:210:LEU:HD11	12:I:214:LEU:HD23	1.96	0.48
1:A:823:ILE:HG22	1:A:824:ASP:H	1.78	0.48
1:A:1103:PRO:HD2	1:A:1143:ALA:HB2	1.96	0.48
1:A:1114:ARG:HB3	1:A:1116:THR:HG23	1.95	0.48
1:A:1653:ALA:O	1:A:1655:THR:N	2.42	0.48
1:A:1745:PRO:HB2	9:O:609:ALA:HB1	1.94	0.48
5:J:617:LEU:HD23	5:J:648:GLN:HE21	1.79	0.48
7:L:19:THR:HG23	7:L:21:THR:HG22	1.96	0.48
7:L:79:ILE:HD11	7:L:153:MET:SD	2.53	0.48
9:O:480:GLN:HG3	12:I:512:LEU:HD11	1.95	0.48
11:Z:253:ASN:O	11:Z:257:VAL:HG23	2.14	0.48
13:N:340:ARG:HB3	13:N:361:LEU:HD22	1.96	0.48
13:N:538:GLU:O	13:N:542:VAL:HG13	2.12	0.48
9:O:445:LEU:HD23	9:O:469:ALA:HB2	1.96	0.48
5:P:502:LEU:HD23	5:P:502:LEU:HA	1.68	0.48
6:Q:27:ASP:HA	6:Q:43:LEU:HD22	1.96	0.48
11:Z:248:PHE:HB2	11:Z:280:LEU:HD11	1.95	0.48
1:A:1033:ARG:HG2	1:A:1566:PHE:HZ	1.78	0.47
9:O:477:HIS:NE2	12:I:510:SER:OG	2.33	0.47
9:O:742:GLN:OE1	9:O:742:GLN:N	2.32	0.47
13:N:63:ARG:HH12	13:N:140:LEU:HA	1.79	0.47
13:N:512:LYS:HG2	13:N:549:PHE:CD1	2.49	0.47
13:N:689:VAL:O	13:N:693:ARG:N	2.43	0.47
1:A:1247:HIS:O	1:A:1251:VAL:HG12	2.14	0.47
6:K:133:CYS:O	6:K:152:SER:OG	2.32	0.47
12:I:113:MET:HG3	12:I:176:LEU:HD11	1.96	0.47
1:A:968:SER:HB2	1:A:1677:LEU:HD23	1.96	0.47
1:A:1520:LEU:HD22	1:A:1542:LEU:HD12	1.96	0.47
5:J:480:ASN:O	5:J:480:ASN:ND2	2.47	0.47
6:K:445:GLU:OE1	3:W:8:ARG:NH1	2.48	0.47
11:Y:59:TYR:HB2	11:Y:115:LEU:HD21	1.96	0.47
11:Y:240:LEU:HD21	11:Y:262:GLN:HB3	1.95	0.47
11:Z:27:LEU:HD12	11:Z:49:HIS:HD2	1.78	0.47
12:I:634:SER:OG	12:I:635:ILE:N	2.48	0.47
9:O:596:SER:O	9:O:596:SER:OG	2.30	0.47
5:P:722:ALA:O	5:P:726:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:134:LEU:HD21	6:Q:165:GLU:HG2	1.97	0.47
6:Q:150:THR:HG22	6:Q:175:MET:HB3	1.96	0.47
10:U:358:LEU:CD2	10:U:371:MET:HE1	2.44	0.47
10:U:449:LEU:O	10:U:453:LYS:HG3	2.15	0.47
1:A:129:CYS:HB3	1:A:187:LEU:HD21	1.97	0.47
1:A:1221:ASP:HB3	1:A:1224:ILE:CG2	2.41	0.47
1:A:1222:MET:SD	10:V:514:ARG:NE	2.88	0.47
7:L:83:TYR:CD2	7:L:115:GLU:HG3	2.38	0.47
9:O:330:ILE:HD11	10:V:414:MET:HG2	1.96	0.47
11:Y:373:LEU:O	11:Y:377:GLU:HG2	2.15	0.47
11:Y:394:VAL:HA	11:Y:397:ASN:ND2	2.29	0.47
12:I:572:PHE:CE2	12:I:589:THR:HG23	2.49	0.47
13:N:289:PHE:O	13:N:293:ILE:HG12	2.14	0.47
11:Z:402:THR:HG23	11:Z:403:LEU:HD12	1.96	0.47
13:N:425:ARG:O	13:N:509:TYR:OH	2.21	0.47
14:C:20:ASP:OD1	14:C:21:GLU:N	2.47	0.47
1:A:795:ARG:NH2	1:A:815:ARG:O	2.48	0.47
1:A:1097:THR:O	9:O:332:GLN:NE2	2.48	0.47
1:A:1301:ALA:O	1:A:1305:VAL:HG23	2.15	0.47
1:A:1496:MET:HE1	13:N:477:PRO:HG3	1.97	0.47
1:A:1733:PHE:CD2	1:A:1776:TYR:HB2	2.50	0.47
5:J:483:GLU:O	5:J:487:ILE:HG22	2.15	0.47
5:J:621:LEU:HG	5:J:625:ARG:HH21	1.79	0.47
6:K:334:GLY:HA3	6:K:364:MET:HE2	1.97	0.47
9:O:430:ARG:CD	9:O:476:LEU:HD11	2.41	0.47
10:U:490:TYR:O	10:U:494:ILE:HG12	2.13	0.47
10:V:420:TYR:OH	10:V:424:ARG:NH1	2.48	0.47
11:Y:50:ALA:HB1	11:Y:66:TYR:HE1	1.73	0.47
11:Y:340:GLN:HE21	11:Y:372:ARG:HH12	1.63	0.47
11:Y:355:VAL:O	11:Y:359:ILE:HG13	2.14	0.47
11:Y:441:TYR:HB3	11:Y:444:ALA:HB3	1.97	0.47
11:Z:293:LEU:O	11:Z:297:LEU:HG	2.15	0.47
12:I:406:VAL:HG21	12:I:478:TYR:HE2	1.80	0.47
13:N:571:ASN:OD1	13:N:622:TYR:OH	2.33	0.47
1:A:89:TYR:HA	9:O:533:THR:HG23	1.95	0.47
1:A:1128:PRO:HG2	1:A:1131:MET:HB2	1.96	0.47
6:K:62:SER:O	6:K:63:ARG:HG2	2.15	0.47
1:A:443:CYS:HB3	1:A:452:LEU:CD2	2.44	0.47
5:J:21:TYR:HE1	5:J:50:ARG:HB3	1.80	0.47
5:J:524:GLU:O	5:J:527:ARG:HG3	2.15	0.47
5:J:625:ARG:NH1	11:Y:495:MET:HE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:492:HIS:HB2	12:I:500:PHE:CZ	2.50	0.47
10:V:301:ASP:OD2	10:V:364:TYR:OH	2.33	0.47
1:A:1014:ASP:HB3	1:A:1044:ALA:HB3	1.97	0.47
1:A:1926:ARG:O	1:A:1930:ARG:NH2	2.48	0.47
4:H:97:LYS:HB3	4:H:102:LEU:CD1	2.45	0.47
5:J:482:LYS:HD2	5:J:482:LYS:HA	1.73	0.47
5:J:581:ARG:HA	5:J:583:HIS:CE1	2.50	0.47
5:J:660:LYS:O	5:J:664:ILE:HD12	2.14	0.47
6:K:275:LEU:HB2	6:K:284:LEU:HD12	1.97	0.47
9:O:159:GLN:O	9:O:163:GLN:HG2	2.15	0.47
9:O:349:VAL:O	9:O:353:LYS:HG2	2.15	0.47
10:V:39:ILE:HG12	10:V:201:LEU:O	2.14	0.47
10:V:79:GLU:HA	10:V:82:GLN:HG2	1.97	0.47
12:I:119:THR:OG1	12:I:212:SER:OG	2.26	0.47
5:P:524:GLU:O	5:P:528:ILE:HG23	2.14	0.46
11:Y:122:ILE:HG23	11:Y:144:LEU:HD23	1.97	0.46
11:Z:255:ASN:O	11:Z:258:LEU:HG	2.15	0.46
13:N:232:TRP:HB2	13:N:235:GLN:NE2	2.28	0.46
13:N:544:LEU:O	13:N:547:LEU:HG	2.15	0.46
9:O:644:LEU:HD22	9:O:648:ILE:HD11	1.96	0.46
5:P:48:TYR:CD1	5:P:56:LYS:HD3	2.50	0.46
6:Q:426:LEU:O	6:Q:430:GLU:HG2	2.15	0.46
10:U:93:TYR:OH	10:V:57:GLU:OE2	2.24	0.46
10:U:467:LYS:HZ1	10:U:506:HIS:HB3	1.81	0.46
10:U:526:TRP:HA	10:U:529:ALA:HB3	1.98	0.46
11:Y:396:ALA:CB	11:Y:416:VAL:HG21	2.44	0.46
11:Z:59:TYR:HB2	11:Z:115:LEU:HD21	1.96	0.46
11:Z:147:LYS:HE2	11:Z:336:SER:HB3	1.97	0.46
11:Z:446:VAL:O	11:Z:450:GLU:HG2	2.15	0.46
13:N:405:LYS:O	13:N:409:VAL:HG12	2.15	0.46
1:A:488:MET:HE2	1:A:500:TYR:HB2	1.97	0.46
1:A:1091:SER:O	1:A:1091:SER:OG	2.28	0.46
1:A:1619:LEU:HD21	1:A:1697:LEU:HD22	1.98	0.46
5:J:32:TYR:OH	5:J:64:HIS:ND1	2.48	0.46
5:P:92:LEU:HD23	5:P:121:LEU:HD22	1.97	0.46
6:Q:184:LEU:O	6:Q:188:LEU:HD23	2.15	0.46
6:Q:489:HIS:ND1	6:Q:497:ASN:HB2	2.30	0.46
11:Y:190:MET:O	11:Y:194:GLN:NE2	2.44	0.46
13:N:542:VAL:HB	13:N:554:MET:HE1	1.97	0.46
13:N:592:TYR:O	14:C:9:ASN:HA	2.15	0.46
14:C:67:GLN:O	14:C:69:VAL:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LEU:HB3	1:A:724:LEU:HD12	1.96	0.46
1:A:1134:TRP:HD1	1:A:1597:THR:HA	1.80	0.46
1:A:1550:MET:HE2	1:A:1558:HIS:HE1	1.80	0.46
5:P:102:SER:OG	5:P:103:HIS:N	2.48	0.46
5:P:473:TYR:HD2	5:P:500:TRP:HZ2	1.64	0.46
6:Q:513:THR:O	6:Q:517:THR:HG23	2.16	0.46
10:U:293:ASP:OD2	10:U:296:ARG:HB2	2.16	0.46
12:I:114:HIS:NE2	12:I:116:MET:HB3	2.29	0.46
13:N:158:ARG:NH1	13:N:251:SER:O	2.48	0.46
13:N:570:ILE:HA	13:N:573:ASN:ND2	2.31	0.46
1:A:263:GLN:HB2	1:A:265:VAL:HG22	1.97	0.46
5:J:142:LEU:HD21	5:J:151:PRO:HB2	1.96	0.46
7:L:74:VAL:HG11	7:L:137:ILE:HD11	1.97	0.46
9:O:416:GLU:HG2	9:O:417:LEU:N	2.31	0.46
5:P:55:TYR:CE2	5:P:56:LYS:HG3	2.50	0.46
11:Y:101:GLU:O	11:Y:105:LYS:HG2	2.16	0.46
11:Y:411:THR:O	11:Y:415:THR:HG23	2.15	0.46
11:Z:323:ARG:HE	11:Z:327:LEU:HD11	1.81	0.46
12:I:688:THR:HB	12:I:691:THR:HG23	1.97	0.46
1:A:12:ILE:O	1:A:510:PHE:N	2.32	0.46
9:O:700:TYR:O	9:O:704:VAL:HG12	2.16	0.46
6:Q:253:LEU:O	6:Q:257:VAL:HG23	2.14	0.46
10:U:26:PHE:CE1	10:U:228:TRP:HB2	2.50	0.46
11:Y:23:SER:HB2	11:Y:49:HIS:CD2	2.48	0.46
13:N:512:LYS:HG2	13:N:549:PHE:HD1	1.79	0.46
1:A:161:MET:SD	1:A:216:PRO:HG3	2.56	0.46
1:A:942:ARG:NH1	1:A:945:GLU:OE2	2.48	0.46
1:A:1867:CYS:HB3	1:A:1885:LEU:HD13	1.97	0.46
5:J:482:LYS:HD3	5:J:512:LEU:HD11	1.98	0.46
7:L:46:ARG:NH1	7:L:156:ILE:O	2.47	0.46
9:O:557:MET:HE1	9:O:593:ARG:NH2	2.31	0.46
11:Y:329:ALA:O	11:Y:332:ILE:HG22	2.16	0.46
12:I:238:THR:HB	12:I:241:LEU:HD13	1.98	0.46
13:N:597:SER:O	13:N:601:TRP:HB2	2.16	0.46
1:A:1084:ARG:NH1	1:A:1139:ASN:OD1	2.39	0.46
5:J:139:GLN:HG3	5:J:161:LYS:NZ	2.31	0.46
5:J:563:ASP:OD2	5:P:55:TYR:OH	2.32	0.46
6:K:160:ASP:OD2	6:Q:13:TYR:OH	2.23	0.46
6:K:227:LEU:HG	6:Q:32:LEU:HD13	1.98	0.46
6:K:301:SER:O	6:K:305:VAL:HG23	2.16	0.46
9:O:95:ILE:HG13	9:O:96:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:173:LEU:HD11	11:Z:205:TRP:HH2	1.80	0.46
12:I:33:ASP:HB3	12:I:728:ARG:HD3	1.98	0.46
1:A:878:ALA:HA	1:A:882:LEU:HD13	1.98	0.46
8:M:49:SER:O	8:M:53:GLN:HG2	2.16	0.46
5:P:671:LEU:O	5:P:675:ILE:HG13	2.15	0.46
5:P:726:LEU:HD11	5:P:742:LEU:HD23	1.97	0.46
11:Y:10:MET:HE2	11:Y:10:MET:HA	1.97	0.46
11:Y:157:SER:O	11:Y:161:VAL:HG23	2.16	0.46
11:Y:451:LEU:O	11:Y:454:ARG:HG2	2.14	0.46
11:Z:139:MET:HE2	11:Z:139:MET:HA	1.98	0.46
11:Z:359:ILE:O	11:Z:363:ARG:HG3	2.15	0.46
11:Z:481:LEU:HD22	11:Z:497:GLN:HG3	1.98	0.46
12:I:434:LEU:HG	12:I:437:LEU:H	1.80	0.46
12:I:602:ARG:NH2	12:I:612:SER:O	2.40	0.46
1:A:248:PHE:HB3	1:A:257:MET:HB3	1.98	0.46
1:A:989:GLU:HG3	1:A:1698:TYR:CE2	2.51	0.46
1:A:1803:ARG:HH12	1:A:1859:TRP:HD1	1.64	0.46
2:D:45:ALA:O	10:U:380:ASN:ND2	2.49	0.46
5:J:27:LEU:HD21	5:P:147:PHE:HB3	1.97	0.46
8:M:55:MET:HA	8:M:55:MET:HE2	1.97	0.46
1:A:11:MET:SD	1:A:510:PHE:HB2	2.56	0.45
1:A:27:HIS:CD2	1:A:113:VAL:HG21	2.51	0.45
1:A:90:ASP:OD1	1:A:106:SER:HB3	2.16	0.45
1:A:211:PHE:HB3	1:A:220:ILE:HG22	1.98	0.45
5:J:18:HIS:O	5:P:73:TYR:OH	2.28	0.45
7:L:18:ARG:HD3	7:L:18:ARG:HA	1.80	0.45
11:Y:430:LEU:HA	11:Y:433:LYS:HD3	1.98	0.45
12:I:12:ARG:HH21	12:I:748:ILE:HD12	1.79	0.45
12:I:21:GLN:HB3	12:I:39:ASN:HB2	1.99	0.45
14:C:53:HIS:HE1	14:C:76:CYS:HB3	1.80	0.45
1:A:597:LEU:HD11	1:A:607:ILE:HD13	1.98	0.45
1:A:1134:TRP:CD1	1:A:1597:THR:HA	2.51	0.45
1:A:1251:VAL:HG23	1:A:1297:ALA:HB2	1.98	0.45
1:A:1925:VAL:HA	1:A:1928:LEU:HB2	1.98	0.45
5:J:92:LEU:HD11	5:J:120:LEU:HG	1.97	0.45
5:J:503:CYS:SG	5:J:535:GLY:HA3	2.56	0.45
6:K:181:GLU:HG3	6:K:209:LEU:CD2	2.46	0.45
9:O:323:ALA:HB2	10:V:416:PHE:CE2	2.52	0.45
5:P:707:PHE:CD1	5:P:707:PHE:C	2.95	0.45
6:Q:330:GLU:HB3	6:Q:333:TYR:HB2	1.99	0.45
6:Q:357:TYR:CE2	6:Q:373:TYR:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:87:TYR:CZ	10:U:113:LYS:HD2	2.51	0.45
11:Z:36:LEU:HG	11:Z:37:PHE:CD2	2.51	0.45
1:A:74:TRP:CH2	1:A:604:MET:HE1	2.52	0.45
1:A:115:LYS:HG2	9:O:267:VAL:HG22	1.99	0.45
1:A:436:LEU:HB2	1:A:638:LEU:HD23	1.98	0.45
5:P:44:LEU:O	5:P:48:TYR:HD2	1.99	0.45
10:V:123:TYR:HD2	10:V:124:LEU:HD22	1.81	0.45
10:V:129:LYS:HA	10:V:129:LYS:HD3	1.69	0.45
11:Y:240:LEU:HG	11:Y:263:ALA:HB2	1.98	0.45
1:A:87:VAL:HB	9:O:544:VAL:HG12	1.99	0.45
1:A:710:LEU:HD11	9:O:715:TYR:CE1	2.51	0.45
1:A:1351:GLN:H	1:A:1351:GLN:HG2	1.60	0.45
1:A:1460:ALA:O	1:A:1464:ILE:HG13	2.16	0.45
6:K:465:LEU:HD21	6:K:485:ILE:HG23	1.98	0.45
9:O:320:ALA:HB3	9:O:350:LEU:HD21	1.98	0.45
5:P:53:LYS:HG3	5:P:55:TYR:CE1	2.51	0.45
5:P:506:GLY:HA3	5:P:522:PHE:CE1	2.52	0.45
11:Y:16:HIS:HA	11:Y:19:VAL:HG22	1.98	0.45
11:Y:209:TYR:O	11:Y:212:VAL:HG12	2.16	0.45
11:Z:20:ARG:HB2	11:Z:52:SER:HB2	1.99	0.45
12:I:558:ARG:HE	12:I:558:ARG:HB2	1.62	0.45
5:P:741:PHE:CE2	5:P:745:LYS:HE3	2.52	0.45
11:Z:158:TYR:HA	11:Z:161:VAL:HG12	1.98	0.45
12:I:290:PHE:CZ	12:I:320:LEU:HD13	2.51	0.45
13:N:401:ILE:HD11	13:N:501:ILE:HG23	1.98	0.45
1:A:790:LEU:HA	1:A:790:LEU:HD23	1.76	0.45
5:P:164:PRO:HG2	5:P:471:LYS:HG2	1.97	0.45
11:Y:163:ARG:HD2	11:Y:163:ARG:C	2.41	0.45
11:Y:481:LEU:O	11:Y:485:LEU:HD13	2.17	0.45
11:Z:109:ALA:O	11:Z:113:THR:HG23	2.17	0.45
12:I:744:PHE:HB2	12:I:746:MET:HE1	1.99	0.45
1:A:1078:MET:O	1:A:1081:PRO:HD2	2.17	0.45
1:A:1794:ASP:O	1:A:1797:ILE:HG13	2.16	0.45
1:A:1810:GLU:HA	1:A:1813:GLN:HG2	1.99	0.45
5:P:170:PHE:O	5:P:456:LYS:NZ	2.40	0.45
6:Q:129:LYS:HB3	6:Q:159:LEU:HD13	1.99	0.45
10:V:122:ARG:NH2	10:V:157:GLU:OE1	2.50	0.45
13:N:351:PHE:HE1	13:N:409:VAL:HG11	1.80	0.45
14:C:30:PHE:HB3	14:C:46:LEU:HD11	1.99	0.45
1:A:756:PHE:HE2	1:A:830:PHE:HB2	1.82	0.45
1:A:966:PRO:HG3	1:A:980:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:50:ALA:HA	11:Y:65:LYS:HE3	1.98	0.45
13:N:626:TYR:HE2	13:N:635:LEU:HG	1.82	0.45
3:G:3:ARG:HG3	3:G:3:ARG:HH11	1.82	0.45
5:J:103:HIS:HD1	5:J:140:LYS:HD3	1.81	0.45
6:K:61:ARG:NH1	6:K:80:HIS:HE1	2.15	0.45
6:K:273:GLY:O	6:K:277:GLU:HG2	2.16	0.45
6:K:386:LEU:HD22	6:K:389:ARG:HH21	1.82	0.45
9:O:727:THR:HG22	9:O:731:ASN:ND2	2.32	0.45
5:P:93:SER:OG	5:P:121:LEU:HD11	2.16	0.45
11:Y:158:TYR:HB3	11:Y:175:LEU:HG	1.98	0.45
11:Y:176:LEU:HD12	11:Y:210:ALA:HA	1.99	0.45
12:I:233:TYR:OH	12:I:235:GLN:OE1	2.30	0.45
12:I:454:GLU:HB3	12:I:455:HIS:HD2	1.82	0.45
1:A:26:ASP:OD1	1:A:26:ASP:N	2.45	0.45
1:A:715:TYR:OH	9:O:712:ASP:OD1	2.31	0.45
1:A:1141:VAL:HG11	1:A:1608:HIS:CG	2.52	0.45
1:A:1328:TYR:CD1	1:A:1363:THR:HG21	2.52	0.45
1:A:1591:HIS:HD2	1:A:1601:TYR:CG	2.35	0.45
5:J:97:PHE:CG	11:Y:252:ASP:HB3	2.52	0.45
5:J:162:PRO:HB3	5:J:474:LEU:HD11	1.97	0.45
6:K:342:HIS:O	6:K:346:VAL:HG13	2.17	0.45
9:O:447:SER:HG	12:I:516:TYR:HH	1.54	0.45
6:Q:16:GLN:O	6:Q:17:GLN:HG2	2.17	0.45
6:Q:61:ARG:HG3	6:Q:61:ARG:HH11	1.82	0.45
10:U:78:GLU:HA	10:V:67:LEU:HD21	1.99	0.45
10:U:323:LEU:HB3	10:U:333:THR:HB	1.99	0.45
11:Z:440:ASP:OD1	11:Z:440:ASP:N	2.50	0.45
12:I:49:LEU:HD13	12:I:730:VAL:HG11	1.98	0.45
1:A:707:TRP:CE3	9:O:730:ARG:HD3	2.52	0.44
1:A:767:HIS:ND1	1:A:806:TYR:OH	2.39	0.44
1:A:775:LEU:HD11	1:A:844:ILE:HD13	1.99	0.44
6:K:190:LEU:O	6:K:198:GLN:NE2	2.25	0.44
9:O:443:GLN:HE22	12:I:514:PHE:H	1.65	0.44
11:Y:377:GLU:O	11:Y:380:ILE:HG12	2.17	0.44
11:Z:23:SER:CB	11:Z:49:HIS:HB2	2.46	0.44
12:I:655:ASP:N	12:I:663:ASP:O	2.39	0.44
13:N:169:PHE:O	13:N:172:MET:HG3	2.17	0.44
13:N:273:MET:HE2	13:N:335:ILE:HG23	2.00	0.44
13:N:351:PHE:HB2	13:N:406:ALA:HB2	1.99	0.44
1:A:224:VAL:HG23	1:A:408:CYS:HB2	1.99	0.44
3:G:11:LEU:HD23	3:G:11:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:37:LYS:NZ	7:L:57:ASP:HB3	2.33	0.44
5:P:125:TYR:HE1	5:P:130:ARG:HH21	1.65	0.44
5:P:150:SER:HA	5:P:153:GLU:HG2	1.98	0.44
11:Y:110:GLU:OE2	11:Y:140:MET:HE2	2.16	0.44
11:Z:297:LEU:HB2	11:Z:307:PRO:HG3	1.99	0.44
12:I:9:PRO:O	12:I:750:ASP:N	2.43	0.44
1:A:350:LEU:HD11	10:V:399:TYR:HE2	1.83	0.44
1:A:953:LEU:HD21	1:A:1821:PHE:CE2	2.53	0.44
1:A:1060:HIS:O	1:A:1063:ILE:HG22	2.18	0.44
5:J:525:VAL:HA	5:J:528:ILE:HG22	1.98	0.44
6:K:174:HIS:CE1	6:K:211:LYS:HD2	2.52	0.44
6:K:503:HIS:O	5:P:625:ARG:HD3	2.17	0.44
7:L:53:TYR:HA	7:L:153:MET:O	2.18	0.44
6:Q:263:PHE:HZ	6:Q:290:LYS:HB3	1.83	0.44
6:Q:407:GLU:O	6:Q:410:VAL:HG12	2.17	0.44
10:V:520:TYR:HA	10:V:523:CYS:SG	2.57	0.44
1:A:89:TYR:HB3	9:O:536:THR:HG23	2.00	0.44
1:A:1251:VAL:HG23	1:A:1297:ALA:CB	2.47	0.44
3:G:23:ARG:HD2	6:Q:525:MET:HE3	2.00	0.44
5:J:485:ILE:HD13	5:J:509:TYR:CE1	2.52	0.44
5:J:641:LEU:HB3	5:J:657:HIS:CD2	2.53	0.44
5:P:685:SER:OG	5:P:716:ASN:OD1	2.25	0.44
6:Q:80:HIS:HB2	6:Q:89:ALA:HB2	1.99	0.44
6:Q:325:LYS:HE2	6:Q:329:LEU:CD2	2.47	0.44
10:V:516:LEU:HD23	10:V:516:LEU:HA	1.83	0.44
11:Y:59:TYR:O	11:Y:63:VAL:HG22	2.17	0.44
13:N:332:PHE:HA	13:N:335:ILE:HG22	1.99	0.44
1:A:1851:THR:O	1:A:1855:THR:HG22	2.17	0.44
6:K:317:GLU:HG2	6:K:318:HIS:N	2.33	0.44
5:P:621:LEU:HD13	5:P:644:ILE:HG21	1.98	0.44
5:P:692:LEU:HD12	5:P:705:CYS:O	2.18	0.44
11:Y:10:MET:HB3	11:Y:19:VAL:HG12	2.00	0.44
11:Y:512:LEU:HA	11:Y:515:MET:HG2	2.00	0.44
11:Z:38:SER:O	11:Z:41:GLN:HG2	2.16	0.44
12:I:8:PHE:HB3	12:I:750:ASP:O	2.18	0.44
13:N:506:VAL:HG11	13:N:512:LYS:HG3	1.99	0.44
1:A:94:TYR:CE1	1:A:96:ALA:HB2	2.53	0.44
5:J:526:ARG:HE	5:J:526:ARG:HB3	1.68	0.44
7:L:76:THR:HG23	7:L:159:TYR:HB2	2.00	0.44
5:P:733:VAL:HG22	5:P:736:GLU:OE1	2.17	0.44
6:Q:60:LEU:HD11	6:Q:75:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:134:THR:HG23	10:V:143:LYS:HG3	1.99	0.44
10:V:327:ASP:O	10:V:333:THR:HG21	2.17	0.44
11:Y:423:THR:HB	11:Y:426:LYS:HE2	1.98	0.44
12:I:20:PRO:HA	12:I:739:ARG:HH21	1.83	0.44
13:N:273:MET:HA	13:N:289:PHE:HZ	1.81	0.44
6:K:155:GLU:O	6:K:158:LYS:HG2	2.18	0.44
9:O:637:PRO:HB2	9:O:674:SER:HB3	1.98	0.44
5:P:58:TYR:HB2	5:P:78:CYS:HB3	1.99	0.44
5:P:161:LYS:HE2	5:P:478:SER:HB3	2.00	0.44
6:Q:459:LYS:HA	6:Q:461:TYR:CE1	2.53	0.44
6:Q:472:LEU:O	6:Q:476:PRO:HA	2.18	0.44
10:V:186:LYS:HB3	10:V:186:LYS:HE2	1.93	0.44
11:Y:232:LEU:HD21	11:Z:33:ASN:CB	2.47	0.44
11:Z:101:GLU:O	11:Z:105:LYS:HG3	2.18	0.44
12:I:258:ILE:HD12	12:I:359:LEU:HD12	1.98	0.44
1:A:83:ILE:HG21	9:O:544:VAL:HG21	1.99	0.44
1:A:628:ILE:HD11	1:A:761:ALA:HB1	2.00	0.44
1:A:853:LYS:HD3	1:A:1819:GLU:OE2	2.18	0.44
5:J:27:LEU:HD11	5:P:147:PHE:O	2.18	0.44
5:J:124:VAL:O	5:J:128:THR:HG22	2.18	0.44
5:J:496:TYR:HA	5:J:501:VAL:HG21	2.00	0.44
5:P:717:GLU:HA	5:P:719:TYR:CE1	2.52	0.44
5:P:731:GLN:OE1	11:Z:152:ARG:NH2	2.50	0.44
6:Q:61:ARG:HG3	6:Q:61:ARG:NH1	2.33	0.44
11:Y:219:ARG:O	11:Y:223:THR:HG22	2.18	0.44
11:Y:260:PHE:HB3	11:Y:277:TYR:HD1	1.82	0.44
11:Z:189:THR:O	11:Z:193:ILE:HG12	2.17	0.44
13:N:82:ASP:OD1	13:N:86:ASN:ND2	2.51	0.44
13:N:404:ILE:HG12	13:N:417:LEU:HD21	1.99	0.44
1:A:1012:GLU:OE1	1:A:1012:GLU:N	2.41	0.44
1:A:1901:PRO:HD3	1:A:1921:LEU:HD11	2.00	0.44
6:K:372:LEU:CD1	6:K:404:VAL:HG23	2.48	0.44
9:O:708:GLU:OE1	9:O:711:ARG:NH2	2.51	0.44
5:P:616:GLU:OE1	5:P:619:LYS:NZ	2.39	0.44
6:Q:485:ILE:O	6:Q:488:ILE:HG22	2.18	0.44
11:Z:100:SER:HB3	11:Z:103:GLU:HG3	2.00	0.44
11:Z:321:TYR:HB2	11:Z:352:MET:HE3	1.99	0.44
13:N:183:VAL:HG13	13:N:233:CYS:HB3	2.00	0.44
1:A:30:HIS:O	9:O:233:PRO:HG2	2.18	0.43
1:A:215:HIS:CG	1:A:216:PRO:HD2	2.53	0.43
5:P:135:SER:O	5:P:139:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:365:LYS:HE2	6:Q:365:LYS:HB2	1.68	0.43
6:Q:441:VAL:HG21	6:Q:444:TRP:CD1	2.52	0.43
10:U:242:GLN:NE2	10:U:429:ARG:HE	2.11	0.43
11:Z:4:ILE:HD12	11:Z:45:LEU:HD21	2.00	0.43
11:Z:102:ILE:HG13	11:Z:103:GLU:H	1.83	0.43
11:Z:224:ILE:HD11	11:Z:239:LEU:HD21	2.00	0.43
13:N:505:LEU:O	13:N:508:ILE:HG12	2.18	0.43
1:A:1076:ARG:HG3	1:A:1559:HIS:HE1	1.84	0.43
1:A:1078:MET:HE3	1:A:1132:THR:HG22	2.00	0.43
1:A:1841:ASN:ND2	13:N:147:GLN:OE1	2.51	0.43
5:J:629:ARG:HH21	11:Y:503:SER:HB2	1.84	0.43
6:K:276:VAL:HG21	3:W:2:LEU:HD11	2.00	0.43
9:O:378:SER:O	9:O:382:GLN:HG2	2.17	0.43
6:Q:194:CYS:HB3	6:Q:197:GLU:OE1	2.18	0.43
11:Y:138:ASN:HD21	11:Y:160:GLU:HB2	1.82	0.43
11:Y:340:GLN:H	11:Y:340:GLN:CD	2.24	0.43
11:Z:120:ASP:O	11:Z:124:ILE:HG22	2.18	0.43
11:Z:397:ASN:C	11:Z:401:LYS:HZ2	2.26	0.43
11:Z:478:HIS:ND1	11:Z:497:GLN:OE1	2.50	0.43
12:I:245:LEU:HB3	12:I:246:PRO:HD3	1.99	0.43
12:I:287:LEU:HD21	12:I:456:PHE:CE1	2.53	0.43
12:I:692:ARG:HG2	12:I:694:ASP:H	1.83	0.43
1:A:1137:PHE:O	1:A:1141:VAL:HG23	2.17	0.43
1:A:1872:LEU:HD23	1:A:1900:LEU:HD11	1.99	0.43
5:J:476:LEU:HD21	5:J:508:ALA:HB2	2.00	0.43
6:K:65:LEU:HB3	6:K:72:CYS:SG	2.58	0.43
6:K:425:PHE:HB3	6:K:451:LEU:HG	2.00	0.43
8:M:5:VAL:O	8:M:7:ARG:HD2	2.17	0.43
8:M:34:ASN:O	8:M:50:VAL:HG22	2.19	0.43
10:V:186:LYS:O	10:V:189:ILE:HG22	2.19	0.43
12:I:143:PRO:HG2	12:I:351:HIS:CD2	2.54	0.43
12:I:444:ASP:O	12:I:448:VAL:HG23	2.17	0.43
1:A:710:LEU:HD11	9:O:715:TYR:CD1	2.52	0.43
2:D:20:LEU:HD23	2:D:20:LEU:HA	1.89	0.43
9:O:108:MET:HE1	9:O:154:LEU:HG	2.00	0.43
9:O:646:MET:HG2	12:I:124:VAL:HG22	1.99	0.43
10:V:180:ARG:NE	10:V:208:GLU:OE1	2.52	0.43
11:Y:321:TYR:O	11:Y:325:LEU:HG	2.19	0.43
11:Y:406:ASN:OD1	11:Y:408:GLN:HG2	2.18	0.43
12:I:644:TYR:O	12:I:726:GLY:HA2	2.18	0.43
13:N:523:LEU:HD12	13:N:524:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:OE2	1:A:185:TYR:OH	2.25	0.43
1:A:172:SER:HB3	10:V:430:PRO:HB3	2.00	0.43
1:A:924:SER:OG	1:A:925:SER:N	2.51	0.43
1:A:1103:PRO:O	1:A:1139:ASN:ND2	2.51	0.43
3:G:11:LEU:HD21	6:Q:456:ARG:NH1	2.30	0.43
5:J:56:LYS:NZ	5:P:531:TYR:O	2.50	0.43
5:J:660:LYS:HE2	11:Y:492:GLN:NE2	2.33	0.43
6:K:171:THR:O	6:K:171:THR:OG1	2.32	0.43
6:K:204:LEU:HD12	6:Q:24:PHE:HZ	1.83	0.43
9:O:581:ILE:HD13	9:O:611:SER:HB2	2.00	0.43
5:P:710:ALA:HB1	5:P:726:LEU:HD11	1.99	0.43
10:U:234:LEU:HA	10:U:237:ILE:HG22	2.01	0.43
10:U:238:TYR:CE2	10:U:250:LYS:HE2	2.54	0.43
10:V:180:ARG:HD3	10:V:212:LEU:HD21	1.99	0.43
11:Y:118:ASP:O	11:Y:122:ILE:HG12	2.18	0.43
11:Z:152:ARG:HA	11:Z:155:VAL:HG12	2.00	0.43
12:I:286:ARG:HA	12:I:286:ARG:HD3	1.71	0.43
12:I:391:THR:HB	12:I:515:PRO:HD3	2.00	0.43
1:A:1461:HIS:O	1:A:1465:ILE:HG23	2.18	0.43
5:J:68:THR:OG1	5:J:71:CYS:SG	2.76	0.43
6:K:6:LEU:HD23	6:K:6:LEU:HA	1.89	0.43
9:O:229:LYS:NZ	9:O:458:VAL:HA	2.34	0.43
9:O:348:TYR:CZ	9:O:361:LEU:HD11	2.53	0.43
6:Q:357:TYR:HB3	6:Q:374:ILE:HG13	2.01	0.43
10:V:304:SER:OG	10:V:339:ASN:ND2	2.36	0.43
11:Y:376:TYR:HD2	11:Y:395:MET:HE1	1.83	0.43
11:Y:395:MET:HA	11:Y:398:ASN:HD21	1.84	0.43
12:I:663:ASP:OD1	12:I:663:ASP:N	2.38	0.43
1:A:1503:ASN:O	1:A:1507:THR:HG22	2.19	0.43
6:K:299:PRO:HB2	6:K:333:TYR:CD2	2.53	0.43
8:M:63:GLN:HA	8:M:67:GLU:HA	2.00	0.43
9:O:644:LEU:O	9:O:648:ILE:HG12	2.19	0.43
5:P:87:GLU:O	5:P:91:ILE:HG22	2.18	0.43
6:Q:19:TYR:CZ	6:Q:49:LEU:HD22	2.53	0.43
10:U:124:LEU:HD23	10:U:124:LEU:HA	1.92	0.43
10:U:295:TYR:HB2	10:V:101:ARG:HG3	2.00	0.43
10:U:358:LEU:HD22	10:U:371:MET:HE1	2.00	0.43
10:V:330:ARG:HB2	10:V:333:THR:HG23	2.01	0.43
11:Y:252:ASP:OD1	11:Y:252:ASP:N	2.49	0.43
11:Y:445:VAL:HA	11:Y:448:LYS:HD2	2.00	0.43
1:A:1493:LYS:HD2	1:A:1493:LYS:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:522:PHE:O	5:P:525:VAL:HG12	2.19	0.43
6:Q:451:LEU:HD13	6:Q:467:TYR:CE2	2.54	0.43
10:U:448:GLN:OE1	10:U:451:GLU:HG3	2.18	0.43
11:Z:240:LEU:HD21	11:Z:262:GLN:NE2	2.34	0.43
12:I:718:LYS:NZ	12:I:736:SER:HB3	2.34	0.43
1:A:857:MET:HE3	1:A:858:PRO:HD2	1.99	0.43
5:J:90:GLN:OE1	5:J:90:GLN:C	2.62	0.43
6:K:201:LEU:HD13	6:Q:25:TRP:HH2	1.84	0.43
6:K:351:ASP:OD1	10:V:550:LEU:HD22	2.19	0.43
8:M:31:ILE:HD13	6:Q:302:TRP:CZ3	2.52	0.43
11:Y:190:MET:HE2	11:Y:190:MET:HB2	1.86	0.43
11:Z:140:MET:HA	11:Z:143:ASN:ND2	2.32	0.43
1:A:352:ARG:NH2	10:V:374:GLU:OE2	2.49	0.43
1:A:629:LEU:HD13	1:A:633:ILE:HG22	2.00	0.43
1:A:1076:ARG:O	1:A:1080:LEU:HG	2.18	0.43
1:A:1709:LYS:HE3	1:A:1709:LYS:HB2	1.87	0.43
1:A:1730:ALA:HA	1:A:1776:TYR:CD2	2.53	0.43
5:J:32:TYR:HH	5:J:64:HIS:CG	2.37	0.43
6:K:7:ARG:HA	6:K:10:VAL:HG12	2.01	0.43
8:M:60:LEU:HD12	8:M:60:LEU:HA	1.86	0.43
5:P:465:LEU:HD13	5:P:495:HIS:CD2	2.54	0.43
5:P:643:MET:HE2	5:P:658:PHE:HZ	1.83	0.43
6:Q:47:LEU:HD23	6:Q:55:ARG:C	2.44	0.43
6:Q:170:LEU:HD22	6:Q:176:LEU:HD11	2.01	0.43
6:Q:179:GLN:O	6:Q:183:GLU:HG2	2.18	0.43
6:Q:190:LEU:HD11	6:Q:201:LEU:HD23	2.01	0.43
10:U:404:GLY:O	10:U:408:THR:HG22	2.19	0.43
11:Y:209:TYR:C	11:Y:211:PHE:H	2.27	0.43
11:Y:414:ALA:O	11:Y:418:LEU:HG	2.18	0.43
11:Y:432:ASP:O	11:Y:436:THR:HG23	2.18	0.43
12:I:671:LEU:HA	12:I:674:VAL:HG12	2.01	0.43
12:I:730:VAL:HG22	12:I:745:GLU:HG2	2.00	0.43
13:N:55:LEU:HD23	13:N:55:LEU:HA	1.88	0.43
13:N:292:TRP:O	13:N:296:VAL:HG22	2.19	0.43
1:A:1363:THR:O	1:A:1363:THR:HG22	2.19	0.42
6:K:291:LEU:HB3	6:K:301:SER:HB2	2.00	0.42
8:M:31:ILE:HD12	6:Q:322:TYR:CE1	2.54	0.42
9:O:408:LEU:HD23	9:O:408:LEU:H	1.84	0.42
9:O:422:ILE:HG21	9:O:445:LEU:HB2	2.01	0.42
6:Q:47:LEU:HB3	6:Q:56:ALA:HB2	2.01	0.42
6:Q:194:CYS:SG	6:Q:195:ASN:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:58:LEU:HD23	10:V:58:LEU:HA	1.80	0.42
11:Y:441:TYR:O	11:Y:445:VAL:HG23	2.19	0.42
11:Z:140:MET:SD	11:Z:144:LEU:HD23	2.59	0.42
11:Z:323:ARG:HH21	11:Z:327:LEU:HD21	1.84	0.42
1:A:669:GLY:HA2	1:A:753:THR:HG21	2.00	0.42
1:A:823:ILE:HG22	1:A:824:ASP:N	2.35	0.42
1:A:1251:VAL:HG13	1:A:1603:LEU:HD22	2.00	0.42
2:D:10:PRO:HG2	9:O:346:TRP:CE2	2.54	0.42
5:J:544:TRP:CD1	5:J:579:LEU:HD13	2.54	0.42
6:K:284:LEU:HD22	6:K:308:TYR:HB2	2.00	0.42
6:Q:395:LEU:HD21	6:Q:405:MET:HB2	2.01	0.42
10:V:281:LYS:HD2	10:V:281:LYS:HA	1.61	0.42
12:I:366:LEU:HD23	12:I:366:LEU:HA	1.89	0.42
12:I:597:LYS:HE3	12:I:617:ALA:HB1	2.01	0.42
13:N:33:PRO:HG3	13:N:124:PRO:HB2	2.01	0.42
13:N:86:ASN:C	13:N:89:PRO:HD2	2.44	0.42
1:A:1396:LEU:HD23	1:A:1396:LEU:HA	1.89	0.42
4:H:67:LEU:HD22	11:Y:308:TRP:CH2	2.54	0.42
5:J:7:PRO:HG3	5:P:455:GLN:HG3	2.00	0.42
7:L:82:ASP:N	7:L:82:ASP:OD1	2.51	0.42
9:O:662:ARG:HG2	9:O:755:LEU:HD12	2.00	0.42
5:P:522:PHE:HB3	5:P:539:TYR:CE2	2.54	0.42
5:P:577:PHE:HD2	5:P:582:GLU:HB3	1.84	0.42
5:P:694:LYS:O	5:P:697:VAL:HG12	2.19	0.42
6:Q:299:PRO:HG3	6:Q:330:GLU:HB2	2.01	0.42
10:U:213:ILE:HG23	10:U:218:MET:HB3	2.00	0.42
11:Z:43:TYR:HE1	11:Z:99:PRO:HD2	1.84	0.42
1:A:633:ILE:HG23	1:A:754:LEU:CD2	2.49	0.42
5:J:546:LEU:HD23	5:J:548:LYS:HE3	2.01	0.42
6:K:66:ASP:OD1	6:K:67:LYS:N	2.53	0.42
7:L:80:TYR:CD2	7:L:154:ARG:HD2	2.54	0.42
5:P:19:TYR:N	5:P:19:TYR:CD1	2.87	0.42
6:Q:185:LEU:HA	6:Q:185:LEU:HD12	1.70	0.42
6:Q:382:ASN:O	6:Q:382:ASN:ND2	2.52	0.42
11:Y:8:ARG:HA	11:Y:48:TYR:CE2	2.55	0.42
11:Y:357:GLU:O	11:Y:360:ILE:HG22	2.19	0.42
11:Z:249:ARG:NH2	11:Z:371:CYS:O	2.51	0.42
12:I:61:ASN:CG	12:I:62:GLU:N	2.77	0.42
12:I:254:LYS:HA	12:I:254:LYS:HD2	1.87	0.42
13:N:188:LYS:HA	13:N:188:LYS:HD3	1.69	0.42
13:N:539:ILE:HA	13:N:542:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:HB3	1:A:457:PHE:CE1	2.54	0.42
1:A:1651:LEU:HD22	6:K:553:LYS:HB2	2.02	0.42
10:U:200:PRO:O	10:U:201:LEU:HB2	2.19	0.42
10:U:516:LEU:HB3	10:U:532:CYS:SG	2.59	0.42
12:I:208:LEU:HD22	12:I:217:LEU:HD11	2.02	0.42
13:N:294:GLU:O	13:N:297:VAL:HG12	2.19	0.42
13:N:622:TYR:HD2	13:N:622:TYR:O	2.03	0.42
1:A:76:LEU:HD12	1:A:589:ASP:CG	2.45	0.42
1:A:707:TRP:CH2	1:A:711:LEU:HD21	2.55	0.42
1:A:1599:ASN:OD1	1:A:1599:ASN:N	2.52	0.42
5:J:104:ASP:OD1	5:J:105:ASP:N	2.53	0.42
5:J:552:LEU:HD12	5:J:552:LEU:HA	1.81	0.42
6:K:406:HIS:HD2	6:K:447:LEU:HD13	1.84	0.42
7:L:80:TYR:HB3	7:L:154:ARG:HB2	2.01	0.42
9:O:326:GLU:OE2	10:V:416:PHE:N	2.43	0.42
10:U:58:LEU:HD23	10:U:58:LEU:HA	1.76	0.42
10:U:62:LEU:HD11	10:U:259:PHE:CE1	2.55	0.42
11:Y:281:LEU:HG	11:Y:290:VAL:HG23	2.01	0.42
11:Z:484:PHE:O	11:Z:488:VAL:HG23	2.20	0.42
1:A:124:GLN:N	1:A:154:LEU:O	2.53	0.42
1:A:168:ASP:OD1	1:A:168:ASP:N	2.42	0.42
1:A:713:SER:O	1:A:717:GLN:HG2	2.19	0.42
1:A:1751:ALA:HA	1:A:1755:CYS:SG	2.59	0.42
2:D:49:ASN:OD1	2:D:49:ASN:N	2.52	0.42
5:J:513:SER:HA	5:J:515:TYR:CE1	2.54	0.42
5:J:517:GLN:HG2	5:J:520:ARG:HE	1.85	0.42
6:K:81:TYR:CD2	6:K:139:ILE:HG12	2.49	0.42
9:O:392:GLY:H	9:O:615:ARG:NH2	2.18	0.42
9:O:608:LEU:HA	9:O:623:THR:HG21	2.02	0.42
5:P:473:TYR:CD2	5:P:500:TRP:HZ2	2.37	0.42
10:U:242:GLN:OE1	10:U:429:ARG:NE	2.53	0.42
12:I:618:ILE:HD12	12:I:705:MET:HE1	2.00	0.42
12:I:745:GLU:C	12:I:746:MET:HE2	2.45	0.42
13:N:536:GLU:O	13:N:539:ILE:HG12	2.19	0.42
14:C:60:ILE:HG12	14:C:80:TRP:CZ2	2.54	0.42
5:J:462:LEU:HD21	5:P:34:GLU:HG2	2.02	0.42
7:L:71:LYS:HD2	7:L:135:PHE:CE2	2.54	0.42
11:Y:410:LEU:HD13	11:Y:433:LYS:HB2	2.01	0.42
11:Z:274:MET:HA	11:Z:277:TYR:HB3	2.02	0.42
11:Z:406:ASN:OD1	11:Z:409:THR:HG23	2.19	0.42
13:N:626:TYR:HE1	13:N:630:LYS:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:OD1	1:A:425:SER:N	2.52	0.42
1:A:628:ILE:CD1	1:A:761:ALA:HB1	2.50	0.42
1:A:961:HIS:ND1	1:A:1830:LEU:HD11	2.35	0.42
1:A:1208:LEU:O	1:A:1212:VAL:HG12	2.20	0.42
5:J:89:GLU:CD	5:J:130:ARG:HH12	2.28	0.42
5:J:639:TYR:HB3	5:J:672:LEU:HD13	2.01	0.42
9:O:63:LEU:HD11	9:O:81:LEU:HB3	2.02	0.42
6:Q:310:LEU:HD11	6:Q:343:SER:HB2	2.01	0.42
6:Q:429:LEU:HD11	6:Q:433:LYS:HE2	2.02	0.42
10:U:33:LYS:HB2	10:U:62:LEU:HD22	2.01	0.42
11:Y:33:ASN:HD21	11:Z:232:LEU:HD23	1.85	0.42
11:Y:108:MET:HE1	11:Y:124:ILE:HG21	2.01	0.42
11:Y:357:GLU:CD	11:Y:357:GLU:H	2.28	0.42
11:Y:431:LEU:HD11	11:Y:448:LYS:HG2	2.02	0.42
12:I:417:PHE:HD1	12:I:448:VAL:HG13	1.84	0.42
13:N:513:ASP:O	13:N:516:ILE:HG13	2.20	0.42
1:A:804:ASP:O	1:A:808:ARG:HG3	2.20	0.42
1:A:857:MET:HE3	1:A:857:MET:HB3	1.73	0.42
1:A:861:PRO:HB3	1:A:899:ILE:HD11	2.02	0.42
1:A:1391:ASP:OD2	1:A:1391:ASP:N	2.38	0.42
6:K:350:HIS:O	6:K:354:MET:HG2	2.20	0.42
9:O:44:MET:CE	12:I:310:TRP:HZ2	2.33	0.42
9:O:360:LEU:HD23	9:O:360:LEU:HA	1.79	0.42
6:Q:285:PHE:HB2	6:Q:308:TYR:CE1	2.55	0.42
10:U:397:ARG:HA	10:U:428:LEU:HD21	2.01	0.42
10:V:379:LYS:HA	10:V:379:LYS:HD3	1.71	0.42
11:Y:190:MET:HA	11:Y:193:ILE:HD12	2.01	0.42
11:Y:319:LYS:HA	11:Y:319:LYS:HD2	1.85	0.42
11:Y:349:LEU:HB3	11:Y:354:ARG:O	2.20	0.42
11:Z:33:ASN:OD1	11:Z:36:LEU:HB2	2.20	0.42
11:Z:418:LEU:HD23	11:Z:418:LEU:HA	1.94	0.42
12:I:79:LEU:HD11	12:I:101:LEU:HD12	2.01	0.42
13:N:519:TYR:O	13:N:523:LEU:HG	2.20	0.42
13:N:552:ALA:N	13:N:553:PRO:HD2	2.35	0.42
1:A:115:LYS:HD3	9:O:267:VAL:HG21	2.02	0.41
5:J:106:ILE:HD13	5:J:106:ILE:HA	1.93	0.41
6:K:484:ALA:O	6:K:488:ILE:HG22	2.20	0.41
5:P:468:GLU:HG2	5:P:491:LEU:HD23	2.01	0.41
5:P:667:GLN:HG3	5:P:698:ILE:HD12	2.01	0.41
10:U:127:GLU:OE2	10:U:181:LYS:NZ	2.49	0.41
10:V:405:LEU:HA	10:V:408:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:196:VAL:HG12	11:Z:199:LEU:HD11	2.02	0.41
11:Z:349:LEU:HD11	11:Z:354:ARG:HB2	2.02	0.41
12:I:47:HIS:ND1	12:I:54:ARG:HA	2.35	0.41
12:I:379:LEU:HA	12:I:379:LEU:HD12	1.85	0.41
12:I:632:ARG:O	12:I:636:TYR:OH	2.38	0.41
13:N:627:GLU:HG2	13:N:633:ARG:O	2.20	0.41
1:A:74:TRP:HA	1:A:93:LEU:O	2.20	0.41
1:A:357:ALA:HA	10:V:395:ASN:HD21	1.84	0.41
1:A:637:MET:HB2	1:A:667:MET:HE1	2.02	0.41
1:A:650:GLY:N	1:A:651:PRO:HD3	2.34	0.41
1:A:848:VAL:O	1:A:852:LEU:HG	2.21	0.41
1:A:1631:TYR:HB2	1:A:1708:TYR:HB2	2.01	0.41
3:G:18:GLU:OE1	6:Q:457:LYS:NZ	2.44	0.41
4:H:79:MET:SD	5:P:580:GLN:NE2	2.93	0.41
6:K:252:LYS:O	6:K:256:VAL:HG13	2.20	0.41
7:L:12:ASP:OD2	7:L:14:LYS:HE3	2.20	0.41
5:P:113:SER:O	5:P:117:THR:HG23	2.19	0.41
6:Q:57:ALA:HB1	6:Q:80:HIS:NE2	2.35	0.41
11:Y:330:LYS:O	11:Y:334:LEU:HG	2.20	0.41
12:I:210:LEU:HB2	12:I:217:LEU:HD13	2.02	0.41
12:I:262:LEU:HD23	12:I:262:LEU:HA	1.88	0.41
13:N:293:ILE:HD12	13:N:328:VAL:HG12	2.02	0.41
13:N:527:LEU:HD11	13:N:560:MET:HE2	2.02	0.41
1:A:1084:ARG:NH2	1:A:1142:ALA:HB3	2.35	0.41
1:A:1663:LEU:HB3	1:A:1680:LEU:HD22	2.02	0.41
1:A:1860:LEU:HD22	1:A:1865:ASP:OD1	2.19	0.41
9:O:283:LEU:HA	9:O:283:LEU:HD12	1.83	0.41
9:O:365:VAL:O	9:O:369:VAL:HG22	2.20	0.41
9:O:642:SER:O	9:O:646:MET:HG3	2.20	0.41
6:Q:6:LEU:O	6:Q:10:VAL:HG12	2.20	0.41
10:V:392:ILE:HG21	10:V:402:TRP:CZ2	2.55	0.41
11:Y:46:LEU:HD11	11:Y:68:MET:HB2	2.02	0.41
11:Y:498:TYR:HB3	11:Y:515:MET:SD	2.60	0.41
11:Y:499:SER:HA	11:Y:502:LEU:HG	2.02	0.41
12:I:426:LEU:HB3	12:I:433:VAL:HG22	2.01	0.41
1:A:257:MET:HE1	1:A:444:PHE:CG	2.55	0.41
1:A:352:ARG:HG3	10:V:308:TYR:HD2	1.86	0.41
1:A:1328:TYR:HB3	1:A:1363:THR:HG22	2.02	0.41
1:A:1369:LEU:HD22	1:A:1585:LEU:HD22	2.02	0.41
5:J:138:TYR:CD1	5:J:151:PRO:HB3	2.52	0.41
6:K:355:ALA:O	6:K:359:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:132:VAL:HG11	12:I:310:TRP:CZ3	2.55	0.41
9:O:631:GLN:HB3	9:O:636:ILE:HG13	2.01	0.41
6:Q:6:LEU:O	6:Q:6:LEU:HD12	2.20	0.41
10:U:512:ALA:O	10:U:516:LEU:HG	2.21	0.41
11:Y:25:LEU:HD21	11:Z:205:TRP:CD1	2.55	0.41
11:Z:447:LYS:HD3	11:Z:447:LYS:HA	1.74	0.41
12:I:195:ILE:HD11	12:I:252:ALA:HB2	2.02	0.41
12:I:427:ARG:HH21	12:I:438:ASN:HD21	1.67	0.41
13:N:105:PRO:HG3	13:N:232:TRP:CD2	2.55	0.41
13:N:273:MET:HE1	13:N:335:ILE:HG12	2.03	0.41
1:A:661:VAL:O	1:A:665:MET:HG3	2.21	0.41
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.92	0.41
1:A:1033:ARG:HG2	1:A:1566:PHE:CZ	2.54	0.41
5:J:8:VAL:HG12	5:J:31:LEU:HD22	2.02	0.41
5:J:549:ASP:HB2	8:M:60:LEU:HD21	2.03	0.41
6:K:60:LEU:HD22	6:K:72:CYS:SG	2.60	0.41
6:K:473:VAL:CG2	5:P:130:ARG:HH12	2.32	0.41
5:P:103:HIS:O	5:P:107:VAL:HG12	2.19	0.41
10:U:31:GLU:HA	10:U:34:LYS:HG2	2.02	0.41
11:Y:401:LYS:HA	11:Y:401:LYS:HD3	1.80	0.41
12:I:299:SER:N	12:I:302:ASP:OD2	2.53	0.41
13:N:350:ASP:OD1	13:N:350:ASP:N	2.53	0.41
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.67	0.41
1:A:444:PHE:CE2	1:A:453:ARG:HB2	2.55	0.41
2:D:51:LEU:HD23	2:D:51:LEU:HA	1.83	0.41
8:M:11:ILE:O	8:M:15:ILE:HD12	2.20	0.41
5:P:102:SER:N	5:P:105:ASP:OD2	2.48	0.41
5:P:516:MET:HE3	5:P:516:MET:HB2	1.92	0.41
10:V:123:TYR:CD2	10:V:124:LEU:HD22	2.55	0.41
11:Z:204:VAL:HB	11:Z:227:LEU:HD21	2.02	0.41
1:A:477:LYS:N	1:A:491:LEU:O	2.52	0.41
1:A:1930:ARG:NH2	13:N:77:GLU:OE2	2.40	0.41
5:J:142:LEU:CD2	5:J:151:PRO:HB2	2.51	0.41
5:J:641:LEU:HA	5:J:644:ILE:CG2	2.49	0.41
7:L:75:LYS:HE3	7:L:161:PRO:HB3	2.03	0.41
8:M:35:GLU:O	6:Q:325:LYS:NZ	2.49	0.41
9:O:65:LEU:HB3	9:O:66:PRO:HD3	2.02	0.41
10:U:379:LYS:HD2	10:U:379:LYS:HA	1.69	0.41
11:Y:21:LEU:HG	11:Z:169:LEU:HD23	2.03	0.41
11:Y:481:LEU:HD23	11:Y:485:LEU:HD13	2.02	0.41
13:N:79:LEU:HG	13:N:156:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:PHE:CE2	1:A:443:CYS:HB2	2.55	0.41
1:A:591:VAL:HG22	1:A:606:ARG:HH22	1.84	0.41
1:A:1811:LEU:HD12	1:A:1811:LEU:HA	1.86	0.41
2:D:53:PRO:HB3	10:U:385:ILE:HG21	2.03	0.41
5:J:8:VAL:HG22	5:P:147:PHE:HE2	1.86	0.41
9:O:361:LEU:HB3	9:O:384:LEU:HG	2.02	0.41
9:O:532:VAL:HG22	9:O:546:ARG:HB3	2.02	0.41
6:Q:169:LEU:HD23	6:Q:169:LEU:HA	1.85	0.41
10:V:203:TRP:CD1	10:V:207:LEU:HD12	2.56	0.41
11:Y:275:ASP:HB2	11:Y:306:GLU:OE1	2.21	0.41
1:A:266:HIS:CE1	1:A:427:ALA:HB2	2.56	0.41
1:A:852:LEU:HB3	1:A:881:ILE:HD13	2.03	0.41
2:D:37:HIS:NE2	9:O:144:SER:OG	2.53	0.41
2:D:54:ILE:HG12	6:Q:510:ARG:NH2	2.35	0.41
5:J:103:HIS:O	5:J:107:VAL:HG23	2.20	0.41
6:K:263:PHE:O	6:Q:55:ARG:HD3	2.21	0.41
6:K:377:GLU:OE2	3:W:4:ARG:NH2	2.40	0.41
7:L:5:ASN:OD1	7:L:5:ASN:N	2.54	0.41
9:O:509:LEU:HD13	9:O:538:LEU:HB2	2.03	0.41
5:P:118:LEU:HD13	5:P:140:LYS:HG3	2.03	0.41
5:P:726:LEU:HD21	5:P:742:LEU:HD23	2.02	0.41
5:P:749:LYS:HB2	5:P:749:LYS:HE2	1.75	0.41
10:U:419:LEU:HD13	10:U:442:CYS:HB3	2.03	0.41
10:U:460:TYR:HE2	10:U:470:LEU:HD21	1.85	0.41
10:V:192:PHE:O	10:V:196:THR:HG23	2.21	0.41
10:V:525:LEU:HB3	10:V:528:GLU:OE1	2.21	0.41
11:Y:105:LYS:HA	11:Y:108:MET:HG3	2.03	0.41
11:Y:332:ILE:HD12	11:Y:332:ILE:HA	1.82	0.41
11:Z:305:ALA:HB1	11:Z:331:ALA:HB1	2.03	0.41
12:I:44:VAL:HG22	12:I:58:PHE:HB3	2.03	0.41
12:I:622:SER:HB3	12:I:633:ARG:HE	1.85	0.41
12:I:679:ASP:OD1	12:I:682:GLU:HB3	2.20	0.41
13:N:287:ARG:O	13:N:291:LYS:HD3	2.21	0.41
1:A:1053:GLN:HG3	1:A:1057:LEU:HD23	2.03	0.41
1:A:1176:LEU:HD13	1:A:1208:LEU:HD13	2.03	0.41
1:A:1617:ARG:HA	1:A:1691:LEU:HD13	2.03	0.41
5:J:476:LEU:HG	5:J:484:ALA:HB1	2.02	0.41
5:J:499:GLY:HA2	5:J:525:VAL:HG23	2.02	0.41
5:J:653:LEU:HA	5:J:653:LEU:HD23	1.81	0.41
9:O:33:TYR:CE2	9:O:73:ILE:HG12	2.56	0.41
11:Z:16:HIS:HA	11:Z:19:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:344:ILE:O	12:I:348:VAL:HG23	2.21	0.41
13:N:368:THR:HG22	13:N:369:ASP:N	2.36	0.41
1:A:150:CYS:HA	1:A:163:SER:HA	2.03	0.40
1:A:152:CYS:SG	1:A:187:LEU:HD11	2.60	0.40
1:A:982:ASP:HB2	1:A:1698:TYR:O	2.20	0.40
1:A:1019:MET:HE1	1:A:1087:PHE:CZ	2.56	0.40
1:A:1390:PRO:HB2	1:A:1396:LEU:HD23	2.02	0.40
3:G:12:LYS:HE3	3:G:12:LYS:HB2	1.87	0.40
9:O:378:SER:HB2	9:O:417:LEU:HD13	2.03	0.40
5:P:628:ILE:HD13	5:P:628:ILE:HA	1.79	0.40
5:P:658:PHE:HB3	5:P:675:ILE:HG12	2.03	0.40
6:Q:155:GLU:OE2	6:Q:159:LEU:HG	2.21	0.40
10:V:228:TRP:H	10:V:228:TRP:HD1	1.68	0.40
10:V:323:LEU:HD23	10:V:323:LEU:HA	1.87	0.40
10:V:537:CYS:HA	10:V:543:ARG:HA	2.02	0.40
11:Y:146:LYS:HE3	11:Y:146:LYS:HB2	1.75	0.40
11:Y:206:ILE:HD12	11:Y:206:ILE:HA	1.93	0.40
11:Z:282:ALA:HB2	11:Z:290:VAL:HG21	2.02	0.40
11:Z:312:GLY:HA3	11:Z:344:LEU:HD21	2.03	0.40
12:I:138:LEU:HA	12:I:138:LEU:HD23	1.87	0.40
13:N:182:ARG:HB3	13:N:223:GLY:HA2	2.03	0.40
1:A:953:LEU:HD21	1:A:1821:PHE:HE2	1.87	0.40
6:K:48:TYR:HB2	6:K:79:CYS:SG	2.62	0.40
6:K:232:ASP:OD1	6:K:264:HIS:NE2	2.54	0.40
9:O:97:ILE:HD12	9:O:97:ILE:HA	1.94	0.40
6:Q:84:LYS:HD3	6:Q:84:LYS:HA	1.83	0.40
6:Q:93:LEU:HD13	6:Q:136:ARG:HG2	2.03	0.40
6:Q:298:ASN:OD1	6:Q:299:PRO:HD2	2.22	0.40
10:U:35:GLN:O	10:U:38:LEU:HG	2.21	0.40
10:U:39:ILE:HG12	10:U:201:LEU:O	2.20	0.40
10:U:376:MET:HB3	10:U:376:MET:HE3	1.77	0.40
10:V:45:GLU:OE2	10:V:45:GLU:HA	2.20	0.40
10:V:91:LYS:NZ	10:V:95:ASP:OD1	2.46	0.40
10:V:209:LEU:HD12	10:V:209:LEU:HA	1.79	0.40
10:V:441:GLU:HG2	10:V:472:LYS:HE2	2.01	0.40
11:Y:412:LEU:O	11:Y:415:THR:OG1	2.29	0.40
12:I:321:LEU:HA	12:I:321:LEU:HD12	1.86	0.40
13:N:59:VAL:HG21	13:N:135:TRP:CZ3	2.56	0.40
13:N:228:LYS:N	13:N:228:LYS:HD3	2.36	0.40
4:H:79:MET:HB2	4:H:79:MET:HE2	1.81	0.40
5:J:498:THR:HG21	5:P:30:ARG:HH12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:50:VAL:HA	8:M:53:GLN:HG2	2.03	0.40
9:O:648:ILE:HD13	9:O:648:ILE:HA	1.85	0.40
5:P:8:VAL:HG23	5:P:27:LEU:HD12	2.02	0.40
5:P:473:TYR:HD2	5:P:500:TRP:CZ2	2.39	0.40
10:U:318:TYR:HA	10:U:321:HIS:CD2	2.57	0.40
11:Y:232:LEU:HD11	11:Z:33:ASN:HB2	2.04	0.40
11:Y:488:VAL:O	11:Y:489:ASN:HB2	2.22	0.40
13:N:180:PHE:HB2	13:N:240:PHE:CZ	2.56	0.40
1:A:1216:LYS:HB3	1:A:1219:THR:OG1	2.22	0.40
1:A:1716:GLN:OE1	13:N:369:ASP:HB3	2.21	0.40
2:D:37:HIS:HD2	9:O:145:LYS:HD3	1.87	0.40
6:K:210:LYS:HB3	6:K:213:ASN:OD1	2.22	0.40
7:L:73:THR:HG23	7:L:133:ARG:HG2	2.03	0.40
9:O:422:ILE:CG2	9:O:445:LEU:HB2	2.52	0.40
9:O:706:CYS:SG	9:O:709:ARG:HD3	2.62	0.40
5:P:160:GLU:O	5:P:162:PRO:HD3	2.21	0.40
10:U:29:LEU:HD12	10:U:62:LEU:HD21	2.04	0.40
10:U:419:LEU:HD21	10:U:443:TYR:CE2	2.56	0.40
10:V:180:ARG:HD3	10:V:212:LEU:CD2	2.50	0.40
11:Y:25:LEU:HD23	11:Z:201:TRP:CZ3	2.57	0.40
11:Z:46:LEU:HD23	11:Z:46:LEU:HA	1.89	0.40
11:Z:140:MET:HE3	11:Z:140:MET:HB3	1.93	0.40
12:I:642:GLN:OE1	12:I:723:ALA:HA	2.21	0.40
13:N:545:LEU:HD23	13:N:545:LEU:O	2.21	0.40
1:A:27:HIS:O	1:A:27:HIS:ND1	2.54	0.40
1:A:1179:LEU:HD23	1:A:1179:LEU:HA	1.93	0.40
1:A:1225:THR:HG21	1:A:1261:TYR:OH	2.22	0.40
1:A:1416:TRP:CH2	1:A:1475:ARG:HA	2.57	0.40
1:A:1702:ARG:HG2	1:A:1782:GLU:OE2	2.21	0.40
6:K:284:LEU:O	6:K:284:LEU:HD23	2.21	0.40
5:P:735:LYS:HA	5:P:735:LYS:HD2	1.83	0.40
10:U:290:ARG:HD3	10:U:300:MET:SD	2.62	0.40
10:U:423:ARG:HG3	10:U:423:ARG:NH1	2.35	0.40
10:V:128:LYS:HB3	10:V:128:LYS:HE3	1.90	0.40
10:V:274:HIS:ND1	10:V:306:LEU:HD21	2.37	0.40
11:Y:22:LEU:HD12	11:Y:22:LEU:HA	1.82	0.40
11:Z:114:MET:HA	11:Z:114:MET:HE2	2.03	0.40
13:N:615:ILE:HD13	13:N:615:ILE:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1546/1944 (80%)	1493 (97%)	52 (3%)	1 (0%)	48	79
2	D	54/121 (45%)	54 (100%)	0	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
5	J	471/824 (57%)	456 (97%)	15 (3%)	0	100	100
5	P	480/824 (58%)	467 (97%)	13 (3%)	0	100	100
6	K	506/620 (82%)	489 (97%)	17 (3%)	0	100	100
6	Q	500/620 (81%)	490 (98%)	10 (2%)	0	100	100
7	L	175/185 (95%)	167 (95%)	8 (5%)	0	100	100
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	499/597 (84%)	486 (97%)	13 (3%)	0	100	100
10	V	532/597 (89%)	519 (98%)	13 (2%)	0	100	100
11	Y	496/565 (88%)	486 (98%)	10 (2%)	0	100	100
11	Z	483/565 (86%)	475 (98%)	8 (2%)	0	100	100
12	I	710/814 (87%)	695 (98%)	15 (2%)	0	100	100
13	N	596/822 (72%)	579 (97%)	16 (3%)	1 (0%)	43	73
14	C	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
All	All	7961/10291 (77%)	7752 (97%)	207 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	N	689	VAL
1	A	591	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1349/1720 (78%)	1340 (99%)	9 (1%)	76	83
2	D	52/115 (45%)	52 (100%)	0	100	100
3	G	24/77 (31%)	24 (100%)	0	100	100
3	W	24/77 (31%)	24 (100%)	0	100	100
4	H	49/89 (55%)	49 (100%)	0	100	100
5	J	343/727 (47%)	340 (99%)	3 (1%)	70	81
5	P	414/727 (57%)	412 (100%)	2 (0%)	81	85
6	K	439/548 (80%)	438 (100%)	1 (0%)	87	89
6	Q	425/548 (78%)	422 (99%)	3 (1%)	76	83
7	L	163/170 (96%)	160 (98%)	3 (2%)	51	74
8	M	52/67 (78%)	52 (100%)	0	100	100
9	O	582/650 (90%)	580 (100%)	2 (0%)	86	88
10	U	431/520 (83%)	430 (100%)	1 (0%)	87	89
10	V	464/520 (89%)	464 (100%)	0	100	100
11	Y	423/484 (87%)	419 (99%)	4 (1%)	70	81
11	Z	412/484 (85%)	411 (100%)	1 (0%)	87	89
12	I	634/736 (86%)	629 (99%)	5 (1%)	73	82
13	N	458/724 (63%)	455 (99%)	3 (1%)	76	83
14	C	48/75 (64%)	48 (100%)	0	100	100
All	All	6786/9058 (75%)	6749 (100%)	37 (0%)	78	85

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	MET
1	A	482	VAL
1	A	490	VAL
1	A	492	GLU

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Mol	Chain	Res	Type
1	A	969	ASP
1	A	1453	ASN
1	A	1455	GLU
1	A	1609	LEU
1	A	1899	HIS
5	J	633[A]	ARG
5	J	633[B]	ARG
5	J	636	ASN
6	K	62	SER
7	L	45	LEU
7	L	101	ASN
7	L	177	ASP
9	O	267	VAL
9	O	636	ILE
5	P	468	GLU
5	P	723	LEU
6	Q	340	TYR
6	Q	351	ASP
6	Q	426	LEU
10	U	467	LYS
11	Y	233	LEU
11	Y	306	GLU
11	Y	344	LEU
11	Y	481	LEU
11	Z	26	LEU
12	I	164	ILE
12	I	300	VAL
12	I	302	ASP
12	I	454	GLU
12	I	663	ASP
13	N	86	ASN
13	N	302	LYS
13	N	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	124	GLN
1	A	155	GLN
1	A	266	HIS
1	A	619	GLN

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Mol	Chain	Res	Type
1	A	671	ASN
1	A	1072	GLN
1	A	1327	GLN
1	A	1351	GLN
1	A	1591	HIS
1	A	1604	GLN
1	A	1627	ASN
1	A	1795	GLN
1	A	1841	ASN
1	A	1899	HIS
4	H	101	GLN
5	J	166	GLN
5	J	545	HIS
5	J	547	GLN
5	J	583	HIS
5	J	648	GLN
6	K	12	GLN
6	K	16	GLN
6	K	54	HIS
6	K	80	HIS
6	K	86	HIS
6	K	415	ASN
6	K	449	ASN
6	K	478	ASN
6	K	557	ASN
7	L	60	GLN
7	L	65	ASN
7	L	67	GLN
7	L	138	GLN
7	L	145	HIS
7	L	146	GLN
8	M	66	HIS
9	O	237	GLN
9	O	261	ASN
9	O	306	ASN
9	O	332	GLN
9	O	492	HIS
9	O	512	GLN
9	O	556	GLN
9	O	671	GLN
9	O	717	GLN
9	O	731	ASN

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Mol	Chain	Res	Type
9	O	754	HIS
5	P	100	GLN
5	P	480	ASN
5	P	530	ASN
5	P	575	ASN
5	P	599	ASN
5	P	626	ASN
5	P	667	GLN
5	P	674	HIS
5	P	679	GLN
5	P	680	HIS
5	P	716	ASN
6	Q	20	GLN
6	Q	45	GLN
6	Q	54	HIS
6	Q	88	GLN
6	Q	316	ASN
6	Q	414	GLN
6	Q	468	HIS
10	U	71	GLN
10	U	104	HIS
10	U	347	HIS
10	U	407	GLN
10	U	426	HIS
10	U	479	GLN
10	U	534	GLN
10	V	145	GLN
10	V	252	GLN
10	V	373	HIS
10	V	431	ASN
10	V	479	GLN
11	Y	213	HIS
11	Y	255	ASN
11	Y	264	GLN
11	Y	299	ASN
11	Y	335	ASN
11	Y	337	ASN
11	Y	408	GLN
11	Z	31	ASN
11	Z	143	ASN
11	Z	150	GLN
11	Z	213	HIS

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Mol	Chain	Res	Type
11	Z	236	ASN
11	Z	262	GLN
11	Z	264	GLN
11	Z	387	ASN
12	I	102	HIS
12	I	362	HIS
12	I	405	GLN
12	I	455	HIS
12	I	502	GLN
12	I	535	GLN
12	I	584	HIS
12	I	668	GLN
13	N	86	ASN
13	N	147	GLN
13	N	170	GLN
13	N	235	GLN
13	N	241	HIS
13	N	245	GLN
13	N	373	GLN
13	N	573	ASN
14	C	31	ASN
14	C	58	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

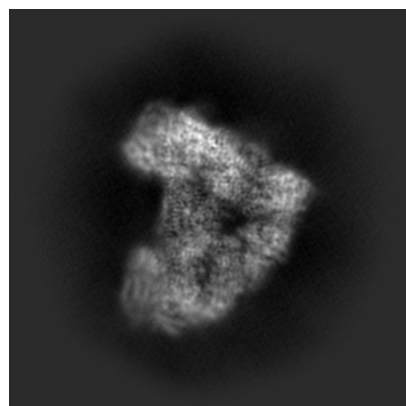
6 Map visualisation [i](#)

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

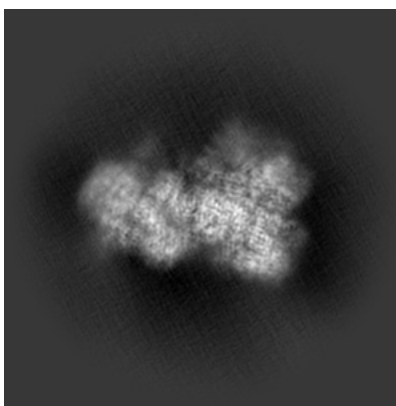
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

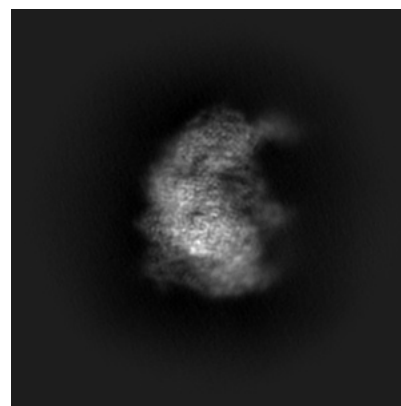
6.1.1 Primary map



X

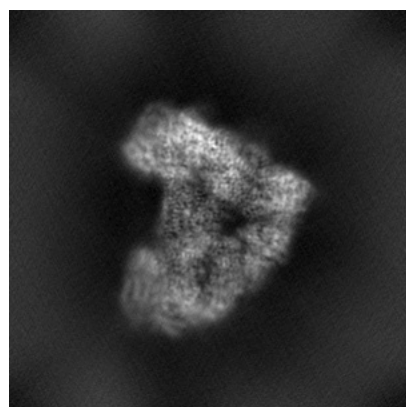


Y

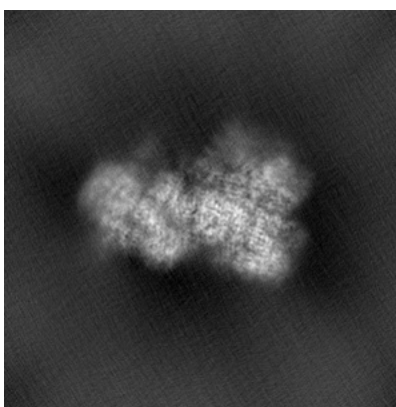


Z

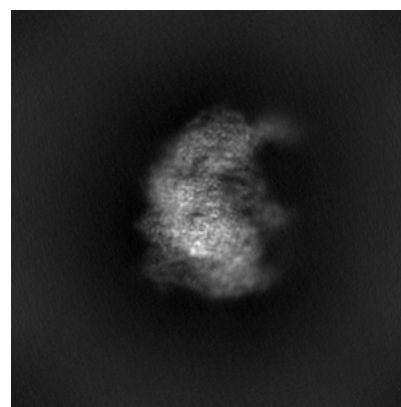
6.1.2 Raw map



X



Y

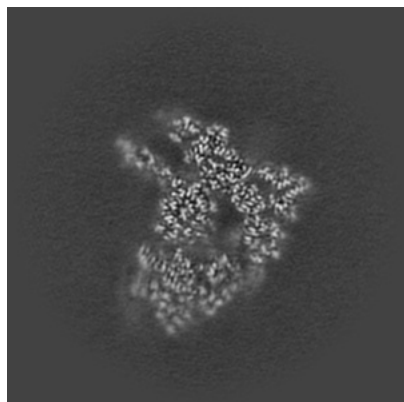


Z

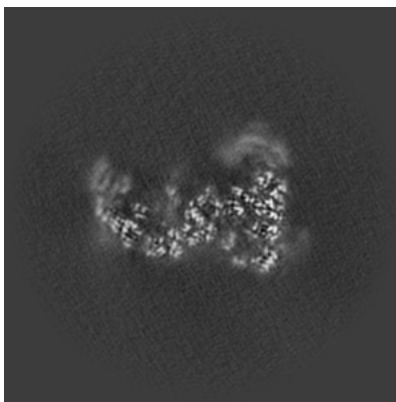
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

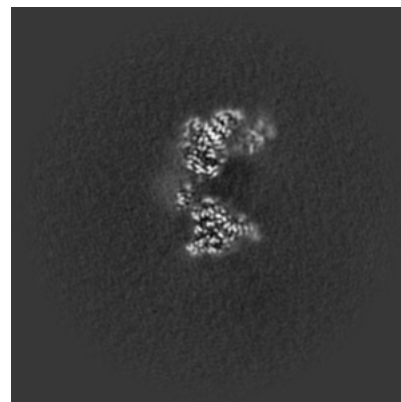
6.2.1 Primary map



X Index: 180

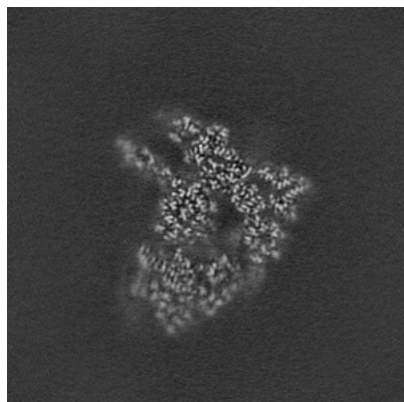


Y Index: 180

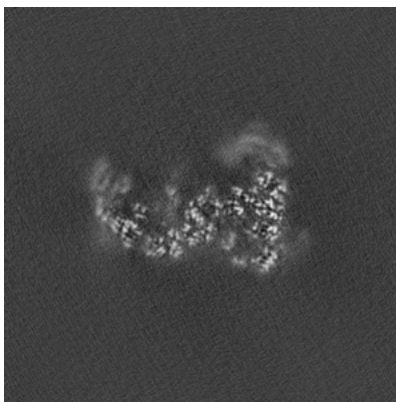


Z Index: 180

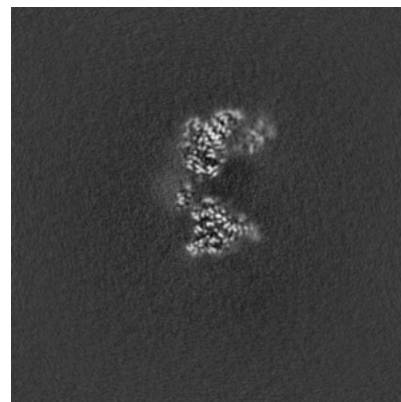
6.2.2 Raw map



X Index: 180



Y Index: 180

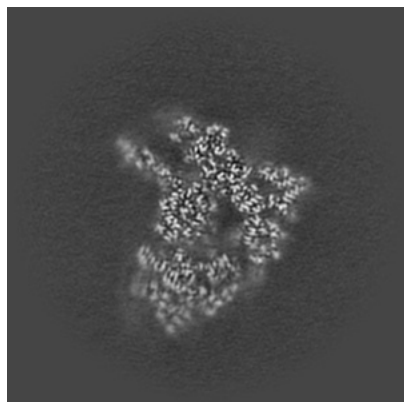


Z Index: 180

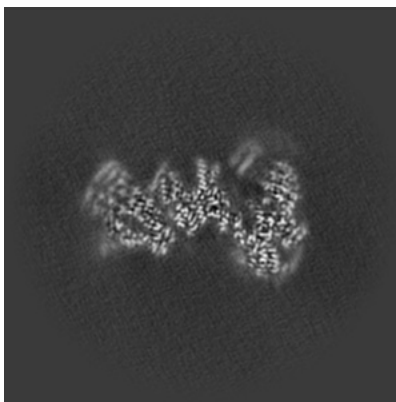
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

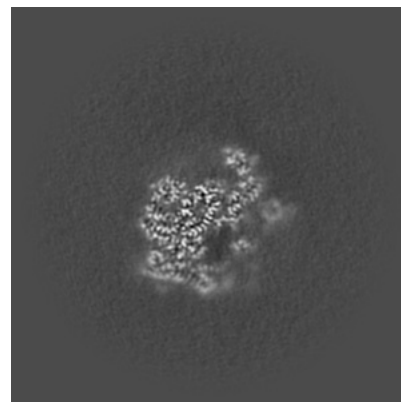
6.3.1 Primary map



X Index: 179

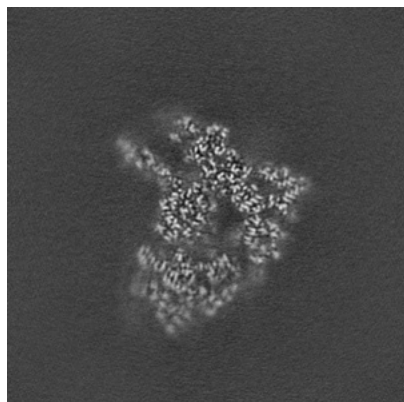


Y Index: 160

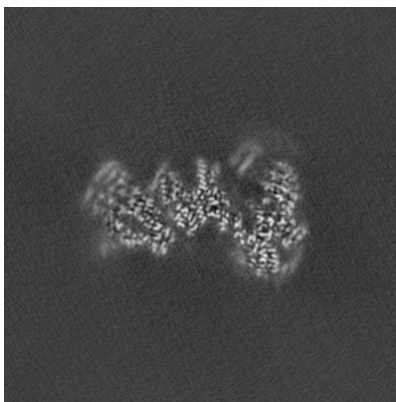


Z Index: 232

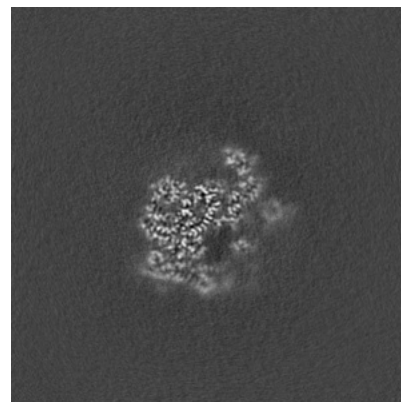
6.3.2 Raw map



X Index: 179



Y Index: 160

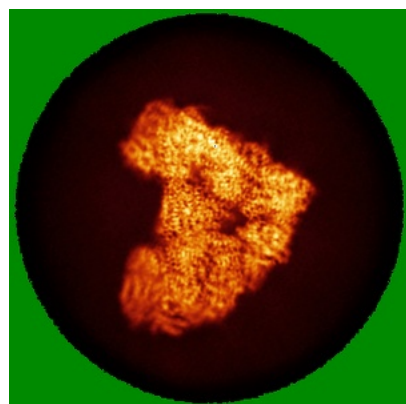


Z Index: 232

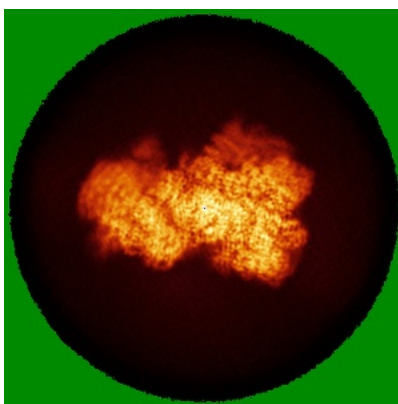
The images above show the largest variance slices of the map in three orthogonal directions.

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

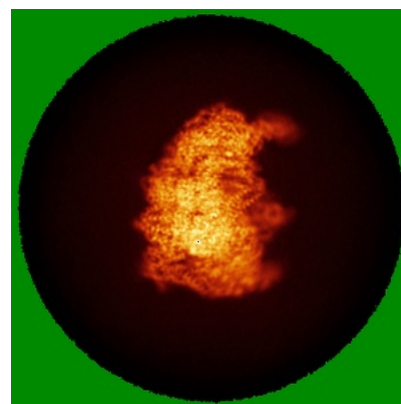
6.4.1 Primary map



X

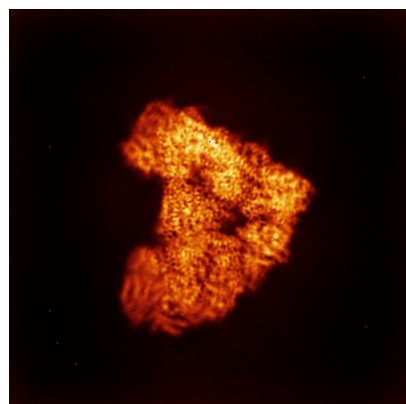


Y

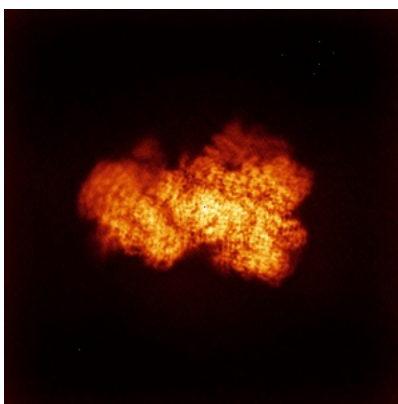


Z

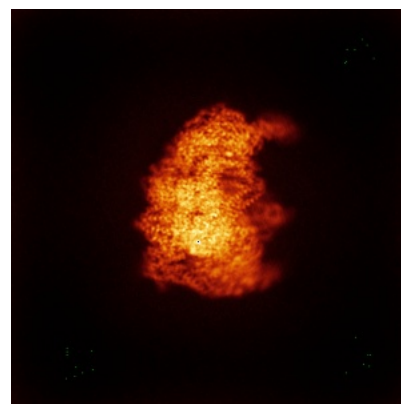
6.4.2 Raw map



X



Y

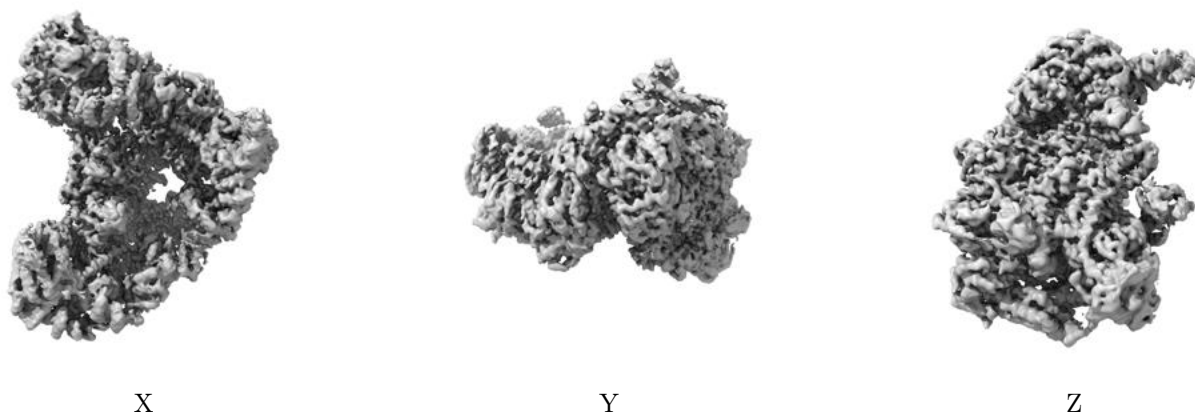


Z

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.

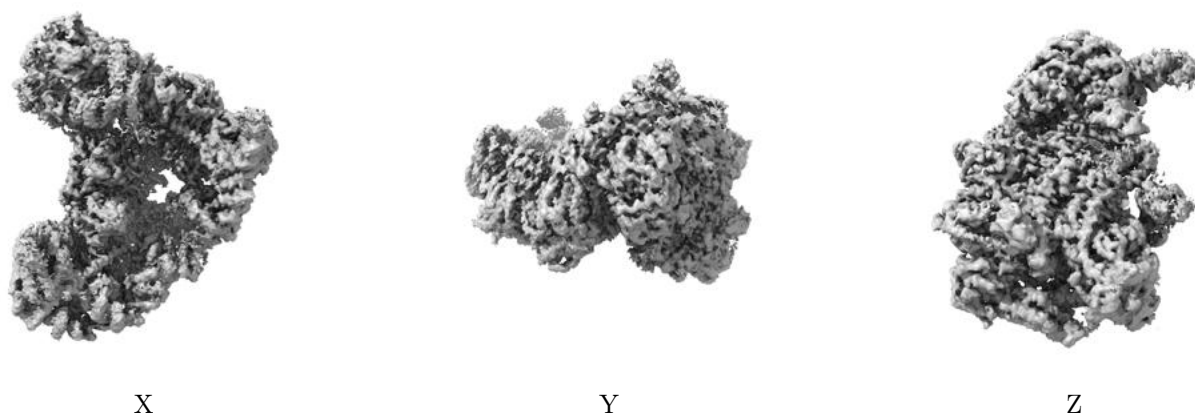
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

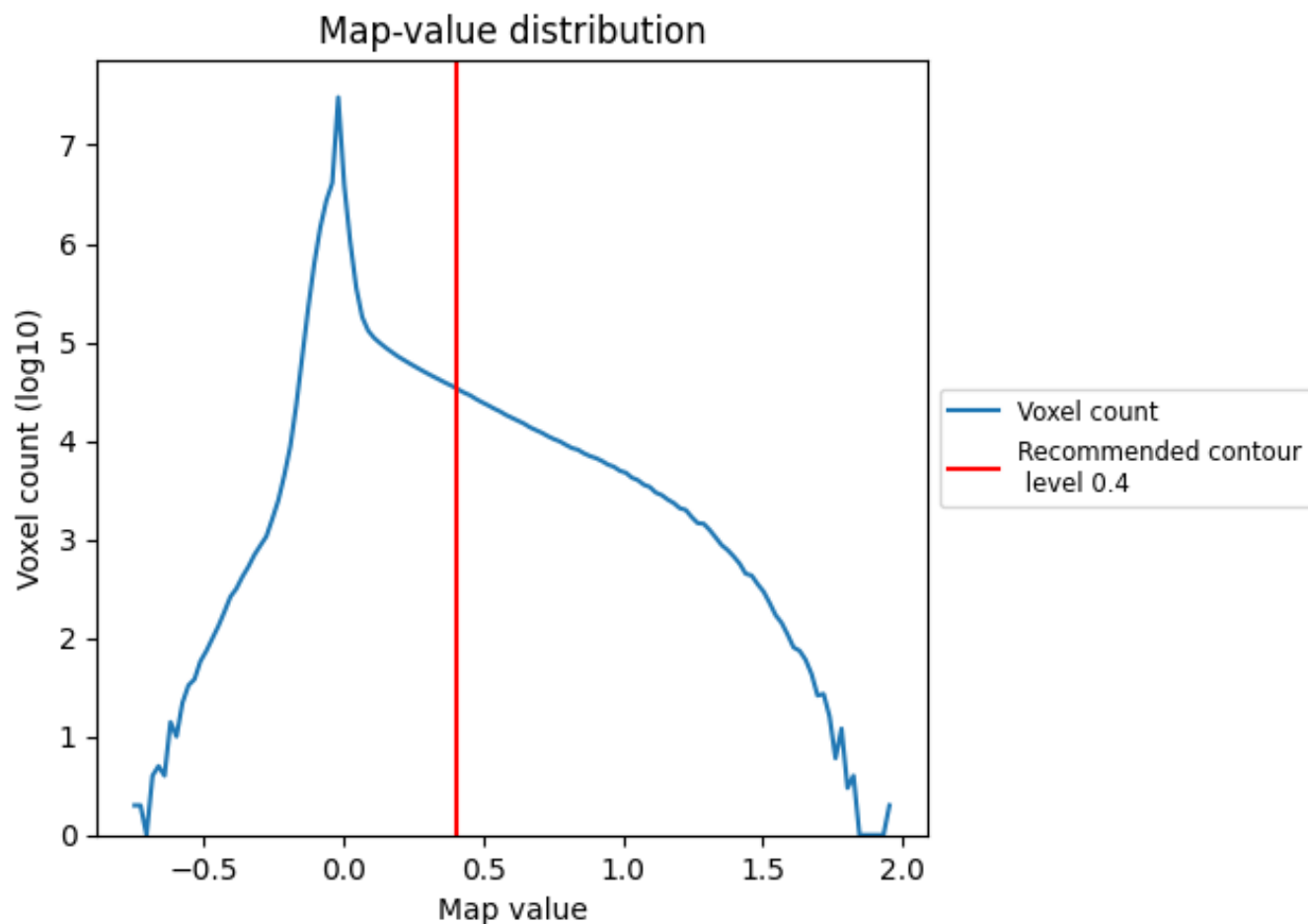
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

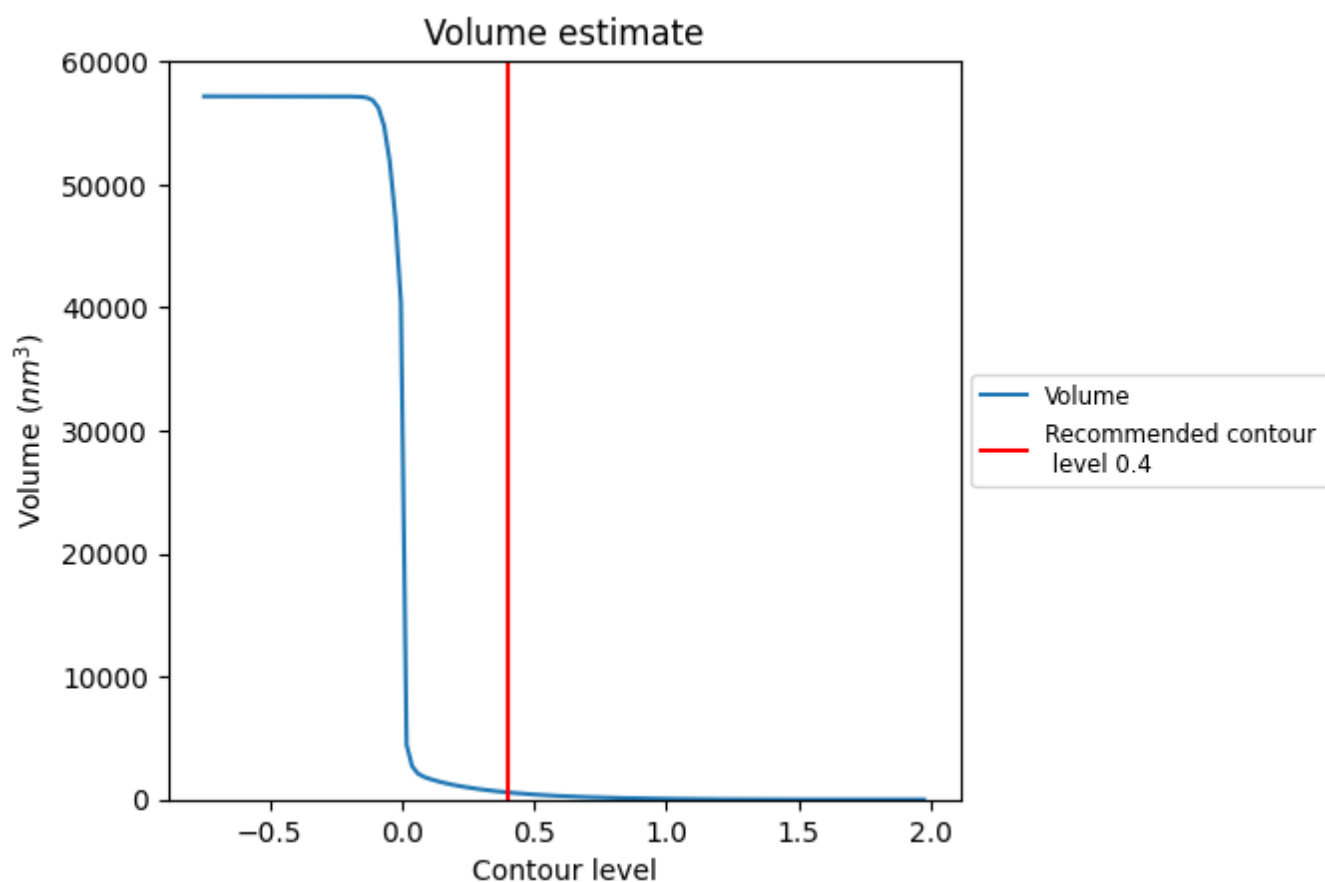
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

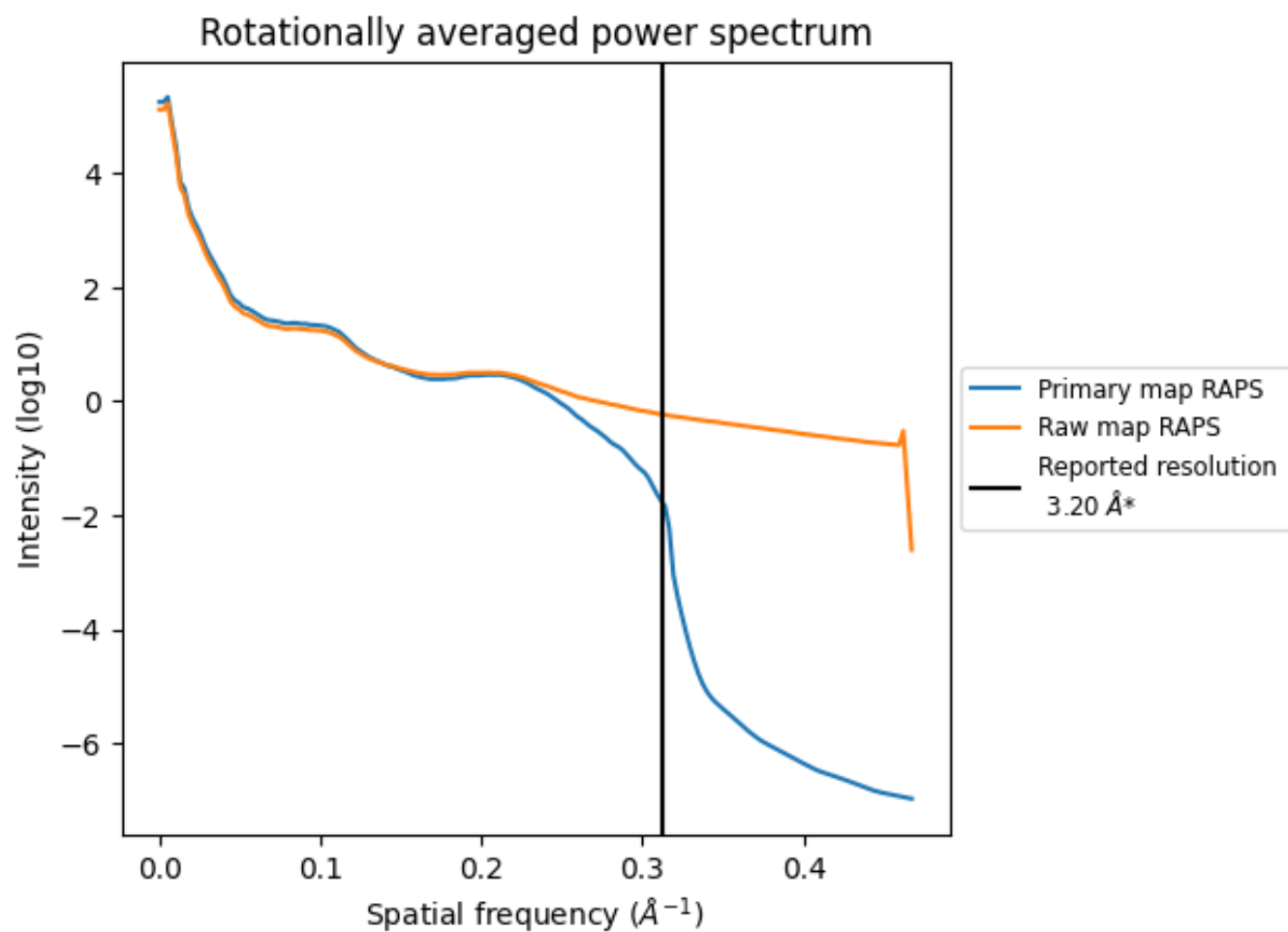
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 582 nm³; 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 ⓘ

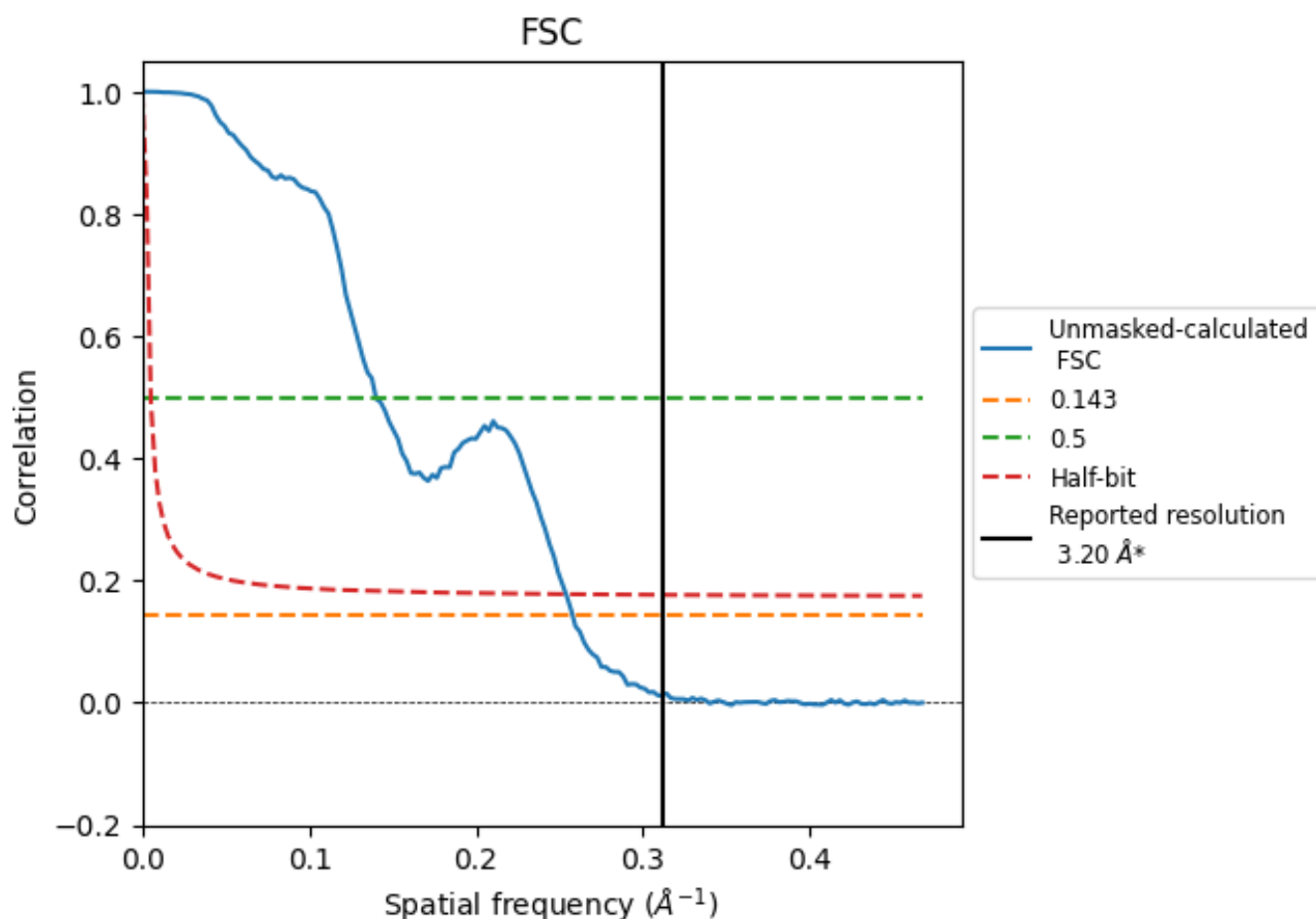


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

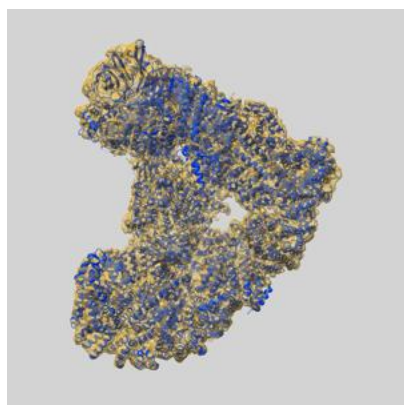
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	7.14	3.94

*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 %

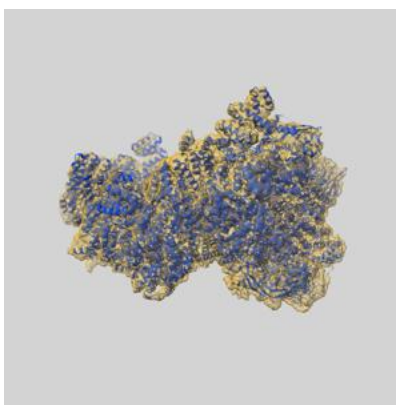
9 Map-model fit [i](#)

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](#).

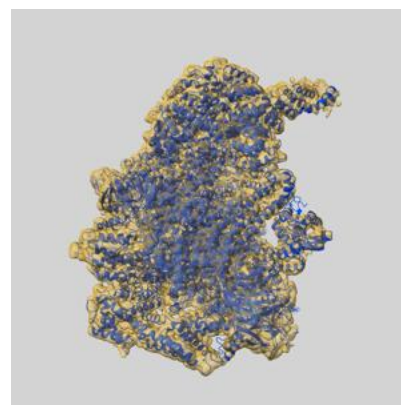
9.1 Map-model overlay [i](#)



X



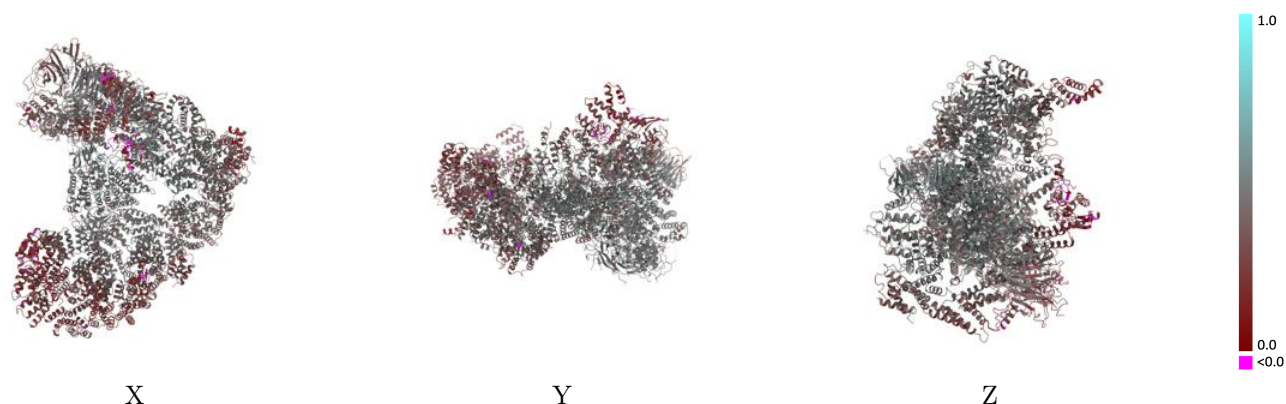
Y



Z

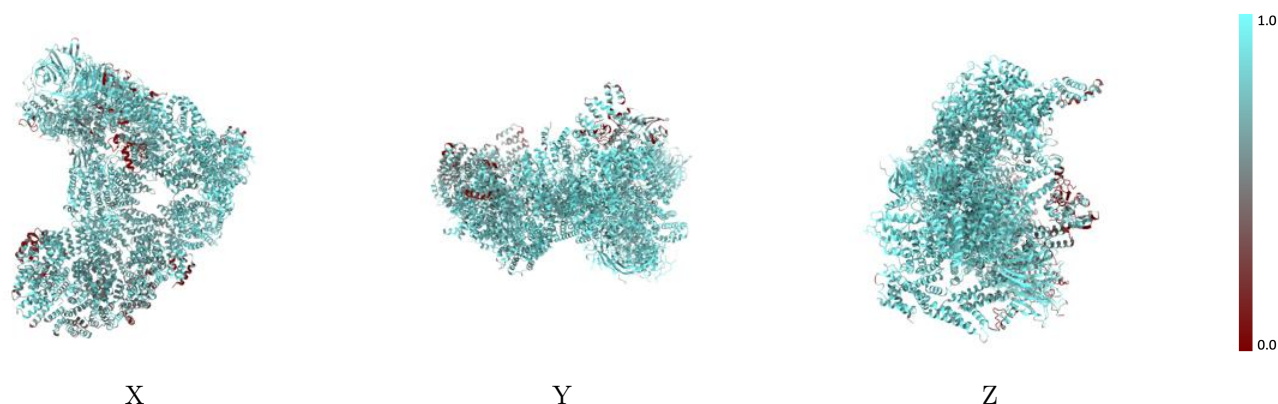
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



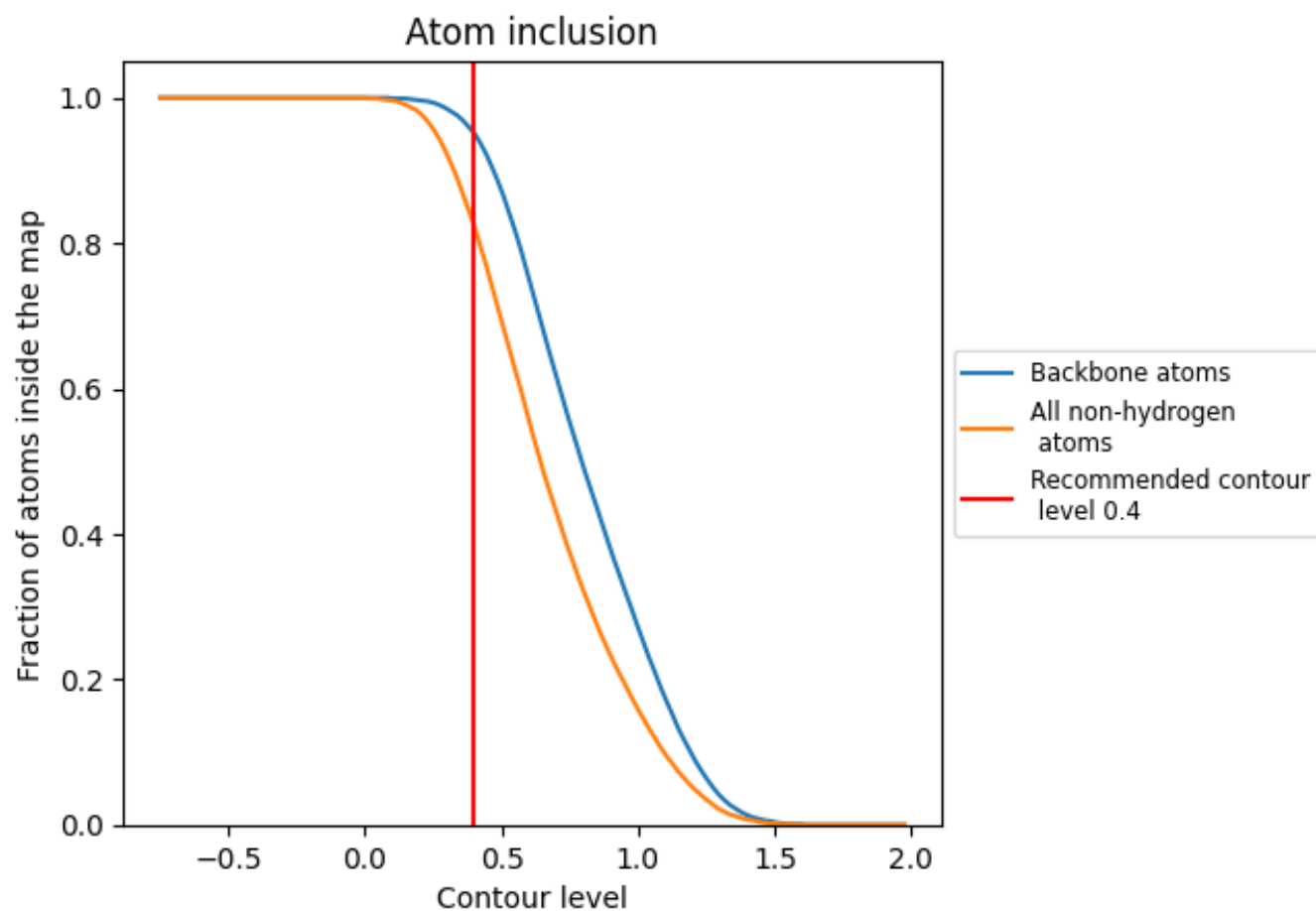
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 82% 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	 0.8230	 0.4120
A	 0.8960	 0.4790
C	 0.1200	 0.0950
D	 0.7850	 0.4610
G	 0.7750	 0.4240
H	 0.7700	 0.3860
I	 0.8440	 0.4220
J	 0.7870	 0.3830
K	 0.8610	 0.4400
L	 0.8370	 0.4390
M	 0.7270	 0.4500
N	 0.7210	 0.3460
O	 0.8840	 0.4750
P	 0.8630	 0.4310
Q	 0.8640	 0.4160
U	 0.8490	 0.4080
V	 0.8800	 0.4690
W	 0.7800	 0.4850
Y	 0.6740	 0.2670
Z	 0.6870	 0.2610

