



## Full wwPDB EM Validation Report ⓘ

Jan 21, 2025 – 07:17 pm GMT

PDB ID : 9GAW  
EMDB ID : EMD-51190  
Title : High-resolution structure of the Anaphase-promoting complex/cyclosome (APC/C) bound to co-activator Cdh1  
Authors : Hoefler, A.; Yu, J.; Chang, L.; Zhang, Z.; Yang, J.; Boland, A.; Barford, D.  
Deposited on : 2024-07-29  
Resolution : 2.90 Å(reported)  
Based on initial model : 4UI9

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

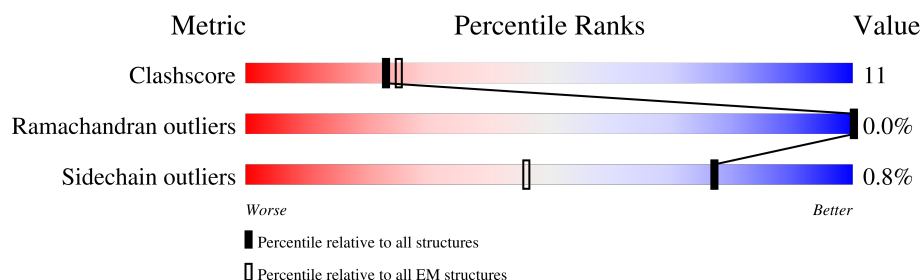
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	L	185	
2	D	121	
3	A	1944	
4	N	822	
5	I	814	
6	O	755	
7	S	447	
8	K	620	

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Mol	Chain	Length	Quality of chain
8	Q	620	
9	G	85	
9	W	85	
10	M	74	
11	H	110	
12	J	824	
12	P	824	
13	Y	599	
13	Z	599	
14	U	597	
14	V	597	
15	R	496	
16	C	84	

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 66640 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 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	178	Total	C	N	O	S	0	0
			1404	882	254	261	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	56	Total	C	N	O	1	0
			446	286	75	85		

- Molecule 3 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1602	Total	C	N	O	S	0	0
			12378	7932	2079	2284	83		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	632	Total	C	N	O	S	0	0
			4632	2942	828	840	22		

- Molecule 5 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	721	Total	C	N	O	S	0	0
			5675	3641	948	1054	32		

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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	812	TYR	-	expression tag	UNP Q9UJX5
I	813	PHE	-	expression tag	UNP Q9UJX5
I	814	GLN	-	expression tag	UNP Q9UJX5

- Molecule 6 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	699	Total	C	N	O	S	0	0
			5473	3492	954	999	28		

- Molecule 7 is a protein called F-box only protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	94	Total	C	N	O	S	0	0
			655	399	123	125	8		

- Molecule 8 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	518	Total	C	N	O	S	0	0
			4164	2676	702	760	26		
8	Q	505	Total	C	N	O	S	1	0
			4064	2606	691	743	24		

- Molecule 9 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	26	Total	C	N	O	S	0	0
			221	137	41	42	1		
9	W	26	Total	C	N	O	S	0	0
			222	139	42	40	1		

- Molecule 10 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	64	Total	C	N	O	S	0	0
			514	323	83	106	2		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	58	Total	C	N	O	S	0	0
			469	298	79	90	2		

- Molecule 12 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	499	Total	C	N	O	S	0	0
			3957	2545	667	719	26		
12	P	491	Total	C	N	O	S	0	0
			3929	2526	660	717	26		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	499	Total	C	N	O	S	0	0
			3696	2335	637	701	23		
13	Z	455	Total	C	N	O	S	1	0
			3247	2044	569	613	21		

- Molecule 14 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	488	Total	C	N	O	S	0	0
			3888	2501	659	709	19		
14	V	493	Total	C	N	O	S	1	0
			4012	2588	677	726	21		

- Molecule 15 is a protein called Fizzy-related protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	415	Total	C	N	O	S	0	0
			3015	1904	542	559	10		

- Molecule 16 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	81	Total	C	N	O	S	0	0
			573	368	102	91	12		

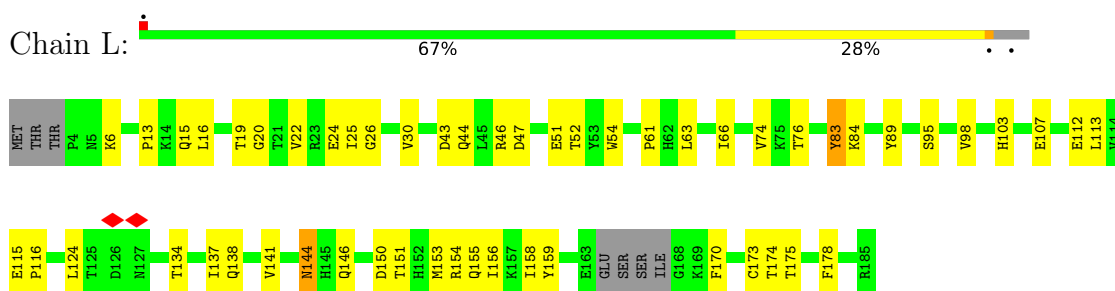
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	N	1	Total 1	Zn 1	0
17	S	2	Total 2	Zn 2	0
17	C	3	Total 3	Zn 3	0

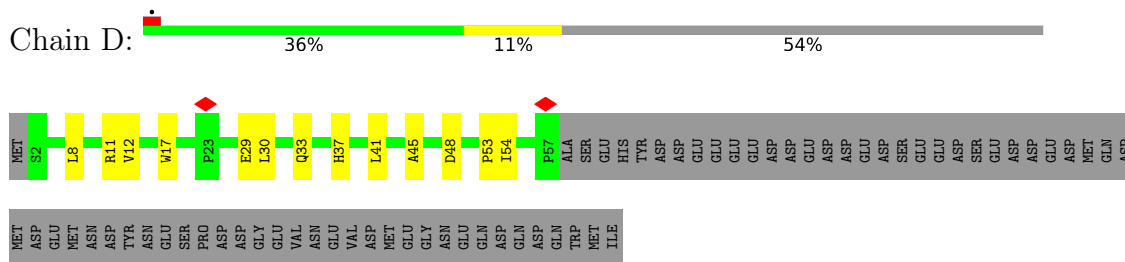
### 3 Residue-property plots

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.

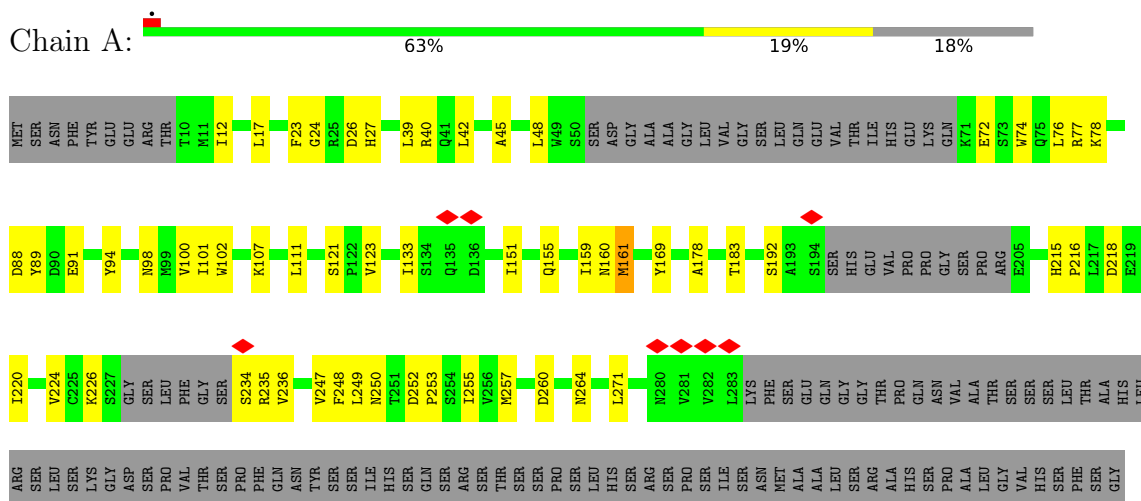
- Molecule 1: Anaphase-promoting complex subunit 10



- Molecule 2: Anaphase-promoting complex subunit 15



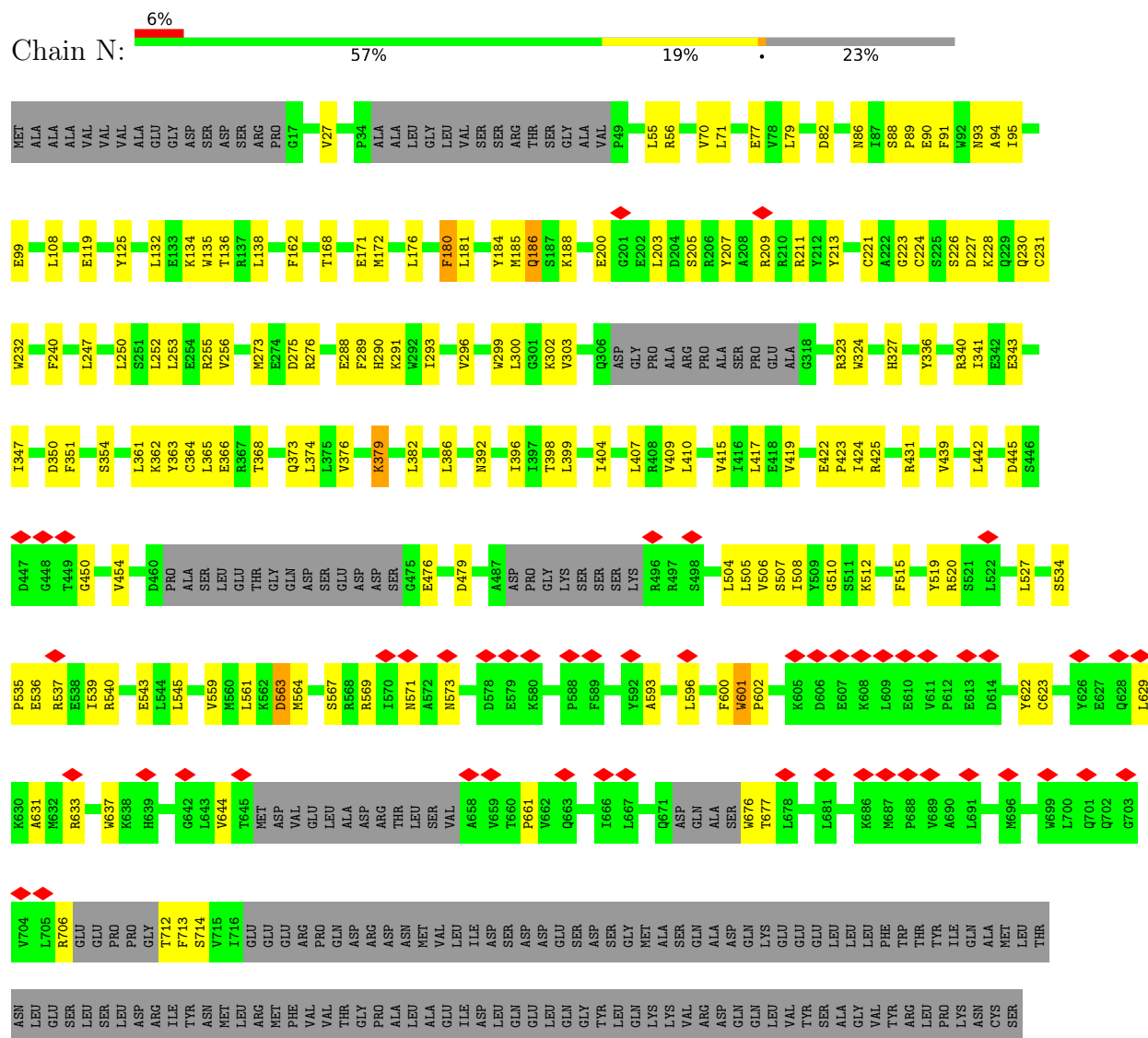
- Molecule 3: Anaphase-promoting complex subunit 1



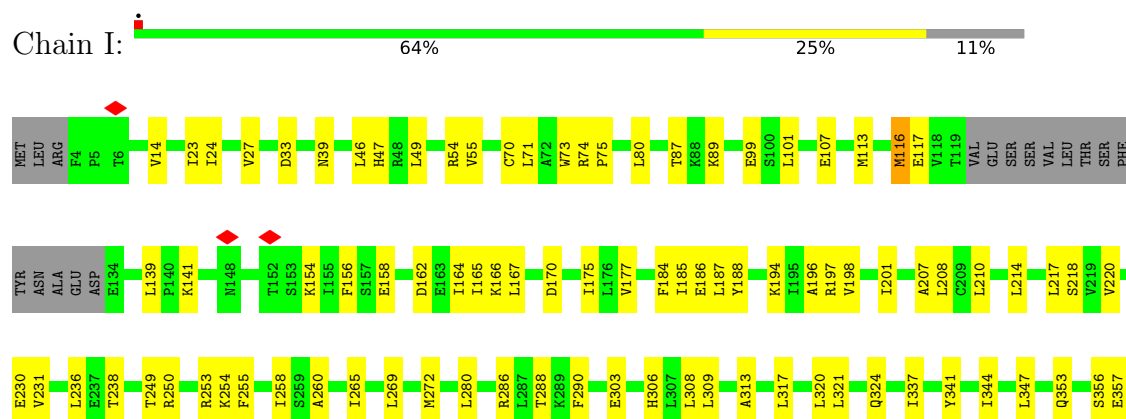


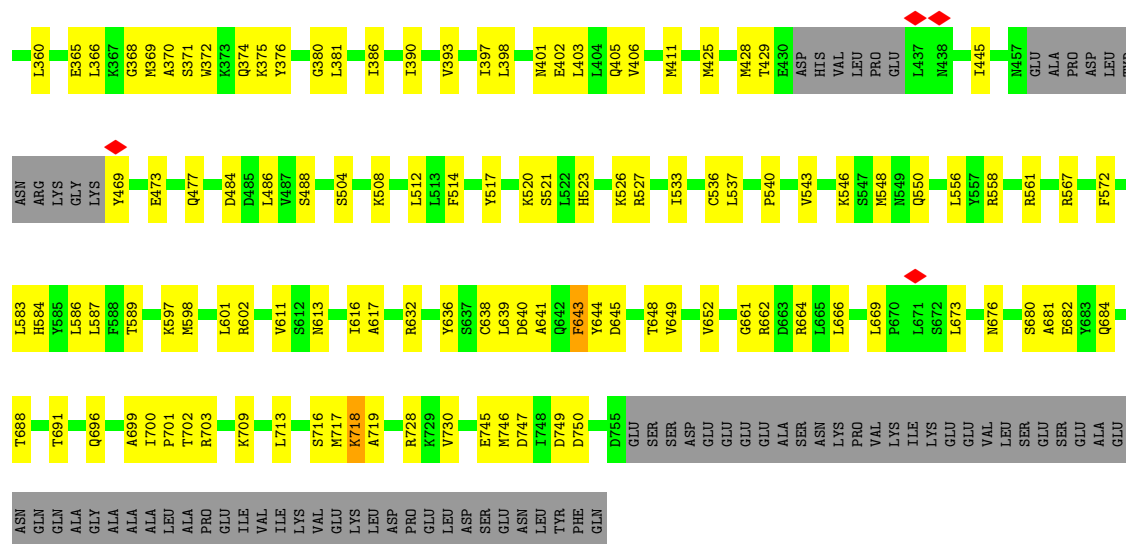


• Molecule 4: Anaphase-promoting complex subunit 2

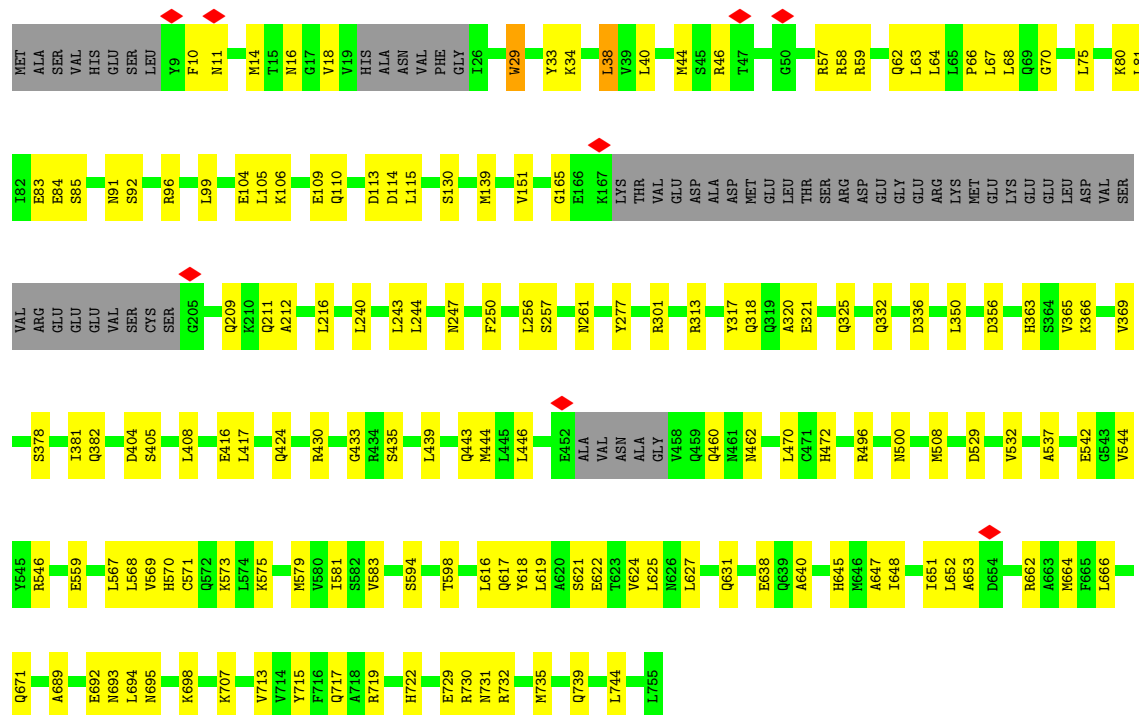


• Molecule 5: Anaphase-promoting complex subunit 4





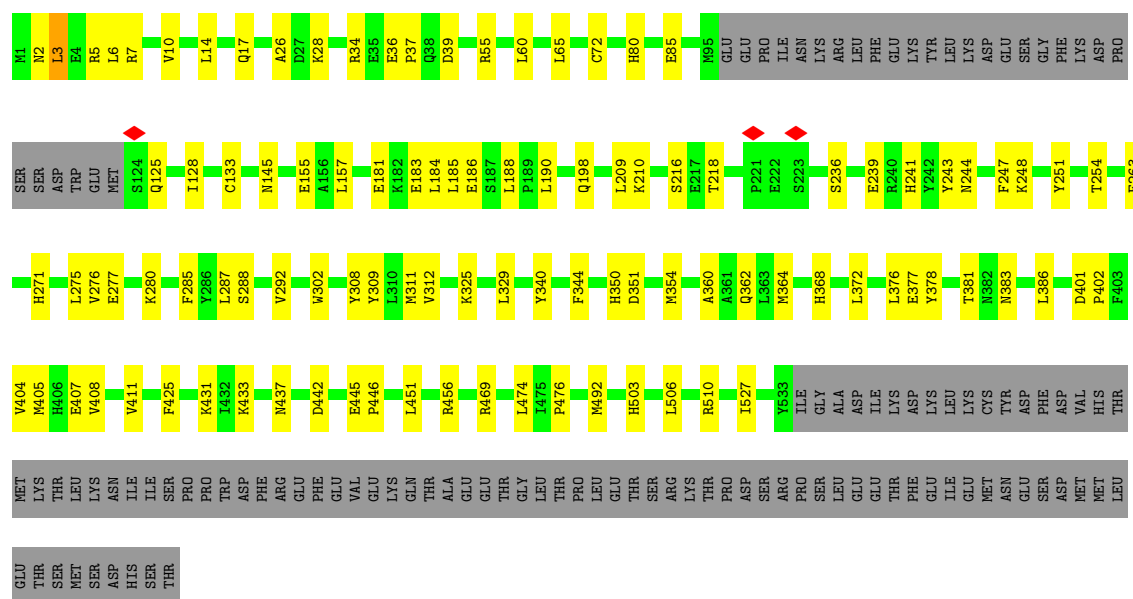
### • Molecule 6: Anaphase-promoting complex subunit 5



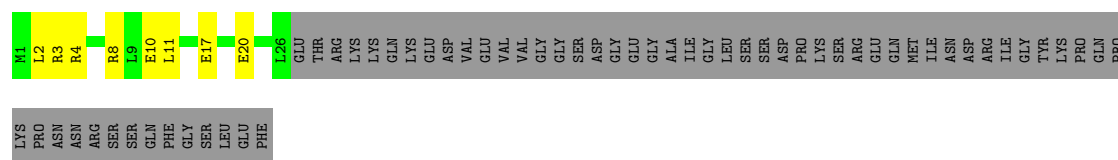
### • Molecule 7: F-box only protein 5



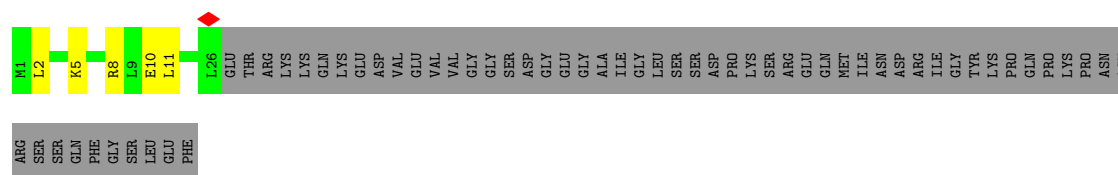




- Molecule 9: Anaphase-promoting complex subunit CDC26



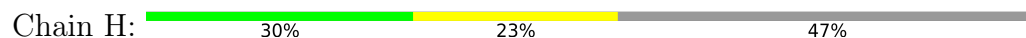
- Molecule 9: Anaphase-promoting complex subunit CDC26

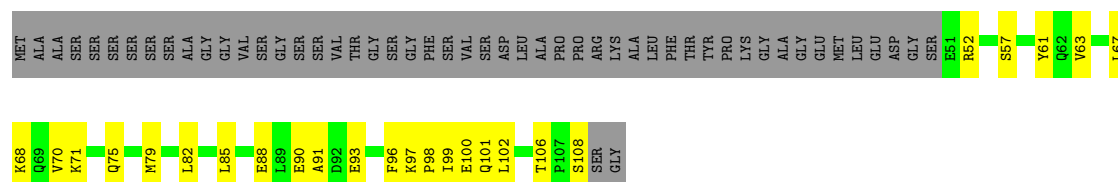


- Molecule 10: Anaphase-promoting complex subunit 13

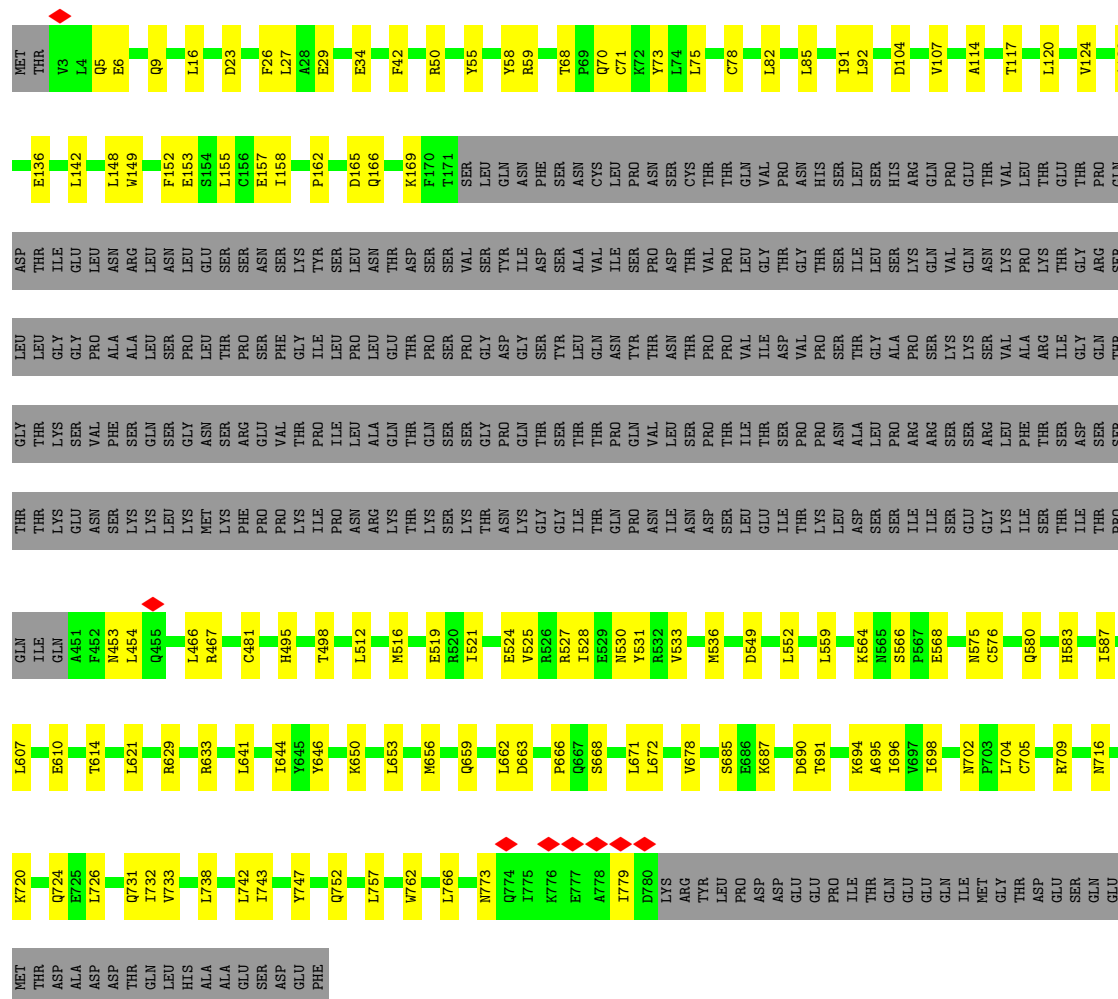


- Molecule 11: Anaphase-promoting complex subunit 16

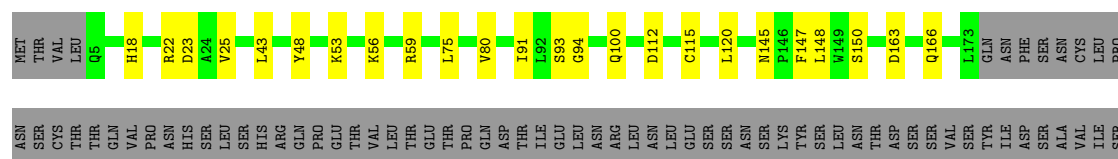


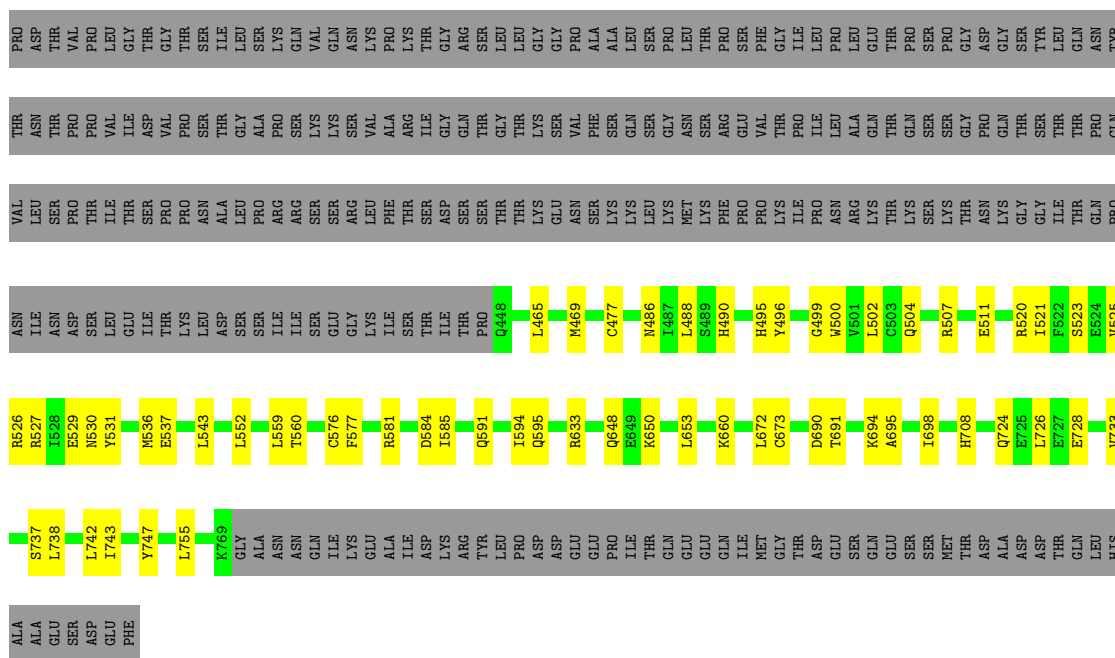


• Molecule 12: Cell division cycle protein 27 homolog

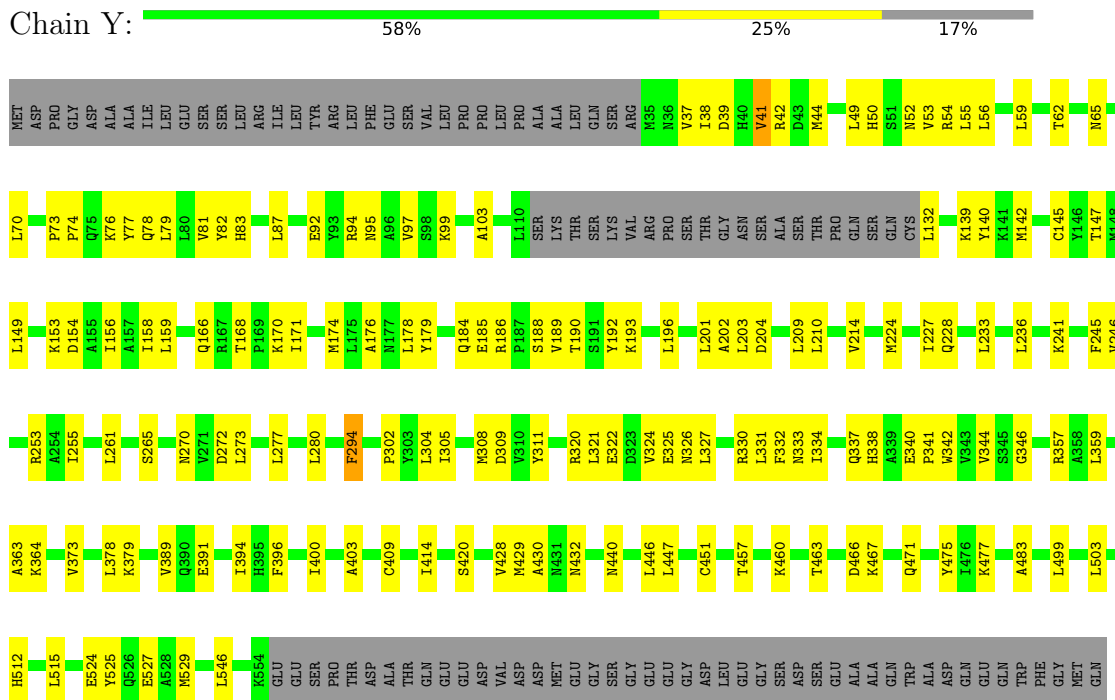


• Molecule 12: Cell division cycle protein 27 homolog

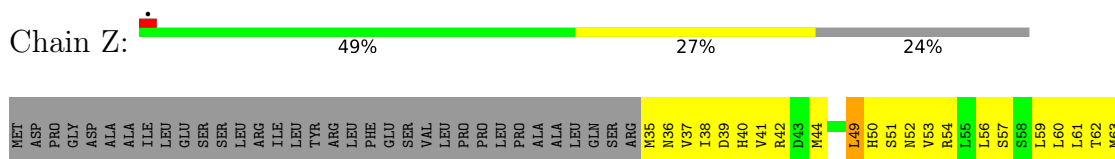


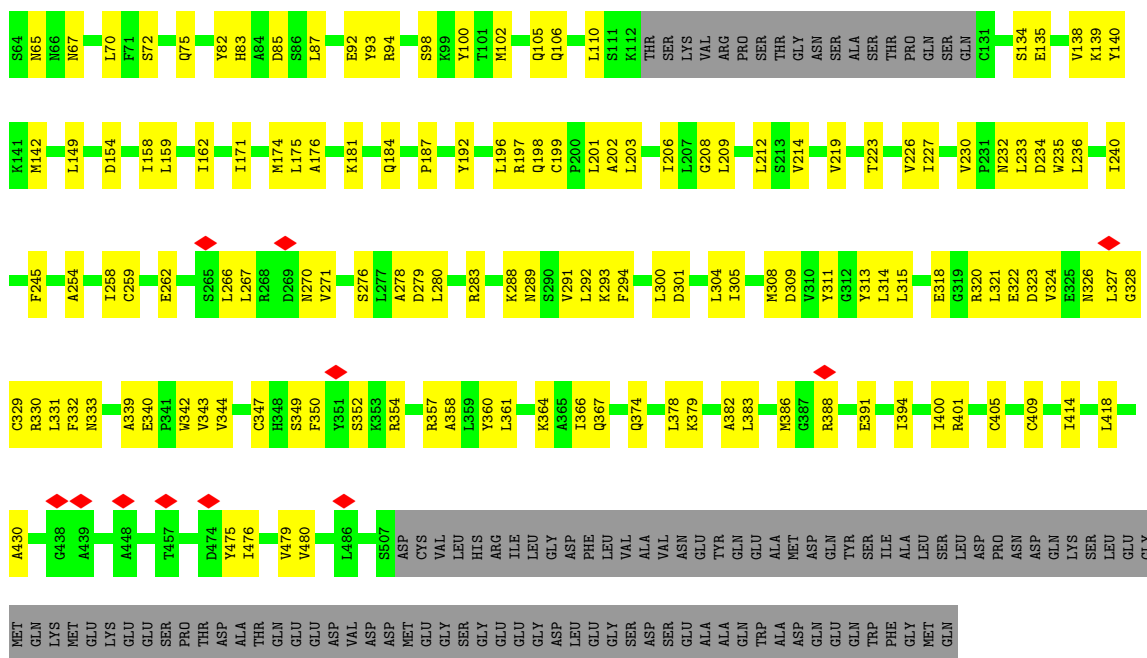


- Molecule 13: Anaphase-promoting complex subunit 7

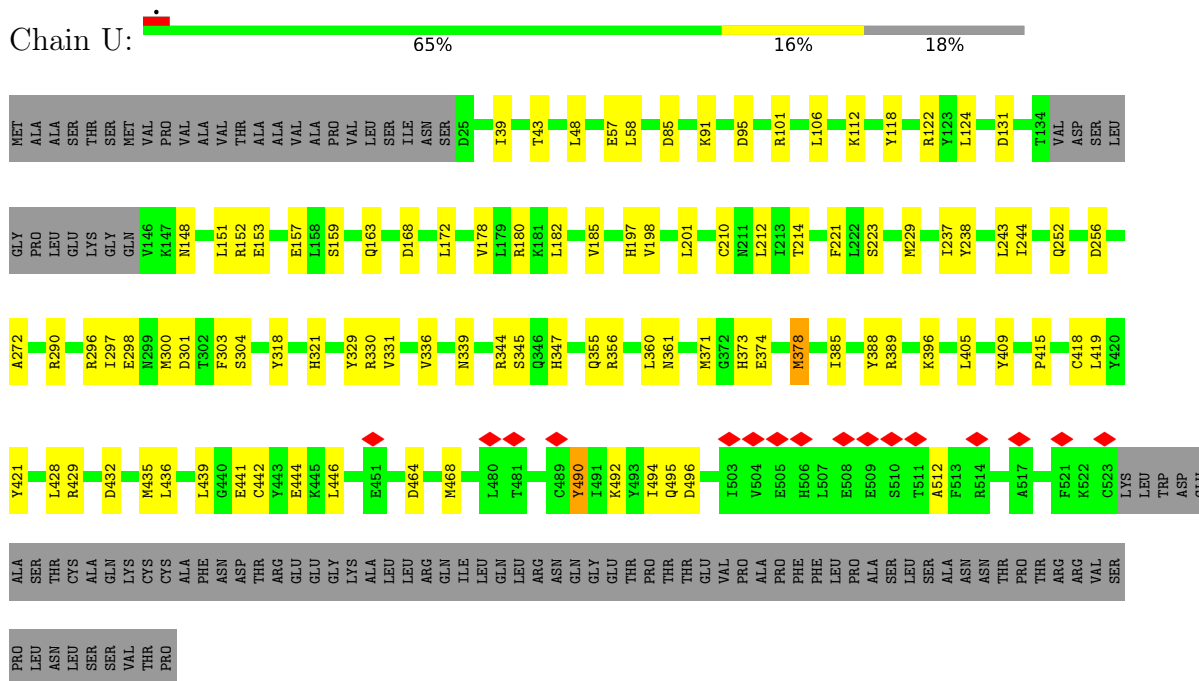


- Molecule 13: Anaphase-promoting complex subunit 7

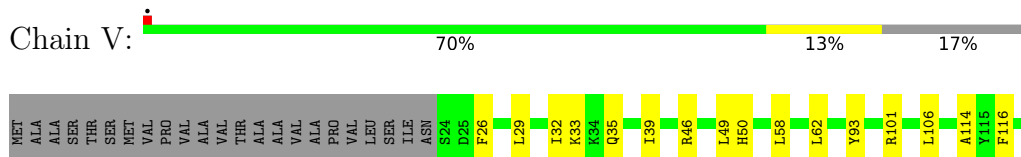




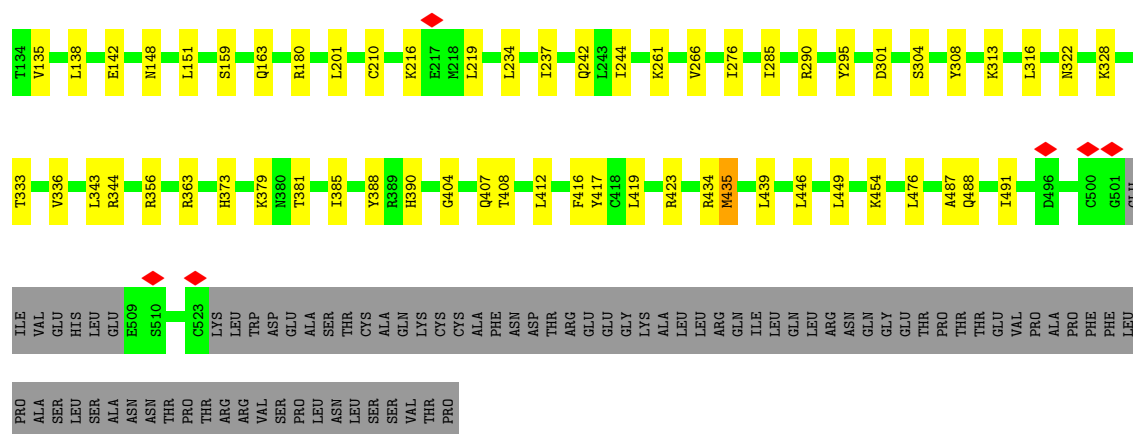
- Molecule 14: Cell division cycle protein 23 homolog



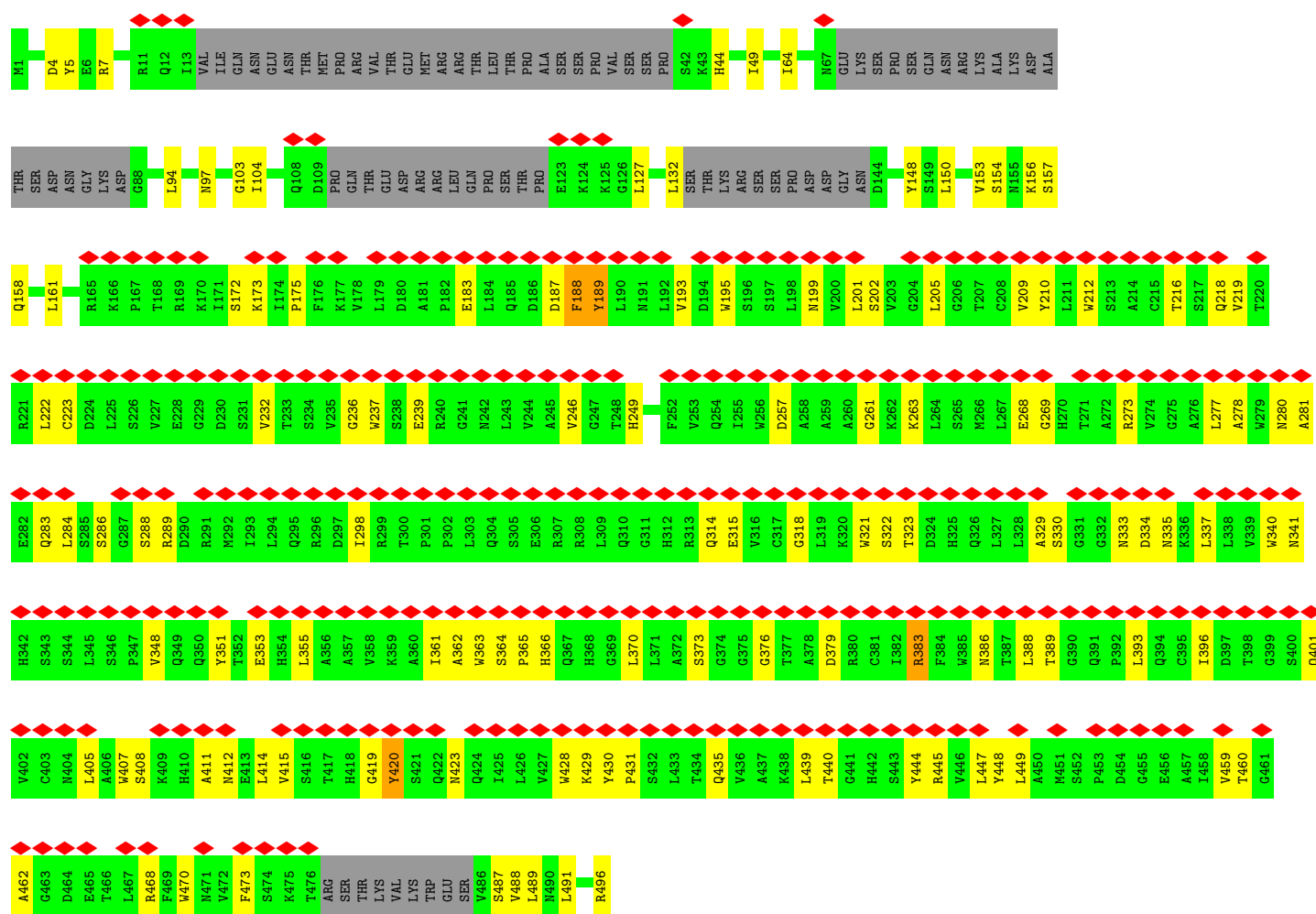
- Molecule 14: Cell division cycle protein 23 homolog





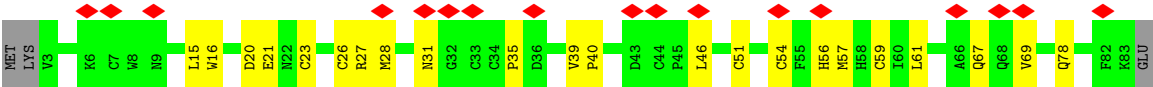


• Molecule 15: Fizzy-related protein homolog



• Molecule 16: 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	364331	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	2.000	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.065	Depositor
Map size ( $\text{\AA}$ )	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	L	0.31	0/1436	0.60	0/1949
2	D	0.38	0/460	0.66	0/630
3	A	0.27	0/12662	0.48	0/17244
4	N	0.30	0/4717	0.52	0/6429
5	I	0.30	0/5795	0.51	0/7855
6	O	0.29	0/5574	0.46	0/7538
7	S	0.37	0/662	0.64	0/896
8	K	0.27	0/4265	0.45	0/5777
8	Q	0.28	0/4165	0.46	0/5640
9	G	0.30	0/222	0.62	0/295
9	W	0.35	0/223	0.63	0/295
10	M	0.32	0/523	0.57	0/711
11	H	0.35	0/477	0.61	0/642
12	J	0.27	0/4051	0.46	0/5482
12	P	0.29	0/4023	0.45	0/5440
13	Y	0.28	0/3753	0.52	0/5113
13	Z	0.30	0/3298	0.53	0/4498
14	U	0.29	0/3975	0.46	0/5380
14	V	0.28	0/4108	0.46	0/5552
15	R	0.31	0/3075	0.53	0/4192
16	C	0.25	0/595	0.48	0/822
All	All	0.29	0/68059	0.49	0/92380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	L	1404	0	1359	36	0
2	D	446	0	414	14	0
3	A	12378	0	12145	266	0
4	N	4632	0	4265	122	0
5	I	5675	0	5585	144	0
6	O	5473	0	5491	114	0
7	S	655	0	557	27	0
8	K	4164	0	4077	72	0
8	Q	4064	0	3961	80	0
9	G	221	0	224	11	0
9	W	222	0	233	7	0
10	M	514	0	479	20	0
11	H	469	0	462	28	0
12	J	3957	0	3876	88	0
12	P	3929	0	3866	70	0
13	Y	3696	0	3569	121	0
13	Z	3247	0	3015	135	0
14	U	3888	0	3745	75	0
14	V	4012	0	3949	57	0
15	R	3015	0	2800	97	0
16	C	573	0	457	14	0
17	C	3	0	0	0	0
17	N	1	0	0	0	0
17	S	2	0	0	0	0
All	All	66640	0	64529	1432	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1432) 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)
3:A:703:SER:HB3	6:O:731:ASN:HB3	1.50	0.94
3:A:1802:ARG:HG3	3:A:1804:GLU:HG2	1.48	0.94
5:I:664:ARG:NH1	5:I:718:LYS:HA	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:414:ILE:HD12	13:Y:446:LEU:HD21	1.51	0.90
8:K:371:MET:HA	8:K:374:ILE:HD12	1.59	0.82
14:U:374:GLU:O	14:U:378:MET:HB2	1.80	0.81
8:Q:360:ALA:O	8:Q:364:MET:HB2	1.79	0.81
4:N:56:ARG:HH22	4:N:138:LEU:HD12	1.46	0.80
15:R:401:GLN:HE21	15:R:419:GLY:HA3	1.47	0.80
11:H:97:LYS:HZ3	11:H:101:GLN:HB3	1.45	0.79
3:A:594:ARG:HG2	3:A:608:THR:HG22	1.65	0.78
5:I:512:LEU:HB3	6:O:439:LEU:HD11	1.65	0.78
13:Z:49:LEU:HD13	13:Z:52:ASN:HB3	1.65	0.78
8:Q:527:ILE:HD12	14:U:419:LEU:HD12	1.66	0.77
11:H:85:LEU:HD21	12:P:560:THR:HG21	1.65	0.77
13:Z:201:LEU:HD21	13:Z:233:LEU:HD21	1.68	0.76
4:N:224:CYS:SG	4:N:231:CYS:HA	2.25	0.76
13:Z:343:VAL:HG11	13:Z:374:GLN:HG2	1.68	0.76
6:O:631:GLN:HB2	6:O:640:ALA:HB2	1.68	0.75
8:Q:350:HIS:O	8:Q:354:MET:HG2	1.87	0.75
15:R:401:GLN:HE22	15:R:445:ARG:HH11	1.33	0.75
2:D:8:LEU:HD11	6:O:424:GLN:HE22	1.51	0.75
3:A:23:PHE:HB2	3:A:111:LEU:HD13	1.68	0.75
3:A:1096:PRO:O	6:O:332:GLN:NE2	2.20	0.74
12:P:552:LEU:HD21	12:P:576:CYS:HA	1.70	0.74
13:Y:414:ILE:CD1	13:Y:446:LEU:HD21	2.17	0.73
13:Z:280:LEU:HA	13:Z:283:ARG:HD3	1.69	0.73
12:P:94:GLY:HA3	12:P:100:GLN:HA	1.69	0.73
13:Y:400:ILE:HD13	13:Y:409:CYS:SG	2.27	0.73
14:U:290:ARG:HD3	14:U:300:MET:SD	2.29	0.73
13:Y:224:MET:O	13:Y:228:GLN:NE2	2.22	0.73
13:Z:44:MET:HB3	13:Z:49:LEU:HD21	1.69	0.73
15:R:189:TYR:HB3	15:R:273:ARG:HH22	1.54	0.72
3:A:1764:LYS:HA	3:A:1767:ILE:HD13	1.70	0.72
13:Y:233:LEU:HD11	13:Y:236:LEU:HB2	1.71	0.72
8:Q:445:GLU:HG3	8:Q:446:PRO:HD3	1.70	0.72
14:U:490:TYR:HE2	14:U:512:ALA:HA	1.53	0.72
3:A:1054:TYR:HB2	3:A:1057:LEU:HG	1.71	0.72
3:A:1357:THR:HG22	3:A:1358:ILE:N	2.04	0.72
5:I:321:LEU:HB3	5:I:425:MET:HE1	1.72	0.72
3:A:39:LEU:HD12	6:O:244:LEU:HB3	1.72	0.71
13:Z:386:MET:HG3	13:Z:388:ARG:HH21	1.54	0.71
5:I:187:LEU:HB2	5:I:196:ALA:HB3	1.72	0.71
11:H:100:GLU:N	11:H:100:GLU:OE2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:78:ARG:HH12	8:Q:17:GLN:HB2	1.55	0.71
3:A:948:PRO:HD2	3:A:951:ILE:HD11	1.73	0.71
3:A:795:ARG:NH2	3:A:815:ARG:O	2.23	0.71
3:A:760:PRO:HD3	3:A:831:MET:HE3	1.72	0.70
11:H:97:LYS:HD3	11:H:98:PRO:HD2	1.73	0.70
3:A:1357:THR:HG22	3:A:1358:ILE:H	1.56	0.70
12:J:533:VAL:HA	12:J:536:MET:HG2	1.74	0.70
16:C:20:ASP:OD1	16:C:21:GLU:N	2.24	0.70
6:O:38:LEU:HD21	6:O:139:MET:HG3	1.73	0.70
1:L:51:GLU:N	1:L:51:GLU:OE2	2.25	0.69
3:A:1766:GLU:OE1	3:A:1798:ARG:NH1	2.26	0.69
3:A:1767:ILE:HG13	3:A:1798:ARG:NH1	2.06	0.69
4:N:227:ASP:HB2	4:N:230:GLN:HG2	1.74	0.69
12:J:732:ILE:HG22	12:J:733:VAL:HG13	1.72	0.69
14:V:435:MET:SD	14:V:435:MET:N	2.66	0.69
15:R:376:GLY:H	15:R:379:ASP:HB3	1.57	0.69
4:N:162:PHE:O	4:N:255:ARG:NH2	2.26	0.69
5:I:254:LYS:NZ	5:I:365:GLU:OE1	2.25	0.69
8:K:157:LEU:HD12	8:K:170:LEU:HD12	1.75	0.68
12:J:16:LEU:HD12	12:J:50:ARG:HD2	1.73	0.68
4:N:623:CYS:SG	4:N:637:TRP:NE1	2.66	0.68
6:O:695:ASN:OD1	6:O:717:GLN:NE2	2.26	0.68
5:I:231:VAL:HG23	5:I:556:LEU:HB2	1.75	0.68
2:D:45:ALA:HA	14:U:378:MET:CE	2.24	0.68
3:A:161:MET:HB2	3:A:169:TYR:HB2	1.76	0.68
12:J:549:ASP:OD1	12:J:580:GLN:NE2	2.24	0.68
5:I:175:ILE:HD11	5:I:187:LEU:HB3	1.74	0.68
3:A:45:ALA:O	14:V:180:ARG:NH1	2.26	0.68
13:Z:94:ARG:HE	13:Z:149:LEU:HD13	1.58	0.68
1:L:144:ASN:ND2	1:L:150:ASP:O	2.26	0.67
5:I:664:ARG:HD3	5:I:719:ALA:O	1.93	0.67
4:N:445:ASP:O	4:N:537:ARG:NH2	2.26	0.67
5:I:177:VAL:HG22	5:I:208:LEU:HD13	1.74	0.67
13:Y:451:CYS:HB3	13:Y:457:THR:HG23	1.76	0.67
13:Y:440:ASN:HA	13:Y:471:GLN:HE22	1.60	0.67
3:A:1054:TYR:H	3:A:1057:LEU:HD12	1.60	0.67
4:N:382:LEU:HD11	4:N:424:ILE:HD11	1.76	0.67
15:R:330:SER:HG	15:R:340:TRP:HE1	1.42	0.67
13:Z:67:ASN:HD22	13:Z:70:LEU:HB2	1.59	0.67
10:M:7:ARG:HH22	10:M:12:LEU:HB2	1.60	0.67
3:A:617:LEU:HD11	3:A:786:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:99:ILE:HA	11:H:102:LEU:HD12	1.77	0.66
8:K:453:HIS:HE1	9:W:11:LEU:HG	1.60	0.66
3:A:12:ILE:O	3:A:510:PHE:N	2.26	0.66
3:A:1396:LEU:HD11	3:A:1434:ILE:HD11	1.78	0.66
7:S:120:ASN:OD1	15:R:445:ARG:NH2	2.28	0.66
11:H:88:GLU:HA	11:H:91:ALA:HB3	1.77	0.66
15:R:222:LEU:O	15:R:263:LYS:NZ	2.28	0.66
13:Z:379:LYS:O	13:Z:383:LEU:HD12	1.95	0.66
2:D:54:ILE:HD12	8:Q:506:LEU:HD13	1.78	0.66
11:H:90:GLU:OE2	11:H:90:GLU:N	2.21	0.66
5:I:374:GLN:HE21	6:O:692:GLU:HB3	1.61	0.66
5:I:139:LEU:HB2	5:I:165:ILE:HG12	1.77	0.66
3:A:1017:ASN:OD1	3:A:1038:ARG:NH2	2.27	0.65
5:I:75:PRO:HG2	5:I:117:GLU:HB2	1.77	0.65
14:V:373:HIS:HD1	14:V:388:TYR:HH	1.44	0.65
13:Z:318:GLU:OE2	13:Z:320:ARG:NH1	2.29	0.65
3:A:1084:ARG:NH2	3:A:1139:ASN:OD1	2.29	0.65
7:S:406:CYS:HB2	7:S:413:TYR:HD1	1.60	0.65
12:J:85:LEU:HB3	12:J:124:VAL:HG23	1.79	0.65
12:P:520:ARG:NH1	13:Z:154:ASP:OD1	2.30	0.65
13:Y:302:PRO:O	13:Y:330:ARG:NH1	2.29	0.65
13:Z:315:LEU:HD22	13:Z:320:ARG:HH12	1.62	0.65
3:A:1074:CYS:O	3:A:1078:MET:HG3	1.97	0.65
12:J:157:GLU:O	12:J:633:ARG:HD3	1.96	0.65
6:O:404:ASP:OD1	6:O:405:SER:N	2.30	0.64
14:U:419:LEU:HD23	14:U:442:CYS:HB2	1.77	0.64
15:R:64:ILE:HD11	15:R:127:LEU:HD12	1.80	0.64
1:L:175:THR:HG21	12:P:733:VAL:HG11	1.78	0.64
4:N:99:GLU:HA	4:N:172:MET:HE1	1.77	0.64
6:O:570:HIS:HA	6:O:573:LYS:HZ3	1.61	0.64
1:L:66:ILE:HD13	1:L:158:ILE:HD11	1.78	0.64
6:O:671:GLN:OE1	6:O:693:ASN:ND2	2.29	0.64
4:N:365:LEU:HA	4:N:368:THR:HG22	1.79	0.64
1:L:113:LEU:HB3	1:L:116:PRO:HG3	1.78	0.64
3:A:1226:ARG:NH1	15:R:154:SER:OG	2.29	0.64
5:I:166:LYS:HE2	5:I:166:LYS:HA	1.79	0.64
13:Z:313:TYR:HA	13:Z:347:CYS:SG	2.38	0.64
8:K:214:LYS:HB2	8:K:217:GLU:HG3	1.78	0.64
3:A:1717:SER:O	4:N:323:ARG:NH2	2.31	0.63
9:W:5:LYS:HE2	9:W:5:LYS:HA	1.80	0.63
10:M:10:ARG:HD2	14:V:131:ASP:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:236:GLY:HA3	15:R:277:LEU:HD11	1.79	0.63
15:R:341:ASN:ND2	15:R:348:VAL:HB	2.13	0.63
3:A:775:LEU:HD11	3:A:844:ILE:HD13	1.80	0.63
13:Y:83:HIS:HD2	13:Y:99:LYS:HG2	1.63	0.63
8:K:171:THR:HG22	8:K:176:LEU:HD12	1.80	0.63
4:N:211:ARG:NH2	4:N:275:ASP:O	2.30	0.63
13:Y:38:ILE:HG22	13:Y:79:LEU:HD12	1.81	0.63
7:S:324:PRO:HB3	15:R:210:TYR:CZ	2.34	0.63
14:V:26:PHE:HA	14:V:32:ILE:HD11	1.80	0.63
5:I:308:LEU:HD21	5:I:445:ILE:HG23	1.81	0.63
5:I:353:GLN:O	5:I:357:GLU:HG2	1.98	0.63
3:A:979:GLY:O	3:A:1700:LYS:NZ	2.32	0.62
5:I:116:MET:HG2	5:I:210:LEU:HB3	1.81	0.62
8:K:181:GLU:HB2	8:K:209:LEU:HD21	1.81	0.62
3:A:869:ARG:HH12	3:A:946:THR:HG23	1.64	0.62
13:Z:300:LEU:H	13:Z:300:LEU:HD23	1.64	0.62
3:A:1651:LEU:HD22	8:K:553:LYS:HB2	1.80	0.62
11:H:97:LYS:NZ	11:H:101:GLN:HB3	2.15	0.62
5:I:397:ILE:O	5:I:401:ASN:ND2	2.32	0.62
5:I:644:TYR:CE1	5:I:746:MET:HG3	2.35	0.62
11:H:85:LEU:CD2	12:P:560:THR:HG21	2.29	0.62
15:R:195:TRP:HE1	15:R:199:ASN:HA	1.65	0.62
5:I:398:LEU:HA	5:I:401:ASN:HD21	1.64	0.62
5:I:477:GLN:NE2	5:I:488:SER:OG	2.32	0.62
13:Y:49:LEU:HB3	13:Y:52:ASN:HD22	1.65	0.62
3:A:1177:MET:HG3	3:A:1207:GLY:HA2	1.81	0.61
11:H:57:SER:OG	13:Z:357:ARG:NH2	2.33	0.61
15:R:341:ASN:HD21	15:R:348:VAL:HB	1.65	0.61
12:P:502:LEU:HB3	12:P:525:VAL:HG22	1.82	0.61
15:R:366:HIS:NE2	15:R:411:ALA:O	2.29	0.61
13:Y:201:LEU:HB2	13:Z:44:MET:HE1	1.83	0.61
15:R:460:THR:HG1	15:R:470:TRP:HE1	1.48	0.61
15:R:330:SER:OG	15:R:340:TRP:NE1	2.30	0.61
13:Z:181:LYS:O	13:Z:401:ARG:NH1	2.32	0.61
3:A:1672:ARG:NH2	3:A:1713:MET:O	2.34	0.61
13:Z:322:GLU:O	13:Z:326:ASN:ND2	2.34	0.61
13:Z:339:ALA:O	13:Z:343:VAL:HG23	2.00	0.61
3:A:178:ALA:HB2	3:A:192:SER:HB3	1.83	0.61
1:L:84:LYS:HE2	1:L:84:LYS:N	2.16	0.61
13:Y:337:GLN:OE1	13:Y:337:GLN:N	2.33	0.61
3:A:1430:VAL:O	3:A:1435:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:293:ILE:HA	4:N:296:VAL:HG22	1.83	0.61
6:O:694:LEU:HD12	6:O:713:VAL:HG13	1.82	0.61
7:S:321:PHE:HD1	7:S:322:ARG:HG3	1.64	0.61
8:K:284:LEU:HG	8:K:308:TYR:HB2	1.82	0.61
13:Y:308:MET:HG3	13:Y:331:LEU:HD21	1.81	0.61
6:O:257:SER:O	6:O:261:ASN:ND2	2.34	0.60
6:O:698:LYS:HB2	6:O:713:VAL:HG11	1.82	0.60
5:I:662:ARG:O	5:I:662:ARG:HG3	2.01	0.60
8:Q:276:VAL:HA	8:Q:311:MET:SD	2.41	0.60
9:G:10:GLU:OE2	9:G:10:GLU:N	2.34	0.60
11:H:96:PHE:HB3	12:P:595:GLN:HB3	1.83	0.60
4:N:571:ASN:ND2	4:N:593:ALA:O	2.29	0.60
12:J:149:TRP:N	12:P:23:ASP:OD2	2.29	0.60
12:P:80:VAL:HG11	12:P:120:LEU:HD11	1.83	0.60
13:Y:185:GLU:N	13:Y:185:GLU:OE1	2.35	0.60
3:A:1767:ILE:H	3:A:1767:ILE:HD12	1.66	0.60
12:J:530:ASN:OD1	12:P:59:ARG:NH1	2.35	0.60
13:Y:204:ASP:H	13:Z:52:ASN:HD22	1.49	0.60
11:H:75:GLN:O	11:H:79:MET:HG2	2.02	0.60
12:P:163:ASP:HB3	12:P:166:GLN:HB2	1.84	0.60
8:Q:401:ASP:O	8:Q:405:MET:HG3	2.02	0.60
13:Z:342:TRP:HE3	13:Z:361:LEU:HG	1.66	0.60
5:I:87:THR:HB	5:I:89:LYS:HG2	1.84	0.59
3:A:1357:THR:CG2	3:A:1358:ILE:H	2.15	0.59
3:A:1635:GLU:OE2	3:A:1648:LYS:NZ	2.34	0.59
5:I:255:PHE:HE1	5:I:366:LEU:HD21	1.67	0.59
8:K:419:LYS:HZ1	8:K:423:LYS:HB2	1.68	0.59
15:R:239:GLU:N	15:R:239:GLU:OE2	2.35	0.59
3:A:1409:LEU:HD22	3:A:1470:LEU:HD23	1.85	0.59
6:O:216:LEU:HD22	6:O:256:LEU:HD22	1.83	0.59
6:O:542:GLU:OE1	6:O:546:ARG:NH1	2.34	0.59
5:I:374:GLN:NE2	6:O:689:ALA:O	2.31	0.59
5:I:586:LEU:HB3	5:I:601:LEU:HB3	1.85	0.59
5:I:613:ASN:HB3	5:I:616:ILE:HD11	1.85	0.59
3:A:102:TRP:CE3	3:A:151:ILE:HD11	2.38	0.59
5:I:504:SER:O	5:I:508:LYS:NZ	2.35	0.59
5:I:664:ARG:CD	5:I:719:ALA:O	2.50	0.59
4:N:247:LEU:HG	4:N:253:LEU:HA	1.83	0.59
13:Z:342:TRP:CE3	13:Z:361:LEU:HG	2.38	0.59
8:K:279:ASN:HA	8:K:311:MET:HE1	1.85	0.59
15:R:257:ASP:OD1	15:R:261:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:314:LEU:O	13:Z:318:GLU:HG3	2.02	0.59
12:J:726:LEU:HD13	12:J:743:ILE:HG12	1.84	0.59
8:Q:236:SER:HA	8:Q:239:GLU:OE2	2.02	0.59
13:Y:142:MET:SD	13:Y:142:MET:N	2.76	0.59
3:A:248:PHE:HB2	3:A:430:VAL:HB	1.84	0.58
3:A:1636:VAL:HG12	3:A:1666:ILE:HG22	1.83	0.58
8:Q:476:PRO:HG2	14:U:182:LEU:HD22	1.85	0.58
15:R:94:LEU:HD11	15:R:161:LEU:HD21	1.85	0.58
15:R:216:THR:O	15:R:218:GLN:NE2	2.35	0.58
11:H:82:LEU:HB3	12:P:577:PHE:HE2	1.67	0.58
14:U:252:GLN:NE2	14:U:256:ASP:OD1	2.36	0.58
13:Z:309:ASP:HB3	13:Z:374:GLN:HG3	1.84	0.58
3:A:1718:LEU:O	4:N:323:ARG:NH1	2.36	0.58
3:A:1595:HIS:ND1	3:A:1596:SER:O	2.37	0.58
12:J:633:ARG:O	12:J:633:ARG:HG2	2.04	0.58
12:P:502:LEU:HD22	12:P:521:ILE:HG23	1.85	0.58
13:Y:322:GLU:O	13:Y:326:ASN:ND2	2.36	0.58
13:Z:223:THR:O	13:Z:227:ILE:HG12	2.03	0.58
13:Z:358:ALA:HB1	13:Z:378:LEU:HD11	1.85	0.58
2:D:29:GLU:N	2:D:29:GLU:OE1	2.34	0.58
5:I:380:GLY:HA3	5:I:543:VAL:HG21	1.84	0.58
12:P:726:LEU:HD21	12:P:742:LEU:HB3	1.85	0.58
8:Q:7:ARG:O	8:Q:10:VAL:HG12	2.02	0.58
16:C:15:LEU:HD12	16:C:31:ASN:HD21	1.67	0.58
3:A:972:GLU:OE2	3:A:972:GLU:N	2.24	0.58
6:O:46:ARG:HH22	6:O:96:ARG:HH22	1.51	0.58
15:R:487:SER:OG	15:R:488:VAL:N	2.37	0.58
13:Z:308:MET:HA	13:Z:311:TYR:HB3	1.86	0.58
4:N:186:GLN:HG3	4:N:223:GLY:N	2.18	0.58
6:O:735:MET:HG2	6:O:739:GLN:NE2	2.19	0.58
13:Z:201:LEU:HD21	13:Z:233:LEU:CD2	2.32	0.58
3:A:1792:ALA:HB2	6:O:598:THR:HG21	1.85	0.58
9:G:2:LEU:HD21	8:Q:276:VAL:HG11	1.86	0.58
3:A:27:HIS:HB3	3:A:101:ILE:HD13	1.86	0.58
3:A:731:SER:O	6:O:719:ARG:NH2	2.37	0.58
4:N:162:PHE:HE2	4:N:252:LEU:HD13	1.69	0.58
5:I:286:ARG:HG2	5:I:324:GLN:HE22	1.69	0.58
12:P:690:ASP:OD1	12:P:691:THR:N	2.37	0.58
14:V:33:LYS:HD2	14:V:62:LEU:HB2	1.86	0.58
16:C:51:CYS:SG	16:C:78:GLN:NE2	2.77	0.58
3:A:74:TRP:O	3:A:588:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:139:LYS:NZ	13:Z:158:ILE:O	2.37	0.57
5:I:217:LEU:HD23	5:I:236:LEU:HD12	1.85	0.57
5:I:368:GLY:HA3	6:O:653:ALA:HB2	1.85	0.57
12:J:650:LYS:HB3	12:J:653:LEU:HD12	1.86	0.57
13:Y:145:CYS:O	13:Y:149:LEU:HB2	2.04	0.57
14:V:142:GLU:OE1	14:V:142:GLU:N	2.35	0.57
3:A:1635:GLU:HB3	3:A:1669:LYS:HD2	1.84	0.57
4:N:336:TYR:HD2	4:N:364:CYS:HG	1.51	0.57
13:Z:476:ILE:O	13:Z:480:VAL:HG13	2.02	0.57
4:N:386:LEU:HD13	4:N:399:LEU:HD23	1.84	0.57
5:I:523:HIS:HB3	5:I:527:ARG:HH12	1.69	0.57
12:J:691:THR:HA	12:J:694:LYS:HE3	1.85	0.57
13:Z:414:ILE:HD11	13:Z:430:ALA:HB2	1.85	0.57
16:C:57:MET:O	16:C:61:LEU:HG	2.05	0.57
4:N:93:ASN:OD1	4:N:94:ALA:N	2.38	0.57
4:N:224:CYS:SG	4:N:231:CYS:CA	2.89	0.57
7:S:119:GLU:HB3	15:R:333:ASN:HD21	1.70	0.57
13:Y:189:VAL:HG13	13:Y:209:LEU:HD11	1.85	0.57
13:Y:204:ASP:H	13:Z:52:ASN:ND2	2.03	0.57
13:Y:246:VAL:HG22	13:Y:280:LEU:HD11	1.86	0.57
13:Z:38:ILE:HA	13:Z:41:VAL:HG12	1.87	0.57
6:O:301:ARG:NH1	6:O:336:ASP:OD2	2.33	0.57
8:Q:401:ASP:HB3	8:Q:404:VAL:HG22	1.87	0.57
14:U:43:THR:HB	14:U:48:LEU:HB2	1.85	0.57
5:I:583:LEU:HD12	5:I:602:ARG:HG3	1.86	0.57
12:J:6:GLU:HB2	12:J:9:GLN:HB2	1.86	0.57
13:Z:201:LEU:CD2	13:Z:233:LEU:HD21	2.34	0.57
6:O:70:GLY:O	6:O:211:GLN:NE2	2.38	0.56
13:Y:41:VAL:HG23	13:Y:82:TYR:HD2	1.70	0.56
14:U:106:LEU:HB3	14:U:118:TYR:HB2	1.87	0.56
15:R:401:GLN:HG3	15:R:420:TYR:H	1.70	0.56
13:Z:271:VAL:HG11	13:Z:301:ASP:HB2	1.87	0.56
3:A:1925:VAL:HG11	4:N:70:VAL:HB	1.86	0.56
12:P:526:ARG:NH1	12:P:530:ASN:O	2.38	0.56
12:P:648:GLN:OE1	12:P:650:LYS:NZ	2.38	0.56
4:N:291:LYS:N	4:N:291:LYS:HE2	2.21	0.56
7:S:117:ASN:HB3	7:S:119:GLU:HG3	1.86	0.56
13:Y:525:TYR:O	13:Y:529:MET:HG2	2.05	0.56
1:L:74:VAL:HG11	1:L:137:ILE:HD11	1.87	0.56
3:A:42:LEU:HD13	14:V:363:ARG:HG2	1.86	0.56
3:A:1617:ARG:HA	3:A:1691:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:356:ASP:OD1	6:O:356:ASP:N	2.37	0.56
8:K:236:SER:OG	8:K:240:ARG:NH1	2.39	0.56
4:N:506:VAL:HA	4:N:515:PHE:CE2	2.41	0.56
15:R:373:SER:HB3	15:R:383:ARG:HB2	1.87	0.56
1:L:170:PHE:HB3	12:P:738:LEU:HD11	1.87	0.56
6:O:378:SER:HB2	6:O:417:LEU:HD13	1.87	0.56
8:K:94:ASP:OD1	8:K:95:MET:N	2.38	0.56
9:G:11:LEU:HD21	8:Q:456:ARG:HH12	1.70	0.56
13:Y:272:ASP:OD1	13:Y:273:LEU:N	2.38	0.56
13:Z:139:LYS:HA	13:Z:142:MET:HG3	1.88	0.56
8:K:523:ILE:HD13	12:P:653:LEU:HG	1.87	0.56
10:M:38:GLU:N	10:M:38:GLU:OE1	2.39	0.56
12:J:155:LEU:HD12	12:J:158:ILE:HD11	1.87	0.56
12:J:524:GLU:OE2	12:J:527:ARG:NH2	2.37	0.56
10:M:52:GLU:OE1	10:M:52:GLU:N	2.30	0.56
5:I:184:PHE:HA	5:I:198:VAL:O	2.06	0.56
13:Y:460:LYS:HA	13:Y:463:THR:HG22	1.88	0.56
14:V:290:ARG:NH2	14:V:322:ASN:OD1	2.38	0.56
15:R:44:HIS:HD2	15:R:132:LEU:HD13	1.70	0.56
5:I:561:ARG:NH1	5:I:589:THR:O	2.27	0.56
6:O:80:LYS:NZ	6:O:84:GLU:OE1	2.39	0.56
8:K:61:ARG:HH12	8:K:88:GLN:HE22	1.54	0.56
8:K:371:MET:HB2	8:K:390:PHE:HD1	1.70	0.56
12:J:685:SER:HB3	12:J:716:ASN:HD21	1.69	0.56
13:Y:309:ASP:OD1	13:Y:309:ASP:N	2.39	0.56
15:R:370:LEU:HD11	15:R:430:TYR:CZ	2.41	0.56
5:I:107:GLU:OE1	5:I:197:ARG:NH2	2.39	0.55
8:K:78:ARG:NH2	8:Q:17:GLN:OE1	2.37	0.55
8:K:496:GLU:OE2	12:P:660:LYS:NZ	2.35	0.55
14:V:316:LEU:HD23	14:V:343:LEU:HD12	1.88	0.55
12:J:58:TYR:HB2	12:J:78:CYS:HB3	1.88	0.55
1:L:95:SER:OG	1:L:107:GLU:OE2	2.24	0.55
2:D:37:HIS:O	2:D:41:LEU:HD22	2.06	0.55
3:A:770:TYR:OH	3:A:809:ASP:OD2	2.23	0.55
5:I:360:LEU:HD13	5:I:393:VAL:HB	1.87	0.55
12:J:731:GLN:O	8:Q:145:ASN:ND2	2.40	0.55
13:Y:166:GLN:N	13:Y:166:GLN:OE1	2.39	0.55
13:Y:245:PHE:HE2	13:Y:253:ARG:HD2	1.71	0.55
3:A:1794:ASP:O	3:A:1798:ARG:HG3	2.07	0.55
3:A:1796:ALA:HB1	3:A:1810:GLU:CD	2.27	0.55
7:S:379:ILE:H	7:S:379:ILE:HD12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:153:LYS:O	13:Y:156:ILE:HG13	2.06	0.55
4:N:350:ASP:O	4:N:354:SER:HB2	2.06	0.55
14:U:415:PRO:HB2	14:U:446:LEU:HD13	1.88	0.55
15:R:405:LEU:HD12	15:R:414:LEU:HD12	1.87	0.55
13:Z:100:TYR:HB3	13:Z:142:MET:HE2	1.88	0.55
13:Z:234:ASP:OD1	13:Z:235:TRP:N	2.40	0.55
12:P:477:CYS:O	12:P:633:ARG:NH2	2.40	0.55
12:P:673:CYS:SG	12:P:708:HIS:ND1	2.78	0.55
13:Y:176:ALA:HB1	13:Y:192:TYR:CE2	2.42	0.55
13:Z:35:MET:HG2	13:Z:40:HIS:CE1	2.42	0.55
3:A:436:LEU:HD23	3:A:638:LEU:HD13	1.89	0.55
3:A:641:TRP:HA	3:A:644:VAL:HG22	1.88	0.55
3:A:716:HIS:ND1	6:O:715:TYR:OH	2.33	0.55
3:A:1470:LEU:HA	3:A:1522:SER:OG	2.07	0.55
8:Q:368:HIS:NE2	8:Q:401:ASP:OD2	2.40	0.55
13:Z:245:PHE:HB2	13:Z:254:ALA:HB2	1.89	0.55
14:U:355:GLN:HG3	14:U:371:MET:HE1	1.88	0.55
3:A:161:MET:HG2	3:A:216:PRO:HG3	1.88	0.54
13:Y:429:MET:HA	13:Y:432:ASN:HD21	1.72	0.54
14:U:91:LYS:NZ	14:U:95:ASP:OD1	2.39	0.54
3:A:411:HIS:NE2	3:A:414:THR:OG1	2.28	0.54
3:A:1357:THR:CG2	3:A:1358:ILE:N	2.69	0.54
3:A:1067:GLU:OE2	3:A:1124:ASN:ND2	2.40	0.54
6:O:113:ASP:OD2	14:U:344:ARG:NH2	2.40	0.54
8:K:205:PHE:O	8:K:209:LEU:HB2	2.07	0.54
12:J:166:GLN:O	12:J:169:LYS:NZ	2.32	0.54
12:P:691:THR:HA	12:P:694:LYS:HE3	1.88	0.54
14:V:304:SER:HB3	14:V:336:VAL:HG22	1.87	0.54
13:Z:44:MET:HB3	13:Z:49:LEU:HD11	1.89	0.54
3:A:234:SER:OG	3:A:235:ARG:N	2.41	0.54
4:N:27:VAL:HG11	4:N:71:LEU:HD11	1.89	0.54
12:J:165:ASP:HA	12:J:467:ARG:HD3	1.88	0.54
3:A:1141:VAL:HG11	3:A:1608:HIS:CG	2.42	0.54
3:A:1163:PRO:O	3:A:1164:LYS:HG2	2.08	0.54
4:N:539:ILE:HG22	4:N:561:LEU:HD23	1.89	0.54
14:U:490:TYR:O	14:U:494:ILE:HG12	2.07	0.54
13:Z:279:ASP:O	13:Z:283:ARG:HG3	2.08	0.54
3:A:1051:VAL:HG21	3:A:1066:LYS:HG2	1.89	0.54
14:U:151:LEU:HD22	14:U:178:VAL:HG23	1.90	0.54
14:U:304:SER:HB3	14:U:336:VAL:HG22	1.90	0.54
13:Z:278:ALA:HA	13:Z:293:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:39:ILE:O	14:U:43:THR:HG23	2.07	0.54
5:I:188:TYR:HA	5:I:194:LYS:HA	1.89	0.54
6:O:14:MET:HB2	14:V:138:LEU:HD12	1.90	0.54
12:J:646:TYR:HD2	12:J:678:VAL:HG12	1.73	0.54
4:N:706:ARG:N	4:N:714:SER:O	2.35	0.54
6:O:381:ILE:HG21	6:O:405:SER:HB2	1.89	0.54
10:M:7:ARG:HD3	14:U:131:ASP:HB3	1.89	0.54
14:U:197:HIS:NE2	14:U:223:SER:O	2.26	0.54
13:Z:208:GLY:O	13:Z:212:LEU:HG	2.08	0.54
3:A:226:LYS:HB2	3:A:236:VAL:HG12	1.90	0.54
3:A:1839:PHE:HD2	3:A:1840:MET:HG3	1.73	0.54
4:N:362:LYS:NZ	4:N:410:LEU:O	2.34	0.54
10:M:48:GLU:N	10:M:48:GLU:OE2	2.41	0.54
12:P:536:MET:HB3	12:P:559:LEU:HD11	1.90	0.54
14:U:57:GLU:OE1	14:V:93:TYR:OH	2.25	0.54
16:C:23:CYS:HB3	16:C:26:CYS:SG	2.47	0.54
3:A:26:ASP:OD1	6:O:500:ASN:ND2	2.32	0.53
4:N:207:TYR:OH	4:N:276:ARG:O	2.26	0.53
8:K:230:ASN:HD21	8:Q:28:LYS:HE3	1.73	0.53
8:Q:325:LYS:HE3	8:Q:329:LEU:HD11	1.88	0.53
15:R:103:GLY:O	15:R:156:LYS:NZ	2.41	0.53
3:A:107:LYS:O	3:A:111:LEU:HG	2.08	0.53
12:P:527:ARG:HB3	13:Y:302:PRO:HG2	1.90	0.53
12:P:537:GLU:OE1	12:P:537:GLU:N	2.38	0.53
14:V:266:VAL:HG13	14:V:285:ILE:HD11	1.91	0.53
4:N:181:LEU:O	4:N:185:MET:HG2	2.08	0.53
4:N:676:TRP:N	4:N:713:PHE:O	2.41	0.53
5:I:162:ASP:N	5:I:162:ASP:OD1	2.40	0.53
5:I:645:ASP:OD1	5:I:648:THR:OG1	2.21	0.53
15:R:175:PRO:HG3	15:R:468:ARG:HD3	1.91	0.53
13:Z:61:LEU:O	13:Z:65:ASN:ND2	2.42	0.53
6:O:460:GLN:OE1	6:O:496:ARG:NH2	2.40	0.53
12:P:486:ASN:O	12:P:490:HIS:ND1	2.41	0.53
13:Y:140:TYR:HD1	13:Y:171:ILE:HG22	1.74	0.53
14:U:389:ARG:NH2	14:U:421:TYR:OH	2.40	0.53
3:A:78:LYS:HE3	3:A:592:HIS:HD2	1.72	0.53
9:G:17:GLU:OE2	9:G:17:GLU:N	2.21	0.53
13:Y:77:TYR:O	13:Y:81:VAL:HG13	2.09	0.53
1:L:22:VAL:HB	1:L:159:TYR:HB3	1.89	0.53
3:A:879:LEU:HD11	3:A:929:ARG:HD2	1.91	0.53
5:I:749:ASP:OD1	5:I:750:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:4:ARG:NH2	8:Q:377:GLU:OE2	2.41	0.53
13:Y:294:PHE:HB3	13:Y:311:TYR:CD1	2.43	0.53
4:N:108:LEU:HD13	4:N:176:LEU:HD12	1.90	0.53
4:N:224:CYS:SG	4:N:231:CYS:CB	2.97	0.53
4:N:273:MET:HE1	4:N:336:TYR:HA	1.89	0.53
13:Y:322:GLU:O	13:Y:325:GLU:HG3	2.08	0.53
3:A:778:LEU:HD23	6:O:594:SER:HB2	1.91	0.53
3:A:1634:LEU:HB2	3:A:1651:LEU:O	2.09	0.53
5:I:101:LEU:HA	5:I:154:LYS:HE2	1.90	0.53
6:O:581:ILE:HD12	6:O:616:LEU:HD12	1.91	0.53
12:J:726:LEU:HD21	12:J:742:LEU:HD22	1.91	0.53
3:A:1797:ILE:HD13	3:A:1851:THR:HG21	1.91	0.53
12:J:521:ILE:O	12:J:525:VAL:HG23	2.09	0.53
14:U:318:TYR:HA	14:U:321:HIS:CD2	2.43	0.53
13:Z:72:SER:H	13:Z:75:GLN:HE21	1.55	0.53
3:A:98:ASN:HA	3:A:123:VAL:HG23	1.90	0.53
3:A:1527:MET:HG3	3:A:1532:ASN:HD22	1.74	0.53
3:A:1797:ILE:HG22	3:A:1852:ILE:HD11	1.92	0.53
4:N:207:TYR:O	4:N:211:ARG:HG2	2.09	0.53
7:S:388:ASP:O	7:S:392:GLN:CA	2.57	0.53
3:A:615:SER:HB3	3:A:618:VAL:HG23	1.91	0.52
3:A:1276:GLU:HG3	3:A:1294:TYR:HE2	1.73	0.52
12:J:656:MET:SD	13:Y:525:TYR:HB2	2.49	0.52
14:V:381:THR:HG21	14:V:412:LEU:HD21	1.89	0.52
3:A:766:LEU:HB3	3:A:790:LEU:HD21	1.90	0.52
5:I:99:GLU:OE1	5:I:154:LYS:NZ	2.40	0.52
12:J:629:ARG:O	12:J:629:ARG:NH1	2.42	0.52
5:I:23:ILE:HD13	5:I:39:ASN:HB3	1.91	0.52
13:Z:374:GLN:N	13:Z:374:GLN:OE1	2.39	0.52
1:L:44:GLN:HG3	1:L:52:THR:HB	1.92	0.52
3:A:781:GLU:OE1	3:A:781:GLU:N	2.37	0.52
12:J:153:GLU:OE1	12:P:22:ARG:NH2	2.42	0.52
15:R:341:ASN:HD21	15:R:348:VAL:CB	2.23	0.52
15:R:439:LEU:HD12	15:R:470:TRP:CZ3	2.44	0.52
3:A:121:SER:OG	3:A:155:GLN:OE1	2.26	0.52
5:I:24:ILE:HG21	5:I:567:ARG:HH21	1.74	0.52
12:J:73:TYR:OH	12:P:18:HIS:O	2.20	0.52
14:V:449:LEU:HB3	14:V:476:LEU:HD12	1.92	0.52
13:Z:327:LEU:O	13:Z:331:LEU:HG	2.10	0.52
3:A:1016:MET:HG2	3:A:1088:THR:HG21	1.91	0.52
5:I:70:CYS:HB2	5:I:113:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:543:VAL:HA	5:I:546:LYS:HE2	1.91	0.52
5:I:680:SER:O	5:I:684:GLN:NE2	2.43	0.52
5:I:486:LEU:HD23	5:I:486:LEU:H	1.75	0.52
6:O:11:ASN:OD1	6:O:11:ASN:N	2.39	0.52
8:K:211:LYS:HB3	8:K:239:GLU:OE2	2.09	0.52
8:K:400:GLU:HB2	8:K:431:LYS:HE3	1.92	0.52
12:P:726:LEU:HD23	12:P:743:ILE:HG12	1.92	0.52
3:A:247:VAL:HG11	3:A:427:ALA:HB3	1.92	0.52
3:A:1018:ASP:OD1	3:A:1018:ASP:N	2.37	0.52
3:A:1217:LEU:HD22	3:A:1612:LEU:HD22	1.92	0.52
3:A:1885:LEU:O	3:A:1889:LEU:HG	2.10	0.52
5:I:477:GLN:HB2	5:I:486:LEU:HB2	1.92	0.52
13:Y:154:ASP:OD1	13:Y:154:ASP:N	2.43	0.52
13:Z:196:LEU:HD23	13:Z:202:ALA:HB3	1.92	0.52
13:Z:236:LEU:O	13:Z:240:ILE:HD12	2.10	0.52
1:L:16:LEU:O	1:L:19:THR:OG1	2.25	0.52
8:K:193:LEU:O	8:K:198:GLN:NE2	2.42	0.52
8:K:417:GLU:N	8:K:417:GLU:OE1	2.43	0.52
12:J:610:GLU:O	12:J:614:THR:HG22	2.10	0.52
13:Y:414:ILE:HD12	13:Y:446:LEU:HD11	1.92	0.52
14:U:464:ASP:OD2	14:U:468:MET:N	2.41	0.52
15:R:239:GLU:OE1	15:R:281:ALA:N	2.43	0.52
3:A:252:ASP:HB2	3:A:253:PRO:HD3	1.91	0.52
3:A:765:VAL:HA	3:A:768:LEU:HD12	1.92	0.52
3:A:1895:PRO:HD3	3:A:1923:MET:SD	2.50	0.52
13:Y:414:ILE:CD1	13:Y:446:LEU:HD11	2.40	0.52
13:Z:49:LEU:HD12	13:Z:53:VAL:HG23	1.92	0.52
4:N:520:ARG:HH22	4:N:602:PRO:HA	1.74	0.51
7:S:388:ASP:O	7:S:392:GLN:N	2.42	0.51
8:Q:218:THR:HG21	8:Q:241:HIS:CD2	2.44	0.51
13:Y:193:LYS:HA	13:Y:196:LEU:HG	1.92	0.51
3:A:720:GLU:O	3:A:725:ASN:ND2	2.43	0.51
15:R:188:PHE:H	15:R:447:LEU:HD12	1.75	0.51
15:R:193:VAL:HG22	15:R:448:TYR:HB3	1.92	0.51
4:N:299:TRP:O	4:N:303:VAL:HG13	2.09	0.51
4:N:407:LEU:HB2	4:N:417:LEU:HD23	1.92	0.51
8:K:24:PHE:CE1	8:K:28:LYS:HE2	2.46	0.51
2:D:45:ALA:HA	14:U:378:MET:HE3	1.92	0.51
3:A:941:LEU:HG	3:A:977:LEU:HD12	1.92	0.51
11:H:61:TYR:HD1	13:Z:360:TYR:CG	2.28	0.51
13:Y:94:ARG:NH2	13:Z:333:ASN:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:338:HIS:CE1	13:Z:92:GLU:OE2	2.63	0.51
14:U:95:ASP:HB3	14:V:49:LEU:HD22	1.91	0.51
4:N:540:ARG:O	4:N:543:GLU:HG3	2.09	0.51
5:I:47:HIS:CE1	5:I:54:ARG:HB2	2.45	0.51
8:K:174:HIS:O	8:K:366:GLY:N	2.43	0.51
12:J:566:SER:OG	12:J:568:GLU:OE1	2.29	0.51
12:P:93:SER:OG	12:P:94:GLY:N	2.42	0.51
13:Z:98:SER:O	13:Z:102:MET:HG3	2.09	0.51
8:K:512:ASP:HB3	8:K:515:SER:HB2	1.93	0.51
5:I:682:GLU:OE2	5:I:703:ARG:NH1	2.43	0.51
5:I:700:ILE:HD12	5:I:701:PRO:HD2	1.93	0.51
7:S:376:LYS:HG2	7:S:377:ALA:H	1.74	0.51
14:U:432:ASP:HB3	14:U:435:MET:HE2	1.92	0.51
14:V:216:LYS:HA	14:V:219:LEU:HB3	1.92	0.51
3:A:1794:ASP:OD1	3:A:1798:ARG:NE	2.42	0.51
4:N:276:ARG:NH2	4:N:288:GLU:OE1	2.44	0.51
6:O:529:ASP:O	6:O:532:VAL:HG12	2.11	0.51
7:S:375:LEU:HG	16:C:28:MET:HE1	1.91	0.51
8:Q:442:ASP:N	8:Q:442:ASP:OD1	2.44	0.51
2:D:45:ALA:HA	14:U:378:MET:HE2	1.93	0.51
4:N:132:LEU:O	4:N:136:THR:HG23	2.11	0.51
6:O:435:SER:HG	6:O:618:TYR:HH	1.55	0.51
9:G:11:LEU:HD21	8:Q:456:ARG:NH1	2.25	0.51
12:P:145:ASN:HB3	12:P:148:LEU:HD23	1.93	0.51
14:V:385:ILE:HG13	14:V:408:THR:HG21	1.93	0.51
4:N:425:ARG:NH2	4:N:507:SER:OG	2.43	0.51
7:S:388:ASP:O	7:S:392:GLN:HA	2.11	0.50
10:M:10:ARG:HG2	14:V:135:VAL:HG21	1.92	0.50
12:J:27:LEU:HD21	12:P:147:PHE:HB3	1.93	0.50
13:Y:524:GLU:OE2	13:Y:524:GLU:N	2.44	0.50
14:U:441:GLU:O	14:U:444:GLU:HG2	2.10	0.50
15:R:284:LEU:HD11	15:R:298:ILE:HG12	1.92	0.50
5:I:356:SER:HB2	5:I:397:ILE:HG12	1.94	0.50
7:S:361:GLU:O	7:S:365:VAL:HG13	2.11	0.50
12:J:23:ASP:OD1	12:P:150:SER:N	2.25	0.50
8:Q:157:LEU:HG	8:Q:188:LEU:HD11	1.94	0.50
14:V:29:LEU:HD23	14:V:32:ILE:HD12	1.93	0.50
13:Z:159:LEU:HD22	13:Z:171:ILE:HG23	1.94	0.50
3:A:971:PRO:HG2	3:A:974:VAL:HG13	1.93	0.50
4:N:119:GLU:HA	4:N:250:LEU:HD21	1.94	0.50
6:O:110:GLN:NE2	6:O:114:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:568:LEU:HB2	6:O:583:VAL:HG11	1.92	0.50
8:K:173:HIS:O	8:K:364:MET:HE2	2.12	0.50
6:O:622:GLU:OE1	6:O:662:ARG:NH2	2.44	0.50
12:J:752:GLN:OE1	12:J:752:GLN:N	2.44	0.50
8:Q:2:ASN:ND2	8:Q:5:ARG:HG2	2.26	0.50
13:Y:270:ASN:HA	13:Z:62:THR:HG21	1.92	0.50
13:Y:359:LEU:HD12	13:Y:379:LYS:HD2	1.92	0.50
3:A:1306:CYS:HB2	3:A:1374:ILE:HG12	1.93	0.50
13:Y:331:LEU:HD23	13:Y:334:ILE:HD11	1.94	0.50
15:R:97:ASN:OD1	15:R:104:ILE:N	2.35	0.50
4:N:184:TYR:CD1	4:N:299:TRP:HB2	2.46	0.50
4:N:224:CYS:HB2	4:N:232:TRP:CD1	2.47	0.50
6:O:594:SER:O	6:O:594:SER:OG	2.24	0.50
3:A:464:THR:OG1	3:A:465:GLN:OE1	2.29	0.50
6:O:462:ASN:OD1	6:O:496:ARG:NE	2.36	0.50
12:P:543:LEU:HB3	12:P:552:LEU:HB2	1.94	0.50
8:Q:251:TYR:HA	8:Q:254:THR:HG22	1.93	0.50
15:R:202:SER:OG	15:R:237:TRP:NE1	2.44	0.50
2:D:53:PRO:O	8:Q:510[B]:ARG:NH2	2.44	0.50
4:N:350:ASP:O	4:N:354:SER:CB	2.60	0.50
4:N:504:LEU:O	4:N:508:ILE:HG23	2.11	0.50
1:L:98:VAL:HB	1:L:134:THR:HG21	1.93	0.50
8:K:284:LEU:HD21	8:K:307:CYS:SG	2.52	0.50
14:U:301:ASP:OD1	14:U:301:ASP:N	2.45	0.50
3:A:959:ILE:HG23	3:A:978:ILE:HA	1.93	0.49
5:I:33:ASP:OD1	5:I:728:ARG:NE	2.43	0.49
5:I:303:GLU:HB3	5:I:317:LEU:HD11	1.93	0.49
5:I:313:ALA:HB3	5:I:428:MET:HE1	1.93	0.49
6:O:729:GLU:HA	6:O:732:ARG:HG2	1.94	0.49
10:M:3:SER:OG	14:U:180:ARG:NH2	2.45	0.49
3:A:183:THR:HG22	3:A:249:LEU:HD11	1.94	0.49
3:A:218:ASP:OD2	14:V:454:LYS:NZ	2.38	0.49
3:A:1767:ILE:HG13	3:A:1798:ARG:HH12	1.78	0.49
4:N:186:GLN:HG3	4:N:223:GLY:H	1.77	0.49
6:O:58:ARG:HG3	6:O:62:GLN:HE22	1.77	0.49
7:S:119:GLU:HB2	15:R:188:PHE:CE2	2.47	0.49
13:Z:315:LEU:CB	13:Z:324:VAL:HG12	2.42	0.49
1:L:6:LYS:HD3	1:L:115:GLU:HG2	1.95	0.49
3:A:1794:ASP:O	3:A:1797:ILE:HG13	2.13	0.49
8:K:342:HIS:NE2	9:W:2:LEU:O	2.41	0.49
10:M:12:LEU:HD13	14:U:360:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:142:LEU:HD11	12:J:152:PHE:HB2	1.94	0.49
13:Z:56:LEU:O	13:Z:60:LEU:HD12	2.12	0.49
13:Z:258:ILE:HD12	13:Z:259:CYS:N	2.27	0.49
6:O:378:SER:O	6:O:382:GLN:HG2	2.12	0.49
11:H:68:LYS:HB3	11:H:68:LYS:NZ	2.27	0.49
14:V:416:PHE:HA	14:V:446:LEU:HD11	1.95	0.49
6:O:63:LEU:HD11	6:O:81:LEU:HD23	1.94	0.49
6:O:209:GLN:OE1	6:O:247:ASN:ND2	2.46	0.49
8:K:443:LYS:HG3	9:W:5:LYS:NZ	2.28	0.49
8:Q:503:HIS:CD2	14:U:389:ARG:HH12	2.30	0.49
5:I:587:LEU:HD21	5:I:643:PHE:HE1	1.77	0.49
7:S:398:ARG:HG3	7:S:401:CYS:H	1.78	0.49
13:Y:320:ARG:O	13:Y:324:VAL:HG13	2.13	0.49
11:H:70:VAL:HG22	13:Y:357:ARG:HD3	1.95	0.49
8:Q:372:LEU:HD13	8:Q:404:VAL:HG12	1.95	0.49
13:Y:41:VAL:HG23	13:Y:82:TYR:CD2	2.47	0.49
15:R:212:TRP:CD1	15:R:219:VAL:HG22	2.48	0.49
15:R:444:TYR:HB2	15:R:462:ALA:HB1	1.95	0.49
6:O:75:LEU:HB3	6:O:165:GLY:HA3	1.94	0.49
12:J:536:MET:HB3	12:J:559:LEU:HD11	1.94	0.49
13:Y:147:THR:HG22	13:Y:178:LEU:HD21	1.94	0.49
14:U:495:GLN:NE2	14:U:496:ASP:OD1	2.46	0.49
3:A:1222:MET:O	3:A:1226:ARG:HD3	2.12	0.49
13:Y:430:ALA:HB1	13:Y:447:LEU:HD23	1.95	0.49
15:R:4:ASP:OD1	15:R:7:ARG:NH1	2.45	0.49
3:A:248:PHE:HZ	3:A:250:ASN:HD22	1.59	0.48
3:A:1086:MET:HE3	3:A:1560:MET:HG3	1.94	0.48
3:A:1326:TYR:HA	3:A:1329:MET:HG2	1.95	0.48
3:A:1527:MET:HA	3:A:1527:MET:HE3	1.95	0.48
3:A:1719:LEU:O	4:N:323:ARG:NH2	2.46	0.48
5:I:306:HIS:CG	6:O:57:ARG:HH21	2.30	0.48
8:K:254:THR:OG1	8:K:267:CYS:SG	2.66	0.48
13:Y:203:LEU:N	13:Z:52:ASN:HD21	2.11	0.48
3:A:443:CYS:HB3	3:A:452:LEU:HD11	1.96	0.48
5:I:288:THR:HG1	5:I:469:TYR:N	2.11	0.48
4:N:340:ARG:HB3	4:N:361:LEU:HD12	1.96	0.48
12:J:42:PHE:HB2	12:J:71:CYS:SG	2.53	0.48
12:J:68:THR:OG1	12:J:71:CYS:SG	2.70	0.48
12:J:762:TRP:CE2	8:Q:362:GLN:HB2	2.48	0.48
8:Q:405:MET:HA	8:Q:408:VAL:HG22	1.94	0.48
15:R:209:VAL:H	15:R:223:CYS:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:LEU:HA	2:D:33:GLN:OE1	2.14	0.48
12:J:453:ASN:OD1	12:J:454:LEU:N	2.47	0.48
13:Y:333:ASN:O	13:Z:94:ARG:NH1	2.44	0.48
15:R:153:VAL:HG12	15:R:158:GLN:HG3	1.95	0.48
13:Z:294:PHE:HB3	13:Z:311:TYR:HD1	1.78	0.48
3:A:1019:MET:SD	3:A:1088:THR:HG22	2.54	0.48
3:A:1060:HIS:O	3:A:1064:GLU:HG2	2.12	0.48
12:J:621:LEU:CD2	12:J:644:ILE:HG21	2.43	0.48
12:P:465:LEU:O	12:P:469:MET:HG3	2.13	0.48
14:V:234:LEU:HA	14:V:237:ILE:HG22	1.95	0.48
14:V:488:GLN:HA	14:V:491:ILE:HG12	1.94	0.48
3:A:77:ARG:NH2	3:A:91:GLU:OE1	2.34	0.48
3:A:1313:LEU:HB3	3:A:1316:MET:SD	2.53	0.48
4:N:56:ARG:NH2	4:N:138:LEU:HD12	2.22	0.48
5:I:101:LEU:HD11	5:I:164:ILE:HG23	1.94	0.48
12:J:668:SER:OG	12:J:671:LEU:HB2	2.13	0.48
13:Z:140:TYR:HD1	13:Z:171:ILE:HG12	1.78	0.48
3:A:1376:LEU:HG	3:A:1377:LYS:HG3	1.95	0.48
12:J:5:GLN:N	12:J:5:GLN:OE1	2.45	0.48
12:P:672:LEU:HB3	12:P:695:ALA:HB2	1.95	0.48
8:Q:309:TYR:HA	8:Q:312:VAL:HG22	1.96	0.48
8:Q:433:LYS:NZ	8:Q:437:ASN:O	2.29	0.48
15:R:187:ASP:C	15:R:189:TYR:H	2.15	0.48
13:Z:323:ASP:HA	13:Z:326:ASN:ND2	2.29	0.48
8:K:180:GLU:N	8:K:180:GLU:OE1	2.47	0.48
11:H:90:GLU:HA	11:H:93:GLU:HB2	1.95	0.48
12:J:92:LEU:HD11	12:J:120:LEU:HD23	1.96	0.48
12:J:702:ASN:HB3	12:J:705:CYS:SG	2.54	0.48
13:Y:414:ILE:HD12	13:Y:446:LEU:CD2	2.34	0.48
13:Z:400:ILE:HD13	13:Z:409:CYS:HB2	1.95	0.48
2:D:17:TRP:O	6:O:277:TYR:OH	2.31	0.48
3:A:625:ILE:O	3:A:629:LEU:HG	2.13	0.48
4:N:168:THR:O	4:N:171:GLU:HG3	2.13	0.48
5:I:632:ARG:HH12	5:I:713:LEU:HB2	1.79	0.48
6:O:109:GLU:HB3	14:U:344:ARG:CZ	2.43	0.48
6:O:625:LEU:HD22	6:O:666:LEU:HD23	1.96	0.48
7:S:437:THR:HG23	7:S:440:SER:H	1.79	0.48
12:J:34:GLU:OE1	12:P:495:HIS:NE2	2.32	0.48
8:Q:80:HIS:ND1	8:Q:85:GLU:OE2	2.45	0.48
3:A:133:ILE:HG22	3:A:215:HIS:CD2	2.49	0.48
3:A:862:TYR:CZ	3:A:864:PRO:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1926:ARG:HA	4:N:77:GLU:HG2	1.95	0.48
4:N:56:ARG:HH21	4:N:135:TRP:HD1	1.58	0.48
12:P:53:LYS:HG3	12:P:56:LYS:HE2	1.96	0.48
1:L:20:GLY:HA3	12:P:581:ARG:NH2	2.28	0.47
3:A:628:ILE:HB	3:A:765:VAL:HG11	1.96	0.47
3:A:880:TYR:HB2	3:A:930:LEU:HD22	1.96	0.47
3:A:1912:ALA:O	3:A:1915:LEU:HG	2.14	0.47
5:I:664:ARG:NH1	5:I:718:LYS:CA	2.68	0.47
8:Q:157:LEU:HD23	8:Q:184:LEU:HD21	1.95	0.47
13:Y:308:MET:HB3	13:Y:331:LEU:HD11	1.96	0.47
13:Z:197:ARG:HH21	13:Z:198:GLN:HB2	1.78	0.47
3:A:1292:GLU:HG3	3:A:1362:VAL:HG22	1.96	0.47
3:A:1875:GLN:N	3:A:1875:GLN:OE1	2.46	0.47
4:N:351:PHE:CE1	4:N:409:VAL:HG11	2.49	0.47
5:I:272:MET:HE3	5:I:347:LEU:HB3	1.95	0.47
5:I:533:ILE:HG22	5:I:537:LEU:HD23	1.97	0.47
10:M:60:LEU:HD11	12:J:549:ASP:HB3	1.96	0.47
13:Y:59:LEU:HD12	13:Z:270:ASN:HD21	1.78	0.47
1:L:112:GLU:HA	1:L:112:GLU:OE1	2.15	0.47
3:A:1271:GLU:HB2	3:A:1319:LEU:HD21	1.96	0.47
3:A:1816:LEU:HD23	3:A:1816:LEU:HA	1.79	0.47
4:N:290:HIS:O	4:N:293:ILE:HG12	2.13	0.47
15:R:289:ARG:HA	15:R:315:GLU:CB	2.45	0.47
3:A:1201:HIS:HB3	3:A:1204:THR:HB	1.96	0.47
4:N:564:MET:O	4:N:567:SER:HB3	2.13	0.47
5:I:71:LEU:HD23	5:I:80:LEU:HD11	1.96	0.47
5:I:290:PHE:HB2	5:I:320:LEU:HD13	1.97	0.47
12:J:59:ARG:HD2	12:P:531:TYR:HB3	1.97	0.47
13:Y:87:LEU:HD13	13:Y:95:ASN:HB3	1.96	0.47
14:U:244:ILE:HG23	14:U:272:ALA:HB1	1.96	0.47
3:A:1300:LEU:O	3:A:1304:MET:HE3	2.14	0.47
3:A:1725:ASN:OD1	4:N:255:ARG:HD3	2.14	0.47
4:N:398:THR:HG23	7:S:436:GLY:HA2	1.96	0.47
5:I:236:LEU:HD23	5:I:550:GLN:HA	1.96	0.47
5:I:238:THR:HA	5:I:548:MET:HG2	1.96	0.47
6:O:105:LEU:HD11	6:O:151:VAL:HG12	1.97	0.47
8:K:196:GLU:O	8:K:199:GLU:HG3	2.15	0.47
14:U:210:CYS:HA	14:U:237:ILE:HD13	1.96	0.47
1:L:13:PRO:HA	1:L:16:LEU:HD23	1.96	0.47
4:N:184:TYR:O	4:N:188:LYS:HG2	2.15	0.47
6:O:318:GLN:O	6:O:321:GLU:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:324:PRO:O	7:S:325:LEU:HD12	2.15	0.47
9:G:4:ARG:NH2	8:Q:376:LEU:HD23	2.30	0.47
12:J:132:ALA:O	12:J:136:GLU:HG2	2.14	0.47
12:P:584:ASP:OD1	12:P:585:ILE:N	2.48	0.47
3:A:628:ILE:HD12	3:A:765:VAL:HG13	1.96	0.47
4:N:90:GLU:HA	4:N:93:ASN:ND2	2.30	0.47
4:N:228:LYS:H	4:N:228:LYS:HD3	1.80	0.47
12:P:53:LYS:HB3	12:P:56:LYS:HG3	1.96	0.47
13:Y:475:TYR:CE2	13:Y:477:LYS:HB2	2.49	0.47
14:U:490:TYR:CE2	14:U:512:ALA:HA	2.41	0.47
15:R:268:GLU:OE1	15:R:269:GLY:N	2.41	0.47
13:Z:206:ILE:HG23	13:Z:219:VAL:HG11	1.96	0.47
13:Z:340:GLU:O	13:Z:344:VAL:HG12	2.14	0.47
3:A:864:PRO:HB3	3:A:898:ARG:HH12	1.80	0.47
4:N:200:GLU:OE1	4:N:276:ARG:NH1	2.47	0.47
4:N:535:PRO:O	4:N:539:ILE:HG23	2.14	0.47
6:O:33:TYR:OH	6:O:67:LEU:O	2.33	0.47
8:Q:425:PHE:HB3	8:Q:451:LEU:HG	1.95	0.47
14:U:297:ILE:HD11	14:U:330:ARG:HD3	1.96	0.47
15:R:189:TYR:HB3	15:R:273:ARG:NH2	2.28	0.47
15:R:277:LEU:HA	15:R:286:SER:HA	1.97	0.47
15:R:420:TYR:O	15:R:423:ASN:ND2	2.48	0.47
3:A:501:THR:HG23	3:A:504:VAL:HB	1.97	0.47
3:A:1793:MET:HG2	3:A:1814:ILE:HG12	1.97	0.47
4:N:631:ALA:O	4:N:633:ARG:NH1	2.48	0.47
5:I:640:ASP:OD1	5:I:641:ALA:N	2.47	0.47
5:I:673:LEU:O	5:I:676:ASN:ND2	2.48	0.47
6:O:212:ALA:HB1	6:O:243:LEU:HD21	1.95	0.47
9:G:17:GLU:HA	9:G:20:GLU:HG2	1.97	0.47
10:M:31:ILE:HG22	10:M:33:LEU:H	1.79	0.47
12:J:587:ILE:HG23	12:J:607:LEU:HD11	1.96	0.47
14:U:122:ARG:HH22	14:U:153:GLU:HG3	1.80	0.47
16:C:67:GLN:O	16:C:69:VAL:N	2.44	0.47
3:A:449:GLN:OE1	3:A:453:ARG:NH1	2.47	0.47
5:I:341:TYR:OH	5:I:473:GLU:OE1	2.28	0.47
9:G:8:ARG:NH1	8:Q:445:GLU:OE2	2.48	0.47
14:U:385:ILE:O	14:U:389:ARG:HG2	2.14	0.47
13:Z:383:LEU:HB3	13:Z:388:ARG:HB2	1.96	0.47
1:L:43:ASP:O	1:L:47:ASP:HB2	2.15	0.46
3:A:628:ILE:CD1	3:A:765:VAL:HG13	2.44	0.46
5:I:255:PHE:CE2	5:I:540:PRO:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:341:TYR:HB3	5:I:411:MET:HE2	1.97	0.46
6:O:109:GLU:OE1	14:U:344:ARG:NH1	2.48	0.46
6:O:664:MET:HE3	6:O:664:MET:HA	1.97	0.46
14:V:35:GLN:HB3	14:V:201:LEU:HD22	1.97	0.46
13:Z:82:TYR:HA	13:Z:85:ASP:OD2	2.15	0.46
14:U:85:ASP:N	14:U:85:ASP:OD1	2.47	0.46
15:R:209:VAL:H	15:R:223:CYS:HB2	1.80	0.46
16:C:23:CYS:HB2	16:C:56:HIS:ND1	2.29	0.46
3:A:485:ILE:HG13	3:A:487:THR:HG23	1.97	0.46
3:A:720:GLU:OE2	6:O:719:ARG:NH1	2.48	0.46
3:A:1799:ARG:HG3	3:A:1804:GLU:HG3	1.98	0.46
6:O:532:VAL:HG23	6:O:546:ARG:HB2	1.97	0.46
8:K:379:GLY:HA3	8:K:411:VAL:HG23	1.98	0.46
16:C:56:HIS:HB2	16:C:59:CYS:SG	2.55	0.46
13:Z:49:LEU:CD1	13:Z:53:VAL:HG23	2.44	0.46
13:Z:364:LYS:O	13:Z:367:GLN:HG3	2.15	0.46
6:O:14:MET:HG3	6:O:29:TRP:HH2	1.81	0.46
8:K:172:SER:O	8:K:175:MET:HG2	2.16	0.46
13:Y:373:VAL:HG11	13:Y:403:ALA:HB2	1.97	0.46
14:V:39:ILE:HG12	14:V:201:LEU:O	2.15	0.46
13:Z:36:ASN:OD1	13:Z:39:ASP:N	2.41	0.46
13:Z:308:MET:HB2	13:Z:340:GLU:OE2	2.15	0.46
13:Z:315:LEU:HD22	13:Z:320:ARG:NH1	2.27	0.46
4:N:186:GLN:NE2	4:N:221:CYS:SG	2.88	0.46
4:N:300:LEU:HA	4:N:303:VAL:HG22	1.97	0.46
5:I:269:LEU:HD22	5:I:526:LYS:HD3	1.98	0.46
5:I:717:MET:C	5:I:719:ALA:H	2.18	0.46
8:Q:37:PRO:HB3	8:Q:65:LEU:HD11	1.98	0.46
8:Q:210:LYS:HB3	8:Q:210:LYS:HE2	1.78	0.46
13:Y:466:ASP:OD1	13:Y:467:LYS:N	2.48	0.46
14:V:129:LYS:O	14:V:133:GLU:HG2	2.15	0.46
15:R:388:LEU:HG	15:R:389:THR:HG23	1.98	0.46
13:Z:321:LEU:HD21	13:Z:352:SER:HB2	1.96	0.46
3:A:40:ARG:HD3	14:V:142:GLU:OE2	2.16	0.46
3:A:1086:MET:HE1	3:A:1610:TYR:CG	2.49	0.46
3:A:1318:ASP:N	3:A:1318:ASP:OD1	2.48	0.46
5:I:186:GLU:HB3	5:I:188:TYR:HE1	1.80	0.46
5:I:652:VAL:HG22	5:I:666:LEU:HD12	1.98	0.46
12:J:773:ASN:OD1	12:J:773:ASN:N	2.49	0.46
3:A:48:LEU:HD22	14:V:50:HIS:CE1	2.51	0.46
5:I:230:GLU:HB2	5:I:558:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:672:LEU:HB3	12:J:695:ALA:HB2	1.98	0.46
12:P:25:VAL:HG13	12:P:48:TYR:HE1	1.81	0.46
15:R:201:LEU:N	15:R:212:TRP:O	2.49	0.46
15:R:212:TRP:HD1	15:R:219:VAL:HG22	1.80	0.46
13:Z:294:PHE:HB3	13:Z:311:TYR:CD1	2.51	0.46
3:A:411:HIS:CE1	3:A:414:THR:HG1	2.25	0.46
3:A:1230:ILE:HA	3:A:1236:LEU:HD21	1.98	0.46
6:O:91:ASN:OD1	6:O:92:SER:N	2.49	0.46
13:Y:186:ARG:O	13:Y:190:THR:HG23	2.15	0.46
13:Y:210:LEU:HA	13:Y:214:VAL:HG12	1.97	0.46
13:Z:266:LEU:HB2	13:Z:267:LEU:HD22	1.97	0.46
3:A:707:TRP:CD2	6:O:730:ARG:HD3	2.51	0.46
3:A:791:VAL:HG21	3:A:814:VAL:HG22	1.98	0.46
3:A:1635:GLU:HG3	3:A:1667:LYS:HB3	1.98	0.46
3:A:1735:PRO:HB2	3:A:1756:LYS:HG3	1.98	0.46
4:N:343:GLU:O	4:N:347:ILE:HG13	2.15	0.46
5:I:269:LEU:HA	5:I:272:MET:HG3	1.98	0.46
5:I:514:PHE:H	6:O:443:GLN:HE22	1.63	0.46
8:K:408:VAL:O	8:K:411:VAL:HG12	2.16	0.46
10:M:7:ARG:HB3	10:M:7:ARG:NH1	2.30	0.46
8:Q:185:LEU:HD12	8:Q:209:LEU:HD21	1.98	0.46
8:Q:285:PHE:HB2	8:Q:308:TYR:CE1	2.50	0.46
14:V:379:LYS:HD2	15:R:64:ILE:HB	1.97	0.46
15:R:249:HIS:HA	15:R:273:ARG:HB2	1.98	0.46
15:R:284:LEU:HD12	15:R:284:LEU:H	1.81	0.46
3:A:88:ASP:N	3:A:88:ASP:OD1	2.47	0.46
4:N:55:LEU:HG	4:N:135:TRP:CH2	2.51	0.46
4:N:404:ILE:HA	4:N:417:LEU:HD21	1.98	0.46
7:S:373:GLU:O	16:C:27:ARG:NH2	2.49	0.46
8:Q:383:ASN:ND2	8:Q:386:LEU:HD12	2.31	0.46
15:R:278:ALA:HB1	15:R:321:TRP:HD1	1.81	0.46
13:Z:49:LEU:HB2	13:Z:52:ASN:HB3	1.98	0.46
13:Z:139:LYS:HZ3	13:Z:158:ILE:HG13	1.82	0.46
3:A:1163:PRO:HB2	3:A:1168:LEU:HB2	1.98	0.45
3:A:1634:LEU:HD12	3:A:1653:ALA:HB2	1.98	0.45
4:N:79:LEU:HD13	4:N:125:TYR:CD1	2.51	0.45
4:N:563:ASP:OD1	4:N:596:LEU:HA	2.16	0.45
4:N:677:THR:HA	4:N:712:THR:HA	1.98	0.45
5:I:583:LEU:HD11	5:I:611:VAL:HG11	1.98	0.45
8:K:35:GLU:HB3	8:K:40:ILE:HD11	1.98	0.45
12:J:516:MET:O	12:J:519:GLU:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:168:THR:O	13:Y:171:ILE:HG12	2.16	0.45
14:V:244:ILE:HG21	14:V:276:ILE:HG12	1.98	0.45
14:V:434:ARG:HH21	15:R:49:ILE:HD12	1.81	0.45
4:N:350:ASP:N	4:N:350:ASP:OD1	2.49	0.45
12:P:523:SER:OG	12:P:527:ARG:NH1	2.49	0.45
15:R:173:LYS:NZ	15:R:440:THR:O	2.49	0.45
2:D:54:ILE:O	14:U:409:TYR:OH	2.30	0.45
3:A:663:CYS:O	3:A:667:MET:HG2	2.16	0.45
3:A:982:ASP:HB2	3:A:1676:LEU:HD21	1.97	0.45
4:N:398:THR:OG1	7:S:436:GLY:N	2.49	0.45
5:I:597:LYS:HG3	5:I:598:MET:H	1.81	0.45
12:J:552:LEU:HG	12:J:576:CYS:HB2	1.99	0.45
13:Y:227:ILE:HD11	13:Y:236:LEU:HB3	1.99	0.45
14:U:436:LEU:HD23	14:U:439:LEU:HD12	1.99	0.45
1:L:76:THR:HG22	1:L:159:TYR:HB2	1.97	0.45
3:A:941:LEU:H	3:A:941:LEU:HD12	1.82	0.45
3:A:1016:MET:SD	3:A:1084:ARG:HG3	2.56	0.45
3:A:1037:VAL:HG13	3:A:1562:LEU:HD21	1.99	0.45
3:A:1910:SER:O	3:A:1913:GLU:HG2	2.16	0.45
4:N:302:LYS:NZ	4:N:302:LYS:HB2	2.32	0.45
4:N:505:LEU:O	4:N:508:ILE:HG12	2.16	0.45
6:O:318:GLN:HA	6:O:321:GLU:OE2	2.16	0.45
7:S:411:CYS:O	7:S:412:ASN:C	2.55	0.45
8:Q:248:LYS:HG2	14:U:153:GLU:OE2	2.16	0.45
13:Y:159:LEU:HD11	13:Y:174:MET:HE3	1.98	0.45
3:A:1208:LEU:HD23	3:A:1208:LEU:HA	1.83	0.45
3:A:1452:LEU:HD12	3:A:1452:LEU:O	2.17	0.45
3:A:1503:ASN:O	3:A:1507:THR:HG22	2.16	0.45
8:K:28:LYS:HA	8:K:28:LYS:HD3	1.74	0.45
12:P:672:LEU:HD11	12:P:698:ILE:HD12	1.98	0.45
8:Q:288:SER:O	8:Q:292:VAL:HG22	2.15	0.45
8:Q:506:LEU:HD23	8:Q:506:LEU:HA	1.78	0.45
13:Y:179:TYR:HB2	13:Y:188:SER:HB2	1.99	0.45
14:V:159:SER:O	14:V:163:GLN:HG2	2.17	0.45
13:Z:219:VAL:O	13:Z:223:THR:HG23	2.16	0.45
13:Z:315:LEU:HB3	13:Z:324:VAL:HG12	1.98	0.45
3:A:768:LEU:HD21	3:A:861:PRO:HB2	1.99	0.45
5:I:33:ASP:OD2	5:I:728:ARG:NH2	2.48	0.45
6:O:575:LYS:HA	6:O:575:LYS:HD2	1.85	0.45
12:J:524:GLU:O	12:J:528:ILE:HG22	2.17	0.45
13:Y:245:PHE:CE2	13:Y:253:ARG:HD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:46:ARG:HB3	14:V:116:PHE:CE2	2.52	0.45
13:Z:42:ARG:HG3	13:Z:82:TYR:OH	2.16	0.45
3:A:591:VAL:HB	3:A:606:ARG:HH22	1.82	0.45
3:A:1865:ASP:HA	3:A:1868:VAL:HG12	1.99	0.45
4:N:224:CYS:O	4:N:226:SER:N	2.50	0.45
5:I:141:LYS:HA	5:I:141:LYS:HD3	1.60	0.45
8:K:15:ASP:O	8:K:17:GLN:NE2	2.50	0.45
11:H:102:LEU:HD13	12:P:594:ILE:HG22	1.99	0.45
13:Y:332:PHE:CD1	13:Y:341:PRO:HB2	2.52	0.45
13:Y:440:ASN:HA	13:Y:471:GLN:NE2	2.31	0.45
14:V:343:LEU:HD23	14:V:343:LEU:HA	1.82	0.45
15:R:318:GLY:O	15:R:361:ILE:HD12	2.16	0.45
1:L:141:VAL:HG11	1:L:151:THR:HG21	1.99	0.45
3:A:1041:LEU:HD13	3:A:1084:ARG:HA	1.99	0.45
4:N:247:LEU:HD11	4:N:252:LEU:HB2	1.98	0.45
9:G:3:ARG:HH21	8:Q:243:TYR:HA	1.82	0.45
12:J:466:LEU:HD12	12:J:466:LEU:O	2.17	0.45
12:J:733:VAL:HG23	12:J:733:VAL:O	2.17	0.45
8:Q:271:HIS:HD2	8:Q:287:LEU:HD22	1.81	0.45
8:Q:351:ASP:OD1	8:Q:351:ASP:N	2.47	0.45
13:Y:331:LEU:HD12	13:Y:344:VAL:HG21	1.99	0.45
1:L:24:GLU:OE2	1:L:25:ILE:N	2.50	0.45
3:A:790:LEU:HD23	3:A:790:LEU:HA	1.82	0.45
3:A:1489:HIS:O	3:A:1493:LYS:HG2	2.17	0.45
4:N:569:ARG:O	4:N:573:ASN:ND2	2.50	0.45
12:J:766:LEU:HA	12:J:766:LEU:HD23	1.82	0.45
14:U:185:VAL:HG13	14:U:212:LEU:HD22	1.99	0.45
14:V:93:TYR:OH	14:V:101:ARG:NH2	2.50	0.45
13:Z:49:LEU:O	13:Z:51:SER:N	2.50	0.45
13:Z:57:SER:HB2	13:Z:83:HIS:HB2	1.98	0.45
3:A:942:ARG:O	3:A:945:GLU:HB3	2.17	0.45
6:O:240:LEU:HD11	6:O:256:LEU:HD23	1.99	0.45
10:M:5:VAL:HG12	14:U:124:LEU:HD22	1.98	0.45
12:P:536:MET:HG3	12:P:559:LEU:HD21	1.99	0.45
8:Q:402:PRO:HG3	8:Q:431:LYS:HB3	1.98	0.45
14:U:492:LYS:O	14:U:495:GLN:HG3	2.16	0.45
13:Z:135:GLU:HA	13:Z:138:VAL:HG22	1.99	0.45
13:Z:360:TYR:HD2	13:Z:361:LEU:HD12	1.81	0.45
1:L:98:VAL:HG12	1:L:137:ILE:HG12	1.98	0.44
3:A:1033:ARG:NH1	3:A:1531:GLY:O	2.50	0.44
3:A:1715:TRP:CG	3:A:1715:TRP:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:392:ASN:O	4:N:396:ILE:HG13	2.16	0.44
4:N:442:LEU:HD13	4:N:545:LEU:HD21	1.99	0.44
5:I:255:PHE:HE2	5:I:540:PRO:HG2	1.81	0.44
5:I:517:TYR:HB3	5:I:520:LYS:HB2	1.98	0.44
6:O:444:MET:HE2	6:O:444:MET:HB2	1.91	0.44
13:Y:140:TYR:CE1	13:Y:170:LYS:HB2	2.52	0.44
13:Y:363:ALA:N	13:Y:379:LYS:HD3	2.31	0.44
14:U:296:ARG:HH12	14:U:298:GLU:HB2	1.83	0.44
14:U:418:CYS:SG	14:U:442:CYS:SG	3.15	0.44
14:V:313:LYS:HE2	14:V:343:LEU:HB3	1.98	0.44
15:R:183:GLU:HB3	15:R:205:LEU:C	2.37	0.44
13:Z:305:ILE:HG23	13:Z:340:GLU:CD	2.37	0.44
1:L:154:ARG:O	1:L:155:GLN:NE2	2.50	0.44
3:A:1871:TYR:HB2	3:A:1885:LEU:HD21	1.99	0.44
4:N:91:PHE:O	4:N:95:ILE:HG12	2.16	0.44
4:N:247:LEU:HD21	4:N:256:VAL:HB	1.99	0.44
4:N:289:PHE:O	4:N:293:ILE:HG23	2.17	0.44
4:N:363:TYR:O	4:N:366:GLU:HG2	2.17	0.44
5:I:540:PRO:HA	5:I:543:VAL:HG22	1.98	0.44
5:I:617:ALA:HB3	5:I:702:THR:HA	2.00	0.44
12:P:724:GLN:O	12:P:728:GLU:HG2	2.17	0.44
8:Q:340:TYR:CE2	8:Q:344:PHE:HE2	2.35	0.44
13:Y:39:ASP:O	13:Y:42:ARG:HB3	2.17	0.44
14:U:201:LEU:H	14:U:229:MET:HG3	1.82	0.44
15:R:188:PHE:HB3	15:R:445:ARG:NH2	2.32	0.44
15:R:232:VAL:HG13	15:R:246:VAL:HG13	1.98	0.44
15:R:415:VAL:HB	15:R:473:PHE:HE1	1.82	0.44
1:L:63:LEU:HD23	1:L:138:GLN:NE2	2.33	0.44
3:A:1718:LEU:HB2	4:N:327:HIS:CE1	2.52	0.44
3:A:1798:ARG:O	3:A:1802:ARG:HG2	2.18	0.44
5:I:533:ILE:HA	5:I:536:CYS:SG	2.57	0.44
6:O:624:VAL:HG11	6:O:647:ALA:HB1	1.99	0.44
6:O:627:LEU:O	6:O:631:GLN:HG2	2.17	0.44
8:K:302:TRP:HB2	8:K:326:ALA:HB2	2.00	0.44
12:P:502:LEU:HD23	12:P:502:LEU:HA	1.78	0.44
13:Y:159:LEU:HD23	13:Y:159:LEU:HA	1.82	0.44
3:A:255:ILE:HD11	3:A:432:ILE:HD11	1.97	0.44
3:A:1463:TYR:HE2	3:A:1511:ASN:HB3	1.83	0.44
4:N:300:LEU:HD11	4:N:324:TRP:CD2	2.52	0.44
8:K:333:TYR:HD2	8:K:336:ALA:HB2	1.82	0.44
13:Y:255:ILE:HG23	13:Y:277:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:429:MET:HA	13:Y:432:ASN:ND2	2.32	0.44
14:U:389:ARG:HD3	14:U:405:LEU:HD11	1.99	0.44
15:R:419:GLY:HA2	15:R:445:ARG:HB2	1.99	0.44
3:A:1663:LEU:HB3	3:A:1680:LEU:HD12	2.00	0.44
6:O:569:VAL:HG12	6:O:573:LYS:HZ1	1.83	0.44
8:K:225:ASP:OD2	8:Q:34:ARG:NH2	2.51	0.44
11:H:67:LEU:HD21	13:Y:332:PHE:HE2	1.82	0.44
12:J:70:GLN:OE1	12:J:70:GLN:N	2.39	0.44
13:Z:226:VAL:O	13:Z:230:VAL:HG22	2.18	0.44
13:Z:331:LEU:HD12	13:Z:344:VAL:HG11	1.99	0.44
3:A:220:ILE:O	15:R:5:TYR:OH	2.28	0.44
3:A:1848:VAL:HA	3:A:1851:THR:HG22	1.99	0.44
5:I:371:SER:OG	6:O:652:LEU:HB3	2.17	0.44
5:I:649:VAL:HG13	5:I:669:LEU:HG	1.98	0.44
11:H:82:LEU:HB3	12:P:577:PHE:CE2	2.51	0.44
12:J:704:LEU:HD11	15:R:491:LEU:HB3	1.98	0.44
8:Q:36:GLU:HB2	8:Q:39:ASP:OD2	2.17	0.44
3:A:76:LEU:HD12	3:A:589:ASP:HB3	2.00	0.44
3:A:1360:VAL:HG13	3:A:1364:CYS:HB2	1.99	0.44
3:A:1813:GLN:O	3:A:1817:VAL:HG23	2.18	0.44
4:N:205:SER:O	4:N:209:ARG:HG3	2.18	0.44
5:I:587:LEU:HD21	5:I:643:PHE:CE1	2.52	0.44
11:H:63:VAL:HG21	13:Y:364:LYS:HB2	1.99	0.44
11:H:71:LYS:HD2	11:H:71:LYS:HA	1.72	0.44
10:M:19:TRP:CH2	14:V:356:ARG:HB3	2.53	0.44
15:R:386:ASN:ND2	15:R:393:LEU:HD13	2.33	0.44
13:Z:291:VAL:HG22	13:Z:314:LEU:HD13	2.00	0.44
13:Z:304:LEU:C	13:Z:305:ILE:HD12	2.38	0.44
3:A:1155:SER:HB2	3:A:1187:LYS:O	2.18	0.44
4:N:203:LEU:HG	4:N:209:ARG:HG2	1.98	0.44
6:O:38:LEU:HB3	6:O:115:LEU:HD11	1.98	0.44
6:O:544:VAL:HG12	6:O:567:LEU:HD22	1.99	0.44
8:K:4:GLU:O	8:K:8:LYS:HG2	2.18	0.44
10:M:13:ASP:OD2	14:U:356:ARG:NH2	2.51	0.44
8:Q:469:ARG:O	8:Q:469:ARG:HD3	2.18	0.44
13:Y:62:THR:HA	13:Y:65:ASN:HD21	1.83	0.44
14:U:58:LEU:HD12	14:U:58:LEU:HA	1.71	0.44
15:R:323:THR:HG21	15:R:365:PRO:HA	1.99	0.44
1:L:54:TRP:HE3	1:L:153:MET:HB2	1.83	0.43
3:A:17:LEU:HD13	3:A:607:ILE:HG22	2.00	0.43
3:A:111:LEU:N	6:O:508:MET:HE3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:155:GLN:NE2	3:A:160:ASN:OD1	2.50	0.43
3:A:871:ARG:HG3	3:A:896:LEU:HD11	2.00	0.43
4:N:55:LEU:HG	4:N:135:TRP:CZ2	2.53	0.43
4:N:442:LEU:HD23	4:N:442:LEU:HA	1.87	0.43
7:S:414:HIS:CD2	7:S:414:HIS:H	2.35	0.43
11:H:101:GLN:HE22	11:H:108:SER:HA	1.82	0.43
13:Y:54:ARG:NE	13:Y:92:GLU:OE2	2.51	0.43
13:Y:241:LYS:O	13:Y:245:PHE:HD1	2.00	0.43
15:R:408:SER:HB2	15:R:473:PHE:CE2	2.53	0.43
16:C:46:LEU:HB3	16:C:54:CYS:SG	2.58	0.43
13:Z:175:LEU:HD12	13:Z:175:LEU:HA	1.81	0.43
3:A:1134:TRP:CD1	3:A:1597:THR:HA	2.53	0.43
3:A:1137:PHE:O	3:A:1141:VAL:HG23	2.18	0.43
4:N:559:VAL:HG23	16:C:39:VAL:HG23	2.00	0.43
5:I:49:LEU:HD13	5:I:730:VAL:HG11	1.99	0.43
5:I:317:LEU:HD23	5:I:317:LEU:HA	1.91	0.43
6:O:430:ARG:HD3	6:O:472:HIS:CD2	2.54	0.43
6:O:707:LYS:HB3	6:O:744:LEU:HD11	2.00	0.43
12:J:564:LYS:HB3	12:J:564:LYS:HE2	1.67	0.43
12:J:646:TYR:CD2	12:J:678:VAL:HG12	2.54	0.43
8:Q:247:PHE:CZ	8:Q:277:GLU:HG3	2.53	0.43
15:R:273:ARG:HG2	15:R:289:ARG:HG3	2.00	0.43
3:A:1090:PHE:HB3	3:A:1149:PRO:HD3	2.01	0.43
3:A:1159:VAL:O	3:A:1162:LYS:HG3	2.18	0.43
3:A:1329:MET:HG3	3:A:1330:VAL:HG23	1.99	0.43
3:A:1474:PHE:HD2	3:A:1581:ILE:HD12	1.83	0.43
3:A:1691:LEU:HA	3:A:1695:GLY:HA2	1.99	0.43
4:N:373:GLN:HA	4:N:376:VAL:HG22	2.00	0.43
4:N:534:SER:HB2	4:N:537:ARG:HB3	2.00	0.43
6:O:559:GLU:OE1	6:O:559:GLU:N	2.48	0.43
12:J:659:GLN:NE2	12:J:663:ASP:OD1	2.51	0.43
8:Q:14:LEU:HD12	8:Q:14:LEU:HA	1.81	0.43
13:Y:38:ILE:O	13:Y:41:VAL:HG22	2.17	0.43
14:U:112:LYS:HD3	14:U:168:ASP:HB3	2.00	0.43
13:Z:349:SER:HA	13:Z:354:ARG:NH2	2.33	0.43
13:Z:475:TYR:O	13:Z:479:VAL:HG13	2.18	0.43
3:A:1053:GLN:HG3	3:A:1062:PHE:CD1	2.54	0.43
3:A:1216:LYS:HA	3:A:1216:LYS:HD3	1.73	0.43
3:A:1619:LEU:HD22	3:A:1657:LEU:HD11	1.99	0.43
3:A:1860:LEU:HD11	3:A:1888:PHE:CE2	2.53	0.43
5:I:696:GLN:HB3	5:I:699:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:59:ARG:NH2	6:O:85:SER:O	2.45	0.43
6:O:735:MET:CG	6:O:739:GLN:NE2	2.81	0.43
8:K:171:THR:O	8:K:171:THR:OG1	2.36	0.43
8:Q:181:GLU:OE2	8:Q:209:LEU:HA	2.18	0.43
13:Y:78:GLN:HA	13:Y:81:VAL:HG22	1.98	0.43
13:Y:391:GLU:HA	13:Y:394:ILE:HG12	1.99	0.43
13:Z:184:GLN:O	13:Z:187:PRO:HD2	2.18	0.43
3:A:248:PHE:HB3	3:A:257:MET:HB3	2.01	0.43
3:A:786:LEU:HD23	3:A:790:LEU:HG	2.00	0.43
3:A:1100:LEU:HD22	3:A:1147:ILE:HD11	2.00	0.43
3:A:1651:LEU:HD13	8:K:553:LYS:HD2	1.99	0.43
3:A:1839:PHE:CD2	3:A:1840:MET:HG3	2.54	0.43
7:S:323:THR:OG1	7:S:326:ALA:HB2	2.18	0.43
12:J:641:LEU:O	12:J:644:ILE:HG22	2.18	0.43
14:U:428:LEU:HA	14:U:428:LEU:HD23	1.80	0.43
14:V:404:GLY:O	14:V:407:GLN:HG2	2.19	0.43
15:R:322:SER:HA	15:R:363:TRP:CG	2.53	0.43
3:A:1031:ASP:OD1	3:A:1031:ASP:N	2.48	0.43
3:A:1656:LEU:HD23	3:A:1656:LEU:HA	1.80	0.43
8:K:251:TYR:CZ	8:K:280:LYS:HE3	2.54	0.43
8:K:261:ASP:OD2	8:Q:55:ARG:NH2	2.52	0.43
12:J:696:ILE:HD12	12:J:709:ARG:HH11	1.84	0.43
12:P:521:ILE:O	12:P:525:VAL:HG23	2.18	0.43
15:R:362:ALA:HB1	15:R:407:TRP:HD1	1.84	0.43
3:A:89:TYR:HB2	6:O:537:ALA:HB2	2.00	0.43
5:I:375:LYS:HD2	6:O:645:HIS:CE1	2.54	0.43
5:I:402:GLU:OE1	5:I:405:GLN:NE2	2.52	0.43
6:O:34:LYS:O	6:O:38:LEU:HD22	2.19	0.43
12:P:507:ARG:O	12:P:511:GLU:HG2	2.18	0.43
13:Y:503:LEU:HD13	13:Y:512:HIS:HE1	1.83	0.43
13:Y:527:GLU:OE2	13:Y:527:GLU:N	2.48	0.43
14:V:261:LYS:HB2	14:V:261:LYS:HE3	1.81	0.43
15:R:449:LEU:HA	15:R:459:VAL:O	2.19	0.43
13:Z:139:LYS:HD3	13:Z:162:ILE:HD11	2.01	0.43
1:L:74:VAL:HG22	1:L:124:LEU:HD13	2.00	0.43
3:A:455:VAL:HB	3:A:471:VAL:HG12	2.01	0.43
3:A:611:GLU:OE2	3:A:612:ILE:HG22	2.19	0.43
3:A:1114:ARG:HB2	3:A:1116:THR:HG23	2.01	0.43
3:A:1656:LEU:O	8:K:553:LYS:HE2	2.19	0.43
3:A:1809:SER:O	3:A:1813:GLN:HG2	2.19	0.43
5:I:166:LYS:HZ3	5:I:170:ASP:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:272:MET:HE1	5:I:344:ILE:HG23	2.00	0.43
5:I:688:THR:HG23	5:I:691:THR:HG22	2.01	0.43
8:K:23:LEU:HD11	8:K:47:LEU:HD23	2.00	0.43
8:K:559:ILE:O	8:K:561:PRO:HD3	2.18	0.43
12:J:142:LEU:HD23	12:J:142:LEU:HA	1.83	0.43
15:R:337:LEU:HB2	15:R:351:TYR:HB2	2.00	0.43
15:R:419:GLY:O	15:R:423:ASN:ND2	2.52	0.43
3:A:1328:TYR:HA	3:A:1358:ILE:HG21	2.01	0.43
3:A:1573:SER:HB2	3:A:1656:LEU:HD13	2.00	0.43
3:A:1793:MET:O	3:A:1797:ILE:HG23	2.19	0.43
4:N:180:PHE:CE2	4:N:240:PHE:HB3	2.54	0.43
4:N:415:VAL:O	4:N:419:VAL:HG23	2.19	0.43
4:N:439:VAL:HG21	4:N:519:TYR:HA	2.00	0.43
6:O:10:PHE:HD1	14:V:390:HIS:CD2	2.37	0.43
8:K:194:CYS:SG	8:K:195:ASN:N	2.91	0.43
12:P:75:LEU:HG	12:P:91:ILE:HD13	1.99	0.43
8:Q:275:LEU:HD22	8:Q:280:LYS:HB2	2.01	0.43
14:U:153:GLU:OE1	14:U:157:GLU:HG3	2.19	0.43
3:A:271:LEU:HD11	3:A:407:LEU:HD23	2.00	0.43
3:A:1130:ASN:OD1	3:A:1130:ASN:N	2.51	0.43
4:N:527:LEU:HD13	4:N:564:MET:HE2	2.01	0.43
5:I:425:MET:O	5:I:429:THR:OG1	2.33	0.43
6:O:446:LEU:HD21	6:O:470:LEU:HG	2.01	0.43
6:O:542:GLU:O	6:O:546:ARG:HG2	2.19	0.43
7:S:375:LEU:HD11	7:S:384:PRO:HB3	2.01	0.43
12:J:158:ILE:O	12:J:633:ARG:NH1	2.52	0.43
12:J:662:LEU:HD22	12:J:666:PRO:HA	2.00	0.43
14:U:238:TYR:CD1	14:U:243:LEU:HD12	2.53	0.43
15:R:415:VAL:HB	15:R:473:PHE:CE1	2.54	0.43
13:Z:289:ASN:O	13:Z:292:LEU:HG	2.19	0.43
5:I:214:LEU:O	5:I:238:THR:OG1	2.37	0.42
5:I:309:LEU:O	6:O:130:SER:HB3	2.19	0.42
5:I:381:LEU:HD12	5:I:381:LEU:HA	1.70	0.42
5:I:681:ALA:HA	5:I:684:GLN:HE21	1.84	0.42
8:K:74:TYR:HB2	8:K:132:ILE:HD11	2.00	0.42
8:K:168:ASP:O	8:K:172:SER:HB3	2.19	0.42
11:H:101:GLN:OE1	11:H:106:THR:OG1	2.37	0.42
12:J:27:LEU:HD11	12:P:147:PHE:O	2.19	0.42
12:P:496:TYR:CZ	13:Z:105:GLN:HG3	2.54	0.42
13:Y:76:LYS:HB3	13:Y:76:LYS:HE2	1.79	0.42
13:Y:142:MET:HB2	13:Y:158:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:483:ALA:HB2	13:Y:499:LEU:HD11	2.01	0.42
14:U:172:LEU:HD12	14:U:198:VAL:HG11	2.01	0.42
13:Z:476:ILE:O	13:Z:479:VAL:HG22	2.19	0.42
1:L:174:THR:HG22	12:P:737:SER:H	1.84	0.42
3:A:159:ILE:HG12	3:A:161:MET:HE3	2.00	0.42
3:A:628:ILE:HD12	3:A:765:VAL:CG1	2.49	0.42
3:A:762:ILE:HD12	3:A:763:PHE:N	2.34	0.42
3:A:1434:ILE:HG21	3:A:1461:HIS:HB2	2.01	0.42
3:A:1845:LEU:HD23	3:A:1845:LEU:HA	1.89	0.42
4:N:422:GLU:HB3	4:N:423:PRO:HD3	2.01	0.42
4:N:573:ASN:OD1	4:N:629:LEU:HD21	2.19	0.42
5:I:370:ALA:HB2	5:I:381:LEU:HG	2.01	0.42
5:I:393:VAL:O	5:I:397:ILE:HG13	2.18	0.42
11:H:67:LEU:HD11	13:Y:332:PHE:CZ	2.54	0.42
13:Y:154:ASP:O	13:Y:158:ILE:HG12	2.18	0.42
13:Y:321:LEU:O	13:Y:324:VAL:HG22	2.19	0.42
13:Z:203:LEU:N	13:Z:203:LEU:HD12	2.35	0.42
3:A:224:VAL:O	3:A:408:CYS:HA	2.19	0.42
3:A:627:PHE:CZ	3:A:864:PRO:HG2	2.54	0.42
3:A:773:LEU:HD23	3:A:783:ILE:HG12	2.00	0.42
3:A:953:LEU:HD22	3:A:1817:VAL:HG13	2.01	0.42
5:I:290:PHE:CG	5:I:320:LEU:HD22	2.54	0.42
6:O:365:VAL:O	6:O:369:VAL:HG22	2.19	0.42
9:W:10:GLU:OE1	9:W:10:GLU:HA	2.19	0.42
14:U:304:SER:OG	14:U:339:ASN:ND2	2.51	0.42
13:Z:54:ARG:HH21	13:Z:87:LEU:HD23	1.85	0.42
4:N:450:GLY:O	4:N:454:VAL:HG23	2.20	0.42
5:I:207:ALA:H	5:I:220:VAL:HG13	1.84	0.42
5:I:662:ARG:O	5:I:662:ARG:CG	2.66	0.42
11:H:99:ILE:HG12	12:P:591:GLN:HG2	2.00	0.42
12:J:738:LEU:HB2	15:R:489:LEU:HD12	2.01	0.42
13:Y:50:HIS:HA	13:Y:53:VAL:HB	2.01	0.42
13:Z:60:LEU:O	13:Z:63:MET:HB2	2.20	0.42
13:Z:328:GLY:O	13:Z:332:PHE:HD2	2.02	0.42
3:A:1255:VAL:HG11	3:A:1606:LEU:HD22	2.01	0.42
4:N:134:LYS:O	4:N:138:LEU:HG	2.20	0.42
5:I:254:LYS:O	5:I:258:ILE:HG12	2.20	0.42
5:I:747:ASP:N	5:I:747:ASP:OD1	2.48	0.42
8:K:157:LEU:HD11	8:K:167:PHE:HA	2.01	0.42
12:J:694:LYS:O	12:J:698:ILE:HG23	2.19	0.42
13:Y:304:LEU:HD12	13:Y:308:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:172:SER:O	15:R:439:LEU:HD11	2.19	0.42
15:R:280:ASN:HB3	15:R:283:GLN:HB2	2.01	0.42
13:Z:37:VAL:HG11	13:Z:60:LEU:HD21	2.01	0.42
1:L:83:TYR:OH	1:L:146:GLN:NE2	2.52	0.42
1:L:173:CYS:HB3	1:L:178:PHE:HB3	2.00	0.42
4:N:379:LYS:HD2	4:N:423:PRO:HG2	2.01	0.42
4:N:396:ILE:HD11	4:N:431:ARG:HH21	1.85	0.42
4:N:510:GLY:O	4:N:512:LYS:NZ	2.52	0.42
5:I:27:VAL:HG13	5:I:73:TRP:HE1	1.83	0.42
5:I:250:ARG:O	5:I:254:LYS:HG2	2.19	0.42
6:O:80:LYS:O	6:O:83:GLU:HG3	2.20	0.42
6:O:366:LYS:HA	6:O:366:LYS:HD3	1.74	0.42
8:K:338:ILE:HD11	8:K:370:PRO:HG3	2.02	0.42
8:K:441:VAL:HB	8:K:474:LEU:HD22	2.00	0.42
9:G:11:LEU:HD23	9:G:11:LEU:HA	1.80	0.42
11:H:52:ARG:NH2	13:Z:333:ASN:OD1	2.53	0.42
13:Y:41:VAL:HG12	13:Y:56:LEU:CD1	2.48	0.42
14:U:347:HIS:ND1	14:U:374:GLU:OE1	2.47	0.42
13:Z:418:LEU:HD23	13:Z:418:LEU:HA	1.86	0.42
3:A:1154:ASP:OD1	3:A:1154:ASP:N	2.50	0.42
4:N:95:ILE:O	4:N:99:GLU:HG3	2.20	0.42
5:I:14:VAL:HG21	5:I:745:GLU:HG3	2.01	0.42
5:I:249:THR:O	5:I:253:ARG:HG3	2.19	0.42
5:I:403:LEU:HA	5:I:406:VAL:HG12	2.02	0.42
12:P:488:LEU:HD23	12:P:488:LEU:HA	1.82	0.42
13:Y:55:LEU:HG	13:Z:203:LEU:HD23	2.01	0.42
13:Y:81:VAL:HG12	13:Y:103:ALA:HB1	2.01	0.42
13:Y:304:LEU:HD13	13:Y:305:ILE:N	2.35	0.42
14:U:159:SER:O	14:U:163:GLN:HG2	2.20	0.42
14:U:214:THR:HG21	14:U:396:LYS:HD3	2.00	0.42
13:Z:38:ILE:HD12	13:Z:38:ILE:H	1.85	0.42
13:Z:39:ASP:OD1	13:Z:42:ARG:NH1	2.41	0.42
3:A:1787:LEU:O	3:A:1791:ILE:HG12	2.20	0.42
4:N:644:VAL:HG23	4:N:661:PRO:HG3	2.02	0.42
5:I:116:MET:SD	5:I:210:LEU:HD23	2.59	0.42
6:O:96:ARG:O	6:O:99:LEU:HG	2.19	0.42
8:K:445:GLU:OE2	9:W:8:ARG:NH1	2.48	0.42
12:P:726:LEU:HD12	12:P:726:LEU:HA	1.93	0.42
8:Q:3:LEU:H	8:Q:3:LEU:HG	1.72	0.42
8:Q:183:GLU:O	8:Q:186:GLU:HG2	2.20	0.42
13:Y:37:VAL:O	13:Y:41:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:301:ASP:N	14:V:301:ASP:OD1	2.53	0.42
14:V:419:LEU:HB3	14:V:423:ARG:NH2	2.35	0.42
15:R:355:LEU:HD12	15:R:379:ASP:HA	2.02	0.42
13:Z:283:ARG:NH2	13:Z:405:CYS:SG	2.82	0.42
13:Z:329:CYS:O	13:Z:333:ASN:ND2	2.52	0.42
3:A:1153:ILE:HD13	3:A:1153:ILE:HA	1.88	0.42
5:I:484:ASP:O	5:I:521:SER:N	2.52	0.42
5:I:523:HIS:HB3	5:I:527:ARG:NH1	2.34	0.42
12:J:720:LYS:O	12:J:724:GLN:HG2	2.20	0.42
14:U:221:PHE:N	14:U:221:PHE:CD1	2.87	0.42
3:A:72:GLU:HG3	3:A:94:TYR:CZ	2.55	0.42
3:A:506:VAL:HG22	3:A:639:VAL:HG22	2.02	0.42
3:A:1094:PRO:HG2	3:A:1153:ILE:HD11	2.01	0.42
6:O:14:MET:HG3	6:O:29:TRP:CH2	2.55	0.42
6:O:433:GLY:HA3	6:O:617:GLN:HB3	2.01	0.42
8:K:367:CYS:O	8:K:370:PRO:HD2	2.20	0.42
8:K:419:LYS:O	8:K:419:LYS:NZ	2.40	0.42
10:M:36:LEU:HD21	8:Q:302:TRP:CZ3	2.54	0.42
15:R:329:ALA:HB3	15:R:361:ILE:HG21	2.01	0.42
3:A:972:GLU:H	3:A:972:GLU:CD	2.14	0.41
3:A:1125:ILE:HD13	3:A:1125:ILE:HA	1.90	0.41
5:I:166:LYS:NZ	5:I:170:ASP:HB2	2.35	0.41
5:I:280:LEU:HA	5:I:337:ILE:HD11	2.01	0.41
6:O:569:VAL:HG12	6:O:573:LYS:NZ	2.35	0.41
8:K:55:ARG:HD2	8:Q:263:PHE:O	2.19	0.41
8:K:551:THR:OG1	8:K:553:LYS:HG3	2.20	0.41
12:J:55:TYR:HA	12:J:82:LEU:HD11	2.02	0.41
12:J:621:LEU:HD21	12:J:644:ILE:HG21	2.02	0.41
12:P:500:TRP:O	12:P:504:GLN:HG2	2.20	0.41
12:P:530:ASN:OD1	12:P:530:ASN:N	2.52	0.41
8:Q:445:GLU:HB3	8:Q:474:LEU:HD23	2.02	0.41
14:V:308:TYR:CD2	14:V:343:LEU:HG	2.55	0.41
15:R:94:LEU:HD22	15:R:157:SER:HB3	2.02	0.41
4:N:571:ASN:ND2	4:N:593:ALA:H	2.18	0.41
6:O:40:LEU:O	6:O:44:MET:HG3	2.21	0.41
6:O:104:GLU:HB3	6:O:106:LYS:HG2	2.02	0.41
6:O:571:CYS:SG	6:O:579:MET:HG2	2.61	0.41
8:Q:133:CYS:SG	8:Q:155:GLU:HB3	2.60	0.41
14:V:242:GLN:HA	14:V:244:ILE:HD11	2.02	0.41
15:R:288:SER:OG	15:R:289:ARG:N	2.53	0.41
15:R:314:GLN:HE22	15:R:334:ASP:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:364:SER:HA	15:R:365:PRO:HD3	1.94	0.41
13:Z:93:TYR:HB2	13:Z:149:LEU:HD21	2.01	0.41
13:Z:288:LYS:O	13:Z:288:LYS:HD3	2.19	0.41
1:L:61:PRO:HG2	1:L:63:LEU:HD11	2.01	0.41
1:L:89:TYR:OH	7:S:329:GLN:HB3	2.20	0.41
3:A:433:THR:HG22	3:A:441:PHE:HB2	2.03	0.41
3:A:855:GLU:H	3:A:855:GLU:HG2	1.71	0.41
3:A:867:CYS:HB3	3:A:870:SER:OG	2.20	0.41
3:A:1364:CYS:O	3:A:1368:THR:HG22	2.21	0.41
3:A:1574:LEU:O	3:A:1617:ARG:NH1	2.42	0.41
4:N:347:ILE:HG23	4:N:354:SER:HB3	2.01	0.41
5:I:313:ALA:HB3	5:I:428:MET:CE	2.49	0.41
6:O:624:VAL:HG11	6:O:647:ALA:CB	2.51	0.41
12:J:155:LEU:HD23	12:J:162:PRO:HB3	2.02	0.41
12:J:621:LEU:HD23	12:J:621:LEU:HA	1.92	0.41
12:P:499:GLY:HA3	12:P:529:GLU:OE2	2.19	0.41
13:Y:270:ASN:HD21	13:Z:59:LEU:HA	1.85	0.41
13:Y:428:VAL:O	13:Y:432:ASN:ND2	2.53	0.41
15:R:428:TRP:CZ3	15:R:435:GLN:HB2	2.55	0.41
4:N:227:ASP:O	4:N:230:GLN:N	2.52	0.41
4:N:351:PHE:HE1	4:N:409:VAL:HG11	1.86	0.41
4:N:601:TRP:CD1	4:N:602:PRO:HD2	2.56	0.41
5:I:185:ILE:HG12	5:I:201:ILE:HG13	2.02	0.41
8:K:309:TYR:OH	10:M:59:ASP:OD2	2.25	0.41
12:J:104:ASP:HA	12:J:107:VAL:HG12	2.02	0.41
12:J:114:ALA:HA	12:J:117:THR:HG22	2.01	0.41
12:P:672:LEU:HD13	12:P:695:ALA:HA	2.02	0.41
8:Q:60:LEU:HD22	8:Q:72:CYS:HB3	2.01	0.41
14:U:300:MET:SD	14:U:303:PHE:HD2	2.43	0.41
14:U:429:ARG:O	14:U:435:MET:HE1	2.21	0.41
15:R:353:GLU:N	15:R:353:GLU:OE2	2.53	0.41
15:R:366:HIS:CE1	15:R:412:ASN:HA	2.55	0.41
13:Z:315:LEU:HB2	13:Z:324:VAL:HG12	2.02	0.41
13:Z:326:ASN:O	13:Z:330:ARG:HG2	2.20	0.41
1:L:46:ARG:NH1	1:L:156:ILE:O	2.54	0.41
2:D:48:ASP:O	2:D:48:ASP:OD1	2.38	0.41
3:A:827:GLN:O	3:A:831:MET:HG2	2.21	0.41
3:A:1422:ASN:OD1	3:A:1425:TRP:N	2.37	0.41
4:N:600:PHE:CE1	16:C:40:PRO:HG3	2.56	0.41
5:I:46:LEU:O	5:I:55:VAL:N	2.53	0.41
5:I:158:GLU:OE1	5:I:158:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:63:LEU:O	6:O:66:PRO:HD2	2.20	0.41
6:O:64:LEU:O	6:O:68:LEU:HG	2.21	0.41
11:H:67:LEU:HD13	13:Y:342:TRP:CZ3	2.55	0.41
12:J:575:ASN:OD1	15:R:496:ARG:NH1	2.53	0.41
12:J:779:ILE:HD13	12:J:779:ILE:HA	1.88	0.41
12:P:112:ASP:N	12:P:112:ASP:OD1	2.53	0.41
8:Q:378:TYR:HA	8:Q:381:THR:HG22	2.01	0.41
13:Y:340:GLU:N	13:Y:341:PRO:HD2	2.35	0.41
3:A:1114:ARG:HG3	3:A:1114:ARG:HH11	1.85	0.41
4:N:536:GLU:O	4:N:539:ILE:HG12	2.21	0.41
5:I:74:ARG:HH22	5:I:167:LEU:HD23	1.84	0.41
6:O:16:ASN:OD1	6:O:18:VAL:HG22	2.21	0.41
6:O:722:HIS:HB2	6:O:730:ARG:HG3	2.02	0.41
10:M:9:GLY:HA3	14:U:329:TYR:CG	2.55	0.41
10:M:27:GLU:OE1	14:V:344:ARG:NH1	2.52	0.41
13:Y:94:ARG:HA	13:Y:97:VAL:HG12	2.01	0.41
13:Y:346:GLY:HA3	13:Y:378:LEU:HD21	2.02	0.41
13:Y:389:VAL:HG11	13:Y:420:SER:OG	2.21	0.41
15:R:429:LYS:HG3	15:R:431:PRO:HD2	2.02	0.41
13:Z:176:ALA:HB1	13:Z:192:TYR:CE2	2.56	0.41
13:Z:223:THR:O	13:Z:226:VAL:HG12	2.20	0.41
13:Z:352:SER:HB3	13:Z:354:ARG:HH21	1.86	0.41
1:L:103:HIS:ND1	3:A:1594:ALA:HB2	2.36	0.41
3:A:951:ILE:HD12	3:A:952:ALA:N	2.36	0.41
4:N:273:MET:HA	4:N:289:PHE:HZ	1.84	0.41
5:I:644:TYR:HE1	5:I:746:MET:HG3	1.84	0.41
5:I:661:GLY:O	5:I:716:SER:N	2.52	0.41
12:J:687:LYS:HA	12:J:690:ASP:OD2	2.21	0.41
8:Q:185:LEU:HD23	8:Q:185:LEU:HA	1.84	0.41
13:Y:261:LEU:O	13:Y:265:SER:HB2	2.19	0.41
14:U:101:ARG:HG3	14:V:295:TYR:HB2	2.02	0.41
13:Z:106:GLN:O	13:Z:110:LEU:HD23	2.20	0.41
2:D:12:VAL:HG12	6:O:313:ARG:CZ	2.51	0.41
3:A:94:TYR:O	3:A:100:VAL:HA	2.20	0.41
3:A:161:MET:HG2	3:A:216:PRO:CG	2.49	0.41
3:A:1499:LEU:HA	3:A:1499:LEU:HD23	1.83	0.41
4:N:82:ASP:OD1	4:N:86:ASN:ND2	2.49	0.41
6:O:321:GLU:O	6:O:325:GLN:HG2	2.20	0.41
8:K:423:LYS:NZ	8:K:427:ASP:OD2	2.50	0.41
10:M:63:GLN:HG2	10:M:64:TYR:CD1	2.56	0.41
12:J:26:PHE:O	12:J:29:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:75:LEU:HG	12:J:91:ILE:HD13	2.01	0.41
12:J:495:HIS:O	12:J:498:THR:OG1	2.30	0.41
8:Q:10:VAL:HG21	8:Q:26:ALA:HB2	2.02	0.41
8:Q:190:LEU:HB3	8:Q:198:GLN:HG3	2.02	0.41
8:Q:372:LEU:HD11	8:Q:407:GLU:HG3	2.01	0.41
14:V:148:ASN:HB3	14:V:151:LEU:HG	2.03	0.41
14:V:328:LYS:HA	14:V:333:THR:HG21	2.03	0.41
13:Z:350:PHE:HE1	13:Z:382:ALA:HA	1.85	0.41
1:L:15:GLN:O	1:L:19:THR:HG23	2.21	0.41
1:L:24:GLU:OE2	1:L:26:GLY:N	2.36	0.41
3:A:489:LEU:HD11	3:A:509:VAL:HG21	2.02	0.41
3:A:665:MET:O	3:A:670:TYR:HB2	2.21	0.41
3:A:1401:PRO:HB2	3:A:1463:TYR:CD2	2.56	0.41
4:N:571:ASN:OD1	4:N:622:TYR:OH	2.39	0.41
5:I:371:SER:HB2	6:O:652:LEU:HD22	2.03	0.41
5:I:372:TRP:CZ3	6:O:648:ILE:HG21	2.56	0.41
6:O:317:TYR:HD1	6:O:350:LEU:HD23	1.86	0.41
6:O:581:ILE:HB	6:O:619:LEU:HD13	2.03	0.41
8:K:190:LEU:HD12	8:K:190:LEU:H	1.86	0.41
8:K:285:PHE:HB2	8:K:308:TYR:CE1	2.56	0.41
8:K:360:ALA:O	8:K:364:MET:HG3	2.20	0.41
12:J:757:LEU:HD13	8:Q:378:TYR:OH	2.21	0.41
12:P:43:LEU:HD23	12:P:43:LEU:HA	1.87	0.41
8:Q:216:SER:O	8:Q:244:ASN:ND2	2.38	0.41
8:Q:354:MET:HG2	8:Q:354:MET:H	1.65	0.41
8:Q:404:VAL:O	8:Q:408:VAL:HG13	2.20	0.41
8:Q:492:MET:HA	8:Q:492:MET:CE	2.51	0.41
13:Y:70:LEU:HD21	13:Z:232:ASN:ND2	2.36	0.41
13:Y:74:PRO:HB3	13:Y:132:LEU:HD11	2.02	0.41
13:Y:139:LYS:HA	13:Y:142:MET:HG2	2.02	0.41
13:Y:202:ALA:C	13:Z:52:ASN:HD21	2.24	0.41
13:Y:311:TYR:HD2	13:Y:327:LEU:HD22	1.85	0.41
14:U:148:ASN:OD1	14:U:152:ARG:NH1	2.54	0.41
14:U:345:SER:O	14:U:345:SER:OG	2.39	0.41
14:U:373:HIS:ND1	14:U:388:TYR:OH	2.45	0.41
14:V:439:LEU:HD23	14:V:439:LEU:HA	1.90	0.41
14:V:487:ALA:O	14:V:491:ILE:HG23	2.20	0.41
3:A:260:ASP:O	3:A:264:ASN:N	2.54	0.41
3:A:779:MET:HE2	3:A:782:GLY:H	1.85	0.41
3:A:1329:MET:HE1	3:A:1387:LEU:HD23	2.02	0.41
3:A:1633:LEU:HD23	3:A:1633:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1900:LEU:HA	3:A:1901:PRO:HD3	1.96	0.41
5:I:386:ILE:O	5:I:390:ILE:HG12	2.22	0.41
5:I:638:CYS:SG	5:I:639:LEU:N	2.94	0.41
7:S:444:LEU:HD23	7:S:444:LEU:HA	1.82	0.41
8:K:453:HIS:CE1	9:W:11:LEU:HG	2.48	0.41
12:J:531:TYR:HD1	12:P:56:LYS:HD2	1.85	0.41
12:J:583:HIS:O	12:J:587:ILE:HG13	2.22	0.41
8:Q:474:LEU:HA	8:Q:474:LEU:HD12	1.81	0.41
13:Y:179:TYR:HB3	13:Y:184:GLN:HG3	2.02	0.41
14:V:210:CYS:HA	14:V:237:ILE:HD13	2.03	0.41
13:Z:134:SER:O	13:Z:138:VAL:HG13	2.20	0.41
3:A:24:GLY:HA3	3:A:94:TYR:CG	2.56	0.40
3:A:1463:TYR:CE2	3:A:1511:ASN:HB3	2.56	0.40
12:J:148:LEU:HA	12:P:23:ASP:OD2	2.21	0.40
12:J:481:CYS:HB2	12:J:512:LEU:HG	2.03	0.40
8:Q:408:VAL:HA	8:Q:411:VAL:HG22	2.04	0.40
13:Y:503:LEU:HD21	13:Y:515:LEU:HD22	2.02	0.40
14:U:223:SER:O	14:U:223:SER:OG	2.33	0.40
14:V:29:LEU:HD23	14:V:29:LEU:HA	1.88	0.40
14:V:58:LEU:HD23	14:V:58:LEU:HA	1.77	0.40
15:R:150:LEU:HD23	15:R:150:LEU:HA	1.94	0.40
15:R:408:SER:OG	15:R:411:ALA:N	2.54	0.40
13:Z:276:SER:HA	13:Z:279:ASP:OD2	2.21	0.40
2:D:11:ARG:NH1	6:O:416:GLU:OE1	2.54	0.40
3:A:725:ASN:OD1	3:A:725:ASN:N	2.55	0.40
3:A:1277:ILE:HD11	3:A:1299:GLY:HA2	2.04	0.40
4:N:341:ILE:HG12	4:N:374:LEU:HD12	2.03	0.40
5:I:265:ILE:HD13	5:I:265:ILE:HA	1.90	0.40
5:I:374:GLN:NE2	6:O:692:GLU:HB3	2.32	0.40
5:I:632:ARG:O	5:I:636:TYR:OH	2.24	0.40
5:I:709:LYS:HE2	5:I:709:LYS:HB3	1.90	0.40
7:S:362:PHE:CD2	16:C:35:PRO:HB3	2.56	0.40
8:K:251:TYR:HA	8:K:254:THR:HG22	2.02	0.40
13:Y:44:MET:SD	13:Z:199:CYS:SG	3.19	0.40
13:Y:308:MET:HA	13:Y:308:MET:CE	2.51	0.40
14:V:39:ILE:HD12	14:V:39:ILE:HA	1.93	0.40
14:V:106:LEU:HD22	14:V:114:ALA:HB1	2.03	0.40
15:R:396:ILE:HD12	15:R:396:ILE:HA	1.93	0.40
13:Z:38:ILE:HD13	13:Z:75:GLN:OE1	2.21	0.40
13:Z:283:ARG:HH22	13:Z:405:CYS:CB	2.33	0.40
1:L:30:VAL:HG12	3:A:1354:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:215:HIS:CG	3:A:216:PRO:HD2	2.56	0.40
3:A:866:ILE:N	3:A:866:ILE:HD12	2.36	0.40
3:A:1897:PRO:HA	3:A:1900:LEU:HD12	2.02	0.40
3:A:1932:ALA:N	3:A:1933:PRO:HD2	2.36	0.40
4:N:88:SER:OG	4:N:89:PRO:HD3	2.22	0.40
4:N:476:GLU:HB2	4:N:479:ASP:HB2	2.03	0.40
5:I:369:MET:HG2	5:I:376:TYR:CZ	2.57	0.40
6:O:621:SER:HB3	6:O:651:ILE:HG12	2.03	0.40
8:Q:125:GLN:O	8:Q:128:ILE:HG22	2.21	0.40
13:Y:73:PRO:HB2	13:Y:74:PRO:HD3	2.04	0.40
14:U:300:MET:HA	14:U:303:PHE:HB3	2.03	0.40
13:Z:262:GLU:HA	13:Z:267:LEU:O	2.21	0.40
13:Z:391:GLU:O	13:Z:394:ILE:HG12	2.21	0.40
3:A:981:GLN:H	3:A:1700:LYS:HZ2	1.70	0.40
3:A:1080:LEU:N	3:A:1081:PRO:HD2	2.36	0.40
3:A:1733:PHE:HE2	3:A:1775:LEU:HD23	1.86	0.40
5:I:156:PHE:HZ	5:I:260:ALA:HB1	1.87	0.40
5:I:309:LEU:HA	5:I:309:LEU:HD23	1.77	0.40
6:O:320:ALA:HB3	6:O:350:LEU:HD21	2.03	0.40
8:K:134:LEU:HD22	8:K:163:CYS:SG	2.61	0.40
12:J:149:TRP:NE1	12:J:153:GLU:HB2	2.36	0.40
12:P:747:TYR:CD2	12:P:755:LEU:HB3	2.56	0.40
8:Q:5:ARG:HD3	8:Q:5:ARG:HA	1.85	0.40
13:Y:396:PHE:O	13:Y:400:ILE:HG12	2.21	0.40
13:Z:209:LEU:O	13:Z:214:VAL:HB	2.21	0.40
3:A:640:LYS:NZ	3:A:667:MET:HB3	2.37	0.40
5:I:186:GLU:HB3	5:I:188:TYR:CE1	2.55	0.40
5:I:218:SER:OG	5:I:584:HIS:ND1	2.54	0.40
8:K:14:LEU:HD23	8:K:14:LEU:HA	1.93	0.40
8:K:502:PHE:CE2	8:K:518:MET:HB3	2.56	0.40
13:Y:503:LEU:HD13	13:Y:512:HIS:CE1	2.56	0.40
14:U:331:VAL:HG11	14:U:361:ASN:HB3	2.04	0.40
15:R:189:TYR:O	15:R:273:ARG:NH2	2.50	0.40
15:R:353:GLU:N	15:R:353:GLU:CD	2.75	0.40
13:Z:366:ILE:HD12	13:Z:366:ILE:HA	1.90	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	L	174/185 (94%)	166 (95%)	8 (5%)	0	100	100
2	D	55/121 (46%)	49 (89%)	6 (11%)	0	100	100
3	A	1574/1944 (81%)	1526 (97%)	48 (3%)	0	100	100
4	N	616/822 (75%)	593 (96%)	23 (4%)	0	100	100
5	I	713/814 (88%)	689 (97%)	23 (3%)	1 (0%)	48	77
6	O	691/755 (92%)	680 (98%)	11 (2%)	0	100	100
7	S	86/447 (19%)	78 (91%)	8 (9%)	0	100	100
8	K	512/620 (83%)	499 (98%)	13 (2%)	0	100	100
8	Q	502/620 (81%)	494 (98%)	8 (2%)	0	100	100
9	G	24/85 (28%)	24 (100%)	0	0	100	100
9	W	24/85 (28%)	24 (100%)	0	0	100	100
10	M	60/74 (81%)	60 (100%)	0	0	100	100
11	H	56/110 (51%)	56 (100%)	0	0	100	100
12	J	495/824 (60%)	484 (98%)	11 (2%)	0	100	100
12	P	487/824 (59%)	477 (98%)	10 (2%)	0	100	100
13	Y	495/599 (83%)	483 (98%)	12 (2%)	0	100	100
13	Z	452/599 (76%)	431 (95%)	20 (4%)	1 (0%)	44	73
14	U	484/597 (81%)	465 (96%)	19 (4%)	0	100	100
14	V	490/597 (82%)	480 (98%)	10 (2%)	0	100	100
15	R	403/496 (81%)	371 (92%)	31 (8%)	1 (0%)	44	73
16	C	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
All	All	8472/11302 (75%)	8203 (97%)	266 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	R	420	TYR
13	Z	50	HIS
5	I	718	LYS

### 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	L	153/170 (90%)	151 (99%)	2 (1%)	65	88
2	D	47/115 (41%)	47 (100%)	0	100	100
3	A	1343/1720 (78%)	1335 (99%)	8 (1%)	84	95
4	N	433/724 (60%)	427 (99%)	6 (1%)	62	86
5	I	619/736 (84%)	616 (100%)	3 (0%)	86	96
6	O	582/650 (90%)	576 (99%)	6 (1%)	73	91
7	S	60/403 (15%)	57 (95%)	3 (5%)	20	52
8	K	441/548 (80%)	437 (99%)	4 (1%)	75	92
8	Q	426/548 (78%)	424 (100%)	2 (0%)	86	96
9	G	24/77 (31%)	24 (100%)	0	100	100
9	W	24/77 (31%)	24 (100%)	0	100	100
10	M	55/67 (82%)	54 (98%)	1 (2%)	54	82
11	H	51/89 (57%)	51 (100%)	0	100	100
12	J	415/727 (57%)	414 (100%)	1 (0%)	92	98
12	P	418/727 (58%)	417 (100%)	1 (0%)	92	98
13	Y	375/513 (73%)	372 (99%)	3 (1%)	79	93
13	Z	303/513 (59%)	301 (99%)	2 (1%)	81	94
14	U	389/520 (75%)	387 (100%)	2 (0%)	86	96
14	V	415/520 (80%)	413 (100%)	2 (0%)	86	96
15	R	292/431 (68%)	287 (98%)	5 (2%)	56	83
16	C	50/75 (67%)	49 (98%)	1 (2%)	50	79
All	All	6915/9950 (70%)	6863 (99%)	52 (1%)	77	93

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	83	TYR
1	L	144	ASN
3	A	161	MET
3	A	766	LEU
3	A	770	TYR
3	A	787	VAL
3	A	961	HIS
3	A	970	TRP
3	A	1078	MET
3	A	1865	ASP
4	N	180	PHE
4	N	186	GLN
4	N	213	TYR
4	N	379	LYS
4	N	563	ASP
4	N	601	TRP
5	I	116	MET
5	I	572	PHE
5	I	643	PHE
6	O	29	TRP
6	O	38	LEU
6	O	250	PHE
6	O	363	HIS
6	O	408	LEU
6	O	638	GLU
7	S	406	CYS
7	S	409	CYS
7	S	414	HIS
8	K	141	ASP
8	K	340	TYR
8	K	358	PHE
8	K	371	MET
10	M	22	ASP
12	J	747	TYR
12	P	115	CYS
8	Q	3	LEU
8	Q	6	LEU
13	Y	41	VAL
13	Y	294	PHE
13	Y	546	LEU
14	U	378	MET
14	U	490	TYR

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Mol	Chain	Res	Type
14	V	417	TYR
14	V	435	MET
15	R	148	TYR
15	R	188	PHE
15	R	189	TYR
15	R	335	ASN
15	R	383	ARG
16	C	16	TRP
13	Z	49	LEU
13	Z	174	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	146	GLN
3	A	264	ASN
3	A	1602	HIS
3	A	1869	HIS
4	N	241	HIS
4	N	327	HIS
4	N	517	ASN
5	I	401	ASN
5	I	676	ASN
5	I	740	HIS
6	O	69	GLN
6	O	424	GLN
6	O	472	HIS
11	H	101	GLN
12	J	659	GLN
12	P	497	ASN
13	Y	36	ASN
13	Y	52	ASN
13	Y	83	HIS
13	Y	106	GLN
13	Y	177	ASN
13	Y	326	ASN
13	Y	471	GLN
14	V	202	HIS
14	V	355	GLN
14	V	477	HIS
15	R	65	ASN
15	R	341	ASN

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Mol	Chain	Res	Type
15	R	401	GLN
15	R	410	HIS
15	R	423	ASN
13	Z	52	ASN
13	Z	67	ASN
13	Z	75	GLN
13	Z	289	ASN
13	Z	296	GLN
13	Z	338	HIS
13	Z	395	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

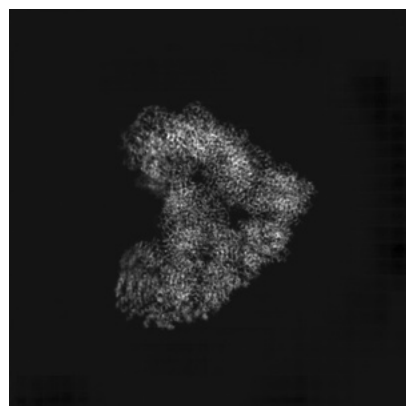
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51190. These allow visual inspection of the internal detail of the map and identification of artifacts.

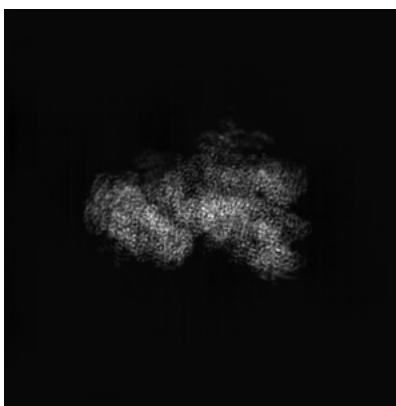
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

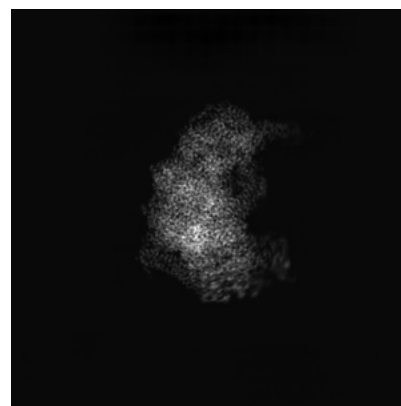
#### 6.1.1 Primary map



X

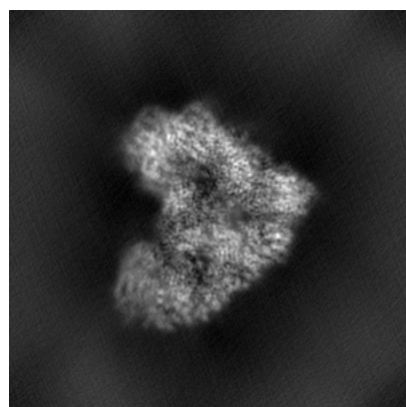


Y

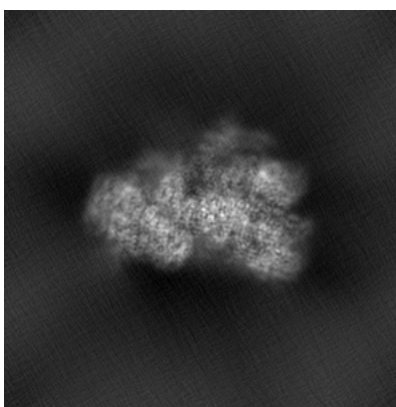


Z

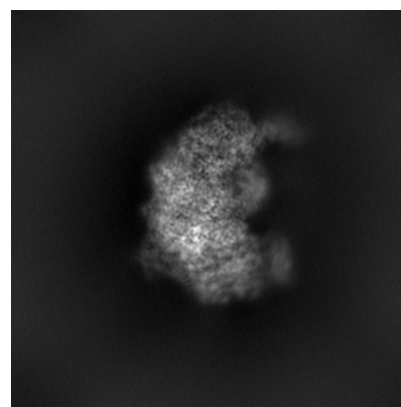
#### 6.1.2 Raw map



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

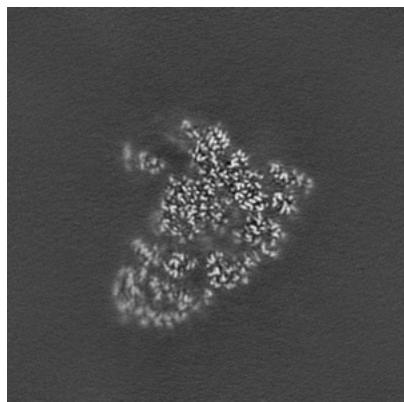


Y Index: 180

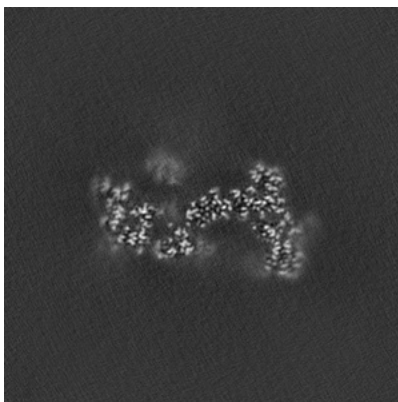


Z Index: 180

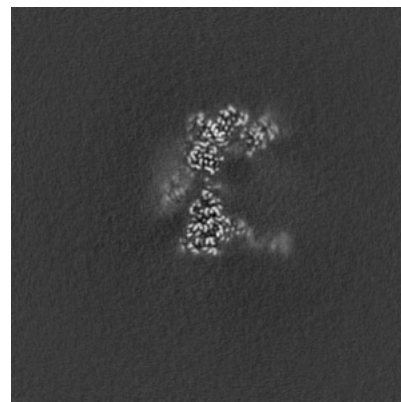
### 6.2.2 Raw map



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: 175

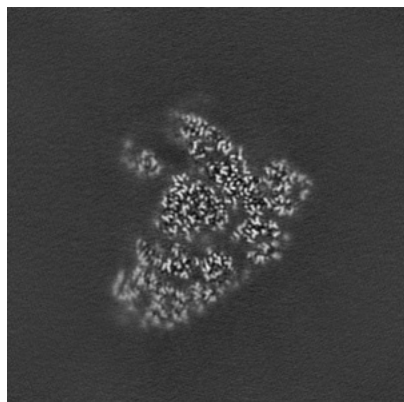


Y Index: 160

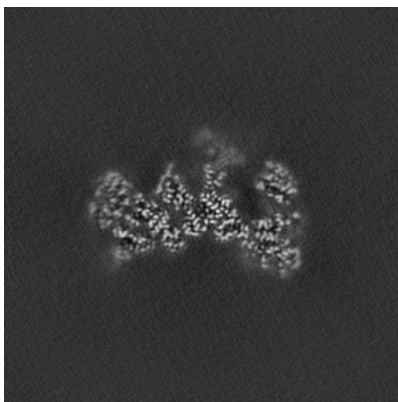


Z Index: 233

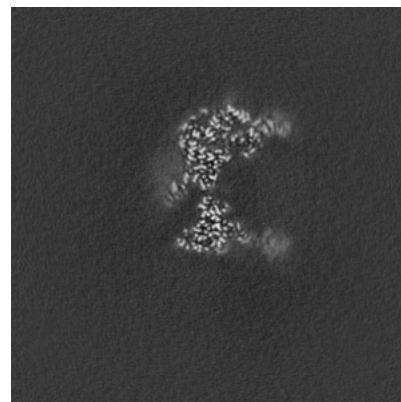
### 6.3.2 Raw map



X Index: 175



Y Index: 154

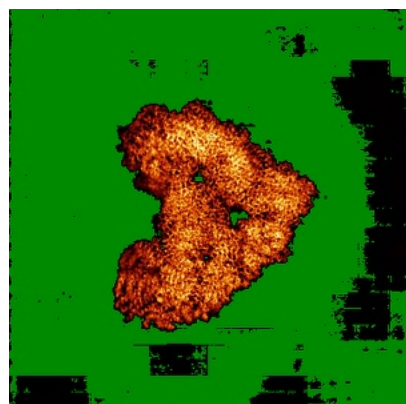


Z Index: 188

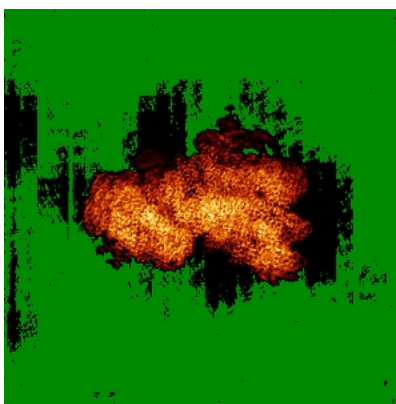
The images above show the largest variance slices of the map in three orthogonal directions.

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

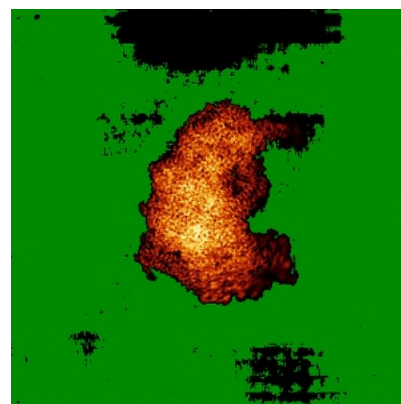
### 6.4.1 Primary map



X

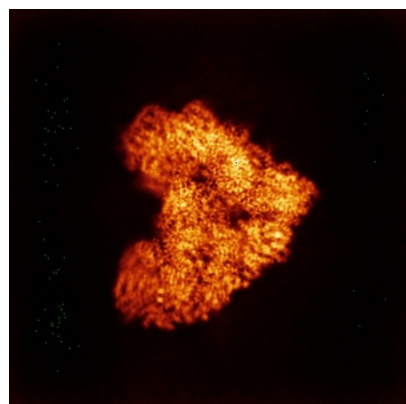


Y

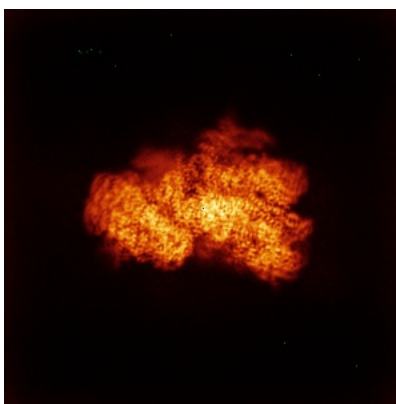


Z

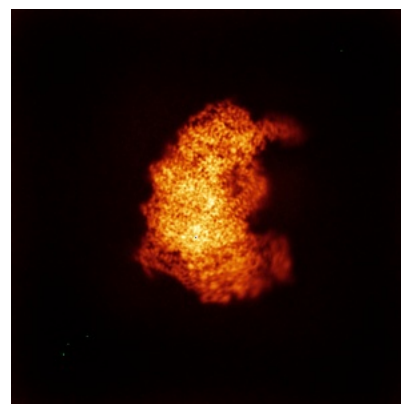
### 6.4.2 Raw map



X



Y

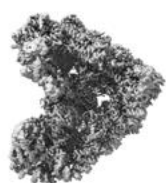


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



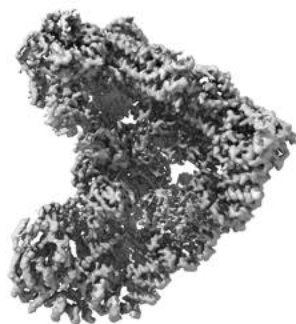
Y



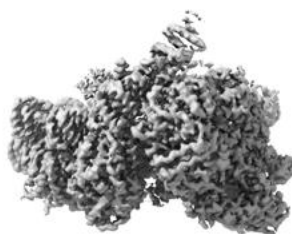
Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

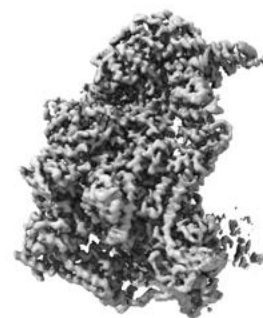
### 6.5.2 Raw map



X



Y



Z

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

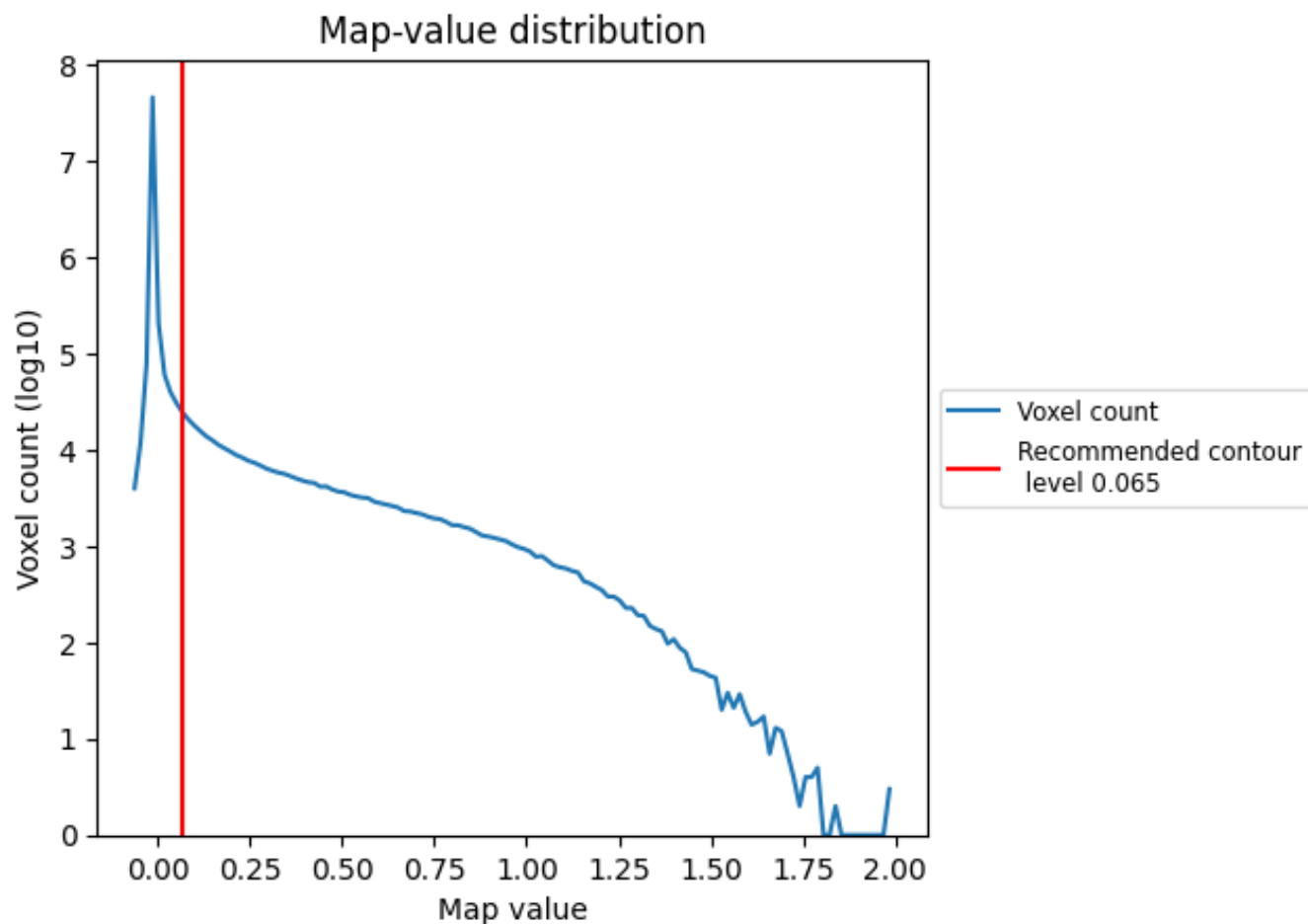
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

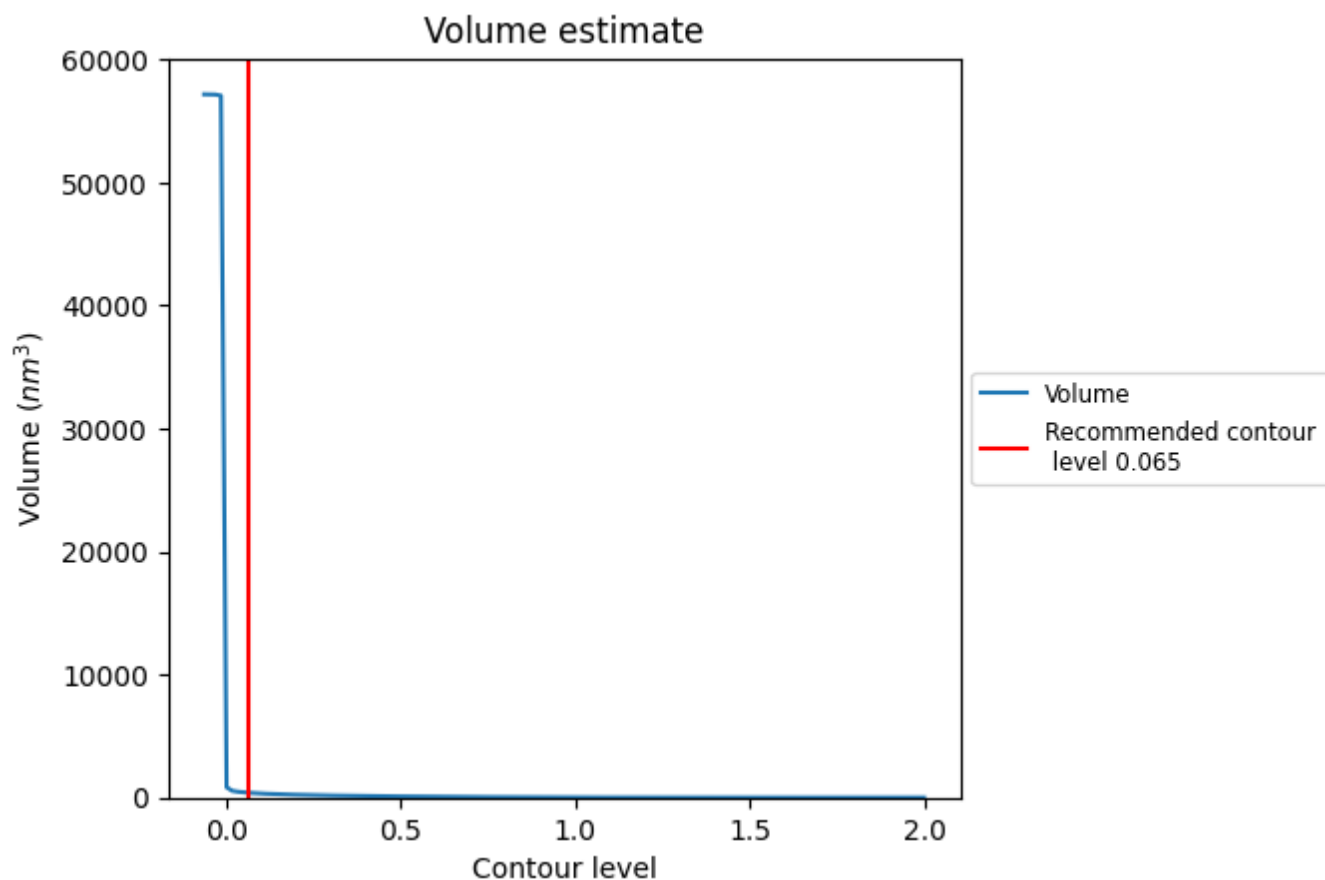
This section contains the results of statistical analysis of the map.

### 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.

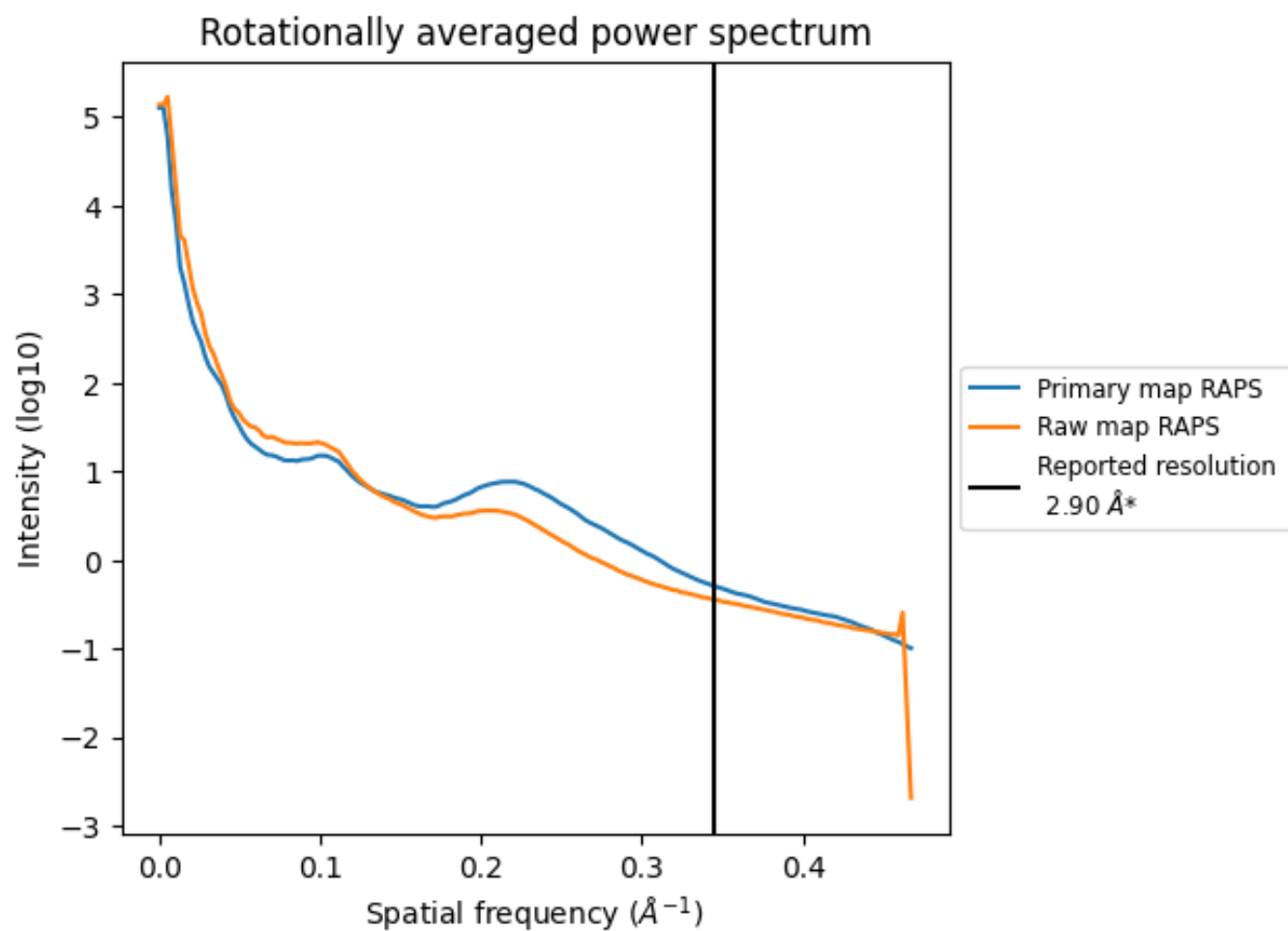
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 392 nm<sup>3</sup>; this corresponds to an approximate mass of 354 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 ⓘ

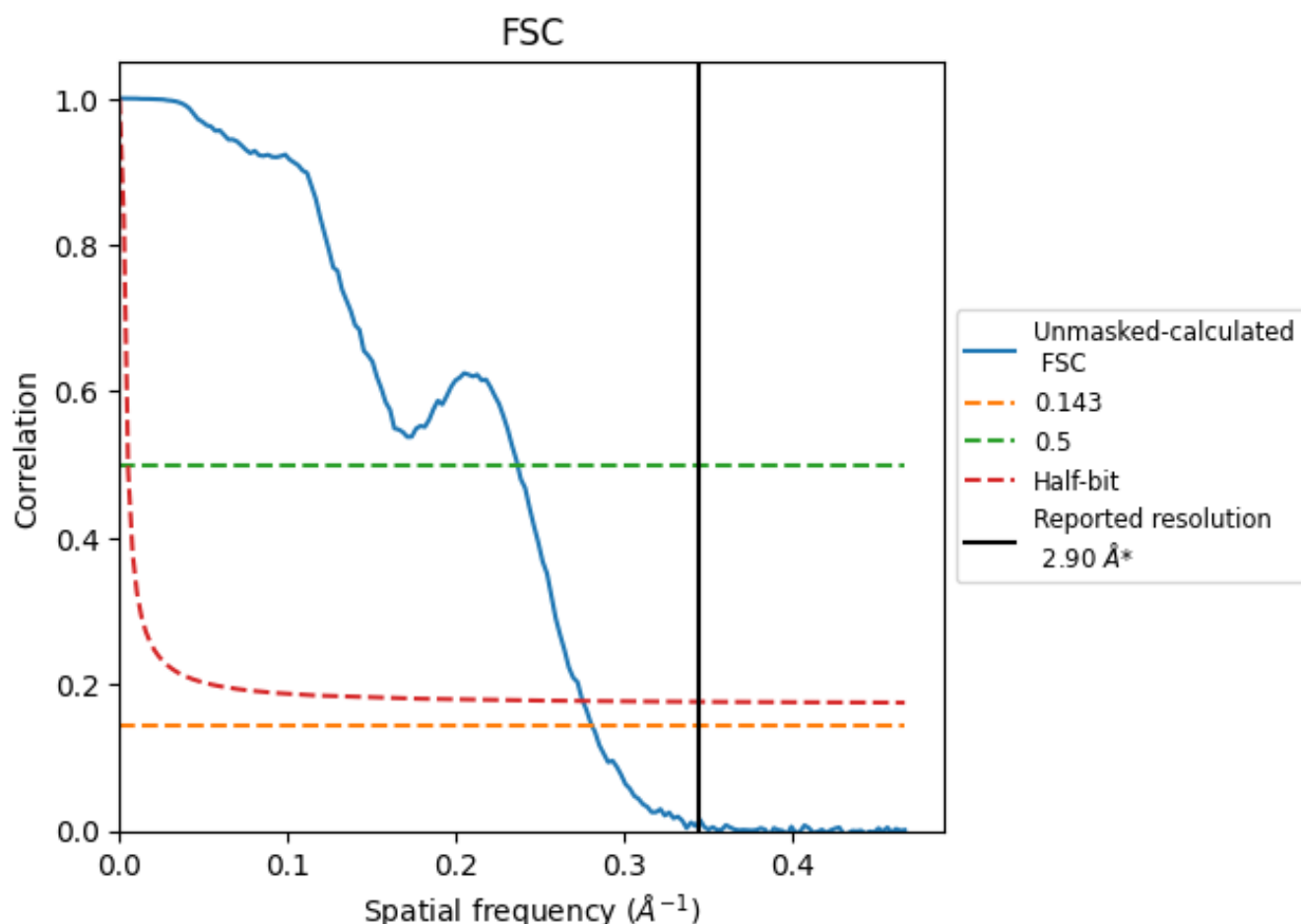


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.56	4.22	3.63

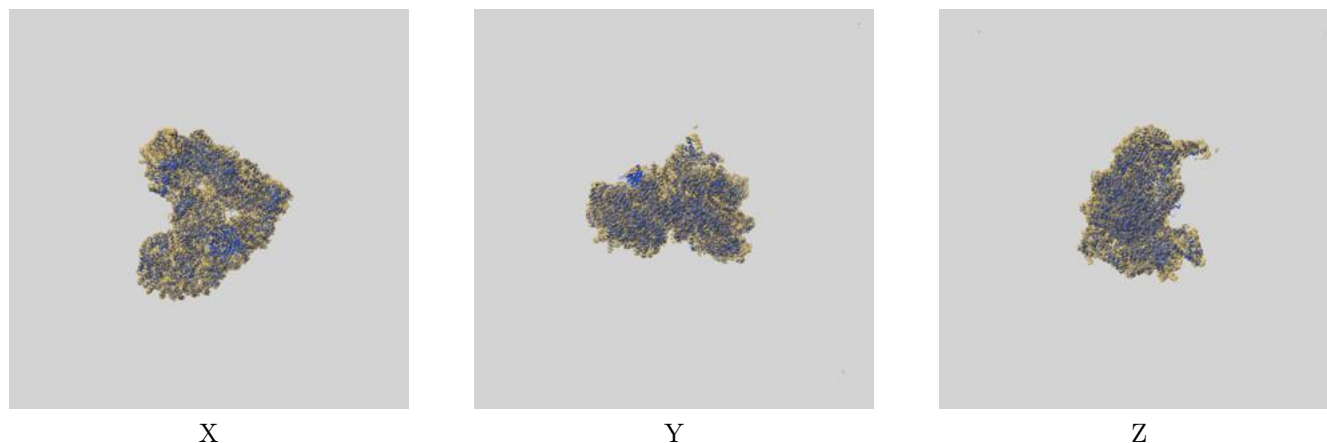
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.56 differs from the reported value 2.9 by more than 10 %



## 9 Map-model fit [i](#)

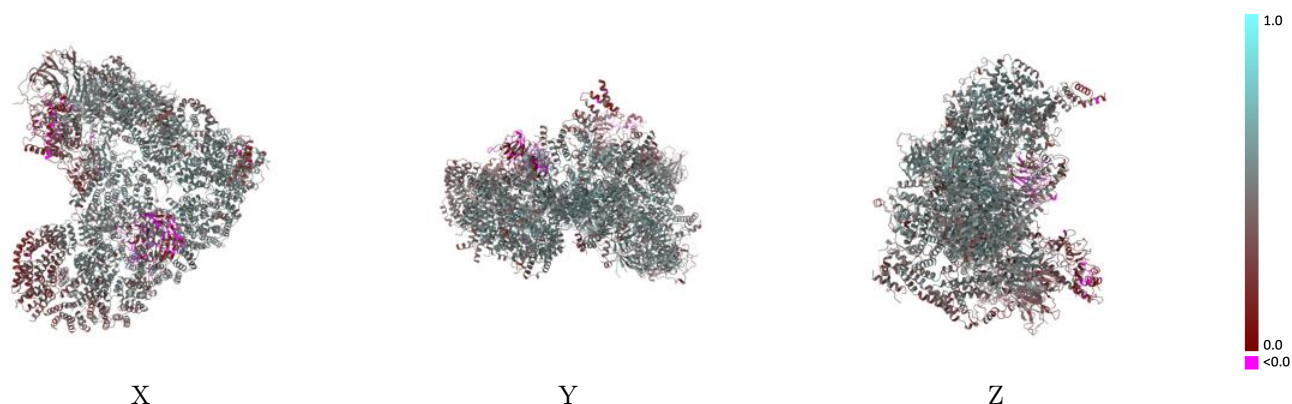
This section contains information regarding the fit between EMDB map EMD-51190 and PDB model 9GAW. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

### 9.1 Map-model overlay [i](#)



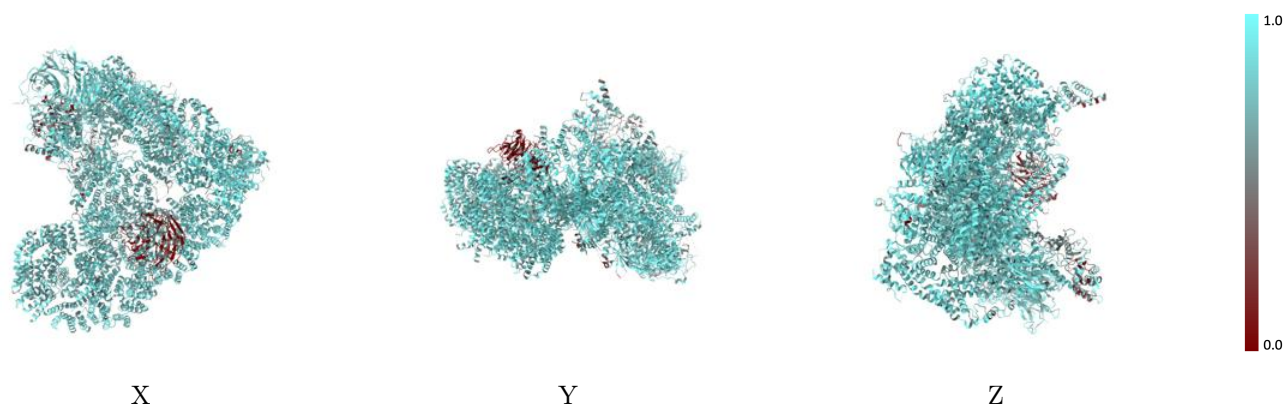
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



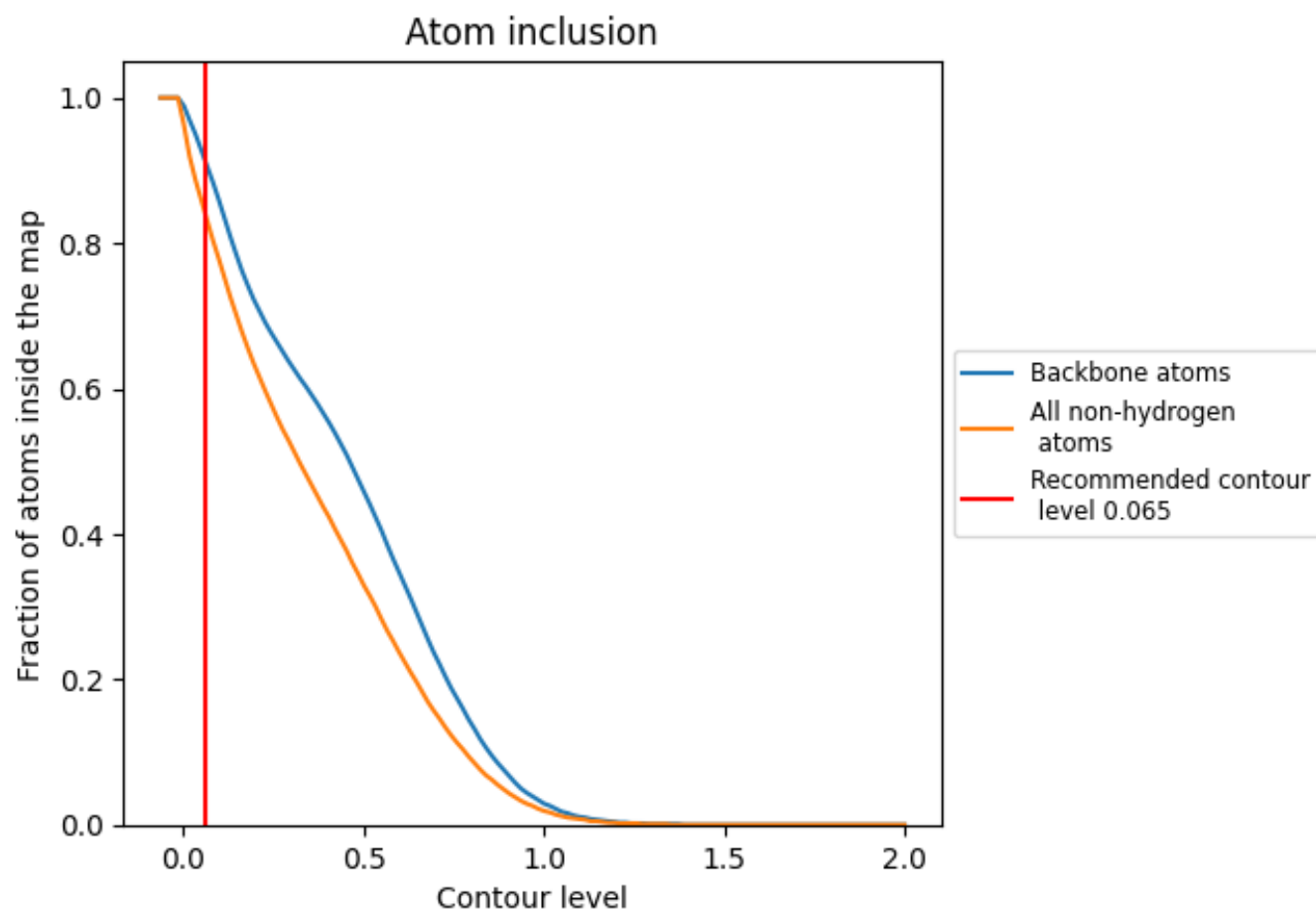
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.4620
A	 0.8830	 0.5130
C	 0.6180	 0.2270
D	 0.8300	 0.4880
G	 0.8220	 0.4490
H	 0.8400	 0.4340
I	 0.8280	 0.4450
J	 0.8920	 0.4980
K	 0.9020	 0.5250
L	 0.8610	 0.4870
M	 0.8270	 0.4800
N	 0.7810	 0.3720
O	 0.8840	 0.5220
P	 0.9020	 0.5160
Q	 0.8990	 0.5200
R	 0.3200	 0.1950
S	 0.4410	 0.2480
U	 0.8720	 0.4890
V	 0.9020	 0.5300
W	 0.8220	 0.4980
Y	 0.8490	 0.3990
Z	 0.7860	 0.3440

