Full wwPDB EM Validation Report

Aug 22, 2022 – 10:36 pm BST

PDB ID	:	8A61
EMDB ID	:	EMD-15201
Title	:	S. cerevisiae apo phosphorylated APC/C
Authors	:	Barford, D.; Fernandez-Vazquez, E.; Zhang, Z.; Yang, J.
Deposited on	:	2022-06-16
Resolution	:	5.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

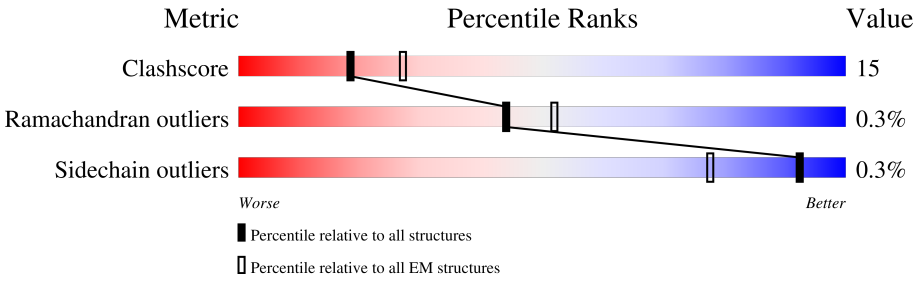
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 5.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	F	758	44% 22% 34%
1	H	758	16% 43% 23% 33%
2	J	850	38% 22% 40%
2	K	850	13% 39% 20% 41%
3	G	124	14% 14% 73%
3	W	124	19% 15% 9% 76%
4	E	265	21% 37% 12% 51%
5	T	853	17% 57% 19% 24%

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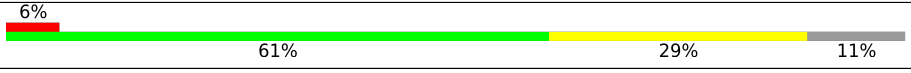
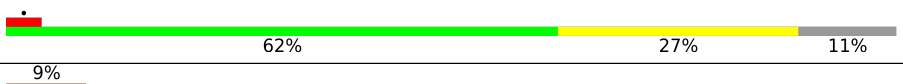
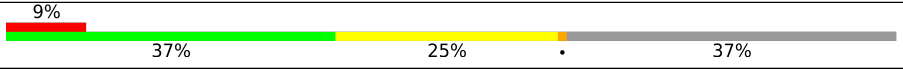
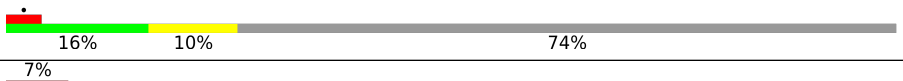
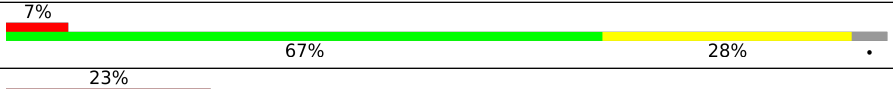
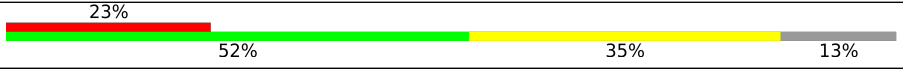
Mol	Chain	Length	Quality of chain
6	U	165	
7	C	1748	
8	O	685	
9	D	626	
9	P	626	
10	I	170	
11	N	368	
12	Q	652	
13	A	250	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 57784 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 CDC27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	502	Total	C	N	O	S	0	0
			3991	2569	656	739	27		
1	H	505	Total	C	N	O	S	0	0
			4038	2599	664	748	27		

- Molecule 2 is a protein called Anaphase-promoting complex subunit CDC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	509	Total	C	N	O	S	0	0
			4124	2658	674	769	23		
2	K	505	Total	C	N	O	S	0	0
			4102	2642	673	764	23		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	841	LYS	-	expression tag	UNP P09798
J	842	SER	-	expression tag	UNP P09798
J	843	SER	-	expression tag	UNP P09798
J	844	ILE	-	expression tag	UNP P09798
J	845	PRO	-	expression tag	UNP P09798
J	846	GLU	-	expression tag	UNP P09798
J	847	ASN	-	expression tag	UNP P09798
J	848	LEU	-	expression tag	UNP P09798
J	849	TYR	-	expression tag	UNP P09798
J	850	PHE	-	expression tag	UNP P09798
K	841	LYS	-	expression tag	UNP P09798
K	842	SER	-	expression tag	UNP P09798
K	843	SER	-	expression tag	UNP P09798
K	844	ILE	-	expression tag	UNP P09798
K	845	PRO	-	expression tag	UNP P09798
K	846	GLU	-	expression tag	UNP P09798
K	847	ASN	-	expression tag	UNP P09798

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Chain	Residue	Modelled	Actual	Comment	Reference
K	848	LEU	-	expression tag	UNP P09798
K	849	TYR	-	expression tag	UNP P09798
K	850	PHE	-	expression tag	UNP P09798

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	34	Total	C	N	O	S	0	0
			275	169	50	55	1		
3	W	30	Total	C	N	O	S	0	0
			242	148	44	49	1		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	130	Total	C	N	O	S	0	0
			1091	678	201	205	7		

- Molecule 5 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	650	Total	C	N	O	S	0	0
			5362	3476	877	985	24		

- Molecule 6 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	114	Total	C	N	O	S	0	0
			912	574	164	162	12		

- Molecule 7 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	1406	Total	C	N	O	S	0	0
			10832	7003	1749	2034	46		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	658	Total	C	N	O	S	0	0
			5285	3399	869	990	27		

- Molecule 9 is a protein called Anaphase-promoting complex subunit CDC23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	560	Total	C	N	O	S	0	0
			4524	2925	729	844	26		
9	P	556	Total	C	N	O	S	0	0
			4520	2923	738	832	27		

- Molecule 10 is a protein called Anaphase-promoting complex subunit SWM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	107	Total	C	N	O	S	0	0
			878	551	154	171	2		

- Molecule 11 is a protein called Anaphase-promoting complex subunit MND2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	96	Total	C	N	O	S	0	0
			784	504	138	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	623	Total	C	N	O	S	0	0
			5086	3279	842	952	13		

- Molecule 13 is a protein called Anaphase-promoting complex subunit DOC1.

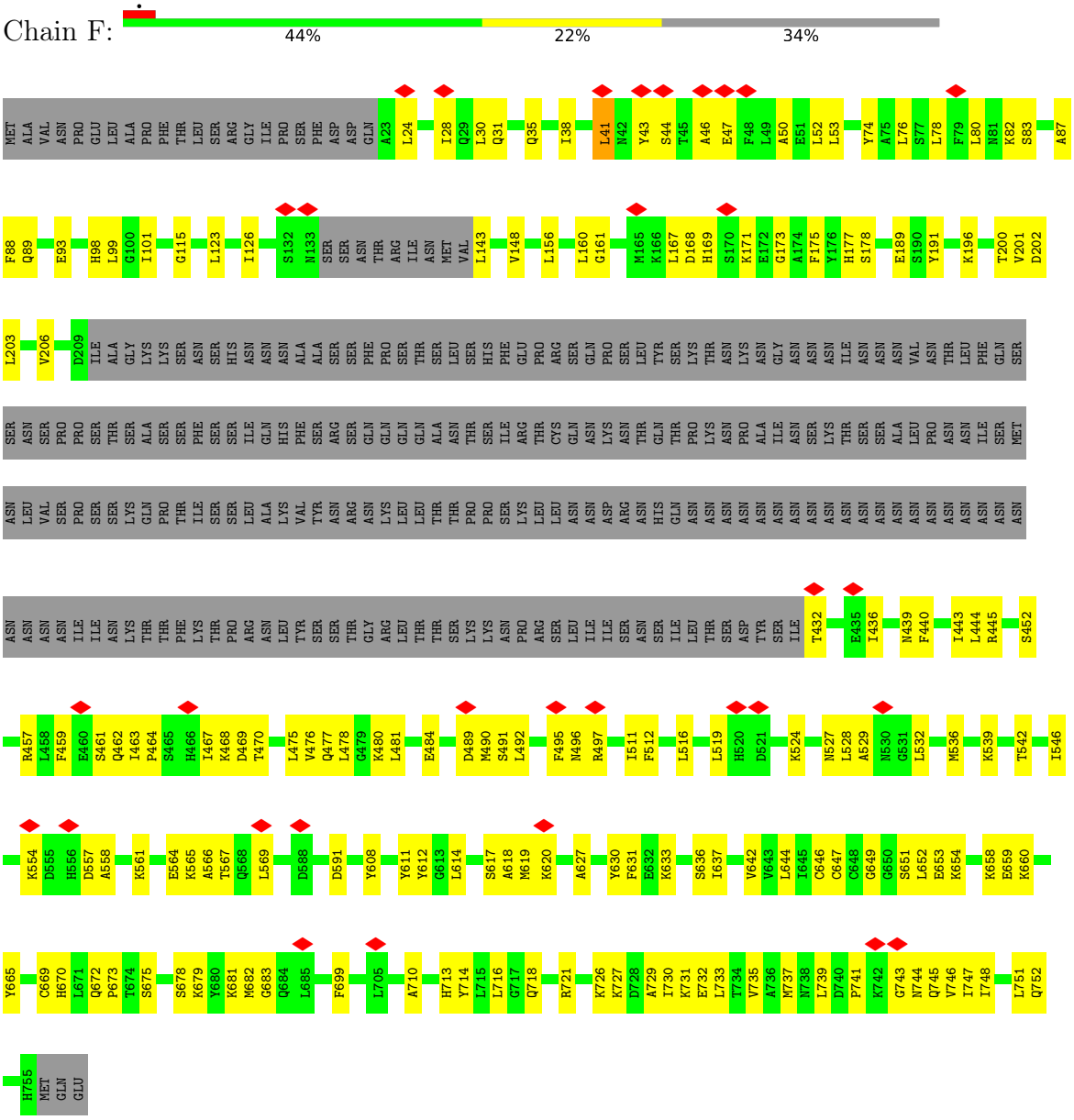
Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	218	Total	C	N	O	S	0	0
			1738	1113	303	312	10		

3 Residue-property plots (i)

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

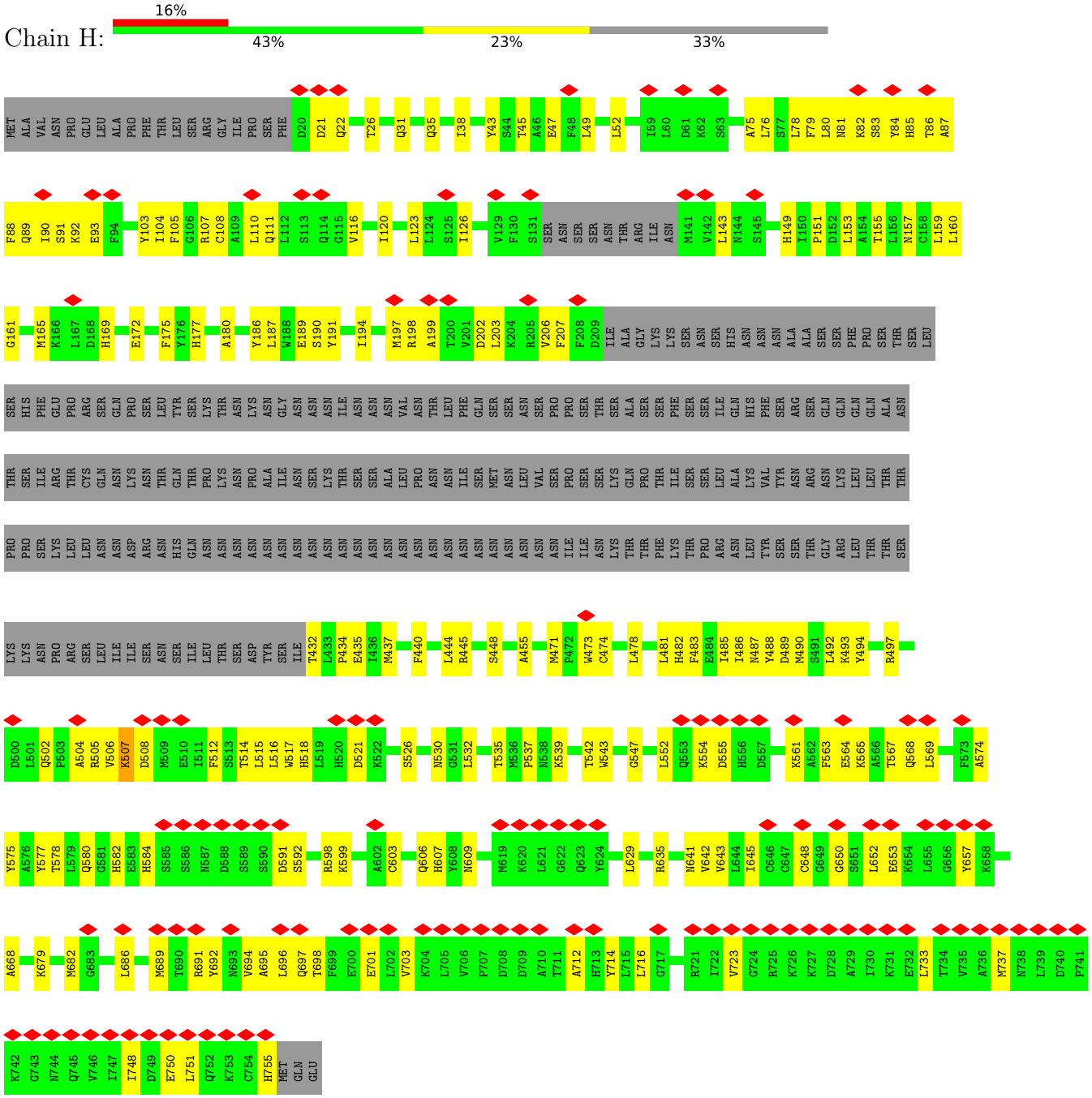
• Molecule 1: Anaphase-promoting complex subunit CDC27

Chain F:



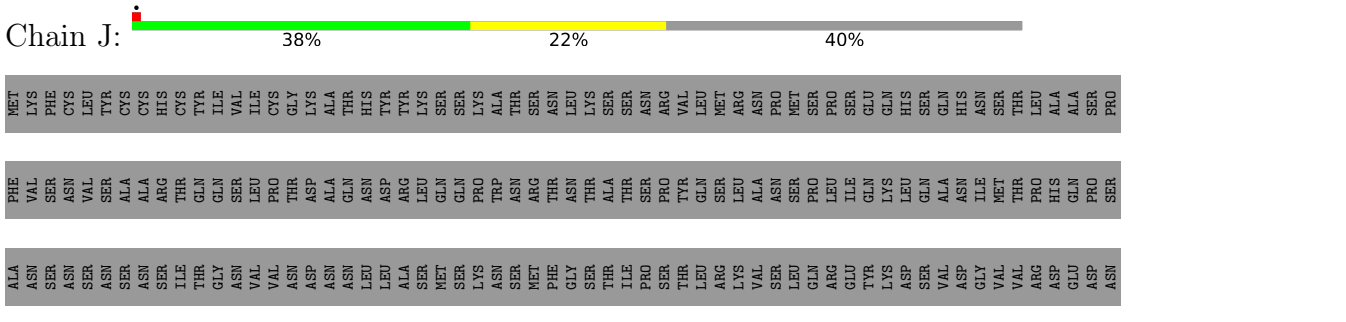
• Molecule 1: Anaphase-promoting complex subunit CDC27

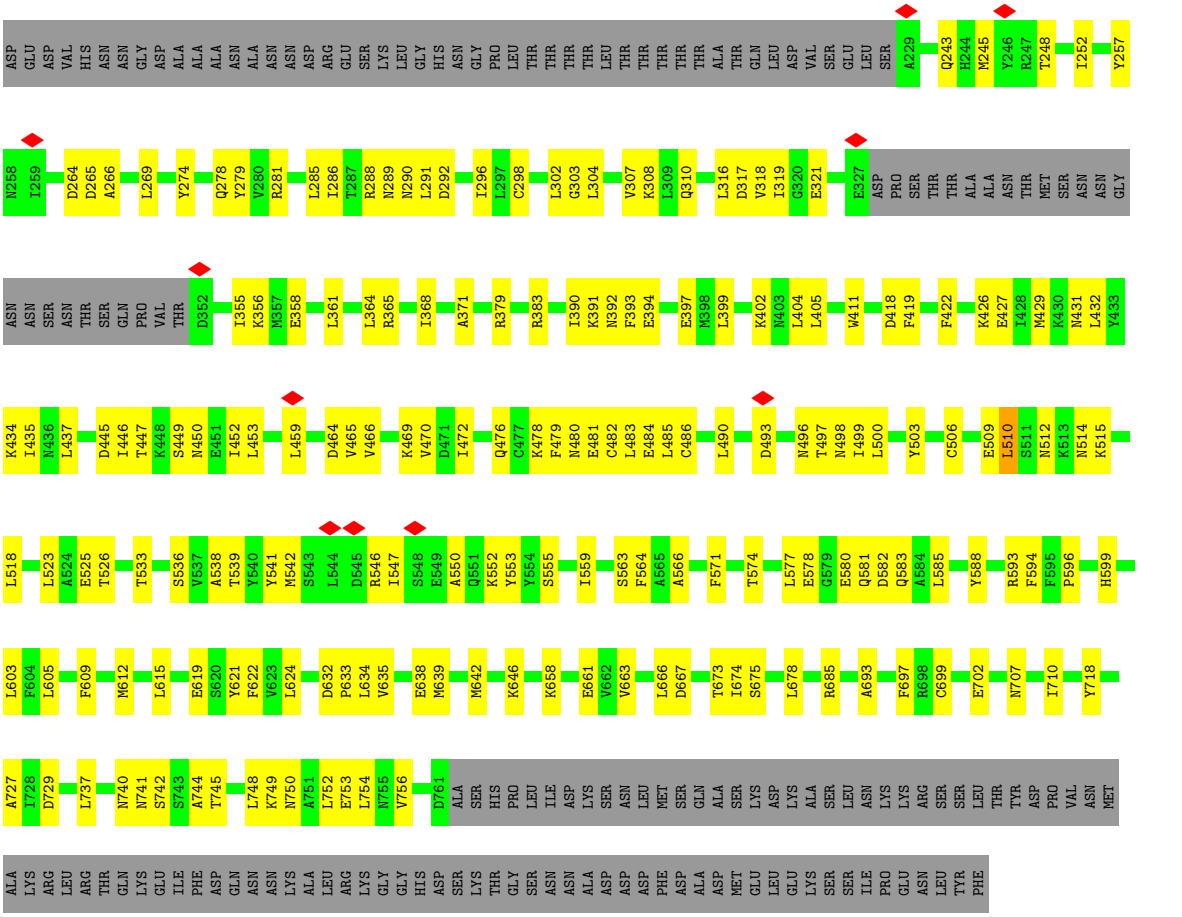
Chain H:



• Molecule 2: Anaphase-promoting complex subunit CDC16

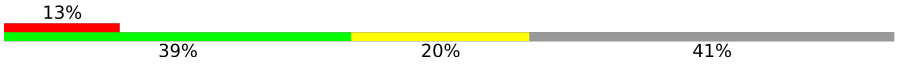
Chain J:

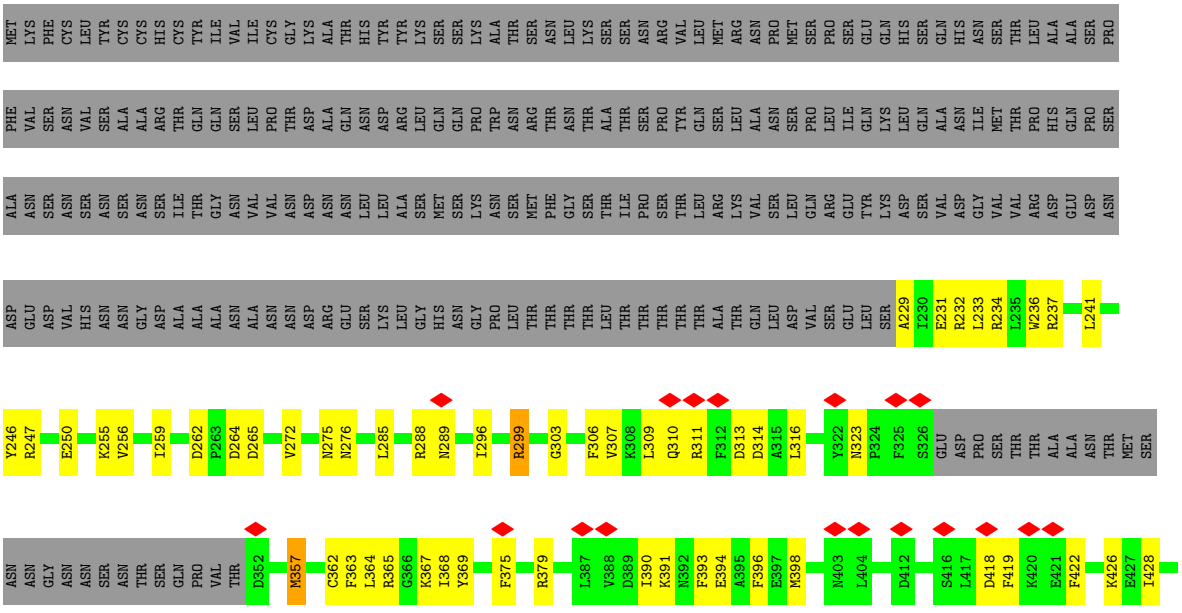


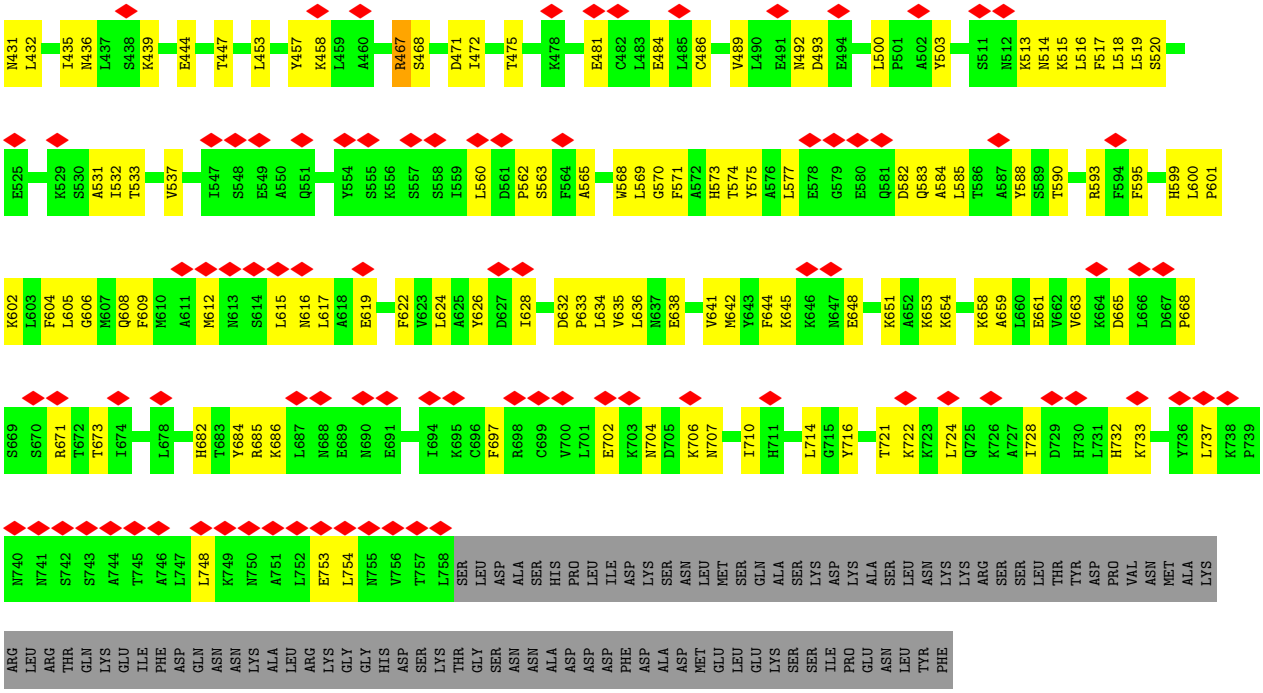


• Molecule 2: Anaphase-promoting complex subunit CDC16

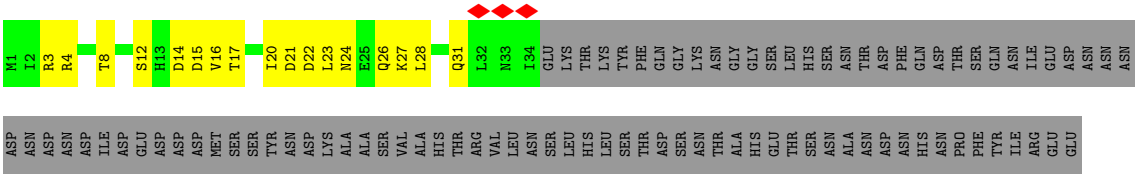
Chain K:



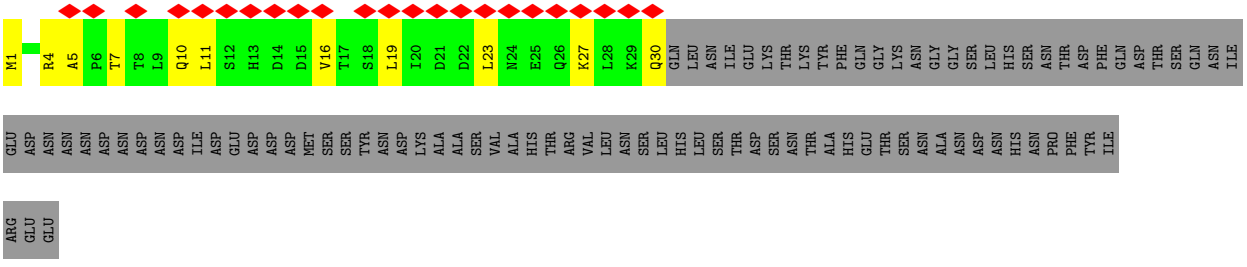




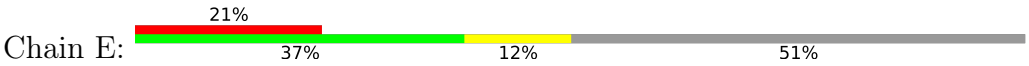
• Molecule 3: Anaphase-promoting complex subunit CDC26

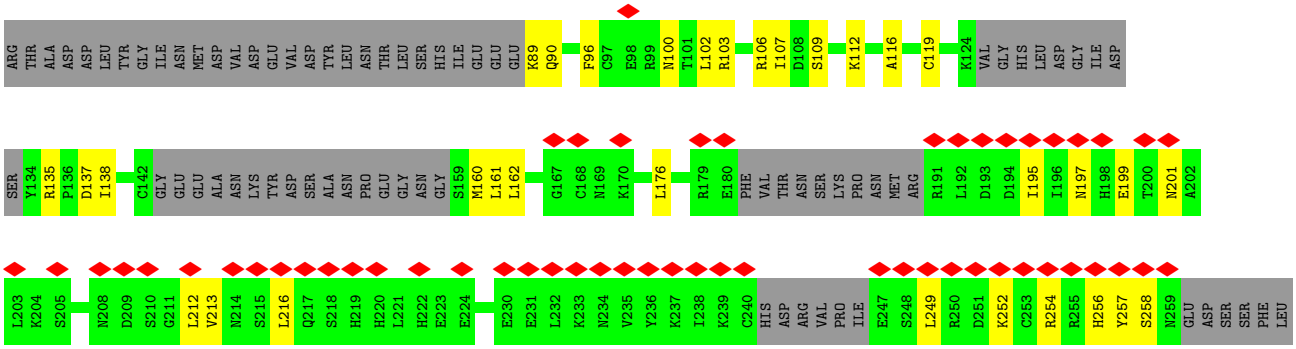


• Molecule 3: Anaphase-promoting complex subunit CDC26



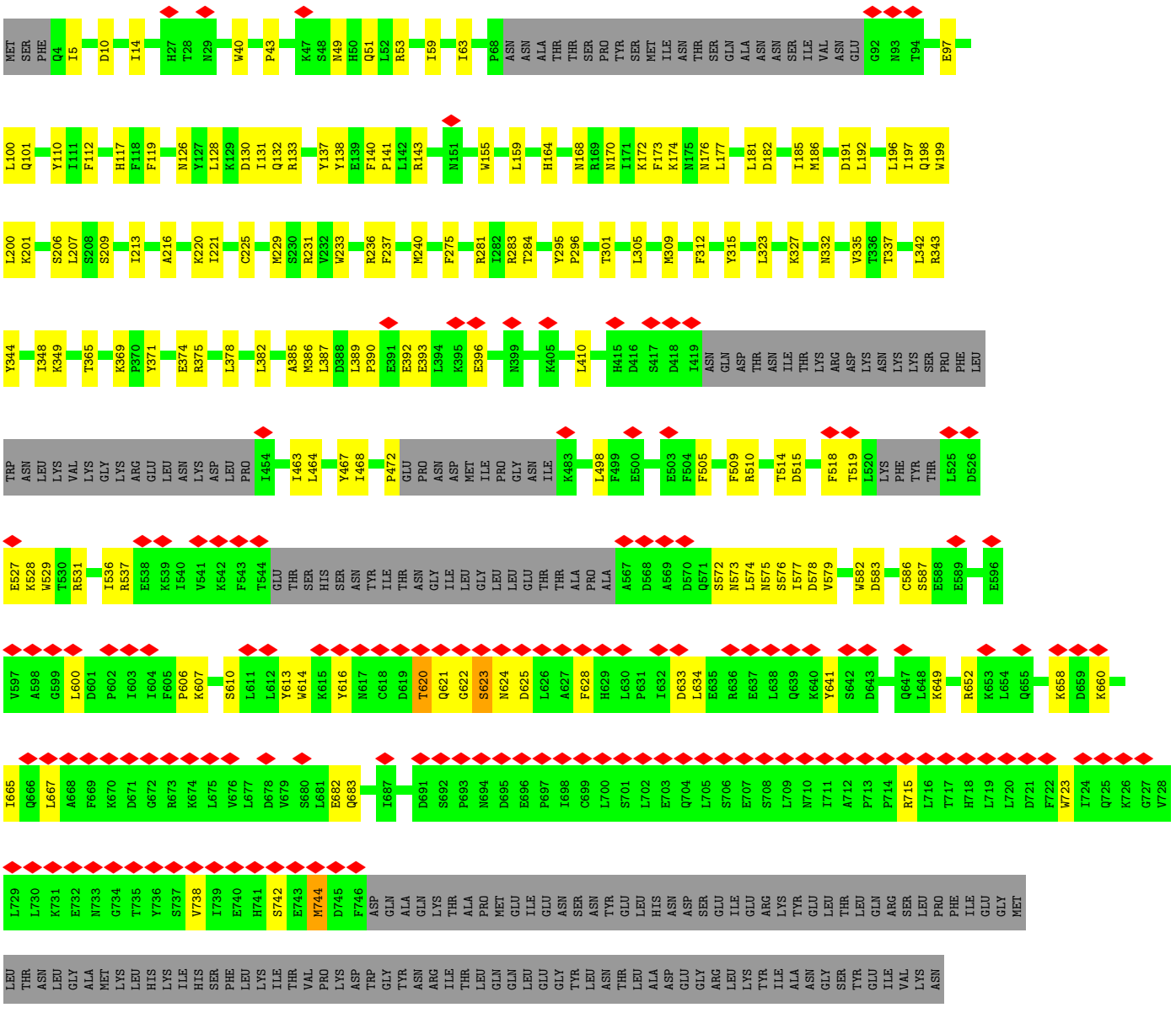
• Molecule 4: Anaphase-promoting complex subunit 9





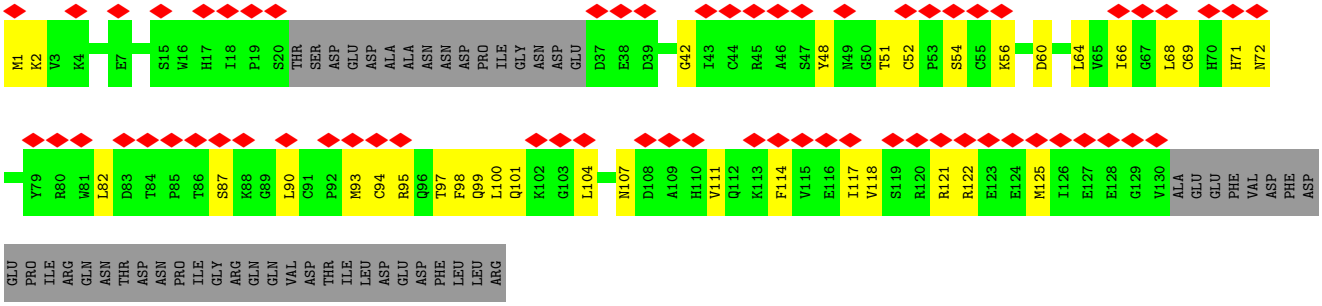
• Molecule 5: Anaphase-promoting complex subunit 2

Chain T:



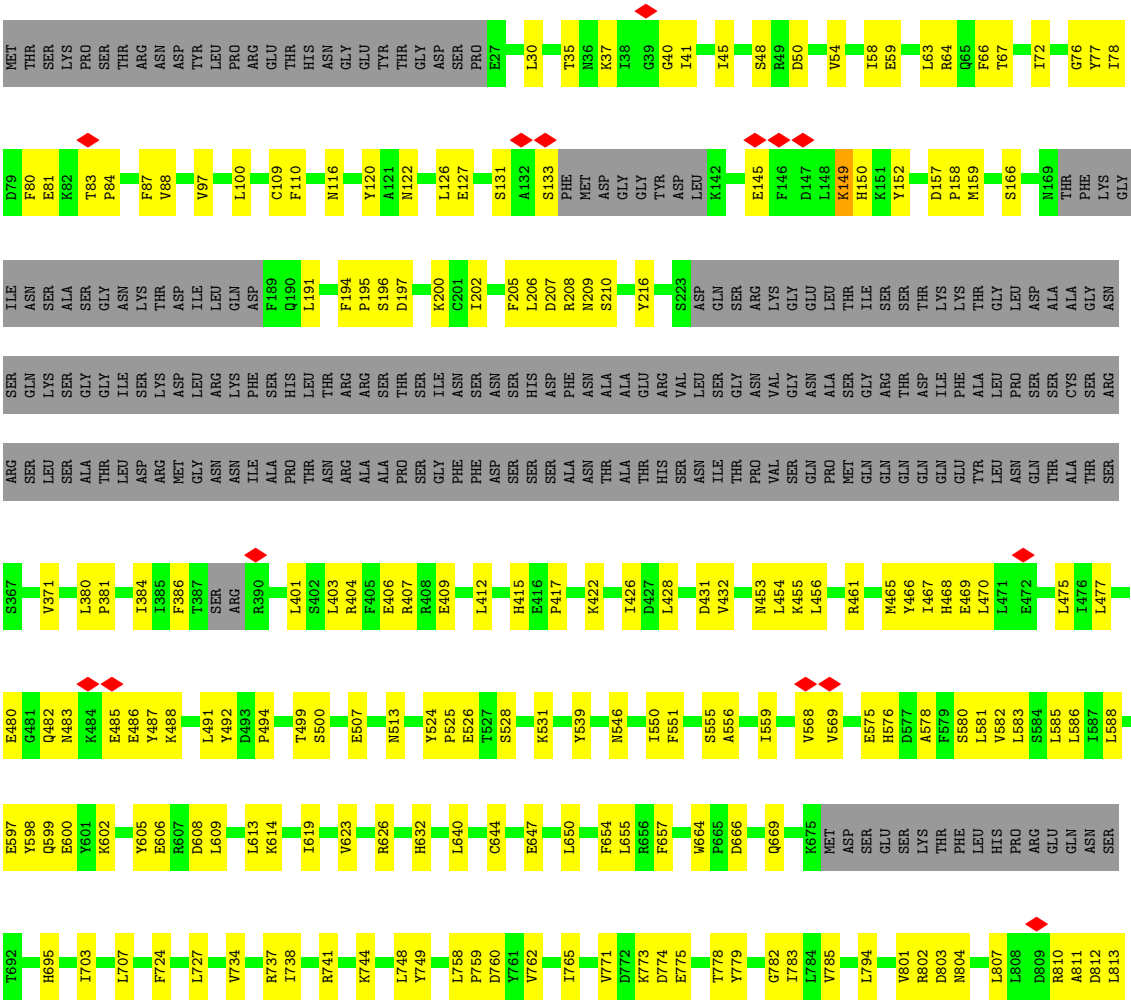
• Molecule 6: Anaphase-promoting complex subunit 11

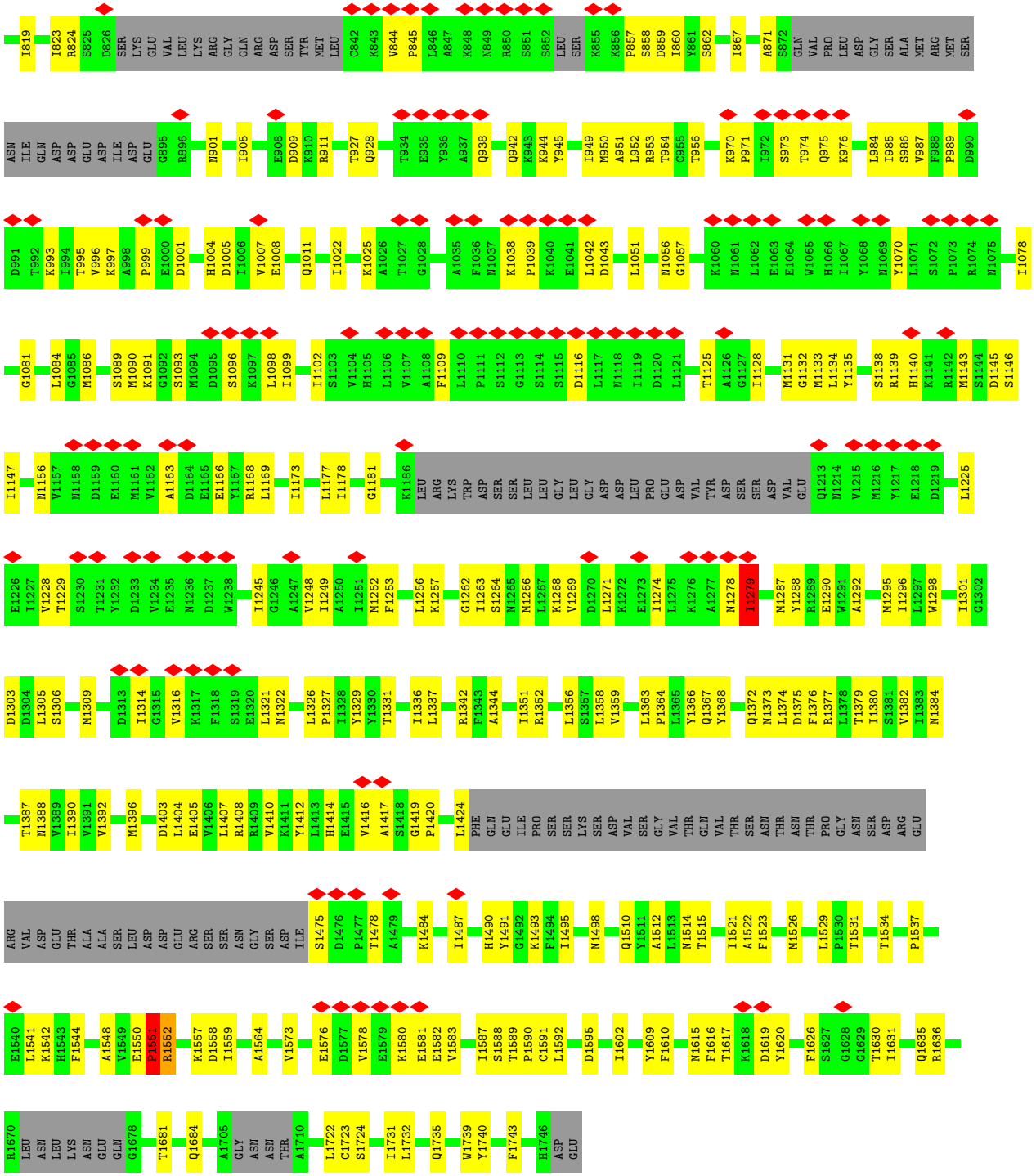
Chain U:



• Molecule 7: Anaphase-promoting complex subunit 1

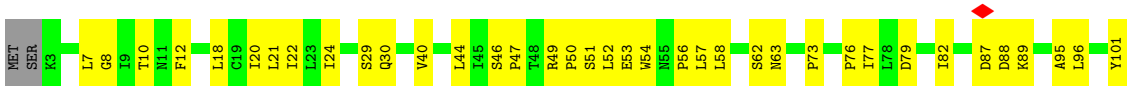
Chain C:

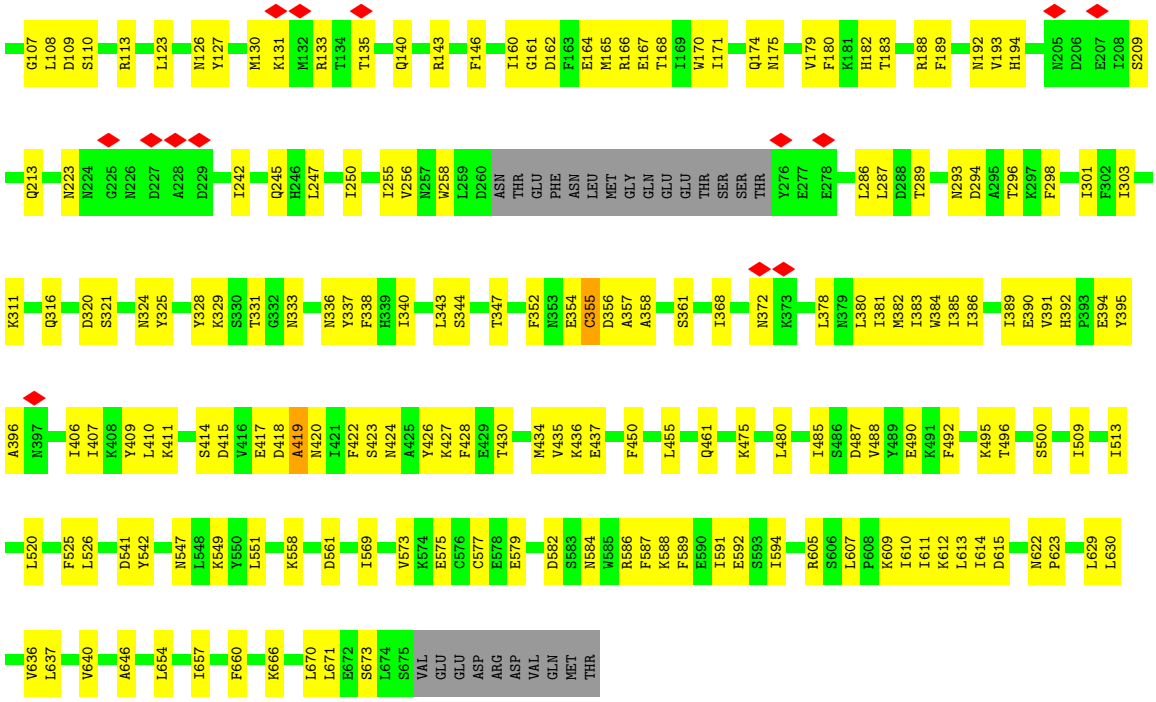




• Molecule 8: Anaphase-promoting complex subunit 5

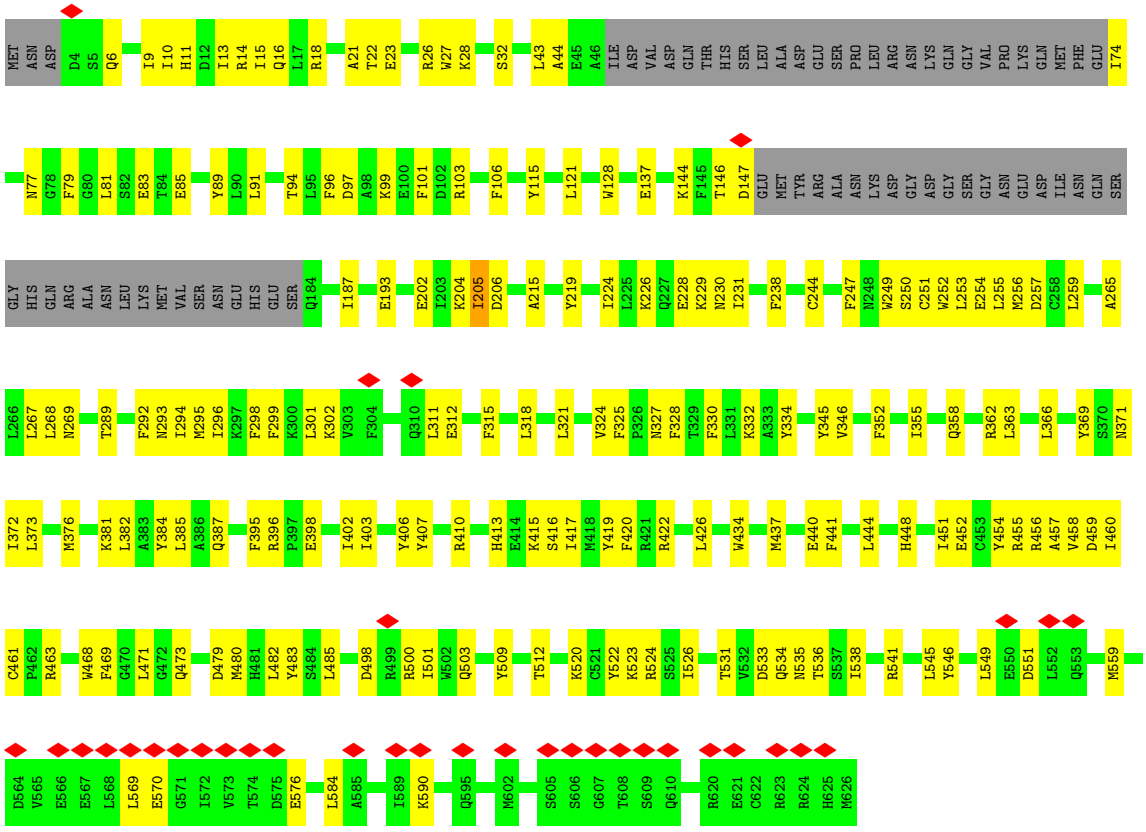
Chain O:





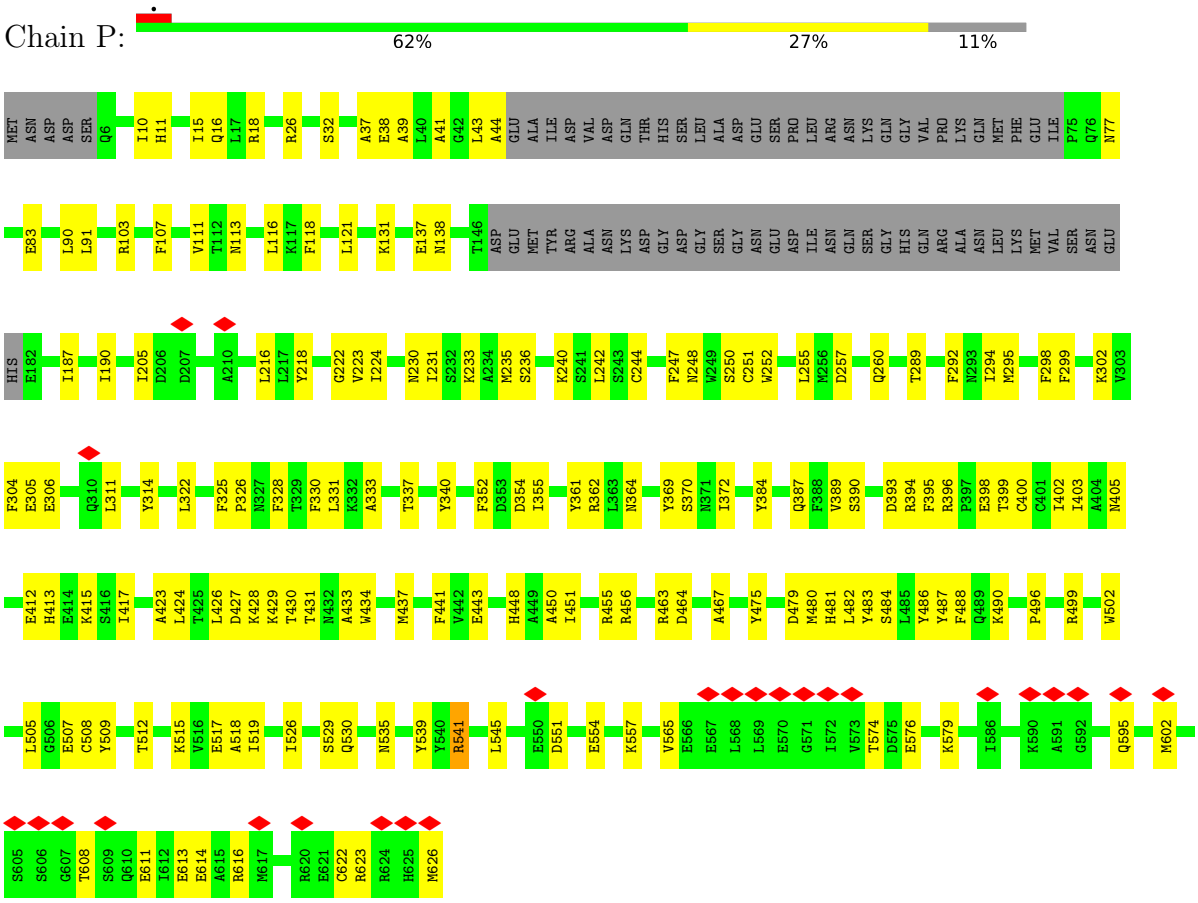
• Molecule 9: Anaphase-promoting complex subunit CDC23

Chain D:



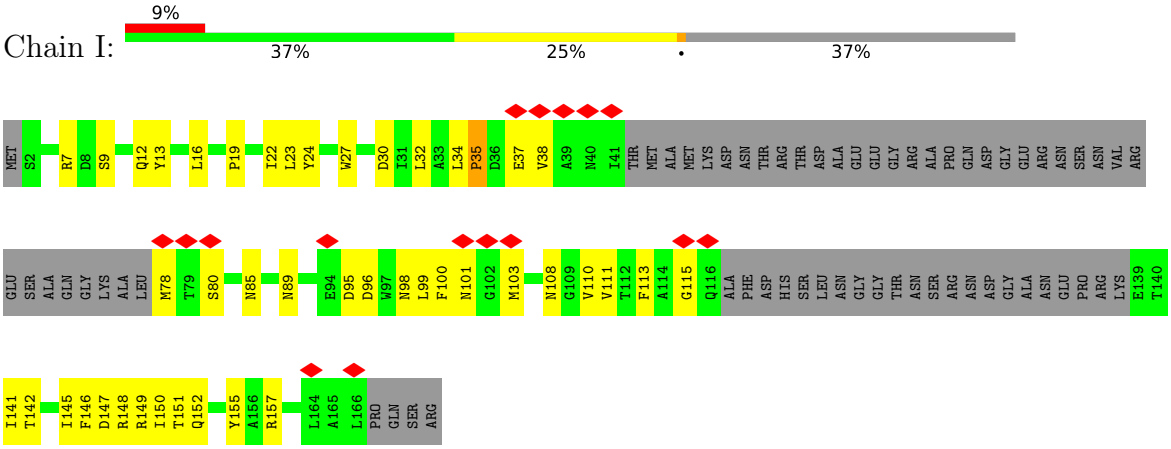
• Molecule 9: Anaphase-promoting complex subunit CDC23

Chain P:



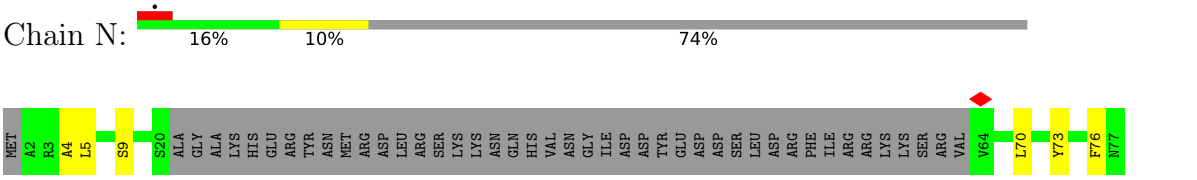
• Molecule 10: Anaphase-promoting complex subunit SWM1

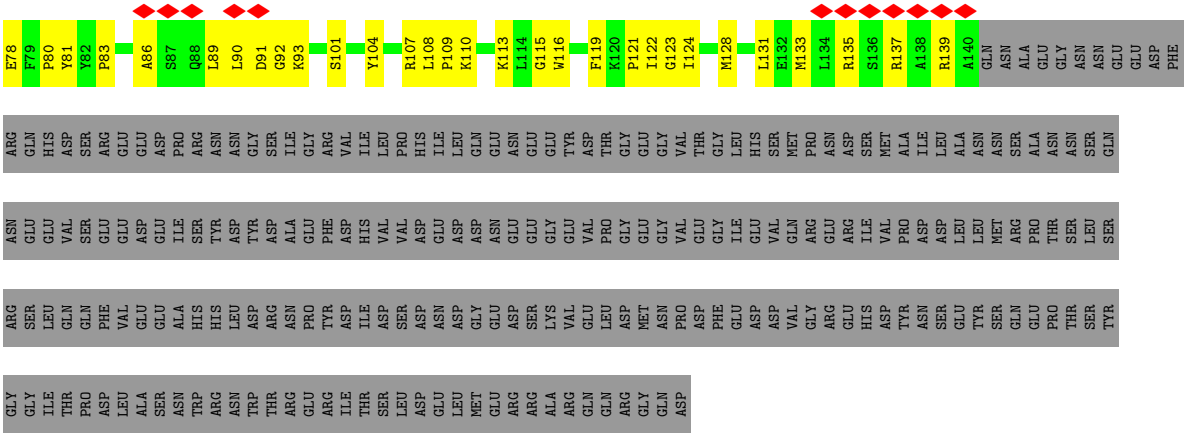
Chain I:



• Molecule 11: Anaphase-promoting complex subunit MND2

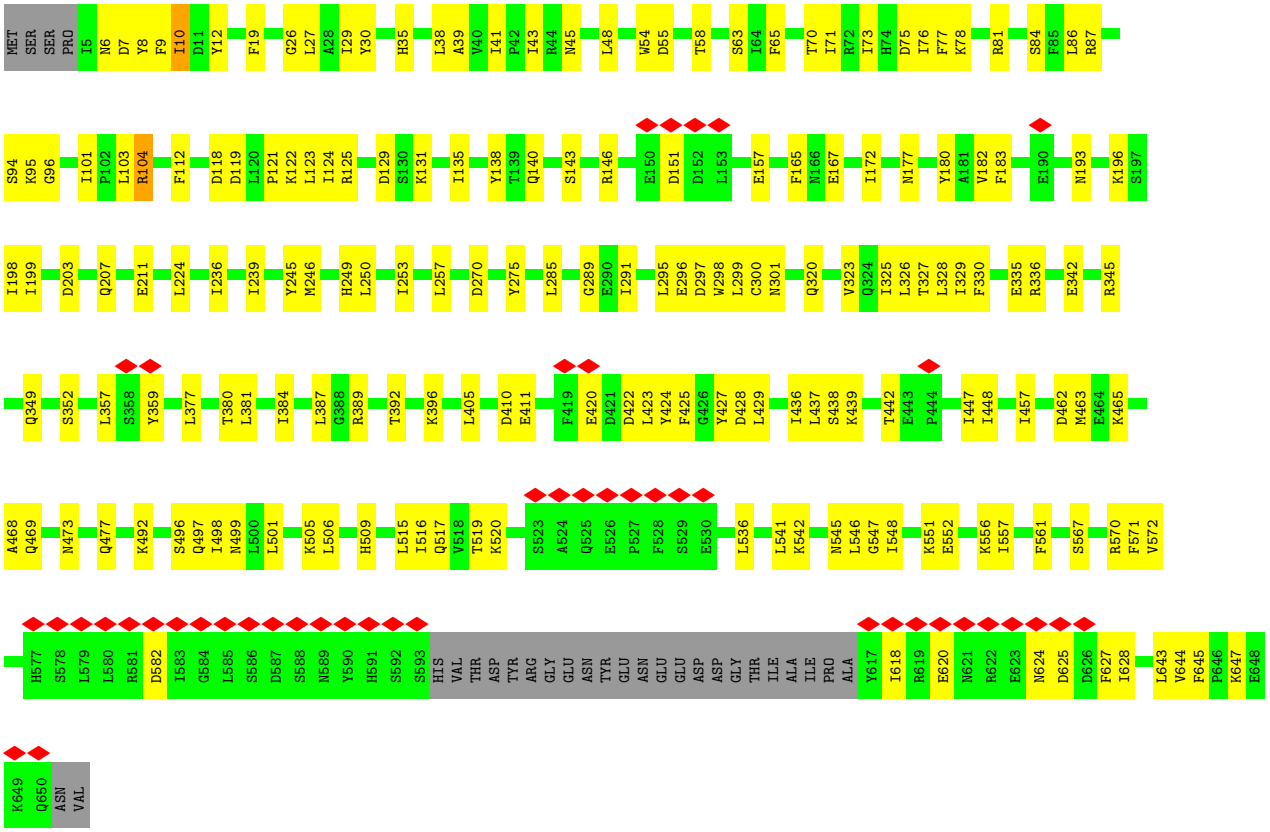
Chain N:





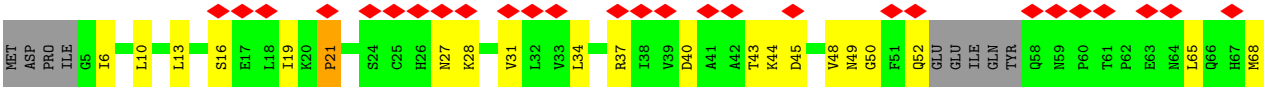
• Molecule 12: Anaphase-promoting complex subunit 4

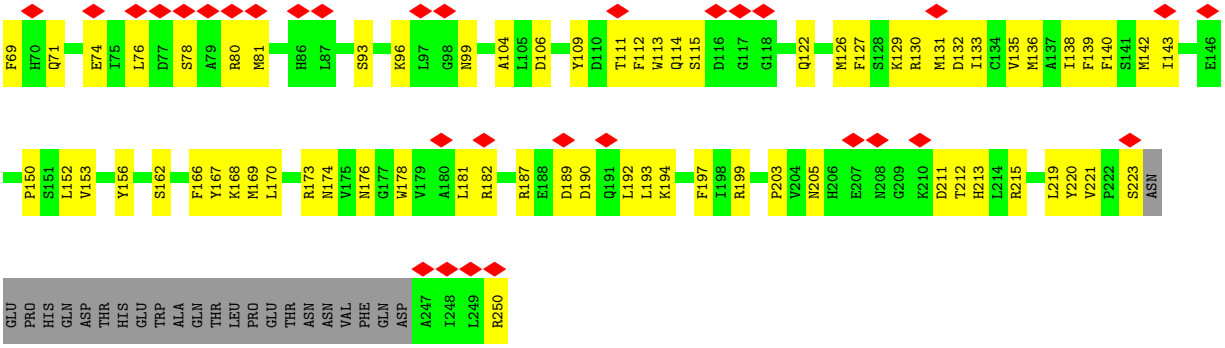
Chain Q:



• Molecule 13: Anaphase-promoting complex subunit DOC1

Chain A:




F69 H70 Q71 E74 L75 L76 D77 S78 A79 R80 M81 H86 L87 S93 K96 L97 G98 N99 A104 L105 D106 Y109 D110 T111 F112 W113 Q114 S115 D116 G117 G118 Q122 M126 F127 S128 K129 R130 M131 D132 I133 C134 V135 M136 A137 I138 F139 F140 S141 M142 I143 E146
P150 S151 L152 V153 Y156 S162 F166 Y167 K168 M169 L170 R173 N174 V175 N176 G177 W178 V179 A180 L181 R182 R187 E188 D189 D190 Q191 L192 L193 K194 F197 I198 R199 P203 V204 N205 H206 E207 N208 G209 K210 D211 T212 H213 L214 R215 L219 Y220 V221 P222 S223 ASN
GLU PRO HIS GLN ASP THR HIS GLU TRP ALA GLN THR LEU PRO GLU THR ASN ASN VAL PHE GLN ASP A247 I248 L249 R250

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	2600	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

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	F	0.27	0/4079	0.50	1/5525 (0.0%)
1	H	0.27	0/4126	0.47	0/5585
2	J	0.30	0/4210	0.53	1/5688 (0.0%)
2	K	0.28	0/4188	0.50	1/5657 (0.0%)
3	G	0.24	0/276	0.62	0/372
3	W	0.28	0/243	0.56	0/327
4	E	0.24	0/1108	0.50	0/1481
5	T	0.26	0/5479	0.45	0/7420
6	U	0.25	0/936	0.47	0/1265
7	C	0.27	0/11057	0.48	2/15038 (0.0%)
8	O	0.30	0/5384	0.47	0/7287
9	D	0.30	0/4621	0.48	0/6243
9	P	0.29	0/4618	0.47	0/6231
10	I	0.31	0/902	0.53	0/1226
11	N	0.29	0/800	0.57	0/1076
12	Q	0.28	0/5193	0.47	0/7024
13	A	0.26	0/1780	0.52	0/2411
All	All	0.28	0/59000	0.49	5/79856 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	T	0	2
7	C	0	1
10	I	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	510	LEU	CA-CB-CG	6.45	130.14	115.30
1	F	41	LEU	CA-CB-CG	5.89	128.84	115.30
7	C	845	PRO	N-CA-CB	5.80	110.26	103.30
7	C	1279	ILE	CG1-CB-CG2	-5.41	99.50	111.40
2	K	357	MET	CB-CG-SD	-5.03	97.32	112.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	1551	PRO	Peptide
10	I	35	PRO	Peptide
5	T	620	THR	Peptide
5	T	623	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3991	0	3947	129	0
1	H	4038	0	4010	145	0
2	J	4124	0	4085	157	0
2	K	4102	0	4065	130	0
3	G	275	0	287	19	0
3	W	242	0	251	14	0
4	E	1091	0	1058	27	0
5	T	5362	0	5336	114	0
6	U	912	0	882	33	0
7	C	10832	0	10637	330	0
8	O	5285	0	5290	175	0
9	D	4524	0	4391	152	0
9	P	4520	0	4415	132	0
10	I	878	0	783	54	0
11	N	784	0	784	29	0
12	Q	5086	0	5095	134	0
13	A	1738	0	1705	81	0
All	All	57784	0	57021	1673	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 15.

All (1673) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:307:VAL:HG22	2:K:368:ILE:HD11	1.51	0.91
5:T:578:ASP:HB2	6:U:56:LYS:HZ1	1.36	0.91
13:A:136:MET:HB3	13:A:181:LEU:HB3	1.57	0.85
8:O:419:ALA:HB2	11:N:4:ALA:H	1.42	0.85
9:P:230:ASN:HD21	9:P:233:LYS:HD3	1.41	0.84
1:F:673:PRO:HG3	4:E:112:LYS:HD2	1.60	0.83
9:P:247:PHE:HA	9:P:295:MET:HE1	1.58	0.83
5:T:518:PHE:HE1	5:T:660:LYS:HB3	1.45	0.82
2:K:241:LEU:HD21	2:K:272:VAL:HG22	1.63	0.80
2:K:367:LYS:HZ1	2:K:398:MET:HG2	1.45	0.80
2:J:434:LYS:HA	2:J:437:LEU:HD13	1.63	0.79
9:D:454:TYR:HB2	9:D:471:LEU:HD13	1.63	0.79
7:C:475:LEU:HD11	7:C:491:LEU:HB3	1.63	0.78
8:O:7:LEU:HD12	8:O:286:LEU:HB3	1.63	0.78
9:D:299:PHE:HA	9:D:302:LYS:HE2	1.64	0.78
7:C:491:LEU:HB2	7:C:500:SER:HB3	1.65	0.78
7:C:1042:LEU:HD12	7:C:1078:ILE:HG12	1.64	0.78
6:U:118:VAL:HA	6:U:121:ARG:HH12	1.48	0.78
1:H:516:LEU:HD11	1:H:521:ASP:HB3	1.66	0.77
7:C:81:GLU:HB2	7:C:122:ASN:HB2	1.66	0.77
2:J:546:ARG:HH22	10:I:37:GLU:CD	1.88	0.77
5:T:309:MET:HG3	5:T:315:TYR:HE1	1.50	0.76
9:D:327:ASN:OD1	9:D:358:GLN:NE2	2.18	0.76
9:P:111:VAL:HG11	9:P:116:LEU:HD22	1.68	0.76
12:Q:26:GLY:HA2	12:Q:43:ILE:HG22	1.68	0.76
12:Q:124:ILE:HD11	12:Q:328:LEU:HD21	1.66	0.76
2:J:546:ARG:NH2	10:I:37:GLU:OE2	2.19	0.75
1:H:194:ILE:HG23	1:H:199:ALA:HB3	1.69	0.75
5:T:112:PHE:HA	7:C:1739:TRP:HZ2	1.51	0.75
5:T:225:CYS:HB3	5:T:229:MET:HE2	1.69	0.75
8:O:434:MET:HG3	8:O:475:LYS:HZ3	1.51	0.75
2:J:379:ARG:HB2	2:J:404:LEU:HD11	1.69	0.75
1:H:169:HIS:ND1	1:H:172:GLU:OE2	2.19	0.75
9:D:295:MET:HA	9:D:298:PHE:HB2	1.69	0.74
1:H:123:LEU:HB3	1:H:160:LEU:HD12	1.70	0.74
1:H:444:LEU:HD21	1:H:473:TRP:HH2	1.51	0.74
1:F:189:GLU:OE1	1:H:45:THR:OG1	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:LEU:HD13	1:H:52:LEU:HD21	1.70	0.74
13:A:31:VAL:HG22	13:A:169:MET:HG2	1.69	0.74
13:A:153:VAL:HB	13:A:170:LEU:HB2	1.70	0.74
1:F:35:GLN:HE22	1:F:148:VAL:H	1.35	0.74
8:O:192:ASN:O	8:O:194:HIS:N	2.17	0.74
2:J:581:GLN:NE2	2:J:612:MET:SD	2.61	0.73
8:O:386:ILE:HA	8:O:389:ILE:HG22	1.70	0.73
2:J:269:LEU:HD22	2:J:285:LEU:HD22	1.68	0.73
8:O:383:ILE:HD11	8:O:424:ASN:HB3	1.70	0.73
2:J:509:GLU:OE2	2:J:510:LEU:HD12	1.89	0.73
13:A:130:ARG:HH21	13:A:194:LYS:HB3	1.55	0.72
7:C:1326:LEU:HD21	7:C:1379:THR:HA	1.71	0.72
7:C:858:SER:HG	7:C:862:SER:HG	1.35	0.72
8:O:10:THR:HG22	8:O:12:PHE:H	1.55	0.72
7:C:159:MET:O	9:D:524:ARG:NH2	2.23	0.72
2:K:728:ILE:O	2:K:732:HIS:ND1	2.20	0.72
12:Q:199:ILE:HD11	12:Q:505:LYS:HB2	1.70	0.72
1:F:714:TYR:HE1	1:F:747:ILE:HG12	1.55	0.71
2:J:278:GLN:OE1	2:J:281:ARG:NH1	2.24	0.71
2:K:753:GLU:HA	1:H:629:LEU:HD11	1.72	0.71
1:F:464:PRO:HG2	1:F:467:ILE:HD13	1.72	0.71
5:T:327:LYS:HE2	12:Q:151:ASP:HA	1.72	0.71
11:N:110:LYS:HA	11:N:113:LYS:HG2	1.73	0.71
2:J:434:LYS:NZ	2:J:445:ASP:OD1	2.20	0.71
7:C:779:TYR:O	8:O:605:ARG:NH2	2.24	0.71
1:F:173:GLY:O	1:F:177:HIS:ND1	2.22	0.70
3:G:24:ASN:HA	3:G:27:LYS:HG2	1.73	0.70
8:O:167:GLU:OE1	9:P:390:SER:OG	2.09	0.70
7:C:1609:TYR:CD1	7:C:1636:ARG:HA	2.27	0.70
5:T:174:LYS:HE3	5:T:207:LEU:HB2	1.71	0.70
9:P:248:ASN:ND2	9:P:251:CYS:SG	2.64	0.70
5:T:742:SER:OG	5:T:744:MET:SD	2.49	0.70
7:C:401:LEU:HD23	7:C:467:ILE:HG23	1.74	0.70
9:D:455:ARG:NH1	9:D:459:ASP:OD1	2.25	0.70
12:Q:436:ILE:HG23	12:Q:437:LEU:HG	1.73	0.70
2:J:402:LYS:HE2	2:J:563:SER:HB2	1.72	0.70
7:C:1374:LEU:HA	7:C:1377:ARG:HB2	1.72	0.70
9:P:352:PHE:HD2	9:P:369:TYR:HD1	1.40	0.70
9:D:32:SER:OG	9:D:250:SER:N	2.18	0.69
6:U:90:LEU:HB2	6:U:95:ARG:HH21	1.56	0.69
1:F:512:PHE:HD2	1:F:528:LEU:HD22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1278:ASN:ND2	13:A:130:ARG:O	2.26	0.69
9:D:269:ASN:ND2	9:D:312:GLU:OE2	2.24	0.69
2:J:547:ILE:HG21	2:J:578:GLU:HG2	1.72	0.69
8:O:96:LEU:HD23	8:O:194:HIS:HB3	1.73	0.69
8:O:368:ILE:HD11	9:D:479:ASP:HB2	1.74	0.69
12:Q:45:ASN:HB3	12:Q:48:LEU:HG	1.74	0.69
8:O:46:SER:HA	8:O:49:ARG:HG3	1.75	0.68
7:C:1099:ILE:HD13	7:C:1134:LEU:HD22	1.74	0.68
7:C:1356:LEU:HD11	7:C:1405:GLU:HG3	1.74	0.68
2:J:476:GLN:HG2	2:J:666:LEU:HD22	1.76	0.68
1:F:463:ILE:O	1:F:468:LYS:NZ	2.25	0.68
9:P:396:ARG:NE	9:P:398:GLU:OE2	2.22	0.68
2:K:563:SER:HA	2:K:595:PHE:HZ	1.59	0.68
1:H:686:LEU:HA	1:H:689:MET:HG2	1.76	0.68
7:C:528:SER:OG	8:O:561:ASP:OD2	2.12	0.68
7:C:905:ILE:HA	7:C:1590:PRO:HB2	1.76	0.68
5:T:464:LEU:HG	5:T:468:ILE:HD12	1.75	0.68
9:P:396:ARG:NH1	10:I:13:TYR:OH	2.27	0.68
6:U:48:TYR:HB3	6:U:64:LEU:HD11	1.75	0.68
8:O:338:PHE:HB3	9:D:480:MET:HE1	1.76	0.68
9:P:608:THR:OG1	9:P:611:GLU:OE1	2.12	0.68
10:I:24:TYR:HB3	10:I:27:TRP:HE1	1.58	0.68
1:F:733:LEU:O	1:F:737:MET:HE2	1.94	0.68
7:C:1051:LEU:HD12	7:C:1081:GLY:HA2	1.75	0.67
13:A:93:SER:HB3	13:A:122:GLN:H	1.58	0.67
7:C:1102:ILE:HG21	7:C:1131:MET:HB2	1.75	0.67
7:C:949:ILE:HG21	7:C:1417:ALA:HB2	1.76	0.67
10:I:99:LEU:HD22	10:I:155:TYR:HE1	1.58	0.67
12:Q:140:GLN:HB2	12:Q:143:SER:HB3	1.75	0.67
2:K:367:LYS:NZ	2:K:398:MET:HG2	2.09	0.67
7:C:1278:ASN:O	7:C:1279:ILE:HG22	1.93	0.67
7:C:1557:LYS:HD3	7:C:1631:ILE:HG21	1.76	0.67
7:C:583:LEU:HB2	7:C:654:PHE:HZ	1.59	0.67
12:Q:542:LYS:HE2	12:Q:545:ASN:HB3	1.77	0.67
1:F:741:PRO:O	1:F:744:ASN:ND2	2.28	0.67
1:H:31:GLN:O	1:H:35:GLN:NE2	2.27	0.67
9:D:387:GLN:HA	10:I:32:LEU:HD11	1.76	0.67
2:K:569:LEU:O	2:K:573:HIS:ND1	2.18	0.67
9:P:121:LEU:HD12	9:P:190:ILE:HG23	1.77	0.67
8:O:50:PRO:HG2	12:Q:420:GLU:HG2	1.77	0.67
11:N:104:TYR:HD1	11:N:107:ARG:HH21	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:668:PRO:O	2:K:673:THR:OG1	2.11	0.66
12:Q:94:SER:HB3	12:Q:167:GLU:HB3	1.77	0.66
12:Q:10:ILE:HG23	12:Q:19:PHE:HB2	1.77	0.66
1:F:642:VAL:HG11	1:F:672:GLN:HE21	1.61	0.66
5:T:537:ARG:NH1	5:T:578:ASP:OD2	2.29	0.66
8:O:325:TYR:OH	8:O:329:LYS:NZ	2.28	0.66
9:D:79:PHE:HB3	9:D:81:LEU:HD23	1.77	0.66
7:C:1038:LYS:HE2	7:C:1070:TYR:HE1	1.59	0.66
12:Q:253:ILE:HG22	12:Q:257:LEU:HD12	1.77	0.66
9:P:255:LEU:HD22	9:P:299:PHE:HZ	1.61	0.66
2:J:756:VAL:HG13	9:P:512:THR:HB	1.78	0.66
5:T:97:GLU:O	5:T:101:GLN:NE2	2.28	0.66
9:D:103:ARG:HH22	9:P:362:ARG:HH11	1.44	0.66
13:A:133:ILE:HA	13:A:221:VAL:HG12	1.78	0.66
5:T:126:ASN:O	5:T:176:ASN:ND2	2.27	0.66
2:J:582:ASP:OD1	2:J:583:GLN:N	2.29	0.65
12:Q:625:ASP:OD1	12:Q:647:LYS:NZ	2.26	0.65
6:U:97:THR:HG21	6:U:122:ARG:HH21	1.60	0.65
7:C:1086:MET:HG3	7:C:1098:LEU:HD11	1.78	0.65
7:C:1373:ASN:O	7:C:1377:ARG:N	2.29	0.65
9:D:226:LYS:HD3	9:D:254:GLU:OE2	1.96	0.65
1:F:492:LEU:O	1:F:496:ASN:HB2	1.97	0.65
1:H:703:VAL:HG12	1:H:712:ALA:HB1	1.78	0.65
8:O:331:THR:HG21	9:D:452:GLU:HB3	1.78	0.65
12:Q:121:PRO:O	12:Q:336:ARG:NH2	2.28	0.65
7:C:454:LEU:HB3	7:C:456:LEU:HD23	1.78	0.65
7:C:1490:HIS:HA	7:C:1493:LYS:HE3	1.78	0.65
10:I:148:ARG:O	10:I:152:GLN:NE2	2.29	0.65
8:O:417:GLU:H	11:N:4:ALA:HB1	1.62	0.65
2:K:721:THR:HG22	2:K:722:LYS:H	1.62	0.65
2:J:523:LEU:HB3	2:J:533:THR:HG22	1.78	0.64
2:J:750:ASN:HD22	3:G:20:ILE:HG13	1.60	0.64
7:C:950:MET:SD	7:C:953:ARG:NH1	2.69	0.64
1:F:646:CYS:HA	1:F:665:TYR:HE1	1.61	0.64
5:T:369:LYS:HE3	5:T:498:LEU:HA	1.78	0.64
2:J:667:ASP:O	2:J:673:THR:OG1	2.14	0.64
5:T:652:ARG:NH2	6:U:60:ASP:OD1	2.31	0.64
5:T:623:SER:O	5:T:625:ASP:N	2.31	0.64
9:D:531:THR:OG1	9:D:534:GLN:NE2	2.30	0.64
2:K:513:LYS:O	2:K:517:PHE:HB2	1.96	0.64
1:H:203:LEU:HD23	1:H:445:ARG:HH12	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:542:MET:HE2	2:J:550:ALA:HB3	1.80	0.64
7:C:35:THR:OG1	7:C:76:GLY:O	2.14	0.64
1:H:198:ARG:HG3	1:H:606:GLN:HE22	1.62	0.64
8:O:324:ASN:CG	9:D:455:ARG:HH21	1.99	0.64
8:O:324:ASN:OD1	9:D:455:ARG:NH2	2.31	0.64
8:O:337:TYR:HD1	8:O:340:ILE:HD12	1.61	0.64
5:T:578:ASP:HB2	6:U:56:LYS:NZ	2.12	0.64
12:Q:299:LEU:HD12	12:Q:405:LEU:HD13	1.79	0.64
2:K:296:ILE:HD12	2:K:299:ARG:HD3	1.80	0.63
8:O:52:LEU:HB2	12:Q:423:LEU:HD11	1.79	0.63
2:K:307:VAL:HG21	2:K:364:LEU:HD11	1.80	0.63
1:H:89:GLN:HA	1:H:92:LYS:HE3	1.80	0.63
5:T:110:TYR:OH	5:T:138:TYR:O	2.16	0.63
1:F:489:ASP:OD1	1:F:490:MET:N	2.32	0.63
5:T:233:TRP:O	5:T:301:THR:OG1	2.16	0.63
5:T:665:ILE:HD12	5:T:667:LEU:HD21	1.80	0.63
7:C:608:ASP:OD1	7:C:609:LEU:N	2.31	0.63
8:O:579:GLU:N	8:O:579:GLU:OE2	2.29	0.63
9:D:301:LEU:HD12	9:D:334:TYR:HE2	1.63	0.63
2:K:288:ARG:NH1	2:K:289:ASN:OD1	2.31	0.63
13:A:68:MET:HA	13:A:71:GLN:CD	2.19	0.63
5:T:49:ASN:OD1	5:T:51:GLN:NE2	2.30	0.63
7:C:1271:LEU:HD13	7:C:1274:ILE:HD11	1.80	0.63
1:H:537:PRO:HB2	4:E:256:HIS:CD2	2.34	0.63
5:T:518:PHE:CE1	5:T:660:LYS:HB3	2.30	0.63
10:I:113:PHE:HB2	10:I:141:ILE:HB	1.80	0.63
7:C:1116:ASP:OD2	7:C:1156:ASN:ND2	2.32	0.62
10:I:34:LEU:HB2	10:I:35:PRO:HD2	1.80	0.62
7:C:1022:ILE:O	7:C:1056:ASN:ND2	2.32	0.62
2:K:585:LEU:HD11	2:K:609:PHE:HE1	1.63	0.62
13:A:31:VAL:HA	13:A:169:MET:HB3	1.79	0.62
5:T:537:ARG:HH21	5:T:574:LEU:HG	1.64	0.62
7:C:811:ALA:N	7:C:1635:GLN:OE1	2.31	0.62
2:K:702:GLU:OE2	1:H:169:HIS:NE2	2.32	0.62
12:Q:236:ILE:HD12	12:Q:239:ILE:HD11	1.79	0.62
1:H:580:GLN:O	1:H:584:HIS:ND1	2.30	0.62
7:C:741:ARG:NH2	7:C:778:THR:OG1	2.30	0.62
8:O:623:PRO:HB2	8:O:660:PHE:HZ	1.65	0.62
2:K:323:ASN:HA	2:K:365:ARG:HH12	1.63	0.62
5:T:387:LEU:HD21	5:T:509:PHE:HE1	1.65	0.62
7:C:774:ASP:OD1	7:C:775:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:142:MET:HG2	13:A:176:ASN:ND2	2.15	0.62
2:J:752:LEU:HD21	9:P:483:TYR:CE1	2.34	0.61
8:O:58:LEU:HD21	8:O:343:LEU:HB2	1.82	0.61
1:F:457:ARG:HH21	4:E:96:PHE:HE2	1.45	0.61
1:H:526:SER:O	1:H:530:ASN:ND2	2.31	0.61
7:C:58:ILE:HG23	7:C:59:GLU:H	1.65	0.61
9:P:481:HIS:O	9:P:484:SER:OG	2.16	0.61
1:F:78:LEU:O	1:F:83:SER:OG	2.15	0.61
1:F:452:SER:OG	1:F:484:GLU:OE2	2.12	0.61
8:O:82:ILE:HD11	8:O:95:ALA:HB1	1.81	0.61
9:D:144:LYS:HG2	9:D:146:THR:HG22	1.81	0.61
1:F:475:LEU:HD21	1:F:497:ARG:HH21	1.65	0.61
1:F:612:TYR:HB2	1:F:644:LEU:HD11	1.82	0.61
2:J:632:ASP:HB3	2:J:635:VAL:HG12	1.83	0.61
5:T:527:GLU:OE2	5:T:531:ARG:NH1	2.32	0.61
1:H:635:ARG:HE	1:H:645:ILE:HD13	1.65	0.61
8:O:347:THR:HG22	8:O:384:TRP:HE1	1.65	0.61
1:H:107:ARG:HD2	1:H:110:LEU:HD21	1.82	0.61
5:T:40:TRP:HA	5:T:49:ASN:HA	1.83	0.61
8:O:338:PHE:HB3	9:D:480:MET:CE	2.30	0.61
7:C:475:LEU:HD21	7:C:491:LEU:HD13	1.81	0.61
9:P:306:GLU:OE2	9:P:463:ARG:NH1	2.34	0.61
11:N:121:PRO:HG2	11:N:124:ILE:HB	1.82	0.61
1:H:444:LEU:HD21	1:H:473:TRP:CH2	2.34	0.61
7:C:480:GLU:O	7:C:488:LYS:N	2.33	0.61
7:C:1090:MET:SD	7:C:1091:LYS:N	2.74	0.61
9:P:515:LYS:HB3	9:P:545:LEU:HD21	1.83	0.61
8:O:258:TRP:HZ2	8:O:311:LYS:HB2	1.65	0.60
2:K:571:PHE:O	2:K:574:THR:OG1	2.15	0.60
8:O:333:ASN:ND2	11:N:91:ASP:O	2.33	0.60
2:J:411:TRP:HZ2	2:J:446:ILE:HD11	1.66	0.60
7:C:54:VAL:HG23	7:C:72:ILE:HD13	1.82	0.60
10:I:108:ASN:OD1	10:I:110:VAL:HG12	2.02	0.60
7:C:588:LEU:O	7:C:614:LYS:NZ	2.23	0.60
7:C:758:LEU:HD23	7:C:760:ASP:H	1.66	0.60
7:C:1587:ILE:HD12	7:C:1591:CYS:HB2	1.83	0.60
9:D:106:PHE:HB2	9:P:361:TYR:HD2	1.66	0.60
10:I:111:VAL:O	10:I:142:THR:HA	2.02	0.60
3:W:4:ARG:HE	3:W:5:ALA:H	1.49	0.60
7:C:1617:THR:HG23	7:C:1619:ASP:H	1.65	0.60
8:O:520:LEU:HD11	8:O:558:LYS:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:419:PHE:HB2	2:J:426:LYS:HE3	1.84	0.60
2:J:447:THR:HA	2:J:450:ASN:HD21	1.67	0.60
7:C:1550:GLU:HG2	7:C:1551:PRO:O	2.02	0.60
1:F:516:LEU:HD11	1:F:524:LYS:HB3	1.84	0.60
8:O:127:TYR:CE1	12:Q:291:ILE:HB	2.36	0.60
5:T:5:ILE:HG13	7:C:1735:GLN:HE22	1.65	0.60
8:O:160:ILE:HD11	11:N:101:SER:HA	1.83	0.60
1:F:735:VAL:HG22	2:J:593:ARG:HG3	1.82	0.60
3:G:12:SER:OG	3:G:14:ASP:OD1	2.19	0.60
1:H:187:LEU:HD23	1:H:189:GLU:H	1.67	0.60
1:H:198:ARG:NH2	1:H:448:SER:O	2.35	0.60
9:P:579:LYS:NZ	9:P:611:GLU:OE2	2.30	0.60
12:Q:357:LEU:HD23	12:Q:359:TYR:H	1.67	0.60
1:H:88:PHE:HB2	1:H:108:CYS:HB3	1.84	0.59
7:C:461:ARG:HG2	7:C:461:ARG:O	2.02	0.59
8:O:320:ASP:OD1	8:O:321:SER:N	2.35	0.59
8:O:338:PHE:C	9:D:480:MET:HE1	2.22	0.59
8:O:409:TYR:HD2	8:O:410:LEU:HD22	1.66	0.59
9:D:256:MET:SD	9:D:302:LYS:HE3	2.41	0.59
2:K:653:LYS:HG3	2:K:684:TYR:HE1	1.67	0.59
2:J:290:ASN:ND2	4:E:100:ASN:OD1	2.35	0.59
12:Q:465:LYS:O	12:Q:469:GLN:NE2	2.35	0.59
13:A:104:ALA:HB2	13:A:113:TRP:HB3	1.83	0.59
8:O:77:ILE:HG22	8:O:79:ASP:H	1.68	0.59
9:D:332:LYS:HB2	9:D:355:ILE:HD11	1.83	0.59
11:N:78:GLU:N	11:N:78:GLU:OE2	2.32	0.59
1:F:171:LYS:HD3	4:E:176:LEU:HD11	1.83	0.59
1:F:741:PRO:HA	1:F:744:ASN:HD21	1.67	0.59
2:J:538:ALA:HB2	2:J:553:TYR:HB3	1.85	0.59
5:T:119:PHE:CD2	7:C:1740:TYR:HD1	2.21	0.59
1:F:710:ALA:HA	1:F:739:LEU:HD13	1.84	0.59
7:C:585:LEU:O	7:C:614:LYS:NZ	2.33	0.59
8:O:422:PHE:CE2	11:N:5:LEU:HD22	2.38	0.59
9:P:519:ILE:HD11	9:P:545:LEU:HD22	1.85	0.59
3:G:14:ASP:OD1	3:G:15:ASP:N	2.35	0.59
2:K:633:PRO:HB3	2:K:663:VAL:HG21	1.85	0.59
5:T:51:GLN:OE1	5:T:53:ARG:NH2	2.28	0.59
9:P:354:ASP:OD1	9:P:355:ILE:N	2.36	0.59
1:H:642:VAL:HG23	1:H:643:VAL:HG23	1.85	0.59
7:C:159:MET:HG2	9:D:520:LYS:HB3	1.83	0.59
1:F:618:ALA:HB3	1:F:627:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:750:ASN:ND2	3:G:20:ILE:HG13	2.17	0.59
2:J:317:ASP:HA	4:E:103:ARG:HB3	1.85	0.58
2:J:427:GLU:O	2:J:431:ASN:ND2	2.36	0.58
3:G:17:THR:O	3:G:20:ILE:HG22	2.03	0.58
6:U:66:ILE:O	6:U:107:ASN:ND2	2.34	0.58
8:O:654:LEU:HD12	8:O:657:ILE:HD11	1.84	0.58
1:F:98:HIS:HB3	1:F:101:ILE:HG13	1.85	0.58
2:K:571:PHE:HE1	2:K:575:TYR:CZ	2.21	0.58
7:C:1420:PRO:O	13:A:27:ASN:ND2	2.36	0.58
9:D:205:ILE:HG13	9:D:206:ASP:H	1.67	0.58
9:P:231:ILE:HG21	9:P:260:GLN:HE22	1.68	0.58
12:Q:63:SER:HA	12:Q:73:ILE:HG22	1.84	0.58
9:P:448:HIS:CD2	11:N:128:MET:HB3	2.38	0.58
9:P:507:GLU:OE2	9:P:541:ARG:NH1	2.36	0.58
10:I:95:ASP:OD1	10:I:96:ASP:N	2.36	0.58
1:F:714:TYR:OH	1:F:746:VAL:HG12	2.03	0.58
2:K:486:CYS:HA	2:K:489:VAL:HG12	1.84	0.58
1:H:177:HIS:O	1:H:190:SER:OG	2.20	0.58
1:H:692:TYR:HA	1:H:695:ALA:HB3	1.84	0.58
12:Q:9:PHE:O	12:Q:10:ILE:HB	2.03	0.58
8:O:161:GLY:HA3	8:O:165:MET:HG2	1.85	0.58
9:P:187:ILE:HA	9:P:190:ILE:HD12	1.84	0.58
13:A:71:GLN:HA	13:A:74:GLU:HG3	1.85	0.58
2:J:466:VAL:HG23	2:J:485:LEU:HD22	1.86	0.58
7:C:208:ARG:HG3	7:C:386:PHE:HE2	1.67	0.58
2:J:304:LEU:HA	2:J:307:VAL:HG22	1.86	0.58
13:A:152:LEU:HD23	13:A:203:PRO:HG2	1.86	0.58
1:F:642:VAL:HG11	1:F:672:GLN:NE2	2.19	0.58
1:F:713:HIS:ND1	1:F:732:GLU:OE2	2.37	0.58
9:D:28:LYS:HB3	9:D:96:PHE:CE2	2.38	0.58
12:Q:291:ILE:HG23	12:Q:295:LEU:HD22	1.86	0.58
1:H:748:ILE:O	1:H:751:LEU:HB2	2.04	0.58
7:C:1626:PHE:HD2	7:C:1630:THR:HA	1.69	0.58
8:O:296:THR:HG21	9:D:456:ARG:NH2	2.19	0.57
13:A:205:ASN:OD1	13:A:212:THR:OG1	2.22	0.57
1:F:436:ILE:HG22	1:F:440:PHE:CE2	2.40	0.57
1:F:561:LYS:O	1:F:564:GLU:HG2	2.04	0.57
1:F:646:CYS:HA	1:F:665:TYR:CE1	2.40	0.57
7:C:381:PRO:HD2	7:C:384:ILE:HD12	1.86	0.57
7:C:568:VAL:HG12	7:C:569:VAL:HG23	1.85	0.57
7:C:985:ILE:HG12	7:C:995:THR:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1329:TYR:OH	13:A:13:LEU:O	2.18	0.57
13:A:93:SER:HA	13:A:122:GLN:HE21	1.70	0.57
7:C:952:LEU:HD11	7:C:1487:ILE:HG13	1.86	0.57
9:D:147:ASP:OD2	9:D:229:LYS:NZ	2.37	0.57
2:J:599:HIS:NE2	2:J:632:ASP:OD2	2.37	0.57
9:P:352:PHE:O	9:P:355:ILE:HG22	2.05	0.57
2:J:754:LEU:HD21	3:G:23:LEU:HG	1.86	0.57
1:H:582:HIS:CE1	13:A:250:ARG:HG3	2.39	0.57
12:Q:78:LYS:HD3	12:Q:81:ARG:HD2	1.87	0.57
12:Q:462:ASP:OD1	12:Q:463:MET:N	2.37	0.57
5:T:221:ILE:HB	5:T:275:PHE:HE1	1.70	0.57
7:C:999:PRO:HB3	7:C:1004:HIS:HB2	1.87	0.57
1:F:670:HIS:HA	4:E:112:LYS:HZ3	1.69	0.57
7:C:1274:ILE:HB	7:C:1279:ILE:HD13	1.86	0.57
7:C:1588:SER:OG	7:C:1591:CYS:SG	2.63	0.57
9:P:242:LEU:HD21	9:P:251:CYS:HB3	1.87	0.57
7:C:526:GLU:O	7:C:531:LYS:NZ	2.39	0.56
8:O:368:ILE:CD1	9:D:479:ASP:HB2	2.34	0.56
10:I:145:ILE:HG23	10:I:146:PHE:CD2	2.40	0.56
1:F:532:LEU:HB3	1:F:542:THR:HG22	1.87	0.56
1:F:557:ASP:OD1	1:F:558:ALA:N	2.37	0.56
9:D:362:ARG:O	9:D:366:LEU:HD23	2.05	0.56
12:Q:515:LEU:HD11	12:Q:536:LEU:HD12	1.87	0.56
1:F:82:LYS:O	1:F:82:LYS:HD3	2.04	0.56
7:C:1384:ASN:O	7:C:1388:ASN:ND2	2.38	0.56
9:D:252:TRP:HB3	9:D:302:LYS:NZ	2.21	0.56
9:P:328:PHE:CE2	9:P:330:PHE:HB3	2.41	0.56
12:Q:125:ARG:HG3	12:Q:138:TYR:HA	1.87	0.56
13:A:114:GLN:HE22	13:A:212:THR:H	1.52	0.56
2:J:302:LEU:HD22	2:J:318:VAL:HG21	1.87	0.56
5:T:164:HIS:CE1	7:C:1732:LEU:HD21	2.40	0.56
7:C:1581:GLU:HG2	7:C:1582:GLU:N	2.21	0.56
8:O:133:ARG:HB2	8:O:140:GLN:HE22	1.71	0.56
1:F:495:PHE:CE2	1:F:512:PHE:HD1	2.24	0.56
8:O:420:ASN:O	8:O:423:SER:OG	2.23	0.56
9:D:16:GLN:HG2	9:D:247:PHE:CE2	2.41	0.56
9:P:328:PHE:HD2	9:P:331:LEU:HG	1.71	0.56
10:I:115:GLY:HA3	10:I:157:ARG:HH12	1.69	0.56
2:J:478:LYS:HB3	2:J:481:GLU:OE1	2.06	0.56
5:T:579:VAL:O	5:T:583:ASP:N	2.32	0.56
9:P:400:CYS:HB2	9:P:423:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:537:PRO:O	1:H:543:TRP:NE1	2.38	0.56
5:T:112:PHE:HA	7:C:1739:TRP:CZ2	2.38	0.56
7:C:707:LEU:HD22	7:C:749:TYR:HD2	1.70	0.56
7:C:1609:TYR:HD1	7:C:1636:ARG:HA	1.68	0.56
9:D:247:PHE:HA	9:D:295:MET:HE1	1.88	0.56
9:P:205:ILE:HG21	9:P:240:LYS:HD2	1.87	0.56
10:I:24:TYR:HB3	10:I:27:TRP:NE1	2.20	0.56
13:A:167:TYR:CD2	13:A:168:LYS:HB2	2.41	0.56
1:F:675:SER:OG	1:F:678:SER:OG	2.23	0.56
1:H:696:LEU:HD11	1:H:723:VAL:HG21	1.88	0.56
5:T:197:ILE:HG22	5:T:201:LYS:NZ	2.20	0.56
7:C:1173:ILE:HG22	7:C:1249:ILE:HG12	1.87	0.56
7:C:1681:THR:HG23	7:C:1684:GLN:H	1.71	0.56
8:O:331:THR:HA	9:D:448:HIS:HB3	1.88	0.56
2:J:619:GLU:HB2	2:J:642:MET:HE1	1.87	0.55
2:K:608:GLN:HG2	2:K:612:MET:SD	2.46	0.55
7:C:48:SER:OG	7:C:50:ASP:O	2.24	0.55
7:C:860:ILE:HG12	12:Q:122:LYS:O	2.06	0.55
7:C:1252:MET:SD	7:C:1292:ALA:HA	2.46	0.55
8:O:107:GLY:HA3	9:P:384:TYR:HE1	1.71	0.55
13:A:109:TYR:O	13:A:215:ARG:NH2	2.38	0.55
2:J:658:LYS:O	2:J:661:GLU:HG2	2.05	0.55
2:K:600:LEU:HD13	3:W:1:MET:HG2	1.87	0.55
2:K:671:ARG:HD2	2:K:671:ARG:O	2.06	0.55
7:C:1366:TYR:CD1	7:C:1387:THR:HG21	2.42	0.55
9:D:413:HIS:HB2	9:D:444:LEU:HD21	1.87	0.55
5:T:505:PHE:HE2	5:T:536:ILE:HG12	1.71	0.55
7:C:588:LEU:HD11	7:C:657:PHE:HZ	1.72	0.55
7:C:1368:TYR:H	7:C:1380:ILE:HD11	1.70	0.55
9:D:406:TYR:OH	9:D:410:ARG:NH1	2.39	0.55
12:Q:422:ASP:OD1	12:Q:424:TYR:N	2.39	0.55
12:Q:422:ASP:HB3	12:Q:425:PHE:HB2	1.88	0.55
9:P:252:TRP:HZ3	9:P:295:MET:HB3	1.70	0.55
5:T:576:SER:HB2	5:T:613:TYR:HB3	1.88	0.55
7:C:944:LYS:NZ	7:C:1001:ASP:OD1	2.29	0.55
7:C:1510:GLN:HA	7:C:1592:LEU:HD11	1.87	0.55
9:D:259:LEU:HD21	9:D:265:ALA:HB2	1.88	0.55
9:P:529:SER:HB2	9:P:535:ASN:HD21	1.72	0.55
7:C:583:LEU:HB2	7:C:654:PHE:CZ	2.41	0.55
12:Q:496:SER:HA	12:Q:520:LYS:HA	1.88	0.55
12:Q:556:LYS:NZ	12:Q:557:ILE:O	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:68:MET:HA	13:A:71:GLN:NE2	2.21	0.55
13:A:99:ASN:ND2	13:A:112:PHE:O	2.40	0.55
1:F:76:LEU:HD23	1:F:80:LEU:HD23	1.87	0.55
2:K:362:CYS:HA	2:K:365:ARG:HE	1.72	0.55
1:H:737:MET:HE1	1:H:751:LEU:HD11	1.87	0.55
7:C:492:TYR:HD2	7:C:499:THR:HB	1.70	0.55
8:O:133:ARG:HH12	8:O:135:THR:HG1	1.53	0.55
10:I:34:LEU:HD11	10:I:37:GLU:OE2	2.06	0.55
10:I:145:ILE:HG13	10:I:146:PHE:H	1.72	0.55
1:F:748:ILE:O	1:F:752:GLN:HG2	2.06	0.55
2:J:447:THR:HA	2:J:450:ASN:ND2	2.22	0.55
7:C:598:TYR:HA	7:C:605:TYR:HE2	1.71	0.55
8:O:355:CYS:HB3	8:O:395:TYR:CE2	2.42	0.55
9:P:427:ASP:O	9:P:428:LYS:HG2	2.07	0.55
10:I:141:ILE:HD11	10:I:157:ARG:NH1	2.22	0.55
2:K:391:LYS:HG2	2:K:422:PHE:HE1	1.72	0.55
2:K:575:TYR:HB3	2:K:584:ALA:HB2	1.89	0.55
7:C:208:ARG:HG3	7:C:386:PHE:CE2	2.42	0.55
8:O:51:SER:OG	12:Q:420:GLU:OE2	2.24	0.55
9:P:205:ILE:HD11	9:P:244:CYS:HB2	1.89	0.55
9:P:412:GLU:HG3	9:P:415:LYS:HB2	1.89	0.55
9:P:427:ASP:HB2	9:P:430:THR:HG22	1.89	0.55
9:P:539:TYR:HE2	9:P:565:VAL:HG21	1.72	0.55
10:I:111:VAL:CG2	10:I:145:ILE:HB	2.37	0.55
12:Q:499:ASN:HB3	12:Q:517:GLN:HB3	1.87	0.55
1:F:38:ILE:HD11	1:F:46:ALA:HB3	1.89	0.54
7:C:583:LEU:HD23	7:C:586:LEU:HD12	1.89	0.54
7:C:1225:LEU:HA	7:C:1228:VAL:HG12	1.88	0.54
7:C:1368:TYR:OH	13:A:21:PRO:HD2	2.08	0.54
9:P:455:ARG:HH12	11:N:122:ILE:HG12	1.71	0.54
10:I:111:VAL:HG21	10:I:145:ILE:HB	1.89	0.54
1:F:660:LYS:HE2	4:E:212:LEU:HB3	1.90	0.54
2:K:648:GLU:HB3	2:K:651:LYS:HZ1	1.71	0.54
1:H:75:ALA:HB1	1:H:104:ILE:HG21	1.89	0.54
4:E:102:LEU:HD23	4:E:107:ILE:HD13	1.88	0.54
5:T:128:LEU:O	5:T:131:ILE:HG22	2.07	0.54
7:C:580:SER:HA	7:C:654:PHE:CE1	2.42	0.54
10:I:100:PHE:HA	10:I:103:MET:HB2	1.89	0.54
2:K:303:GLY:O	2:K:307:VAL:HG23	2.07	0.54
1:H:537:PRO:HB2	4:E:256:HIS:HD2	1.72	0.54
1:H:645:ILE:HG21	1:H:668:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:628:ILE:HB	12:Q:645:PHE:HB2	1.88	0.54
13:A:68:MET:HA	13:A:71:GLN:OE1	2.08	0.54
1:H:187:LEU:HD22	1:H:190:SER:H	1.73	0.54
6:U:82:LEU:HB3	6:U:121:ARG:NH2	2.22	0.54
7:C:1387:THR:HA	7:C:1390:ILE:HG12	1.89	0.54
8:O:110:SER:HA	8:O:113:ARG:HG3	1.88	0.54
9:D:384:TYR:HD2	9:D:385:LEU:HD22	1.73	0.54
12:Q:118:ASP:OD1	12:Q:119:ASP:N	2.40	0.54
2:K:616:ASN:OD1	2:K:617:LEU:N	2.40	0.54
7:C:1133:MET:HA	7:C:1177:LEU:HD22	1.89	0.54
9:P:509:TYR:CE2	9:P:517:GLU:HB3	2.43	0.54
12:Q:253:ILE:HG21	12:Q:325:ILE:HG21	1.90	0.54
5:T:312:PHE:HA	5:T:315:TYR:CD2	2.42	0.54
8:O:127:TYR:CZ	12:Q:291:ILE:HB	2.43	0.54
12:Q:439:LYS:O	12:Q:442:THR:OG1	2.25	0.54
1:H:733:LEU:O	1:H:737:MET:HE2	2.08	0.54
7:C:404:ARG:HA	7:C:409:GLU:HA	1.90	0.54
8:O:29:SER:O	8:O:30:GLN:HG3	2.07	0.54
8:O:294:ASP:O	8:O:298:PHE:N	2.40	0.54
9:P:242:LEU:HG	9:P:252:TRP:HE1	1.73	0.54
1:F:527:ASN:ND2	2:K:518:LEU:HD21	2.23	0.54
1:F:669:CYS:SG	1:F:679:LYS:HD3	2.48	0.54
1:H:455:ALA:HB3	1:H:481:LEU:HD21	1.88	0.54
5:T:128:LEU:HG	5:T:132:GLN:HE22	1.72	0.54
7:C:951:ALA:HB2	7:C:996:VAL:HG21	1.89	0.54
9:P:479:ASP:OD1	9:P:480:MET:N	2.41	0.54
1:F:727:LYS:O	1:F:731:LYS:NZ	2.41	0.54
7:C:647:GLU:HA	7:C:650:LEU:HB2	1.90	0.54
7:C:500:SER:HB2	7:C:551:PHE:CG	2.43	0.54
8:O:247:LEU:HD11	8:O:287:LEU:HD21	1.89	0.54
9:P:111:VAL:HG12	9:P:113:ASN:H	1.73	0.54
9:P:431:THR:O	9:P:433:ALA:N	2.39	0.53
13:A:113:TRP:CZ2	13:A:115:SER:HB3	2.44	0.53
2:K:313:ASP:OD1	2:K:314:ASP:N	2.39	0.53
1:H:478:LEU:HD22	1:H:494:TYR:HD2	1.73	0.53
7:C:1589:THR:HB	7:C:1590:PRO:HD3	1.90	0.53
12:Q:428:ASP:OD1	12:Q:429:LEU:N	2.41	0.53
2:J:588:TYR:OH	3:G:4:ARG:NH2	2.41	0.53
9:D:187:ILE:HG23	9:D:224:ILE:HD11	1.89	0.53
9:P:223:VAL:HG21	10:I:9:SER:HB2	1.89	0.53
9:P:352:PHE:HD2	9:P:369:TYR:CD1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:575:ASN:O	6:U:56:LYS:NZ	2.42	0.53
8:O:109:ASP:OD1	8:O:110:SER:N	2.40	0.53
9:D:14:ARG:HE	9:D:43:LEU:HD22	1.74	0.53
2:K:685:ARG:NH2	3:W:11:LEU:HA	2.23	0.53
1:H:161:GLY:O	1:H:165:MET:HG2	2.08	0.53
7:C:1263:ILE:HG12	7:C:1266:MET:HE2	1.90	0.53
8:O:343:LEU:O	8:O:347:THR:HG23	2.09	0.53
10:I:98:ASN:HA	10:I:101:ASN:ND2	2.24	0.53
13:A:74:GLU:O	13:A:78:SER:N	2.41	0.53
13:A:132:ASP:HB3	13:A:192:LEU:HD13	1.89	0.53
2:J:634:LEU:HD21	3:G:3:ARG:HD2	1.90	0.53
2:K:514:ASN:OD1	2:K:515:LYS:N	2.42	0.53
1:H:157:ASN:HB2	1:H:180:ALA:HB2	1.91	0.53
8:O:336:ASN:HB3	8:O:372:ASN:HD21	1.74	0.53
8:O:356:ASP:OD1	8:O:357:ALA:N	2.42	0.53
9:P:551:ASP:HB3	9:P:554:GLU:HB2	1.90	0.53
12:Q:75:ASP:OD2	12:Q:78:LYS:N	2.42	0.53
1:F:200:THR:OG1	1:F:445:ARG:NH1	2.41	0.53
2:J:514:ASN:OD1	9:D:384:TYR:HD1	1.91	0.53
2:J:729:ASP:OD1	2:J:729:ASP:N	2.40	0.53
7:C:956:THR:HG23	7:C:1498:ASN:HD21	1.74	0.53
9:D:417:ILE:HD13	9:D:440:GLU:HB2	1.89	0.53
12:Q:497:GLN:N	12:Q:519:THR:O	2.41	0.53
13:A:80:ARG:HH12	13:A:223:SER:H	1.57	0.53
1:F:41:LEU:O	1:F:41:LEU:HD23	2.09	0.53
5:T:510:ARG:CZ	5:T:573:ASN:HA	2.39	0.53
8:O:435:VAL:HG13	8:O:582:ASP:HA	1.90	0.53
9:D:106:PHE:HB2	9:P:361:TYR:CD2	2.44	0.53
9:D:498:ASP:HB3	9:D:501:ILE:HG22	1.90	0.53
13:A:81:MET:SD	13:A:220:TYR:HB3	2.48	0.53
13:A:114:GLN:NE2	13:A:211:ASP:HB3	2.24	0.53
2:J:432:LEU:HD12	2:J:435:ILE:HD12	1.91	0.53
2:J:515:LYS:O	2:J:518:LEU:HG	2.09	0.53
3:W:10:GLN:OE1	3:W:10:GLN:N	2.42	0.53
7:C:67:THR:H	8:O:316:GLN:NE2	2.05	0.53
8:O:51:SER:HB3	11:N:90:LEU:HD21	1.90	0.53
12:Q:298:TRP:HE3	12:Q:299:LEU:HD22	1.74	0.53
12:Q:410:ASP:O	12:Q:411:GLU:HG2	2.08	0.53
2:J:310:GLN:OE1	10:I:152:GLN:NE2	2.42	0.53
2:J:752:LEU:HB3	9:P:482:LEU:HD21	1.91	0.53
1:H:471:MET:HB3	1:H:474:CYS:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:694:VAL:O	1:H:697:GLN:HG3	2.09	0.53
4:E:249:LEU:HA	4:E:252:LYS:HE2	1.91	0.53
6:U:68:LEU:HD12	6:U:99:GLN:HB2	1.90	0.53
6:U:87:SER:O	6:U:95:ARG:NH2	2.42	0.53
9:D:91:LEU:HD13	9:P:38:GLU:HA	1.89	0.53
13:A:129:LYS:HB2	13:A:131:MET:SD	2.49	0.53
1:H:490:MET:HA	1:H:493:LYS:NZ	2.24	0.52
7:C:206:LEU:HD11	7:C:380:LEU:HD11	1.91	0.52
7:C:950:MET:SD	7:C:953:ARG:HD3	2.49	0.52
2:J:749:LYS:O	2:J:752:LEU:HB2	2.09	0.52
1:H:703:VAL:HG21	1:H:716:LEU:HD22	1.89	0.52
7:C:166:SER:HB2	7:C:371:VAL:HG12	1.92	0.52
7:C:431:ASP:OD1	7:C:432:VAL:N	2.41	0.52
8:O:18:LEU:O	8:O:22:ILE:HG12	2.10	0.52
13:A:106:ASP:OD2	13:A:111:THR:OG1	2.21	0.52
1:H:107:ARG:O	1:H:110:LEU:HG	2.08	0.52
5:T:185:ILE:HG21	5:T:216:ALA:HB1	1.90	0.52
5:T:649:LYS:NZ	6:U:60:ASP:OD2	2.32	0.52
7:C:109:CYS:SG	7:C:110:PHE:N	2.81	0.52
7:C:1132:GLY:HA2	7:C:1178:ILE:HD11	1.92	0.52
9:D:247:PHE:HA	9:D:295:MET:CE	2.38	0.52
11:N:135:ARG:HH12	11:N:139:ARG:HD2	1.75	0.52
1:F:167:LEU:CD2	1:F:168:ASP:HB2	2.40	0.52
2:K:622:PHE:CE2	2:K:638:GLU:HB3	2.45	0.52
9:D:238:PHE:HB3	9:D:255:LEU:HD12	1.91	0.52
12:Q:101:ILE:HD13	12:Q:224:LEU:HD21	1.91	0.52
2:J:286:ILE:HB	2:J:302:LEU:HD12	1.90	0.52
7:C:762:VAL:HA	7:C:765:ILE:HD12	1.92	0.52
7:C:824:ARG:NH1	7:C:1620:TYR:HB3	2.25	0.52
7:C:1264:SER:O	7:C:1268:LYS:N	2.34	0.52
7:C:1731:ILE:O	7:C:1735:GLN:HG3	2.10	0.52
9:D:498:ASP:OD1	9:D:500:ARG:HG2	2.09	0.52
2:J:621:TYR:HA	2:J:624:LEU:HD12	1.92	0.52
2:K:316:LEU:HG	2:K:368:ILE:HG21	1.90	0.52
5:T:198:GLN:HA	5:T:201:LYS:HG2	1.91	0.52
5:T:332:ASN:HB3	5:T:335:VAL:HG23	1.90	0.52
5:T:587:SER:HB3	5:T:607:LYS:HA	1.92	0.52
7:C:88:VAL:HG23	7:C:97:VAL:HG22	1.90	0.52
7:C:404:ARG:HH12	7:C:428:LEU:HD12	1.75	0.52
7:C:1523:PHE:HA	7:C:1526:MET:HG2	1.91	0.52
12:Q:8:TYR:HA	12:Q:644:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:20:ILE:O	3:G:24:ASN:ND2	2.43	0.52
1:H:502:GLN:HE21	1:H:505:ARG:HD3	1.75	0.52
7:C:1392:VAL:O	7:C:1396:MET:HG2	2.10	0.52
3:W:27:LYS:HA	3:W:30:GLN:HE22	1.74	0.52
8:O:123:LEU:HD11	8:O:143:ARG:HD2	1.92	0.52
9:D:121:LEU:HD21	9:D:193:GLU:HG2	1.91	0.52
12:Q:297:ASP:OD1	12:Q:301:ASN:ND2	2.28	0.52
1:F:161:GLY:HA2	1:F:173:GLY:HA2	1.92	0.52
2:K:468:SER:O	2:K:472:ILE:HG12	2.10	0.52
1:H:565:LYS:O	1:H:568:GLN:HG3	2.09	0.52
8:O:179:VAL:HA	8:O:182:HIS:CE1	2.45	0.52
12:Q:27:LEU:HB2	12:Q:41:ILE:HB	1.90	0.52
2:J:379:ARG:HG2	2:J:383:ARG:HH12	1.74	0.52
2:J:718:TYR:CB	2:J:727:ALA:HB2	2.40	0.52
7:C:1514:ASN:N	7:C:1548:ALA:O	2.43	0.52
9:P:118:PHE:CE2	9:P:216:LEU:HD23	2.45	0.52
12:Q:492:LYS:HD2	12:Q:548:ILE:HD13	1.91	0.52
13:A:142:MET:HE1	13:A:174:ASN:HB2	1.91	0.52
2:J:559:ILE:HD12	10:I:103:MET:HE1	1.92	0.51
1:H:172:GLU:HA	1:H:175:PHE:CD2	2.45	0.51
7:C:782:GLY:H	7:C:1722:LEU:HD12	1.74	0.51
2:K:733:LYS:O	2:K:737:LEU:HG	2.10	0.51
1:H:43:TYR:CE2	1:H:80:LEU:HB3	2.45	0.51
5:T:510:ARG:NH2	5:T:572:SER:O	2.42	0.51
8:O:62:SER:O	8:O:461:GLN:NE2	2.41	0.51
9:P:488:PHE:HB3	9:P:505:LEU:HD12	1.92	0.51
12:Q:387:LEU:HD21	12:Q:448:ILE:HG22	1.92	0.51
2:K:363:PHE:CE1	2:K:394:GLU:HB3	2.45	0.51
2:K:444:GLU:O	2:K:447:THR:OG1	2.20	0.51
1:F:714:TYR:CE1	1:F:747:ILE:HG12	2.41	0.51
1:H:565:LYS:HZ3	1:H:569:LEU:HD21	1.74	0.51
7:C:626:ARG:HH21	7:C:727:LEU:HB2	1.74	0.51
7:C:952:LEU:O	7:C:956:THR:HG22	2.10	0.51
9:D:9:ILE:O	9:D:13:ILE:HG12	2.10	0.51
12:Q:129:ASP:OD1	12:Q:131:LYS:N	2.43	0.51
1:H:89:GLN:HA	1:H:92:LYS:HG2	1.90	0.51
7:C:37:LYS:HG3	7:C:41:ILE:HB	1.91	0.51
7:C:664:TRP:NE1	7:C:695:HIS:HB3	2.25	0.51
7:C:734:VAL:HG22	7:C:737:ARG:HH22	1.75	0.51
12:Q:561:PHE:HD2	12:Q:628:ILE:HD13	1.74	0.51
2:J:464:ASP:OD1	2:J:465:VAL:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:GLN:O	1:H:92:LYS:HG2	2.11	0.51
5:T:515:ASP:O	5:T:518:PHE:HB3	2.11	0.51
5:T:610:SER:O	5:T:614:TRP:HD1	1.94	0.51
11:N:108:LEU:HB3	11:N:109:PRO:HD3	1.93	0.51
2:K:665:ASP:OD1	2:K:665:ASP:N	2.41	0.51
2:K:716:TYR:CZ	3:W:19:LEU:HD13	2.46	0.51
1:H:81:ASN:OD1	1:H:83:SER:OG	2.15	0.51
1:H:84:TYR:CD1	1:H:111:GLN:HG2	2.46	0.51
9:D:27:TRP:CH2	9:D:115:TYR:HB3	2.45	0.51
2:J:479:PHE:O	2:J:482:CYS:HB3	2.10	0.51
2:J:483:LEU:HD12	2:J:484:GLU:N	2.26	0.51
2:K:516:LEU:HD12	2:K:519:LEU:HD11	1.92	0.51
7:C:1166:GLU:HG2	7:C:1537:PRO:HB3	1.92	0.51
9:D:526:ILE:HD11	9:D:535:ASN:HB3	1.93	0.51
11:N:133:MET:O	11:N:137:ARG:HG2	2.10	0.51
12:Q:6:ASN:ND2	12:Q:618:ILE:O	2.44	0.51
12:Q:389:ARG:O	12:Q:392:THR:OG1	2.17	0.51
2:K:615:LEU:HD21	2:K:645:LYS:HB2	1.93	0.51
3:W:23:LEU:O	3:W:27:LYS:HG2	2.09	0.51
5:T:467:TYR:OH	7:C:928:GLN:HB2	2.11	0.51
7:C:80:PHE:CD2	7:C:158:PRO:HD3	2.46	0.51
7:C:194:PHE:CG	7:C:195:PRO:HD2	2.45	0.51
7:C:1096:SER:HA	7:C:1099:ILE:HG22	1.92	0.51
13:A:44:LYS:HZ2	13:A:50:GLY:HA2	1.76	0.51
2:J:321:GLU:O	2:J:365:ARG:HD3	2.10	0.50
2:K:706:LYS:NZ	2:K:737:LEU:HD22	2.26	0.50
7:C:1534:THR:OG1	13:A:162:SER:O	2.29	0.50
9:D:448:HIS:O	9:D:451:ILE:HG12	2.11	0.50
9:P:39:ALA:HA	9:P:328:PHE:HE1	1.77	0.50
7:C:575:GLU:HG2	7:C:576:HIS:N	2.26	0.50
7:C:1099:ILE:HD11	7:C:1131:MET:HG2	1.93	0.50
7:C:1576:GLU:HG2	7:C:1583:VAL:HG12	1.92	0.50
8:O:133:ARG:NH1	8:O:133:ARG:HA	2.26	0.50
8:O:209:SER:HA	8:O:213:GLN:HG3	1.94	0.50
8:O:316:GLN:OE1	8:O:316:GLN:N	2.44	0.50
12:Q:551:LYS:NZ	12:Q:552:GLU:O	2.42	0.50
2:J:541:TYR:HB2	2:J:550:ALA:HB2	1.93	0.50
2:J:748:LEU:O	2:J:752:LEU:HD13	2.10	0.50
4:E:116:ALA:HA	4:E:119:CYS:HB2	1.91	0.50
9:D:536:THR:HG22	9:D:576:GLU:HG2	1.92	0.50
12:Q:124:ILE:HD12	12:Q:135:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:183:PHE:O	12:Q:477:GLN:NE2	2.44	0.50
12:Q:246:MET:CE	12:Q:330:PHE:HA	2.41	0.50
2:J:718:TYR:HB2	2:J:727:ALA:HB2	1.93	0.50
2:J:750:ASN:ND2	3:G:23:LEU:HD23	2.25	0.50
2:K:716:TYR:HE1	3:W:16:VAL:HA	1.76	0.50
5:T:633:ASP:OD2	5:T:634:LEU:N	2.44	0.50
7:C:1475:SER:O	7:C:1478:THR:OG1	2.27	0.50
8:O:591:ILE:HA	8:O:594:ILE:HD12	1.94	0.50
9:P:464:ASP:OD2	9:P:467:ALA:N	2.43	0.50
10:I:37:GLU:HG2	10:I:38:VAL:N	2.26	0.50
12:Q:35:HIS:NE2	12:Q:582:ASP:HB3	2.26	0.50
1:F:43:TYR:CG	1:F:80:LEU:HD13	2.47	0.50
1:F:672:GLN:HE22	1:F:675:SER:CB	2.24	0.50
1:F:716:LEU:HB3	1:F:732:GLU:HG2	1.93	0.50
7:C:996:VAL:HG13	7:C:1001:ASP:HB2	1.92	0.50
7:C:1249:ILE:HA	7:C:1252:MET:HB2	1.92	0.50
8:O:50:PRO:HA	8:O:245:GLN:HG2	1.92	0.50
9:P:39:ALA:HA	9:P:328:PHE:CE1	2.45	0.50
9:P:304:PHE:CE1	9:P:311:LEU:HA	2.46	0.50
12:Q:19:PHE:CZ	12:Q:30:TYR:HB2	2.46	0.50
12:Q:182:VAL:HG13	12:Q:473:ASN:HD22	1.77	0.50
2:J:481:GLU:HA	2:J:484:GLU:HG3	1.94	0.50
2:K:435:ILE:O	2:K:439:LYS:NZ	2.37	0.50
1:H:90:ILE:HA	1:H:93:GLU:OE1	2.11	0.50
1:H:206:VAL:HG13	1:H:207:PHE:HD1	1.77	0.50
1:H:714:TYR:HE1	1:H:750:GLU:HG3	1.76	0.50
7:C:524:TYR:CG	7:C:525:PRO:HD2	2.46	0.50
7:C:1344:ALA:HB3	7:C:1515:THR:HG21	1.93	0.50
9:D:97:ASP:OD1	9:D:97:ASP:N	2.45	0.50
9:D:482:LEU:O	9:D:485:LEU:HG	2.12	0.50
2:J:693:ALA:O	2:J:697:PHE:HD1	1.95	0.50
8:O:108:LEU:HD11	8:O:166:ARG:HB3	1.94	0.50
9:D:268:LEU:HD11	9:D:299:PHE:HZ	1.76	0.50
1:F:529:ALA:HB1	1:F:546:ILE:HD13	1.93	0.50
2:J:431:ASN:O	2:J:435:ILE:HG13	2.10	0.50
2:J:609:PHE:HA	2:J:612:MET:CE	2.42	0.50
5:T:606:PRO:HG3	5:T:641:TYR:CD2	2.47	0.50
7:C:1145:ASP:OD1	7:C:1146:SER:N	2.44	0.50
8:O:386:ILE:HB	8:O:428:PHE:CE2	2.47	0.50
9:P:44:ALA:HB2	9:P:326:PRO:HG2	1.94	0.50
12:Q:342:GLU:OE2	12:Q:345:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:783:ILE:HD12	7:C:783:ILE:H	1.77	0.50
8:O:162:ASP:O	8:O:165:MET:HG3	2.11	0.50
8:O:547:ASN:O	8:O:551:LEU:N	2.43	0.50
2:J:663:VAL:O	2:J:663:VAL:HG12	2.11	0.49
2:K:246:TYR:CZ	2:K:275:ASN:HB3	2.46	0.49
1:H:86:THR:O	1:H:90:ILE:HG12	2.12	0.49
5:T:155:TRP:O	5:T:159:LEU:HD23	2.11	0.49
7:C:1490:HIS:O	7:C:1493:LYS:HG2	2.12	0.49
8:O:394:GLU:HG3	8:O:395:TYR:CD1	2.46	0.49
8:O:587:PHE:HE1	8:O:629:LEU:HD11	1.76	0.49
9:P:370:SER:HB2	9:P:402:ILE:HG13	1.94	0.49
11:N:81:TYR:CZ	11:N:83:PRO:HA	2.47	0.49
2:J:257:TYR:CZ	2:J:266:ALA:HB2	2.47	0.49
7:C:76:GLY:HA3	7:C:88:VAL:HG12	1.94	0.49
7:C:1139:ARG:NH2	7:C:1181:GLY:O	2.41	0.49
7:C:1292:ALA:O	7:C:1296:ILE:HG12	2.12	0.49
7:C:1581:GLU:HG2	7:C:1582:GLU:H	1.77	0.49
8:O:611:ILE:HD13	8:O:614:ILE:HD12	1.94	0.49
12:Q:498:ILE:HD11	12:Q:516:ILE:HB	1.94	0.49
2:K:234:ARG:HG2	2:K:237:ARG:HH12	1.78	0.49
5:T:468:ILE:HG12	7:C:1412:TYR:HB2	1.95	0.49
7:C:744:LYS:O	7:C:748:LEU:HG	2.12	0.49
7:C:975:GLN:NE2	7:C:976:LYS:O	2.45	0.49
8:O:54:TRP:HZ3	8:O:303:ILE:HD13	1.77	0.49
8:O:87:ASP:OD1	8:O:88:ASP:N	2.45	0.49
8:O:168:THR:HA	8:O:171:ILE:HG22	1.94	0.49
12:Q:246:MET:HE3	12:Q:330:PHE:HA	1.93	0.49
2:J:470:VAL:HG11	2:J:499:ILE:HD11	1.94	0.49
2:J:523:LEU:HD12	2:J:533:THR:HG22	1.93	0.49
2:K:428:ILE:HD12	2:K:457:TYR:CD1	2.48	0.49
2:K:472:ILE:O	2:K:475:THR:OG1	2.30	0.49
2:K:531:ALA:HB2	2:K:560:LEU:HB2	1.94	0.49
1:H:194:ILE:HA	1:H:197:MET:HG2	1.94	0.49
1:H:574:ALA:HB2	1:H:603:CYS:HB3	1.93	0.49
5:T:170:ASN:OD1	5:T:172:LYS:HG2	2.12	0.49
8:O:76:PRO:HG3	8:O:242:ILE:CG2	2.42	0.49
9:D:523:LYS:O	9:D:526:ILE:HG22	2.11	0.49
1:H:512:PHE:CE2	1:H:516:LEU:HD22	2.48	0.49
7:C:945:TYR:O	7:C:949:ILE:HG12	2.11	0.49
7:C:1248:VAL:HG11	7:C:1288:TYR:HB3	1.94	0.49
9:D:403:ILE:HD12	9:D:419:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:458:VAL:HG21	9:D:468:TRP:CE2	2.48	0.49
9:P:43:LEU:HD13	9:P:325:PHE:CE1	2.46	0.49
12:Q:349:GLN:O	12:Q:352:SER:OG	2.20	0.49
2:J:547:ILE:CD1	2:J:577:LEU:HB2	2.42	0.49
2:K:599:HIS:HB3	2:K:628:ILE:HD11	1.93	0.49
1:H:79:PHE:CZ	1:H:107:ARG:HB3	2.46	0.49
7:C:133:SER:C	9:D:267:LEU:HG	2.32	0.49
7:C:1252:MET:HE3	7:C:1295:MET:HG2	1.94	0.49
7:C:1414:HIS:HE1	7:C:1498:ASN:OD1	1.95	0.49
8:O:354:GLU:O	8:O:356:ASP:N	2.46	0.49
1:F:168:ASP:HB3	1:F:169:HIS:CD2	2.48	0.49
1:F:461:SER:OG	1:F:462:GLN:OE1	2.28	0.49
1:F:495:PHE:HE2	1:F:512:PHE:HD1	1.61	0.49
1:F:718:GLN:O	1:F:721:ARG:HG3	2.12	0.49
2:J:459:LEU:HD21	2:K:259:ILE:HG12	1.95	0.49
2:J:685:ARG:HH11	2:J:685:ARG:HG2	1.77	0.49
5:T:365:THR:O	5:T:369:LYS:HG2	2.12	0.49
6:U:90:LEU:HB2	6:U:95:ARG:HE	1.77	0.49
7:C:867:ILE:HB	8:O:426:TYR:OH	2.13	0.49
7:C:1309:MET:HG2	13:A:6:ILE:HG23	1.95	0.49
8:O:175:ASN:O	8:O:179:VAL:HG23	2.13	0.49
1:F:665:TYR:CZ	1:F:681:LYS:HG2	2.48	0.49
2:K:296:ILE:HG23	2:K:357:MET:HG2	1.94	0.49
5:T:181:LEU:HD13	5:T:196:LEU:HD22	1.94	0.49
7:C:803:ASP:OD2	7:C:804:ASN:N	2.43	0.49
7:C:1495:ILE:HD11	7:C:1542:LYS:HG3	1.95	0.49
1:F:24:LEU:HD23	1:F:24:LEU:H	1.78	0.49
1:F:476:VAL:O	1:F:480:LYS:HG2	2.13	0.49
2:J:355:ILE:HD11	2:K:236:TRP:HE1	1.77	0.49
9:P:526:ILE:HD13	9:P:539:TYR:CE1	2.48	0.49
7:C:461:ARG:HH11	7:C:482:GLN:HG2	1.78	0.49
10:I:7:ARG:O	10:I:12:GLN:NE2	2.38	0.49
2:J:514:ASN:HD22	9:D:387:GLN:HB3	1.78	0.48
6:U:52:CYS:HG	6:U:54:SER:HG	1.61	0.48
9:D:23:GLU:O	9:D:27:TRP:N	2.45	0.48
12:Q:249:HIS:HB3	12:Q:325:ILE:HD11	1.95	0.48
1:F:191:TYR:HD1	1:F:444:LEU:HD23	1.78	0.48
7:C:1252:MET:CE	7:C:1295:MET:HG2	2.42	0.48
8:O:7:LEU:HD23	8:O:8:GLY:N	2.26	0.48
8:O:344:SER:O	8:O:347:THR:OG1	2.24	0.48
9:D:422:ARG:HD3	10:I:27:TRP:CZ2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:457:ALA:O	9:D:460:ILE:HG22	2.13	0.48
9:P:417:ILE:HG23	9:P:437:MET:SD	2.53	0.48
9:P:509:TYR:HD2	9:P:518:ALA:HB2	1.77	0.48
9:P:622:CYS:HB3	9:P:626:MET:HE3	1.94	0.48
12:Q:71:ILE:HB	12:Q:86:LEU:HB2	1.95	0.48
13:A:127:PHE:HZ	13:A:219:LEU:HD13	1.77	0.48
2:K:648:GLU:HB3	2:K:651:LYS:NZ	2.28	0.48
1:H:577:TYR:HD1	1:H:599:LYS:HZ3	1.60	0.48
5:T:49:ASN:ND2	5:T:137:TYR:OH	2.47	0.48
5:T:623:SER:O	5:T:623:SER:OG	2.29	0.48
7:C:1541:LEU:HD13	7:C:1544:PHE:CE2	2.49	0.48
9:P:426:LEU:HD21	10:I:22:ILE:HD13	1.95	0.48
10:I:98:ASN:HD22	10:I:101:ASN:HD21	1.61	0.48
12:Q:392:THR:O	12:Q:396:LYS:HG2	2.13	0.48
13:A:130:ARG:NH2	13:A:194:LYS:HE3	2.28	0.48
2:K:262:ASP:N	2:K:262:ASP:OD1	2.46	0.48
2:K:500:LEU:HD22	2:K:532:ILE:CG2	2.43	0.48
2:K:632:ASP:OD1	2:K:632:ASP:N	2.46	0.48
5:T:463:ILE:HG12	7:C:1412:TYR:CE1	2.48	0.48
7:C:131:SER:OG	7:C:145:GLU:O	2.26	0.48
7:C:468:HIS:CE1	7:C:470:LEU:HB3	2.48	0.48
8:O:63:ASN:OD1	8:O:461:GLN:NE2	2.46	0.48
8:O:541:ASP:OD1	8:O:542:TYR:N	2.47	0.48
9:D:226:LYS:NZ	9:D:257:ASP:HB3	2.28	0.48
9:P:333:ALA:O	9:P:337:THR:OG1	2.28	0.48
9:P:441:PHE:HB2	9:P:450:ALA:HB2	1.95	0.48
12:Q:542:LYS:NZ	12:Q:547:GLY:HA3	2.29	0.48
1:F:50:ALA:HB1	1:F:74:TYR:HA	1.95	0.48
1:F:480:LYS:HD2	1:F:511:ILE:HG21	1.96	0.48
1:F:651:SER:HA	1:F:654:LYS:HD2	1.95	0.48
2:J:422:PHE:CZ	2:J:429:MET:HG2	2.49	0.48
5:T:97:GLU:OE1	5:T:101:GLN:NE2	2.47	0.48
7:C:157:ASP:OD1	7:C:157:ASP:N	2.44	0.48
7:C:810:ARG:HD3	7:C:813:LEU:HD23	1.95	0.48
7:C:1228:VAL:HG13	7:C:1229:THR:HG23	1.94	0.48
9:P:623:ARG:O	9:P:623:ARG:HD3	2.13	0.48
10:I:78:MET:SD	10:I:78:MET:N	2.86	0.48
13:A:126:MET:HG3	13:A:197:PHE:HD1	1.78	0.48
13:A:142:MET:HG3	13:A:143:ILE:HG23	1.95	0.48
1:H:478:LEU:HD22	1:H:494:TYR:CD2	2.48	0.48
7:C:1326:LEU:HD22	7:C:1382:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1558:ASP:OD1	7:C:1559:ILE:N	2.43	0.48
9:D:407:TYR:HB3	9:D:416:SER:HB2	1.95	0.48
12:Q:572:VAL:HG21	12:Q:644:VAL:HG23	1.94	0.48
1:F:536:MET:O	1:F:542:THR:HG21	2.14	0.48
2:J:319:ILE:HD12	2:J:361:LEU:HD22	1.96	0.48
2:K:565:ALA:HB2	2:K:595:PHE:CD2	2.48	0.48
7:C:200:LYS:HA	7:C:404:ARG:HH21	1.79	0.48
7:C:954:THR:HG21	7:C:984:LEU:H	1.78	0.48
8:O:22:ILE:HG23	8:O:101:TYR:HD2	1.79	0.48
8:O:223:ASN:ND2	9:P:387:GLN:HE22	2.12	0.48
9:P:424:LEU:HD12	9:P:428:LYS:HA	1.94	0.48
13:A:139:PHE:HD2	13:A:215:ARG:HB2	1.78	0.48
1:H:75:ALA:HA	1:H:90:ILE:HD11	1.95	0.48
1:H:116:VAL:O	1:H:120:ILE:HG12	2.14	0.48
7:C:1253:PHE:HE1	7:C:1522:ALA:HA	1.79	0.48
7:C:1352:ARG:NH1	7:C:1403:ASP:OD2	2.46	0.48
7:C:1610:PHE:CZ	7:C:1635:GLN:HB3	2.49	0.48
8:O:610:ILE:O	8:O:614:ILE:HG13	2.14	0.48
9:D:249:TRP:NE1	9:D:253:LEU:HD21	2.29	0.48
2:K:754:LEU:HD13	3:W:27:LYS:HE2	1.95	0.48
1:H:103:TYR:CD2	1:H:151:PRO:HG3	2.49	0.48
7:C:1057:GLY:HA2	7:C:1089:SER:HA	1.95	0.48
2:K:569:LEU:HD11	2:K:601:PRO:HG3	1.96	0.48
1:H:43:TYR:O	1:H:47:GLU:HG2	2.14	0.48
1:H:563:PHE:HB3	1:H:580:GLN:HG3	1.95	0.48
4:E:160:MET:HE3	4:E:162:LEU:H	1.78	0.48
7:C:126:LEU:O	7:C:152:TYR:HA	2.14	0.48
7:C:905:ILE:HD13	7:C:1510:GLN:HB3	1.94	0.48
8:O:495:LYS:O	8:O:496:THR:OG1	2.29	0.48
8:O:549:LYS:NZ	8:O:575:GLU:OE2	2.33	0.48
8:O:569:ILE:HD11	8:O:589:PHE:HB3	1.95	0.48
13:A:142:MET:HG2	13:A:176:ASN:HD21	1.79	0.48
1:H:123:LEU:HA	1:H:126:ILE:HG22	1.96	0.47
7:C:599:GLN:HA	7:C:602:LYS:HZ3	1.79	0.47
7:C:1374:LEU:HD11	13:A:166:PHE:O	2.14	0.47
8:O:56:PRO:O	8:O:57:LEU:HD22	2.14	0.47
9:P:340:TYR:HB2	9:P:372:ILE:HD11	1.94	0.47
3:G:21:ASP:HA	3:G:24:ASN:HD22	1.79	0.47
1:H:91:SER:OG	1:H:105:PHE:HB2	2.14	0.47
6:U:118:VAL:HA	6:U:121:ARG:NH1	2.23	0.47
7:C:524:TYR:CD1	7:C:525:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1723:CYS:SG	7:C:1735:GLN:HG2	2.54	0.47
9:D:77:ASN:HD21	9:P:77:ASN:HD22	1.61	0.47
2:J:588:TYR:HB3	2:J:605:LEU:HG	1.96	0.47
2:J:741:ASN:HB3	2:J:744:ALA:HB3	1.96	0.47
8:O:170:TRP:CH2	8:O:174:GLN:HG3	2.49	0.47
8:O:358:ALA:O	8:O:361:SER:OG	2.28	0.47
9:D:21:ALA:HB3	9:P:90:LEU:HD23	1.97	0.47
12:Q:571:PHE:HA	12:Q:643:LEU:HD13	1.96	0.47
2:J:542:MET:CE	2:J:550:ALA:HB3	2.43	0.47
2:J:547:ILE:HD13	2:J:578:GLU:HG3	1.96	0.47
2:J:552:LYS:O	2:J:555:SER:OG	2.22	0.47
2:K:569:LEU:HD13	2:K:604:PHE:CD2	2.49	0.47
5:T:472:PRO:HB2	7:C:909:ASP:OD1	2.14	0.47
7:C:466:TYR:O	7:C:477:LEU:N	2.47	0.47
7:C:556:ALA:HB1	7:C:581:LEU:HD11	1.96	0.47
8:O:107:GLY:HA3	9:P:384:TYR:CE1	2.49	0.47
9:D:535:ASN:HA	9:D:538:ILE:HD13	1.96	0.47
12:Q:76:ILE:HG13	12:Q:77:PHE:N	2.30	0.47
13:A:49:ASN:OD1	13:A:178:TRP:N	2.47	0.47
2:J:559:ILE:HD11	10:I:113:PHE:HZ	1.80	0.47
1:H:582:HIS:NE2	13:A:250:ARG:HA	2.29	0.47
5:T:463:ILE:HG23	7:C:1412:TYR:HE1	1.80	0.47
7:C:1321:LEU:HD12	7:C:1376:PHE:HE1	1.79	0.47
8:O:180:PHE:O	8:O:183:THR:OG1	2.22	0.47
8:O:289:THR:HG22	9:D:144:LYS:HZ1	1.80	0.47
9:D:295:MET:O	9:D:299:PHE:N	2.43	0.47
9:D:384:TYR:CD2	9:D:385:LEU:HD22	2.50	0.47
9:D:398:GLU:O	9:D:402:ILE:HG12	2.15	0.47
10:I:145:ILE:HG13	10:I:146:PHE:N	2.29	0.47
12:Q:73:ILE:HD11	12:Q:84:SER:HB3	1.96	0.47
1:F:89:GLN:O	1:F:93:GLU:HG2	2.14	0.47
1:F:564:GLU:HA	1:F:567:THR:HG22	1.97	0.47
1:F:745:GLN:HG2	1:F:746:VAL:N	2.30	0.47
2:J:571:PHE:O	2:J:574:THR:OG1	2.27	0.47
2:J:678:LEU:HD11	3:G:8:THR:HB	1.96	0.47
5:T:515:ASP:O	5:T:519:THR:HG23	2.15	0.47
7:C:205:PHE:HB2	7:C:216:TYR:HE1	1.78	0.47
10:I:150:ILE:HG13	10:I:151:THR:N	2.30	0.47
1:F:464:PRO:HG2	1:F:467:ILE:CD1	2.44	0.47
2:J:303:GLY:O	2:J:307:VAL:HG13	2.15	0.47
2:J:514:ASN:ND2	9:D:387:GLN:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:363:PHE:CZ	2:K:394:GLU:HB3	2.50	0.47
2:K:375:PHE:O	2:K:379:ARG:HG3	2.15	0.47
2:K:486:CYS:SG	2:K:503:TYR:HB2	2.55	0.47
2:K:582:ASP:OD1	2:K:583:GLN:N	2.48	0.47
5:T:342:LEU:HD13	5:T:410:LEU:HB3	1.97	0.47
7:C:995:THR:HG22	7:C:997:LYS:HE3	1.96	0.47
7:C:1374:LEU:HD21	13:A:167:TYR:HA	1.95	0.47
8:O:165:MET:O	8:O:168:THR:OG1	2.30	0.47
8:O:434:MET:SD	8:O:584:ASN:ND2	2.87	0.47
8:O:485:ILE:HD11	12:Q:335:GLU:HA	1.97	0.47
10:I:148:ARG:N	10:I:148:ARG:HD2	2.29	0.47
12:Q:12:TYR:CD1	12:Q:19:PHE:HB3	2.49	0.47
12:Q:35:HIS:CE1	12:Q:582:ASP:HB3	2.50	0.47
12:Q:424:TYR:HD1	12:Q:427:TYR:HD2	1.63	0.47
13:A:68:MET:HE3	13:A:176:ASN:O	2.14	0.47
2:J:633:PRO:HB3	2:J:663:VAL:HG21	1.97	0.47
2:K:562:PRO:HA	2:K:568:TRP:HH2	1.80	0.47
1:H:482:HIS:HA	1:H:485:ILE:HG22	1.97	0.47
1:H:502:GLN:HE21	1:H:505:ARG:CD	2.27	0.47
7:C:956:THR:HB	7:C:1491:TYR:CE1	2.50	0.47
7:C:987:VAL:HG22	7:C:993:LYS:HG3	1.95	0.47
9:D:81:LEU:HD12	9:D:85:GLU:HG3	1.97	0.47
10:I:99:LEU:HD22	10:I:155:TYR:CE1	2.45	0.47
12:Q:326:LEU:O	12:Q:330:PHE:HB2	2.15	0.47
1:F:41:LEU:HD12	1:H:149:HIS:ND1	2.29	0.47
1:H:76:LEU:HD11	1:H:149:HIS:HB2	1.96	0.47
4:E:135:ARG:H	4:E:138:ILE:HD11	1.80	0.47
7:C:911:ARG:HH11	7:C:1404:LEU:HD21	1.80	0.47
13:A:44:LYS:NZ	13:A:50:GLY:HA2	2.30	0.47
1:F:123:LEU:HD23	1:F:126:ILE:HD12	1.97	0.47
1:F:565:LYS:HE2	1:F:565:LYS:HB2	1.71	0.47
2:J:392:ASN:OD1	2:J:393:PHE:N	2.48	0.47
2:J:541:TYR:HD1	2:J:546:ARG:HD2	1.80	0.47
2:K:577:LEU:HG	3:W:4:ARG:HH12	1.80	0.47
1:H:87:ALA:HA	1:H:90:ILE:HG12	1.97	0.47
1:H:635:ARG:HE	1:H:645:ILE:CD1	2.27	0.47
7:C:461:ARG:O	7:C:480:GLU:HG3	2.15	0.47
7:C:1084:LEU:HD23	7:C:1544:PHE:HE2	1.80	0.47
1:F:167:LEU:HD22	1:F:168:ASP:HB2	1.97	0.46
1:H:504:ALA:HB1	1:H:535:THR:HG21	1.98	0.46
1:H:679:LYS:NZ	1:H:701:GLU:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:5:ILE:HG13	7:C:1735:GLN:NE2	2.30	0.46
5:T:199:TRP:HE3	5:T:200:LEU:HD22	1.80	0.46
5:T:225:CYS:O	5:T:229:MET:HG2	2.15	0.46
7:C:404:ARG:HG3	7:C:409:GLU:HB3	1.97	0.46
7:C:599:GLN:HG3	7:C:602:LYS:HZ1	1.80	0.46
7:C:1322:ASN:ND2	13:A:189:ASP:OD2	2.47	0.46
11:N:73:TYR:CE2	11:N:80:PRO:HB3	2.50	0.46
1:F:512:PHE:CD2	1:F:528:LEU:HD22	2.44	0.46
2:J:274:TYR:CE1	2:J:279:TYR:HE1	2.34	0.46
2:K:256:VAL:HG12	2:K:265:ASP:OD2	2.15	0.46
2:K:519:LEU:HD12	2:K:520:SER:N	2.30	0.46
2:K:533:THR:O	2:K:537:VAL:HG23	2.15	0.46
4:E:213:VAL:HA	4:E:216:LEU:HG	1.96	0.46
7:C:1298:TRP:CH2	7:C:1342:ARG:HA	2.49	0.46
8:O:21:LEU:HA	8:O:24:ILE:HG22	1.96	0.46
8:O:96:LEU:HD21	8:O:192:ASN:HB3	1.98	0.46
8:O:636:VAL:O	8:O:640:VAL:HG23	2.14	0.46
9:D:26:ARG:HH22	9:P:26:ARG:HD3	1.80	0.46
9:D:231:ILE:H	9:D:231:ILE:HD12	1.80	0.46
12:Q:101:ILE:HG21	12:Q:224:LEU:HD21	1.97	0.46
12:Q:270:ASP:HB2	12:Q:275:TYR:CZ	2.50	0.46
13:A:80:ARG:NH2	13:A:223:SER:OG	2.48	0.46
1:F:78:LEU:HB3	1:F:87:ALA:HB2	1.97	0.46
2:J:603:LEU:HD11	2:J:638:GLU:HG3	1.96	0.46
2:K:390:ILE:HD13	2:K:418:ASP:O	2.14	0.46
1:H:207:PHE:CD2	1:H:437:MET:HG3	2.50	0.46
1:H:650:GLY:O	1:H:653:GLU:HG3	2.16	0.46
1:H:652:LEU:HD22	1:H:657:TYR:HB2	1.97	0.46
5:T:295:TYR:HE2	5:T:349:LYS:HE2	1.80	0.46
6:U:117:ILE:HG12	6:U:121:ARG:NH2	2.31	0.46
7:C:1131:MET:O	7:C:1134:LEU:HB3	2.15	0.46
8:O:88:ASP:OD1	8:O:89:LYS:N	2.48	0.46
8:O:487:ASP:O	8:O:490:GLU:HG3	2.15	0.46
8:O:588:LYS:O	8:O:592:GLU:HG2	2.15	0.46
11:N:115:GLY:HA2	11:N:119:PHE:HD2	1.79	0.46
1:F:554:LYS:HE2	1:F:554:LYS:HA	1.98	0.46
1:F:591:ASP:OD1	1:F:591:ASP:N	2.49	0.46
1:F:670:HIS:HA	4:E:112:LYS:NZ	2.29	0.46
2:J:486:CYS:HB3	2:J:503:TYR:CD1	2.50	0.46
1:H:555:ASP:OD1	1:H:555:ASP:N	2.46	0.46
1:H:694:VAL:O	1:H:698:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:578:ASP:O	5:T:582:TRP:N	2.43	0.46
7:C:1359:VAL:HA	7:C:1390:ILE:HD12	1.98	0.46
13:A:34:LEU:H	13:A:173:ARG:HH12	1.63	0.46
2:J:435:ILE:HD11	2:J:453:LEU:HD13	1.97	0.46
9:D:456:ARG:HH21	11:N:70:LEU:HD23	1.81	0.46
9:D:469:PHE:HE1	9:D:473:GLN:HE21	1.64	0.46
9:D:480:MET:HB3	9:D:483:TYR:HB3	1.98	0.46
1:F:99:LEU:HD23	1:F:143:LEU:HA	1.96	0.46
1:F:469:ASP:OD1	1:F:470:THR:N	2.49	0.46
2:J:699:CYS:O	2:J:702:GLU:HG3	2.15	0.46
2:J:742:SER:O	2:J:745:THR:OG1	2.22	0.46
2:K:432:LEU:HA	2:K:435:ILE:HD12	1.97	0.46
1:H:505:ARG:NH2	1:H:507:LYS:HG2	2.31	0.46
5:T:528:LYS:HG3	5:T:529:TRP:CD1	2.51	0.46
5:T:620:THR:O	5:T:622:GLY:N	2.48	0.46
7:C:1131:MET:CE	7:C:1147:ILE:HD11	2.45	0.46
8:O:406:ILE:HG23	8:O:410:LEU:HD23	1.97	0.46
8:O:612:LYS:HG3	8:O:613:LEU:HD22	1.98	0.46
9:P:448:HIS:NE2	11:N:128:MET:HB3	2.31	0.46
12:Q:180:TYR:HE1	12:Q:468:ALA:HB1	1.81	0.46
1:F:28:ILE:O	1:F:31:GLN:HG2	2.15	0.46
2:K:285:LEU:O	2:K:288:ARG:HG2	2.15	0.46
1:H:79:PHE:O	1:H:84:TYR:HE2	1.99	0.46
1:H:532:LEU:HB3	1:H:542:THR:HG22	1.97	0.46
5:T:231:ARG:HD3	5:T:233:TRP:CH2	2.51	0.46
5:T:281:ARG:O	5:T:284:THR:OG1	2.29	0.46
7:C:116:ASN:N	7:C:127:GLU:OE2	2.49	0.46
7:C:901:ASN:O	7:C:905:ILE:HG13	2.16	0.46
9:D:452:GLU:OE2	11:N:70:LEU:HB2	2.15	0.46
9:D:545:LEU:O	9:D:549:LEU:HG	2.16	0.46
2:K:636:LEU:HB3	2:K:659:ALA:HB2	1.96	0.46
1:H:506:VAL:HG13	1:H:507:LYS:N	2.30	0.46
4:E:89:LYS:HD2	4:E:90:GLN:O	2.16	0.46
7:C:771:VAL:O	7:C:807:LEU:HD11	2.16	0.46
7:C:1279:ILE:O	13:A:130:ARG:HB3	2.16	0.46
9:D:247:PHE:HZ	9:D:294:ILE:HD13	1.81	0.46
9:D:252:TRP:O	9:D:256:MET:HG2	2.16	0.46
9:D:381:LYS:O	9:D:384:TYR:HB3	2.16	0.46
9:P:424:LEU:HD21	9:P:434:TRP:CZ2	2.50	0.46
12:Q:146:ARG:NH1	12:Q:177:ASN:HB3	2.30	0.46
2:J:292:ASP:HA	2:J:298:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:724:LEU:HD21	2:K:754:LEU:HG	1.98	0.46
5:T:231:ARG:HA	5:T:233:TRP:CH2	2.51	0.46
7:C:197:ASP:N	7:C:197:ASP:OD1	2.49	0.46
7:C:938:GLN:HE22	7:C:942:GLN:HE21	1.64	0.46
8:O:255:ILE:HG13	8:O:256:VAL:N	2.30	0.46
12:Q:29:ILE:HG22	12:Q:38:LEU:HB3	1.98	0.46
2:J:740:ASN:OD1	2:J:741:ASN:N	2.40	0.46
5:T:387:LEU:O	5:T:529:TRP:NE1	2.39	0.46
5:T:628:PHE:CE1	5:T:658:LYS:HB3	2.50	0.46
6:U:69:CYS:SG	6:U:71:HIS:ND1	2.88	0.46
7:C:606:GLU:OE1	7:C:606:GLU:N	2.46	0.46
7:C:785:VAL:HG21	7:C:1722:LEU:HD11	1.97	0.46
7:C:1262:GLY:O	7:C:1266:MET:HG2	2.16	0.46
7:C:1292:ALA:O	7:C:1295:MET:HG3	2.16	0.46
8:O:46:SER:OG	8:O:47:PRO:HD3	2.15	0.46
8:O:287:LEU:HB3	8:O:301:ILE:HD11	1.98	0.46
9:P:255:LEU:HD22	9:P:299:PHE:CZ	2.46	0.46
12:Q:8:TYR:HB2	12:Q:570:ARG:HH12	1.80	0.46
1:F:202:ASP:O	1:F:206:VAL:HG23	2.16	0.45
2:J:480:ASN:O	2:J:483:LEU:HG	2.16	0.45
2:K:619:GLU:HA	2:K:642:MET:HE1	1.97	0.45
1:H:486:ILE:HG23	1:H:488:TYR:HE1	1.81	0.45
7:C:77:TYR:HA	7:C:87:PHE:HA	1.98	0.45
7:C:1314:ILE:HG12	7:C:1316:VAL:HG12	1.98	0.45
7:C:1512:ALA:HB3	7:C:1552:ARG:HD2	1.98	0.45
8:O:57:LEU:HD12	8:O:500:SER:OG	2.16	0.45
8:O:355:CYS:HB3	8:O:395:TYR:HE2	1.80	0.45
10:I:141:ILE:HG12	10:I:157:ARG:HD3	1.98	0.45
12:Q:323:VAL:HG23	12:Q:384:ILE:HG23	1.97	0.45
13:A:34:LEU:H	13:A:173:ARG:NH1	2.14	0.45
2:J:741:ASN:O	2:J:745:THR:HG23	2.15	0.45
1:H:508:ASP:N	1:H:508:ASP:OD1	2.49	0.45
1:H:543:TRP:HE3	4:E:257:TYR:HH	1.64	0.45
9:P:32:SER:HB3	9:P:250:SER:HB2	1.98	0.45
9:P:611:GLU:OE1	9:P:611:GLU:N	2.48	0.45
10:I:147:ASP:OD2	10:I:149:ARG:HG2	2.16	0.45
1:F:699:PHE:HB3	1:F:716:LEU:HD22	1.99	0.45
2:J:622:PHE:HB3	2:J:639:MET:SD	2.56	0.45
2:K:697:PHE:HB3	2:K:714:LEU:HD21	1.98	0.45
1:H:591:ASP:OD1	1:H:592:SER:N	2.45	0.45
5:T:375:ARG:HB2	5:T:378:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:738:VAL:HG11	6:U:1:MET:HB2	1.98	0.45
7:C:539:TYR:HE2	7:C:738:ILE:HD11	1.81	0.45
9:D:345:TYR:CE1	9:D:346:VAL:HG23	2.52	0.45
9:D:422:ARG:HB2	10:I:27:TRP:CH2	2.51	0.45
9:D:482:LEU:HD12	9:D:483:TYR:N	2.31	0.45
9:P:11:HIS:HE1	9:P:15:ILE:HD11	1.80	0.45
1:F:196:LYS:HE2	1:F:196:LYS:HB2	1.79	0.45
1:F:726:LYS:O	1:F:730:ILE:HG12	2.16	0.45
2:J:310:GLN:NE2	10:I:148:ARG:HB3	2.31	0.45
2:J:356:LYS:HE3	2:J:358:GLU:HB3	1.98	0.45
7:C:66:PHE:HA	8:O:316:GLN:HE22	1.81	0.45
7:C:640:LEU:HD11	7:C:703:ILE:HG21	1.97	0.45
7:C:927:THR:HG21	7:C:986:SER:HB2	1.98	0.45
7:C:1043:ASP:N	7:C:1043:ASP:OD1	2.50	0.45
8:O:670:LEU:O	8:O:673:SER:OG	2.23	0.45
9:D:77:ASN:ND2	9:P:77:ASN:HD22	2.14	0.45
9:D:328:PHE:CZ	9:D:330:PHE:HB3	2.51	0.45
9:D:434:TRP:HB3	9:D:457:ALA:HB2	1.98	0.45
9:P:554:GLU:HA	9:P:557:LYS:HG2	1.98	0.45
2:J:754:LEU:HD22	3:G:27:LYS:HE3	1.97	0.45
2:K:422:PHE:HB2	2:K:426:LYS:HB3	1.98	0.45
7:C:632:HIS:HA	7:C:655:LEU:HD21	1.99	0.45
8:O:418:ASP:O	8:O:420:ASN:N	2.49	0.45
11:N:128:MET:HA	11:N:131:LEU:HG	1.99	0.45
13:A:80:ARG:NH2	13:A:223:SER:O	2.49	0.45
1:H:191:TYR:HE1	1:H:203:LEU:HD21	1.82	0.45
5:T:236:ARG:HG2	5:T:237:PHE:CD2	2.51	0.45
5:T:600:LEU:HD13	5:T:641:TYR:CE1	2.52	0.45
8:O:509:ILE:O	8:O:513:ILE:HG12	2.16	0.45
9:D:382:LEU:HG	9:D:406:TYR:HB2	1.98	0.45
9:P:137:GLU:HB2	9:P:456:ARG:NH1	2.32	0.45
13:A:140:PHE:CE1	13:A:150:PRO:HG2	2.52	0.45
13:A:190:ASP:HB3	13:A:192:LEU:HG	1.97	0.45
1:F:566:ALA:O	1:F:569:LEU:HG	2.17	0.45
1:H:186:TYR:CE2	1:H:437:MET:HE1	2.51	0.45
1:H:751:LEU:HD22	1:H:755:HIS:HE1	1.81	0.45
7:C:149:LYS:HD2	7:C:150:HIS:HB2	1.97	0.45
7:C:824:ARG:CZ	7:C:1620:TYR:HB3	2.47	0.45
9:P:302:LYS:O	9:P:305:GLU:HG3	2.16	0.45
10:I:37:GLU:HB2	10:I:80:SER:HB2	1.98	0.45
2:J:316:LEU:HD11	2:J:321:GLU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:364:LEU:O	2:J:368:ILE:HG23	2.16	0.45
2:J:674:ILE:HG13	2:J:675:SER:N	2.32	0.45
2:K:431:ASN:HB3	2:K:453:LEU:HD21	1.98	0.45
2:K:590:THR:HA	2:K:593:ARG:HG2	1.98	0.45
2:K:682:HIS:O	2:K:685:ARG:HG2	2.17	0.45
7:C:1084:LEU:HD23	7:C:1544:PHE:CE2	2.52	0.45
8:O:382:MET:HA	8:O:385:ILE:HD12	1.98	0.45
8:O:455:LEU:HB3	12:Q:327:THR:HG21	1.98	0.45
9:D:296:ILE:O	9:D:299:PHE:HB3	2.17	0.45
9:D:325:PHE:HB3	9:D:328:PHE:HB2	1.99	0.45
13:A:37:ARG:NH2	13:A:52:GLN:O	2.50	0.45
2:K:668:PRO:HA	2:K:673:THR:HG21	1.98	0.45
4:E:195:ILE:O	4:E:199:GLU:N	2.48	0.45
5:T:173:PHE:CE2	5:T:177:LEU:HD11	2.52	0.45
7:C:1326:LEU:N	7:C:1327:PRO:HD2	2.32	0.45
9:D:321:LEU:HA	9:D:324:VAL:HG12	1.98	0.45
12:Q:245:TYR:OH	12:Q:329:ILE:HD12	2.17	0.45
13:A:187:ARG:NH2	13:A:190:ASP:OD2	2.44	0.45
5:T:390:PRO:HB2	5:T:392:GLU:CD	2.38	0.45
7:C:1005:ASP:HA	7:C:1008:GLU:OE2	2.16	0.45
8:O:436:LYS:O	8:O:437:GLU:HG3	2.17	0.45
8:O:607:LEU:HA	8:O:610:ILE:HG12	1.99	0.45
9:P:427:ASP:C	9:P:429:LYS:H	2.20	0.45
9:P:595:GLN:HA	9:P:626:MET:HE1	1.99	0.45
2:J:663:VAL:HG13	2:J:666:LEU:HD12	1.99	0.44
3:G:28:LEU:HD12	3:G:31:GLN:HE22	1.82	0.44
1:H:43:TYR:CZ	1:H:80:LEU:HD13	2.52	0.44
1:H:202:ASP:O	1:H:206:VAL:HG12	2.16	0.44
5:T:344:TYR:O	5:T:348:ILE:HG12	2.18	0.44
5:T:683:GLN:OE1	5:T:723:TRP:NE1	2.50	0.44
6:U:122:ARG:O	6:U:125:MET:HG2	2.17	0.44
7:C:83:THR:N	7:C:84:PRO:HD3	2.32	0.44
7:C:927:THR:O	7:C:989:PRO:HD3	2.17	0.44
8:O:333:ASN:OD1	11:N:92:GLY:HA3	2.17	0.44
12:Q:447:ILE:HG22	12:Q:448:ILE:HG23	1.99	0.44
13:A:136:MET:HG3	13:A:138:ILE:HD11	1.99	0.44
2:J:248:THR:O	2:J:252:ILE:HG12	2.17	0.44
2:J:707:ASN:OD1	2:J:710:ILE:N	2.36	0.44
1:H:561:LYS:O	1:H:564:GLU:HG3	2.18	0.44
5:T:231:ARG:HD3	5:T:233:TRP:HH2	1.82	0.44
5:T:505:PHE:CE2	5:T:536:ILE:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:956:THR:HG23	7:C:1498:ASN:ND2	2.32	0.44
7:C:1004:HIS:O	7:C:1007:VAL:HG12	2.16	0.44
7:C:1595:ASP:OD1	7:C:1595:ASP:N	2.48	0.44
8:O:389:ILE:HD11	8:O:396:ALA:N	2.32	0.44
8:O:391:VAL:HG12	8:O:392:HIS:CD2	2.52	0.44
8:O:630:LEU:HD12	12:Q:112:PHE:HD2	1.82	0.44
9:D:373:LEU:HD21	9:D:381:LYS:HG3	2.00	0.44
1:F:633:LYS:O	1:F:636:SER:OG	2.29	0.44
2:J:585:LEU:HD22	2:J:609:PHE:CE1	2.52	0.44
2:K:532:ILE:H	2:K:532:ILE:HD12	1.81	0.44
1:H:434:PRO:HA	1:H:437:MET:HG2	1.99	0.44
1:H:506:VAL:O	1:H:508:ASP:N	2.50	0.44
7:C:1521:ILE:H	7:C:1521:ILE:HD12	1.81	0.44
7:C:1602:ILE:HG22	7:C:1616:PHE:HE1	1.82	0.44
8:O:526:LEU:HD23	8:O:526:LEU:HA	1.83	0.44
9:P:481:HIS:HB3	9:P:508:CYS:SG	2.57	0.44
12:Q:55:ASP:OD2	12:Q:58:THR:OG1	2.33	0.44
1:F:729:ALA:O	1:F:733:LEU:HD23	2.18	0.44
2:J:559:ILE:HD11	10:I:113:PHE:CZ	2.52	0.44
2:J:622:PHE:CZ	2:J:638:GLU:HB3	2.52	0.44
2:K:481:GLU:HA	2:K:484:GLU:HG2	1.98	0.44
1:H:483:PHE:CG	1:H:515:LEU:HD11	2.53	0.44
4:E:197:ASN:O	4:E:201:ASN:HB2	2.16	0.44
4:E:254:ARG:NH2	4:E:258:SER:OG	2.50	0.44
9:D:538:ILE:H	9:D:538:ILE:HD12	1.82	0.44
9:P:480:MET:HE1	9:P:483:TYR:HB2	1.98	0.44
12:Q:300:CYS:SG	12:Q:301:ASN:N	2.90	0.44
1:H:22:GLN:O	1:H:26:THR:HG23	2.17	0.44
1:H:635:ARG:NH2	1:H:648:CYS:HB3	2.32	0.44
7:C:858:SER:OG	7:C:859:ASP:N	2.49	0.44
9:D:219:TYR:CE1	9:D:251:CYS:HA	2.52	0.44
9:P:91:LEU:HD21	9:P:107:PHE:HD2	1.83	0.44
9:P:364:ASN:OD1	9:P:396:ARG:NH2	2.50	0.44
9:P:389:VAL:HG11	9:P:402:ILE:HG21	1.99	0.44
13:A:114:GLN:HB2	13:A:213:HIS:CE1	2.53	0.44
2:J:288:ARG:HG3	2:J:289:ASN:N	2.33	0.44
2:J:490:LEU:HD12	2:J:493:ASP:O	2.17	0.44
1:H:575:TYR:HA	1:H:578:THR:HG22	1.98	0.44
5:T:514:THR:O	5:T:616:TYR:OH	2.35	0.44
6:U:97:THR:HG21	6:U:122:ARG:NH2	2.31	0.44
6:U:121:ARG:NH1	6:U:121:ARG:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:412:LEU:HD21	7:C:465:MET:HG3	1.99	0.44
7:C:1109:PHE:HE1	7:C:1146:SER:HB2	1.82	0.44
7:C:1169:LEU:HD13	7:C:1245:ILE:HG22	2.00	0.44
9:D:18:ARG:O	9:D:22:THR:OG1	2.24	0.44
9:D:91:LEU:HD22	9:P:41:ALA:HB2	1.99	0.44
9:D:407:TYR:CE2	9:D:415:LYS:HG2	2.52	0.44
12:Q:95:LYS:HE3	12:Q:198:ILE:HG13	2.00	0.44
1:F:477:GLN:O	1:F:481:LEU:HG	2.18	0.44
2:J:449:SER:O	2:J:452:ILE:HG22	2.17	0.44
2:J:564:PHE:CE2	2:J:566:ALA:HB3	2.53	0.44
2:K:573:HIS:HD2	3:W:4:ARG:CZ	2.30	0.44
1:H:35:GLN:HA	1:H:38:ILE:HG12	1.98	0.44
1:H:432:THR:O	1:H:435:GLU:HG2	2.17	0.44
9:D:434:TRP:O	9:D:437:MET:HB3	2.18	0.44
9:D:461:CYS:SG	9:D:463:ARG:HG2	2.57	0.44
1:F:699:PHE:HB3	1:F:716:LEU:CD2	2.48	0.44
2:J:615:LEU:HG	2:J:646:LYS:HD3	1.99	0.44
1:H:679:LYS:HA	1:H:682:MET:HE2	1.99	0.44
7:C:67:THR:H	8:O:316:GLN:HE22	1.66	0.44
7:C:578:ALA:O	7:C:582:VAL:HG23	2.18	0.44
9:D:43:LEU:HD23	9:D:44:ALA:O	2.17	0.44
9:P:218:TYR:O	9:P:222:GLY:N	2.47	0.44
9:P:574:THR:HG23	9:P:576:GLU:H	1.82	0.44
12:Q:78:LYS:HB3	12:Q:81:ARG:NE	2.33	0.44
12:Q:285:LEU:HD12	12:Q:289:GLY:HA2	2.00	0.44
12:Q:501:LEU:HD13	12:Q:567:SER:HA	2.00	0.44
2:J:498:ASN:CG	2:K:247:ARG:HH12	2.21	0.44
1:H:514:THR:O	1:H:518:HIS:ND1	2.50	0.44
5:T:140:PHE:HB3	5:T:141:PRO:HD3	2.00	0.44
5:T:682:GLU:OE2	5:T:715:ARG:NH2	2.51	0.44
7:C:576:HIS:NE2	7:C:650:LEU:HB3	2.33	0.44
7:C:759:PRO:O	7:C:762:VAL:HG12	2.18	0.44
7:C:871:ALA:HA	8:O:411:LYS:O	2.17	0.44
9:D:202:GLU:OE1	9:D:202:GLU:N	2.51	0.44
9:D:362:ARG:HG3	9:P:103:ARG:NH2	2.31	0.44
12:Q:101:ILE:HG23	12:Q:203:ASP:HB3	1.99	0.44
13:A:65:LEU:HA	13:A:68:MET:HG3	1.99	0.44
2:J:391:LYS:HD2	2:J:391:LYS:HA	1.88	0.43
2:J:619:GLU:HB2	2:J:642:MET:CE	2.48	0.43
2:K:585:LEU:HD11	2:K:609:PHE:CE1	2.48	0.43
2:K:641:VAL:HG21	3:W:7:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:LEU:HD12	1:H:86:THR:OG1	2.18	0.43
5:T:283:ARG:HG3	5:T:305:LEU:HD21	1.99	0.43
7:C:1007:VAL:O	7:C:1011:GLN:HG3	2.18	0.43
7:C:1256:LEU:HD23	7:C:1257:LYS:HG3	2.01	0.43
7:C:1550:GLU:HB2	7:C:1551:PRO:HD2	2.00	0.43
8:O:133:ARG:NH1	8:O:135:THR:OG1	2.37	0.43
9:P:289:THR:OG1	9:P:292:PHE:HB2	2.18	0.43
13:A:93:SER:HB3	13:A:122:GLN:HG3	2.00	0.43
13:A:219:LEU:HD23	13:A:219:LEU:HA	1.84	0.43
1:F:201:VAL:HG23	1:F:203:LEU:HD22	2.00	0.43
2:J:288:ARG:NH2	2:K:493:ASP:HB2	2.33	0.43
2:J:402:LYS:HA	2:J:402:LYS:HD2	1.64	0.43
3:G:15:ASP:OD1	3:G:16:VAL:N	2.51	0.43
1:H:607:HIS:NE2	1:H:609:ASN:HB2	2.33	0.43
7:C:483:ASN:HB2	7:C:486:GLU:HG2	1.99	0.43
7:C:1257:LYS:HE3	7:C:1521:ILE:HD13	2.00	0.43
8:O:127:TYR:HA	8:O:130:MET:HG2	1.99	0.43
8:O:615:ASP:OD1	8:O:615:ASP:N	2.50	0.43
9:P:10:ILE:HG13	9:P:43:LEU:HD11	2.00	0.43
9:P:43:LEU:HD13	9:P:325:PHE:HE1	1.83	0.43
12:Q:250:LEU:HD22	12:Q:457:ILE:HD12	1.99	0.43
1:F:617:SER:O	1:F:620:LYS:HG2	2.17	0.43
2:J:472:ILE:O	2:J:476:GLN:HG3	2.17	0.43
2:J:737:LEU:HD23	2:J:737:LEU:HA	1.85	0.43
2:K:457:TYR:O	2:K:458:LYS:HG2	2.18	0.43
1:H:489:ASP:OD1	1:H:490:MET:N	2.51	0.43
1:H:497:ARG:HD2	1:H:497:ARG:HA	1.77	0.43
1:H:506:VAL:HG13	1:H:507:LYS:H	1.84	0.43
6:U:100:LEU:HD11	6:U:114:PHE:CD2	2.52	0.43
7:C:422:LYS:HG2	7:C:453:ASN:OD1	2.17	0.43
7:C:1526:MET:O	7:C:1529:LEU:HD22	2.19	0.43
8:O:20:ILE:H	8:O:20:ILE:HD12	1.83	0.43
1:F:608:TYR:N	1:F:637:ILE:HD11	2.34	0.43
2:J:559:ILE:HG21	10:I:100:PHE:HE1	1.82	0.43
2:K:651:LYS:HA	2:K:654:LYS:HD3	2.00	0.43
8:O:49:ARG:O	12:Q:423:LEU:HD22	2.18	0.43
8:O:380:LEU:O	8:O:383:ILE:HG22	2.18	0.43
12:Q:12:TYR:CE1	12:Q:19:PHE:HB3	2.54	0.43
1:H:21:ASP:OD2	1:H:22:GLN:N	2.51	0.43
5:T:97:GLU:HA	5:T:100:LEU:HD12	2.00	0.43
5:T:209:SER:O	5:T:213:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:42:GLY:HA3	6:U:93:MET:HE3	2.00	0.43
7:C:1359:VAL:O	7:C:1363:LEU:HB2	2.19	0.43
7:C:1372:GLN:NE2	13:A:27:ASN:HA	2.33	0.43
8:O:577:CYS:SG	8:O:586:ARG:NH1	2.91	0.43
9:D:252:TRP:HB3	9:D:302:LYS:HZ1	1.83	0.43
9:D:363:LEU:HD23	9:D:363:LEU:HA	1.86	0.43
9:P:484:SER:OG	9:P:508:CYS:SG	2.76	0.43
11:N:86:ALA:O	11:N:89:LEU:HG	2.19	0.43
12:Q:104:ARG:O	12:Q:104:ARG:HG2	2.19	0.43
2:K:255:LYS:HA	2:K:255:LYS:HD3	1.67	0.43
2:K:570:GLY:O	2:K:574:THR:HG23	2.19	0.43
2:K:634:LEU:O	2:K:638:GLU:HG2	2.19	0.43
1:H:539:LYS:HA	1:H:539:LYS:HD2	1.76	0.43
7:C:64:ARG:NH2	8:O:352:PHE:HB3	2.34	0.43
7:C:415:HIS:CE1	7:C:417:PRO:HD2	2.53	0.43
7:C:1407:LEU:HA	7:C:1410:VAL:HG12	1.99	0.43
9:D:228:GLU:OE1	9:D:230:ASN:HB2	2.19	0.43
12:Q:199:ILE:HG23	12:Q:207:GLN:HB2	2.00	0.43
12:Q:298:TRP:CE3	12:Q:299:LEU:HD22	2.54	0.43
12:Q:438:SER:O	12:Q:442:THR:HG23	2.17	0.43
1:F:665:TYR:HB3	1:F:682:MET:SD	2.58	0.43
2:J:394:GLU:HA	2:J:397:GLU:OE2	2.18	0.43
1:H:155:THR:O	1:H:159:LEU:HD23	2.18	0.43
7:C:644:CYS:HB2	7:C:647:GLU:OE2	2.19	0.43
7:C:1367:GLN:HG3	7:C:1419:GLY:HA2	2.00	0.43
8:O:131:LYS:NZ	12:Q:296:GLU:OE1	2.33	0.43
8:O:610:ILE:HG13	8:O:611:ILE:N	2.34	0.43
9:D:74:ILE:N	9:P:83:GLU:OE2	2.52	0.43
9:D:103:ARG:CZ	9:P:362:ARG:HB2	2.49	0.43
9:D:128:TRP:CE2	9:D:187:ILE:HD11	2.54	0.43
12:Q:65:PHE:CE2	12:Q:96:GLY:HA3	2.53	0.43
13:A:48:VAL:HG21	13:A:76:LEU:HD21	1.99	0.43
13:A:135:VAL:HB	13:A:220:TYR:HB2	2.01	0.43
13:A:156:TYR:HB2	13:A:199:ARG:HG3	2.00	0.43
1:F:457:ARG:HH12	4:E:137:ASP:HB3	1.84	0.43
2:J:264:ASP:OD1	2:J:265:ASP:N	2.52	0.43
2:K:264:ASP:OD1	2:K:265:ASP:N	2.52	0.43
2:K:569:LEU:HB2	3:W:1:MET:HE1	2.00	0.43
7:C:666:ASP:N	7:C:666:ASP:OD1	2.51	0.43
9:D:11:HIS:NE2	9:D:15:ILE:HD11	2.33	0.43
9:P:399:THR:O	9:P:403:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:475:TYR:CE2	9:P:487:TYR:HE2	2.37	0.43
12:Q:199:ILE:CG2	12:Q:207:GLN:HB2	2.49	0.43
12:Q:465:LYS:HB3	12:Q:469:GLN:HE22	1.84	0.43
12:Q:506:LEU:HB2	12:Q:509:HIS:HB2	2.01	0.43
12:Q:627:PHE:HD1	12:Q:647:LYS:H	1.67	0.43
1:F:539:LYS:HA	1:F:539:LYS:HD2	1.78	0.43
2:J:291:LEU:HD23	2:J:291:LEU:H	1.83	0.43
2:J:609:PHE:HA	2:J:612:MET:HE2	1.99	0.43
2:K:229:ALA:N	2:K:231:GLU:OE1	2.52	0.43
2:K:658:LYS:O	2:K:661:GLU:HG3	2.19	0.43
1:H:82:LYS:HG2	1:H:82:LYS:O	2.18	0.43
7:C:1301:ILE:HD13	7:C:1342:ARG:HD3	2.01	0.43
8:O:57:LEU:O	8:O:58:LEU:HB2	2.17	0.43
8:O:242:ILE:HD12	8:O:247:LEU:HB2	2.01	0.43
8:O:289:THR:HA	9:D:144:LYS:NZ	2.34	0.43
8:O:328:TYR:OH	9:D:459:ASP:OD2	2.37	0.43
9:D:83:GLU:OE1	9:P:18:ARG:NH1	2.52	0.43
9:D:420:PHE:HB3	9:D:437:MET:HE1	2.01	0.43
9:P:602:MET:HA	9:P:616:ARG:HH22	1.84	0.43
12:Q:123:LEU:HD12	12:Q:123:LEU:H	1.83	0.43
12:Q:193:ASN:HB3	12:Q:211:GLU:HG2	2.00	0.43
12:Q:330:PHE:HB3	12:Q:380:THR:HG21	2.00	0.43
2:J:480:ASN:OD1	2:J:481:GLU:N	2.52	0.43
2:J:580:GLU:HG3	2:J:583:GLN:HE21	1.84	0.43
2:K:644:PHE:CE2	2:K:686:LYS:HG3	2.54	0.43
5:T:323:LEU:O	5:T:327:LYS:HG2	2.19	0.43
7:C:120:TYR:HA	7:C:196:SER:HA	2.01	0.43
7:C:401:LEU:HD13	7:C:412:LEU:HD23	2.01	0.43
7:C:409:GLU:HG3	7:C:426:ILE:HG22	1.99	0.43
8:O:40:VAL:O	8:O:44:LEU:HD23	2.18	0.43
8:O:73:PRO:HG2	8:O:250:ILE:HD12	2.00	0.43
8:O:492:PHE:CZ	12:Q:381:LEU:HB3	2.54	0.43
9:P:131:LYS:HB3	9:P:131:LYS:HE3	1.90	0.43
9:P:260:GLN:HA	9:P:463:ARG:HG3	2.01	0.43
12:Q:165:PHE:CD2	12:Q:172:ILE:HG22	2.54	0.43
2:J:510:LEU:HD22	2:J:512:ASN:OD1	2.19	0.42
5:T:43:PRO:HB2	5:T:117:HIS:CD2	2.54	0.42
5:T:182:ASP:O	5:T:186:MET:HG2	2.19	0.42
7:C:76:GLY:N	7:C:88:VAL:O	2.50	0.42
9:P:496:PRO:O	9:P:502:TRP:NE1	2.39	0.42
13:A:156:TYR:HD1	13:A:166:PHE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:22:ASP:O	3:G:26:GLN:OE1	2.37	0.42
1:H:563:PHE:O	1:H:567:THR:HG23	2.18	0.42
1:H:565:LYS:HA	1:H:568:GLN:HG3	2.01	0.42
1:H:574:ALA:HA	1:H:577:TYR:HD2	1.83	0.42
6:U:114:PHE:HA	6:U:117:ILE:HG22	2.01	0.42
7:C:734:VAL:HA	7:C:737:ARG:NH1	2.34	0.42
9:D:551:ASP:OD1	9:D:551:ASP:N	2.52	0.42
1:F:44:SER:HA	1:F:47:GLU:HB2	2.01	0.42
1:F:123:LEU:HD22	1:F:156:LEU:HD12	2.01	0.42
1:F:519:LEU:HD23	1:F:519:LEU:HA	1.85	0.42
2:J:525:GLU:HG3	2:J:526:THR:HG23	2.00	0.42
2:K:246:TYR:HB3	2:K:276:ASN:OD1	2.19	0.42
2:K:626:TYR:CD1	2:K:635:VAL:HG11	2.54	0.42
2:K:704:ASN:O	2:K:707:ASN:ND2	2.52	0.42
7:C:35:THR:HA	7:C:78:ILE:HG22	2.01	0.42
7:C:597:GLU:HA	7:C:600:GLU:HG2	2.01	0.42
8:O:170:TRP:CZ3	8:O:174:GLN:HG3	2.54	0.42
9:D:363:LEU:O	9:D:396:ARG:NH2	2.52	0.42
9:D:419:TYR:OH	10:I:30:ASP:OD2	2.37	0.42
10:I:85:ASN:O	10:I:89:ASN:HB2	2.20	0.42
12:Q:7:ASP:N	12:Q:7:ASP:OD1	2.52	0.42
13:A:156:TYR:CD1	13:A:166:PHE:HA	2.54	0.42
1:F:175:PHE:O	1:F:178:SER:OG	2.28	0.42
1:H:103:TYR:HE1	1:H:159:LEU:HG	1.84	0.42
7:C:406:GLU:OE1	7:C:407:ARG:HG2	2.20	0.42
7:C:1099:ILE:CD1	7:C:1131:MET:HG2	2.49	0.42
7:C:1135:TYR:CE2	7:C:1143:MET:HG3	2.54	0.42
7:C:1306:SER:HA	7:C:1309:MET:HG3	2.01	0.42
7:C:1336:ILE:HG13	7:C:1337:LEU:N	2.34	0.42
8:O:594:ILE:HD13	8:O:610:ILE:HG22	2.00	0.42
9:D:311:LEU:HD23	9:D:311:LEU:H	1.83	0.42
9:P:451:ILE:O	9:P:455:ARG:HG2	2.20	0.42
12:Q:29:ILE:HD13	12:Q:39:ALA:HB3	2.02	0.42
12:Q:541:LEU:HB3	12:Q:546:LEU:HA	2.02	0.42
13:A:189:ASP:OD1	13:A:189:ASP:N	2.47	0.42
1:F:733:LEU:HD12	1:F:747:ILE:HG23	2.02	0.42
2:J:496:ASN:O	2:J:500:LEU:HG	2.19	0.42
3:G:17:THR:HA	3:G:20:ILE:HG22	2.00	0.42
7:C:63:LEU:HD23	7:C:63:LEU:HA	1.82	0.42
7:C:546:ASN:O	7:C:550:ILE:HD12	2.20	0.42
9:P:322:LEU:HD23	9:P:322:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:395:PHE:CZ	10:I:23:LEU:HD21	2.54	0.42
12:Q:505:LYS:HE3	12:Q:509:HIS:O	2.19	0.42
2:J:371:ALA:HA	10:I:148:ARG:NH1	2.34	0.42
2:J:605:LEU:HD23	2:J:605:LEU:HA	1.71	0.42
2:K:467:ARG:NH1	2:K:471:ASP:HB2	2.34	0.42
1:H:202:ASP:OD1	1:H:202:ASP:N	2.53	0.42
4:E:106:ARG:HA	4:E:109:SER:HB3	2.00	0.42
5:T:130:ASP:O	5:T:133:ARG:HG2	2.19	0.42
6:U:82:LEU:HD11	6:U:98:PHE:CD2	2.55	0.42
7:C:1541:LEU:HD13	7:C:1544:PHE:CD2	2.54	0.42
9:D:215:ALA:HB2	9:D:244:CYS:SG	2.60	0.42
9:D:503:GLN:HG3	9:D:541:ARG:HH12	1.84	0.42
10:I:16:LEU:HD23	10:I:16:LEU:H	1.84	0.42
1:F:491:SER:HB3	1:F:495:PHE:CE1	2.55	0.42
1:F:611:TYR:CE2	1:F:633:LYS:HG3	2.54	0.42
1:F:633:LYS:HA	1:F:633:LYS:HD2	1.87	0.42
1:F:659:GLU:HG2	1:F:660:LYS:N	2.35	0.42
1:F:670:HIS:O	4:E:116:ALA:HB3	2.20	0.42
2:J:243:GLN:HB3	2:J:245:MET:HG2	2.02	0.42
2:K:569:LEU:HD12	3:W:1:MET:CE	2.50	0.42
5:T:10:ASP:O	5:T:14:ILE:HG12	2.20	0.42
7:C:35:THR:HG22	7:C:37:LYS:HG2	2.02	0.42
7:C:576:HIS:CD2	7:C:650:LEU:HB3	2.55	0.42
7:C:819:ILE:O	7:C:823:ILE:HG12	2.19	0.42
9:D:533:ASP:OD1	9:D:534:GLN:N	2.53	0.42
12:Q:381:LEU:HD12	12:Q:384:ILE:HD12	2.02	0.42
1:F:459:PHE:CD2	1:F:478:LEU:HD12	2.55	0.42
1:H:547:GLY:HA3	1:H:563:PHE:CE1	2.55	0.42
5:T:240:MET:HE2	5:T:240:MET:HA	2.00	0.42
7:C:760:ASP:O	7:C:802:ARG:NH1	2.48	0.42
7:C:1269:VAL:HG22	7:C:1274:ILE:HD13	2.00	0.42
8:O:426:TYR:O	8:O:430:THR:HG23	2.20	0.42
9:D:253:LEU:O	9:D:256:MET:N	2.52	0.42
9:D:289:THR:OG1	9:D:292:PHE:HB2	2.20	0.42
9:D:559:MET:HG2	9:D:584:LEU:HD13	2.01	0.42
9:P:242:LEU:HG	9:P:252:TRP:NE1	2.34	0.42
2:J:750:ASN:O	2:J:754:LEU:HD23	2.20	0.42
2:K:247:ARG:O	2:K:250:GLU:HG3	2.20	0.42
2:K:306:PHE:HE1	2:K:311:ARG:HH11	1.68	0.42
5:T:582:TRP:NE1	5:T:586:CYS:SG	2.92	0.42
9:D:6:GLN:O	9:D:10:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:590:LYS:HA	9:D:590:LYS:HD3	1.90	0.42
9:P:295:MET:HA	9:P:298:PHE:HD2	1.85	0.42
12:Q:54:TRP:CH2	12:Q:76:ILE:HD13	2.54	0.42
1:F:191:TYR:CD1	1:F:444:LEU:HD23	2.55	0.42
2:J:296:ILE:H	2:J:296:ILE:HD12	1.85	0.42
2:K:396:PHE:HE2	2:K:436:ASN:HB2	1.85	0.42
1:H:568:GLN:NE2	1:H:569:LEU:HD22	2.35	0.42
5:T:59:ILE:O	5:T:63:ILE:HG12	2.20	0.42
5:T:613:TYR:OH	6:U:51:THR:N	2.49	0.42
7:C:664:TRP:O	7:C:669:GLN:NE2	2.51	0.42
7:C:1578:VAL:HG23	7:C:1580:LYS:H	1.85	0.42
7:C:1616:PHE:HA	7:C:1620:TYR:CE1	2.55	0.42
7:C:1739:TRP:CD1	7:C:1743:PHE:HD2	2.37	0.42
12:Q:87:ARG:HA	12:Q:87:ARG:NE	2.35	0.42
12:Q:275:TYR:CE2	12:Q:442:THR:HG22	2.55	0.42
1:F:439:ASN:O	1:F:443:ILE:HG12	2.19	0.41
1:F:619:MET:SD	1:F:654:LYS:NZ	2.85	0.41
1:F:649:GLY:O	1:F:653:GLU:OE1	2.37	0.41
1:F:743:GLY:O	1:F:747:ILE:HG13	2.20	0.41
2:J:316:LEU:HD13	2:J:368:ILE:HD11	2.02	0.41
2:K:606:GLY:HA3	2:K:622:PHE:CE1	2.54	0.41
1:H:686:LEU:HD22	1:H:691:ARG:HB3	2.02	0.41
7:C:30:LEU:HD12	7:C:45:ILE:O	2.20	0.41
7:C:455:LYS:HD2	7:C:455:LYS:HA	1.89	0.41
7:C:812:ASP:OD1	7:C:812:ASP:N	2.53	0.41
7:C:1138:SER:HB3	7:C:1140:HIS:HB2	2.01	0.41
9:D:395:PHE:O	9:D:426:LEU:HD13	2.20	0.41
13:A:142:MET:N	13:A:176:ASN:OD1	2.53	0.41
1:F:30:LEU:HD13	1:F:52:LEU:HD22	2.01	0.41
2:J:506:CYS:O	2:J:509:GLU:HG3	2.20	0.41
2:K:602:LYS:HD3	2:K:624:LEU:HD22	2.01	0.41
2:K:732:HIS:CE1	2:K:748:LEU:HD11	2.55	0.41
1:H:517:TRP:CD1	1:H:552:LEU:HB2	2.56	0.41
5:T:197:ILE:HG22	5:T:201:LYS:HZ2	1.85	0.41
7:C:1038:LYS:HA	7:C:1039:PRO:HD3	1.94	0.41
8:O:44:LEU:O	8:O:47:PRO:HD2	2.19	0.41
8:O:164:GLU:O	8:O:167:GLU:HG2	2.20	0.41
8:O:386:ILE:HD12	8:O:386:ILE:H	1.86	0.41
8:O:488:VAL:HG11	12:Q:377:LEU:HD23	2.01	0.41
9:D:137:GLU:N	9:D:137:GLU:OE1	2.53	0.41
9:D:226:LYS:HZ1	9:D:257:ASP:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:315:PHE:O	9:D:318:LEU:N	2.52	0.41
9:P:623:ARG:HA	9:P:626:MET:SD	2.60	0.41
2:J:288:ARG:CZ	2:K:492:ASN:HB3	2.50	0.41
2:J:749:LYS:O	2:J:753:GLU:OE1	2.39	0.41
1:H:186:TYR:CZ	1:H:437:MET:HE1	2.55	0.41
1:H:714:TYR:CE1	1:H:750:GLU:HG3	2.54	0.41
7:C:487:TYR:HD1	7:C:507:GLU:HA	1.85	0.41
7:C:613:LEU:HD23	7:C:613:LEU:HA	1.84	0.41
7:C:759:PRO:O	7:C:794:LEU:HD21	2.20	0.41
7:C:1125:THR:HA	7:C:1128:ILE:HG22	2.02	0.41
8:O:126:ASN:OD1	8:O:127:TYR:N	2.46	0.41
8:O:386:ILE:O	8:O:390:GLU:N	2.42	0.41
8:O:480:LEU:HD13	8:O:622:ASN:OD1	2.20	0.41
8:O:630:LEU:HD12	12:Q:112:PHE:CD2	2.55	0.41
9:D:372:ILE:O	9:D:376:MET:HG2	2.19	0.41
9:P:486:TYR:OH	9:P:490:LYS:HD2	2.20	0.41
13:A:69:PHE:CG	13:A:109:TYR:HB2	2.55	0.41
1:F:737:MET:HE1	1:F:751:LEU:HD11	2.02	0.41
2:J:469:LYS:HB3	2:J:485:LEU:HD13	2.01	0.41
6:U:48:TYR:CZ	6:U:72:ASN:HB2	2.55	0.41
6:U:101:GLN:HB3	6:U:104:LEU:HD12	2.01	0.41
7:C:468:HIS:HE1	7:C:470:LEU:HB3	1.85	0.41
7:C:1375:ASP:O	7:C:1379:THR:HG23	2.20	0.41
7:C:1531:THR:HB	7:C:1537:PRO:HD2	2.03	0.41
7:C:1557:LYS:HA	7:C:1564:ALA:HA	2.03	0.41
9:P:311:LEU:HD13	9:P:314:TYR:HB3	2.01	0.41
11:N:9:SER:OG	12:Q:320:GLN:OE1	2.38	0.41
11:N:93:LYS:HA	11:N:93:LYS:HD2	1.87	0.41
12:Q:103:LEU:HG	12:Q:157:GLU:O	2.20	0.41
13:A:93:SER:N	13:A:122:GLN:O	2.53	0.41
1:F:30:LEU:HD22	1:F:53:LEU:HG	2.02	0.41
1:F:43:TYR:CE2	1:F:80:LEU:HB2	2.55	0.41
2:J:675:SER:O	2:J:678:LEU:HG	2.21	0.41
2:K:588:TYR:HB3	2:K:605:LEU:HD12	2.03	0.41
1:H:471:MET:HE2	1:H:473:TRP:HB3	2.02	0.41
6:U:71:HIS:HE1	6:U:94:CYS:HB3	1.85	0.41
7:C:40:GLY:HA3	7:C:469:GLU:OE2	2.20	0.41
7:C:465:MET:HB2	7:C:477:LEU:O	2.20	0.41
7:C:1287:MET:SD	7:C:1288:TYR:N	2.94	0.41
7:C:1351:ILE:HD12	7:C:1351:ILE:H	1.85	0.41
7:C:1364:PRO:HG2	13:A:16:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:427:LYS:HB3	8:O:450:PHE:CD2	2.55	0.41
9:D:509:TYR:HA	9:D:512:THR:HG22	2.02	0.41
13:A:40:ASP:HB3	13:A:43:THR:HG23	2.02	0.41
13:A:133:ILE:HD11	13:A:193:LEU:HD22	2.01	0.41
2:J:497:THR:HA	2:J:500:LEU:HD12	2.02	0.41
2:K:233:LEU:HB3	2:K:256:VAL:CG2	2.51	0.41
2:K:419:PHE:HB3	2:K:426:LYS:HB2	2.03	0.41
2:K:599:HIS:CE1	2:K:600:LEU:HG	2.55	0.41
5:T:382:LEU:O	5:T:386:MET:HG2	2.19	0.41
6:U:90:LEU:HB2	6:U:95:ARG:NH2	2.27	0.41
7:C:209:ASN:N	7:C:209:ASN:OD1	2.54	0.41
7:C:619:ILE:HG23	7:C:623:VAL:HG21	2.01	0.41
7:C:1290:GLU:OE1	7:C:1331:THR:HG23	2.20	0.41
9:P:205:ILE:HD13	9:P:218:TYR:HE2	1.85	0.41
9:P:393:ASP:OD1	9:P:394:ARG:N	2.54	0.41
10:I:24:TYR:HA	11:N:76:PHE:CZ	2.56	0.41
10:I:147:ASP:O	10:I:150:ILE:HG12	2.21	0.41
12:Q:357:LEU:HD23	12:Q:359:TYR:N	2.32	0.41
13:A:45:ASP:OD1	13:A:182:ARG:HD2	2.20	0.41
1:F:432:THR:O	1:F:436:ILE:HG12	2.20	0.41
2:J:248:THR:OG1	2:K:393:PHE:HB3	2.19	0.41
2:J:484:GLU:OE2	2:J:485:LEU:HG	2.20	0.41
1:H:191:TYR:HE2	1:H:444:LEU:HB2	1.86	0.41
7:C:202:ILE:HG13	7:C:409:GLU:OE2	2.21	0.41
8:O:368:ILE:HD13	8:O:368:ILE:HA	1.93	0.41
8:O:414:SER:OG	8:O:415:ASP:N	2.54	0.41
9:D:417:ILE:HG12	9:D:441:PHE:CE2	2.55	0.41
9:P:252:TRP:CZ3	9:P:295:MET:HB3	2.54	0.41
9:P:294:ILE:HG13	9:P:295:MET:N	2.36	0.41
9:P:352:PHE:CE2	9:P:372:ILE:HD12	2.55	0.41
9:P:613:GLU:OE2	9:P:614:GLU:HG3	2.21	0.41
1:F:206:VAL:HG22	4:E:161:LEU:HD13	2.02	0.41
1:F:491:SER:HB3	1:F:495:PHE:HE1	1.85	0.41
1:H:485:ILE:HG23	1:H:487:ASN:HB2	2.03	0.41
7:C:30:LEU:N	7:C:513:ASN:OD1	2.52	0.41
7:C:860:ILE:HD13	12:Q:121:PRO:HB2	2.03	0.41
7:C:1404:LEU:O	7:C:1408:ARG:HG3	2.21	0.41
7:C:1615:ASN:O	7:C:1620:TYR:OH	2.14	0.41
8:O:378:LEU:HA	8:O:381:ILE:HG22	2.02	0.41
8:O:407:ILE:H	8:O:407:ILE:HG12	1.71	0.41
9:D:204:LYS:O	9:D:205:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:116:TRP:HA	11:N:128:MET:SD	2.61	0.41
12:Q:469:GLN:HA	12:Q:473:ASN:OD1	2.20	0.41
12:Q:542:LYS:HG2	12:Q:547:GLY:H	1.86	0.41
1:F:670:HIS:HD2	4:E:112:LYS:HZ1	1.69	0.41
1:F:672:GLN:HE22	1:F:675:SER:HB3	1.86	0.41
2:K:231:GLU:HG2	2:K:232:ARG:N	2.36	0.41
2:K:309:LEU:O	2:K:310:GLN:HB3	2.21	0.41
2:K:365:ARG:HB3	2:K:369:TYR:CZ	2.56	0.41
1:H:85:HIS:O	1:H:89:GLN:OE1	2.39	0.41
1:H:126:ILE:HD11	1:H:143:LEU:HD22	2.03	0.41
1:H:440:PHE:O	1:H:444:LEU:HD23	2.21	0.41
1:H:530:ASN:OD1	4:E:249:LEU:HB2	2.20	0.41
5:T:168:ASN:HD21	5:T:206:SER:HB3	1.86	0.41
5:T:337:THR:HB	5:T:375:ARG:HH11	1.86	0.41
5:T:385:ALA:HB1	5:T:410:LEU:HD13	2.02	0.41
5:T:537:ARG:NE	5:T:577:ILE:HD11	2.35	0.41
7:C:724:PHE:HB2	7:C:727:LEU:HD11	2.02	0.41
7:C:956:THR:HB	7:C:1491:TYR:HE1	1.86	0.41
7:C:1090:MET:HE2	7:C:1093:SER:HB3	2.03	0.41
7:C:1163:ALA:HB1	7:C:1168:ARG:HH12	1.86	0.41
7:C:1305:LEU:HD21	13:A:10:LEU:HD11	2.02	0.41
7:C:1374:LEU:HA	7:C:1374:LEU:HD13	1.91	0.41
7:C:1484:LYS:HA	7:C:1487:ILE:HG22	2.03	0.41
7:C:1724:SER:O	7:C:1724:SER:OG	2.29	0.41
8:O:671:LEU:HD23	8:O:671:LEU:HA	1.85	0.41
9:D:94:THR:HG21	9:P:37:ALA:HB3	2.02	0.41
9:D:96:PHE:CE1	9:D:101:PHE:HE2	2.39	0.41
9:D:99:LYS:HZ2	10:I:19:PRO:HG3	1.86	0.41
9:D:293:ASN:HD22	9:D:296:ILE:CD1	2.34	0.41
9:D:352:PHE:HB3	9:D:369:TYR:HD2	1.85	0.41
12:Q:620:GLU:O	12:Q:624:ASN:HB2	2.21	0.41
1:F:658:LYS:HA	1:F:658:LYS:HD3	1.98	0.41
2:J:308:LYS:HE3	2:J:308:LYS:HB3	1.85	0.41
2:J:536:SER:O	2:J:539:THR:HG22	2.21	0.41
2:K:563:SER:HA	2:K:595:PHE:CZ	2.47	0.41
2:K:651:LYS:O	2:K:654:LYS:HG2	2.21	0.41
2:K:706:LYS:HZ1	2:K:737:LEU:HD22	1.86	0.41
1:H:49:LEU:HA	1:H:52:LEU:HG	2.02	0.41
1:H:471:MET:HG3	1:H:474:CYS:H	1.85	0.41
1:H:565:LYS:O	1:H:569:LEU:HD23	2.21	0.41
7:C:461:ARG:NH1	7:C:482:GLN:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:555:SER:O	7:C:559:ILE:HG12	2.21	0.41
7:C:1099:ILE:HD12	7:C:1099:ILE:HA	1.91	0.41
7:C:1368:TYR:H	7:C:1380:ILE:CD1	2.33	0.41
7:C:1368:TYR:HD1	7:C:1424:LEU:HD23	1.85	0.41
8:O:573:VAL:HG23	8:O:586:ARG:HG3	2.02	0.41
9:D:26:ARG:O	9:D:89:TYR:OH	2.33	0.41
9:D:523:LYS:NZ	9:D:546:TYR:OH	2.53	0.41
12:Q:70:THR:HG23	12:Q:87:ARG:HD2	2.03	0.41
1:F:123:LEU:CB	1:F:160:LEU:HD21	2.51	0.40
1:F:614:LEU:HD13	1:F:630:TYR:CE1	2.56	0.40
2:J:286:ILE:HA	2:J:291:LEU:HD21	2.02	0.40
5:T:295:TYR:CG	5:T:296:PRO:HA	2.56	0.40
5:T:371:TYR:O	5:T:374:GLU:HB2	2.21	0.40
7:C:550:ILE:HD12	7:C:550:ILE:H	1.86	0.40
7:C:599:GLN:HA	7:C:602:LYS:NZ	2.36	0.40
7:C:857:PRO:HG2	12:Q:122:LYS:HE3	2.03	0.40
8:O:49:ARG:HD2	8:O:146:PHE:CE1	2.56	0.40
8:O:609:LYS:HA	8:O:612:LYS:HZ3	1.86	0.40
13:A:19:ILE:HD13	13:A:19:ILE:HA	1.98	0.40
1:F:683:GLY:HA3	1:F:699:PHE:CZ	2.56	0.40
2:J:245:MET:HB3	2:K:394:GLU:OE2	2.22	0.40
2:K:710:ILE:O	2:K:714:LEU:HD23	2.22	0.40
1:H:153:LEU:O	1:H:157:ASN:ND2	2.54	0.40
5:T:464:LEU:O	5:T:468:ILE:HB	2.21	0.40
7:C:100:LEU:HD23	7:C:100:LEU:HA	1.95	0.40
7:C:403:LEU:HD13	7:C:494:PRO:HG3	2.03	0.40
7:C:465:MET:N	7:C:465:MET:SD	2.95	0.40
8:O:188:ARG:HD3	8:O:189:PHE:CE1	2.55	0.40
9:D:522:TYR:CZ	9:D:541:ARG:CZ	3.04	0.40
9:P:486:TYR:CZ	9:P:490:LYS:HD2	2.55	0.40
12:Q:196:LYS:HD3	12:Q:196:LYS:HA	1.93	0.40
1:F:88:PHE:HZ	1:F:115:GLY:HA3	1.84	0.40
1:F:631:PHE:CE2	1:F:647:CYS:HB3	2.57	0.40
1:F:649:GLY:O	1:F:652:LEU:HB2	2.21	0.40
2:J:399:LEU:HD21	2:J:405:LEU:HB2	2.02	0.40
2:J:594:PHE:C	2:J:596:PRO:HD3	2.42	0.40
2:J:634:LEU:HD21	3:G:3:ARG:HH11	1.86	0.40
2:K:590:THR:HG23	2:K:593:ARG:NH2	2.37	0.40
1:H:206:VAL:HG13	1:H:207:PHE:CD1	2.55	0.40
5:T:191:ASP:OD1	5:T:192:LEU:N	2.51	0.40
6:U:100:LEU:HD12	6:U:111:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:107:ASN:O	6:U:111:VAL:HG23	2.21	0.40
7:C:773:LYS:HD2	7:C:773:LYS:HA	1.86	0.40
7:C:970:LYS:HE2	7:C:971:PRO:HD2	2.03	0.40
7:C:973:SER:OG	7:C:974:THR:N	2.55	0.40
7:C:1358:LEU:HD23	7:C:1358:LEU:HA	1.97	0.40
8:O:338:PHE:CB	9:D:480:MET:HE1	2.49	0.40
9:D:538:ILE:HA	9:D:541:ARG:HH21	1.86	0.40
9:D:569:LEU:O	9:D:570:GLU:HG2	2.21	0.40
9:P:413:HIS:CD2	9:P:443:GLU:HG3	2.57	0.40
9:P:499:ARG:NH1	9:P:529:SER:O	2.53	0.40
2:J:288:ARG:NH1	2:K:492:ASN:HB3	2.36	0.40
2:J:390:ILE:HG12	2:J:418:ASP:O	2.21	0.40
2:J:547:ILE:HD11	2:J:574:THR:HA	2.03	0.40
1:H:652:LEU:HD23	1:H:652:LEU:HA	1.94	0.40
5:T:186:MET:O	5:T:220:LYS:NZ	2.55	0.40
5:T:389:LEU:HD22	5:T:393:GLU:OE1	2.21	0.40
5:T:392:GLU:O	5:T:396:GLU:HG3	2.21	0.40
7:C:1303:ASP:HB2	7:C:1351:ILE:HD11	2.02	0.40
7:C:1573:VAL:HA	7:C:1582:GLU:OE2	2.20	0.40
8:O:525:PHE:HE1	8:O:558:LYS:HB2	1.85	0.40
9:P:187:ILE:HB	9:P:224:ILE:HD11	2.04	0.40
9:P:235:MET:SD	9:P:236:SER:N	2.95	0.40
9:P:242:LEU:HD21	9:P:251:CYS:CB	2.50	0.40
9:P:257:ASP:OD2	10:I:7:ARG:NH2	2.54	0.40
1:H:492:LEU:HD22	1:H:515:LEU:HD23	2.03	0.40
1:H:641:ASN:OD1	1:H:642:VAL:N	2.55	0.40
7:C:191:LEU:HD21	7:C:194:PHE:HB2	2.04	0.40
7:C:207:ASP:HB3	7:C:210:SER:OG	2.22	0.40
7:C:485:GLU:OE2	7:C:485:GLU:N	2.52	0.40
8:O:127:TYR:OH	8:O:131:LYS:HE3	2.21	0.40
8:O:378:LEU:O	8:O:381:ILE:HG22	2.20	0.40
8:O:637:LEU:HD23	8:O:646:ALA:HB2	2.04	0.40
8:O:666:LYS:HD2	8:O:666:LYS:HA	1.95	0.40
9:P:483:TYR:CE2	11:N:123:GLY:HA3	2.57	0.40
10:I:24:TYR:CD1	10:I:24:TYR:N	2.89	0.40
10:I:34:LEU:HD11	10:I:37:GLU:CD	2.41	0.40
13:A:205:ASN:ND2	13:A:211:ASP:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	496/758 (65%)	477 (96%)	19 (4%)	0	100	100
1	H	499/758 (66%)	484 (97%)	13 (3%)	2 (0%)	34	72
2	J	505/850 (59%)	481 (95%)	24 (5%)	0	100	100
2	K	501/850 (59%)	491 (98%)	10 (2%)	0	100	100
3	G	32/124 (26%)	32 (100%)	0	0	100	100
3	W	28/124 (23%)	28 (100%)	0	0	100	100
4	E	120/265 (45%)	118 (98%)	2 (2%)	0	100	100
5	T	638/853 (75%)	619 (97%)	17 (3%)	2 (0%)	41	76
6	U	110/165 (67%)	108 (98%)	2 (2%)	0	100	100
7	C	1380/1748 (79%)	1289 (93%)	85 (6%)	6 (0%)	34	72
8	O	654/685 (96%)	619 (95%)	31 (5%)	4 (1%)	25	65
9	D	554/626 (88%)	533 (96%)	20 (4%)	1 (0%)	47	81
9	P	550/626 (88%)	527 (96%)	22 (4%)	1 (0%)	47	81
10	I	101/170 (59%)	94 (93%)	7 (7%)	0	100	100
11	N	92/368 (25%)	86 (94%)	6 (6%)	0	100	100
12	Q	619/652 (95%)	596 (96%)	22 (4%)	1 (0%)	47	81
13	A	212/250 (85%)	204 (96%)	7 (3%)	1 (0%)	29	69
All	All	7091/9872 (72%)	6786 (96%)	287 (4%)	18 (0%)	44	76

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	T	621	GLN
5	T	624	ASN
7	C	844	VAL
7	C	1279	ILE
7	C	1552	ARG

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Mol	Chain	Res	Type
8	O	193	VAL
9	D	205	ILE
1	H	507	LYS
1	H	554	LYS
12	Q	10	ILE
8	O	53	GLU
9	P	530	GLN
7	C	1416	VAL
8	O	419	ALA
7	C	801	VAL
8	O	355	CYS
13	A	21	PRO
7	C	1551	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	433/684 (63%)	433 (100%)	0	100	100
1	H	440/684 (64%)	439 (100%)	1 (0%)	93	96
2	J	450/760 (59%)	450 (100%)	0	100	100
2	K	448/760 (59%)	446 (100%)	2 (0%)	91	94
3	G	33/115 (29%)	33 (100%)	0	100	100
3	W	29/115 (25%)	29 (100%)	0	100	100
4	E	123/246 (50%)	123 (100%)	0	100	100
5	T	608/804 (76%)	605 (100%)	3 (0%)	88	93
6	U	103/149 (69%)	102 (99%)	1 (1%)	76	86
7	C	1177/1568 (75%)	1175 (100%)	2 (0%)	93	96
8	O	597/643 (93%)	596 (100%)	1 (0%)	93	96
9	D	477/560 (85%)	476 (100%)	1 (0%)	93	96
9	P	477/560 (85%)	473 (99%)	4 (1%)	81	89
10	I	92/144 (64%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	N	83/332 (25%)	83 (100%)	0	100 100
12	Q	572/598 (96%)	571 (100%)	1 (0%)	93 96
13	A	190/226 (84%)	188 (99%)	2 (1%)	73 85
All	All	6332/8948 (71%)	6314 (100%)	18 (0%)	92 95

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	299	ARG
2	K	467	ARG
1	H	598	ARG
5	T	143	ARG
5	T	343	ARG
5	T	744	MET
6	U	2	LYS
7	C	149	LYS
7	C	1025	LYS
8	O	293	ASN
9	D	371	ASN
9	P	16	GLN
9	P	138	ASN
9	P	405	ASN
9	P	541	ARG
12	Q	104	ARG
13	A	28	LYS
13	A	96	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	35	GLN
1	F	527	ASN
1	F	609	ASN
1	F	670	HIS
1	F	672	GLN
1	F	697	GLN
1	F	744	ASN
2	J	290	ASN
2	J	310	GLN
2	J	450	ASN

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Mol	Chain	Res	Type
2	K	258	ASN
2	K	271	GLN
2	K	608	GLN
1	H	568	GLN
5	T	101	GLN
7	C	36	ASN
7	C	938	GLN
7	C	1056	ASN
8	O	223	ASN
9	D	77	ASN
9	D	534	GLN
9	P	77	ASN
9	P	230	ASN
9	P	248	ASN
10	I	98	ASN
10	I	101	ASN
10	I	152	GLN
12	Q	469	GLN
13	A	27	ASN
13	A	122	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

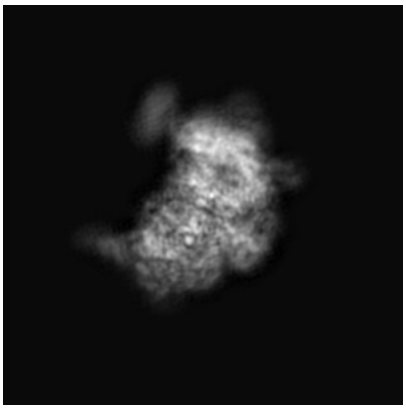
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15201. These allow visual inspection of the internal detail of the map and identification of artifacts.

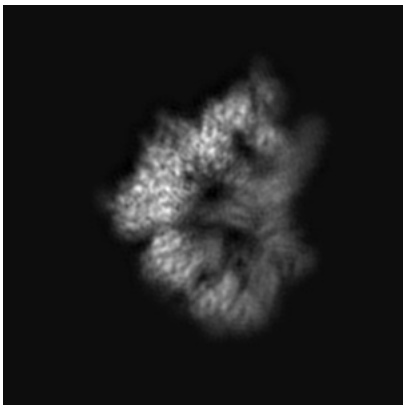
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

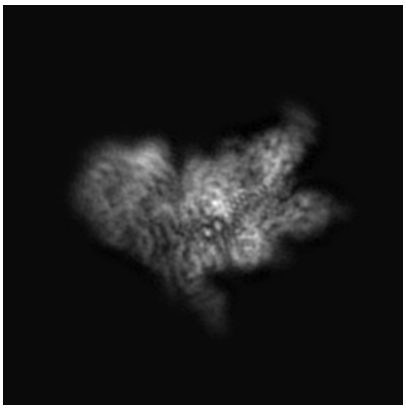
6.1.1 Primary map



X

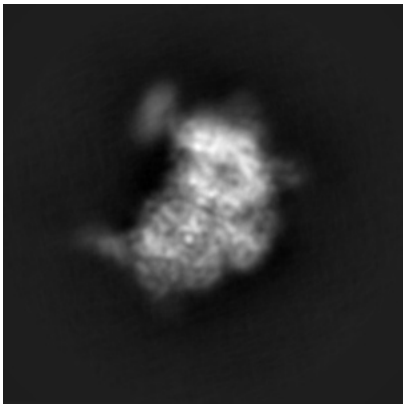


Y

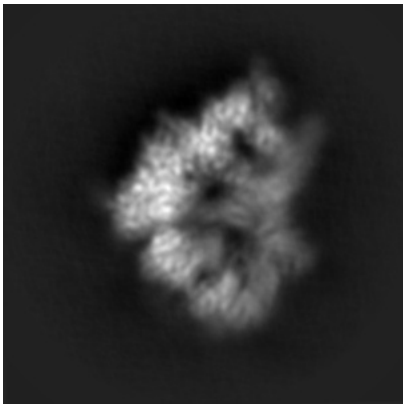


Z

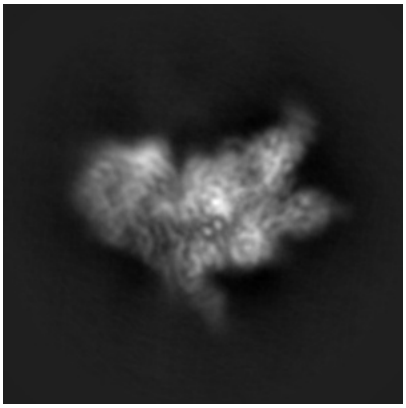
6.1.2 Raw map



X



Y

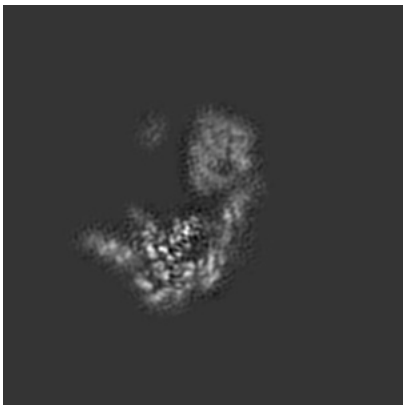


Z

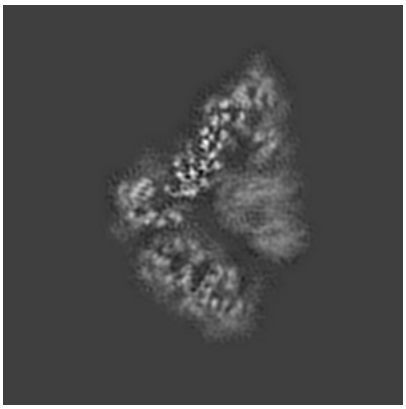
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

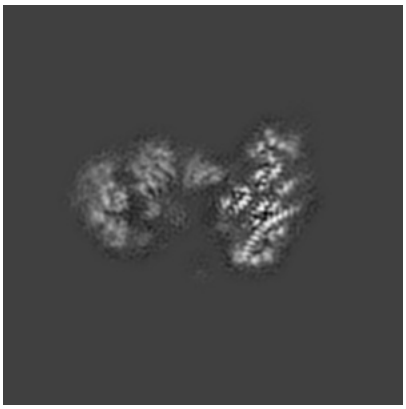
6.2.1 Primary map



X Index: 128

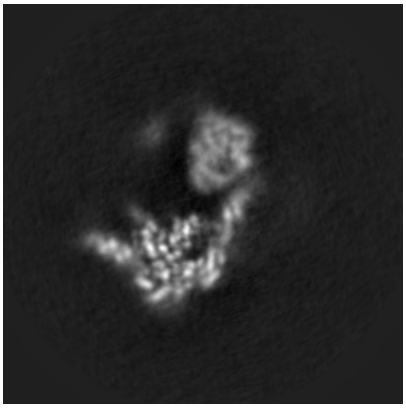


Y Index: 128

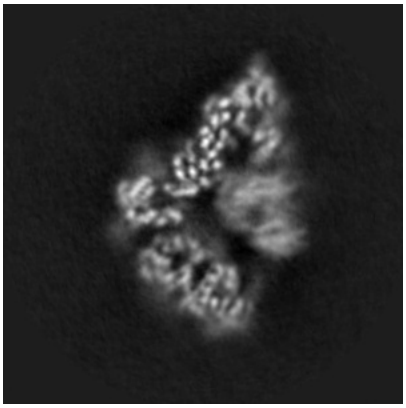


Z Index: 128

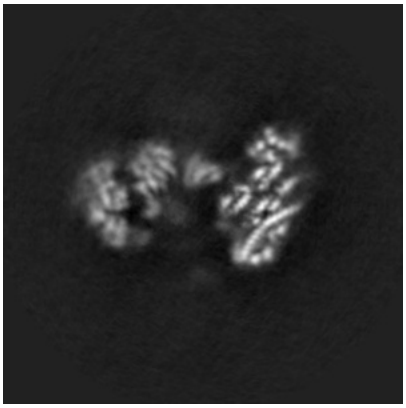
6.2.2 Raw map



X Index: 128



Y Index: 128

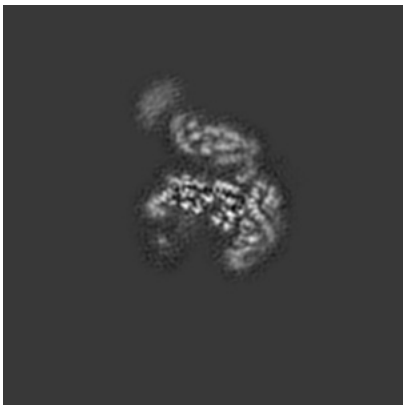


Z Index: 128

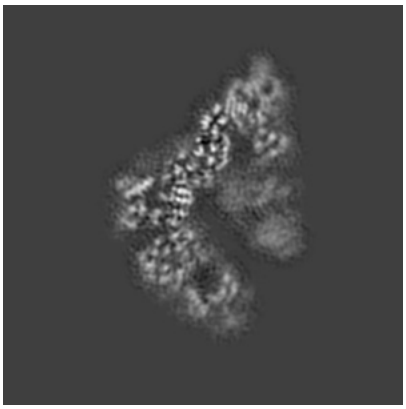
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

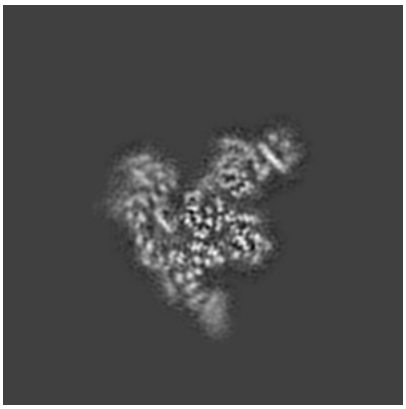
6.3.1 Primary map



X Index: 170

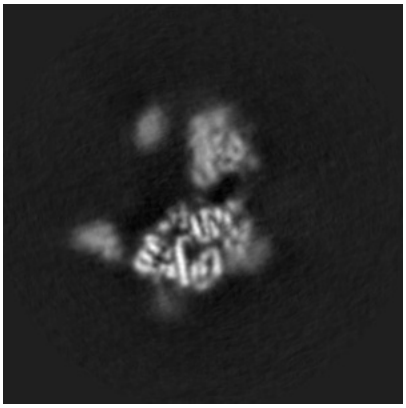


Y Index: 122

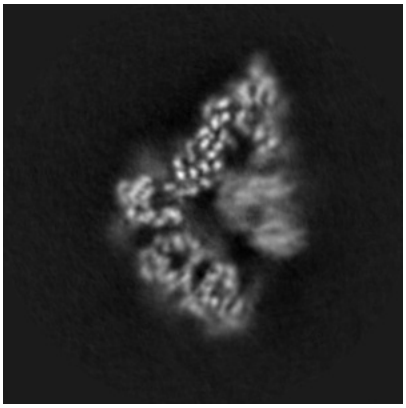


Z Index: 105

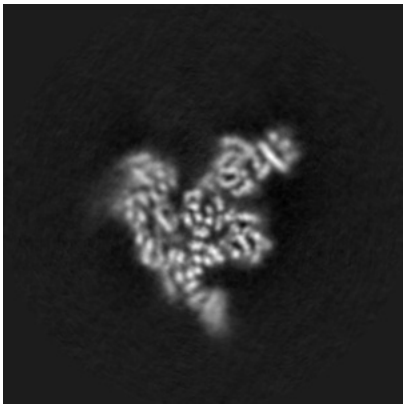
6.3.2 Raw map



X Index: 137



Y Index: 127

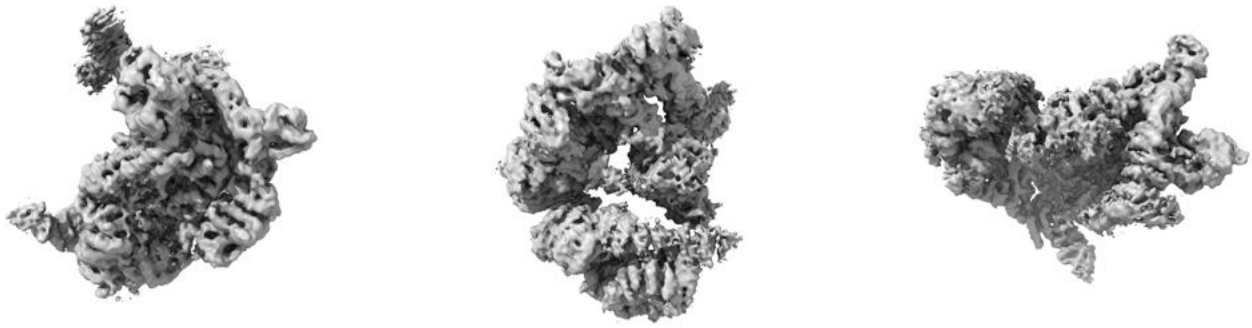


Z Index: 105

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

6.4 Orthogonal surface views (i)

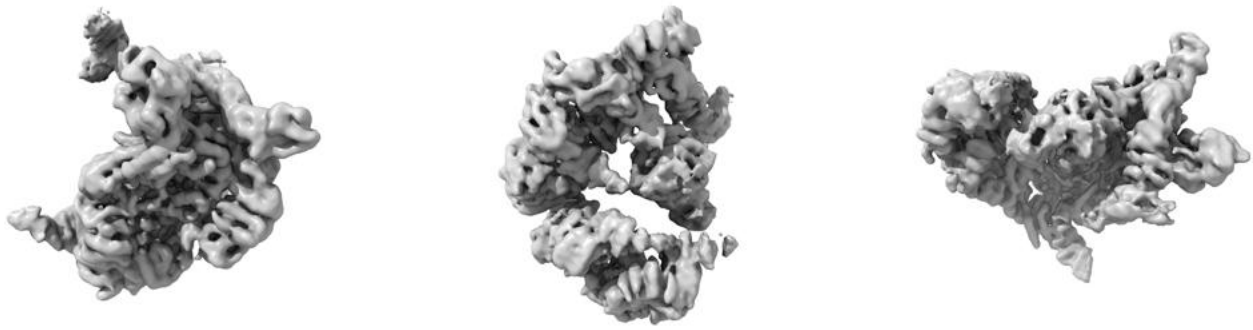
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

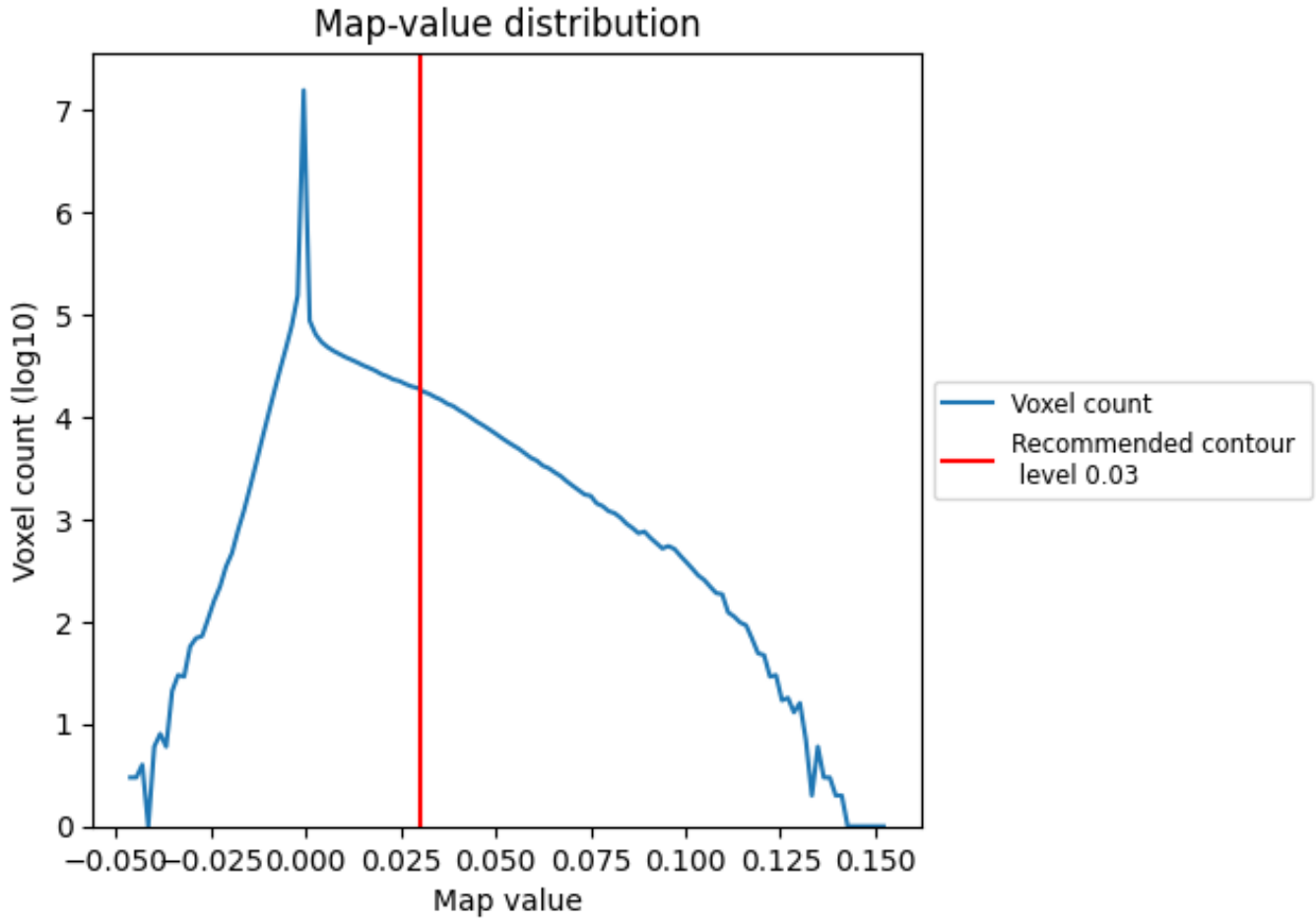
6.5 Mask visualisation (i)

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

7 Map analysis

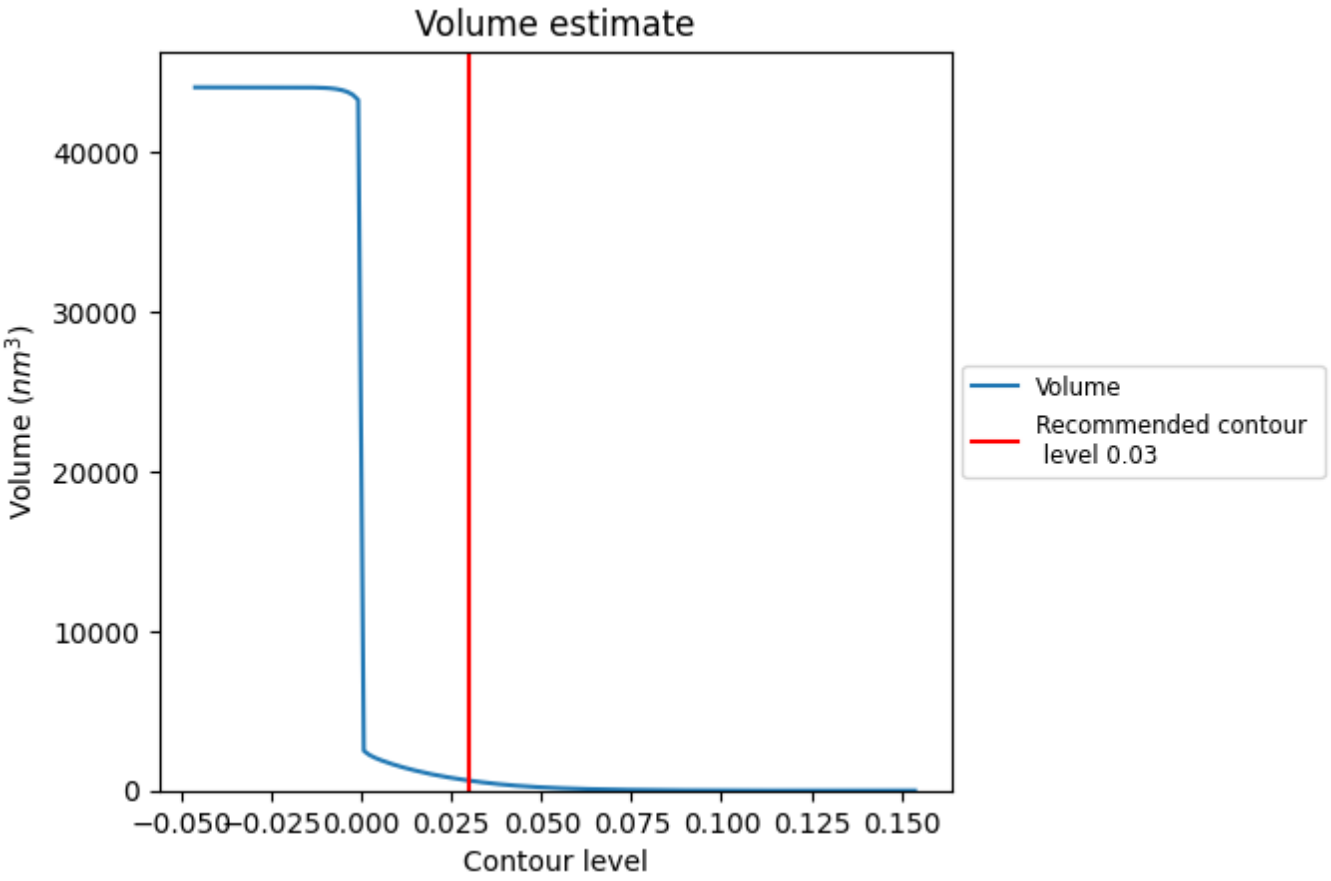
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

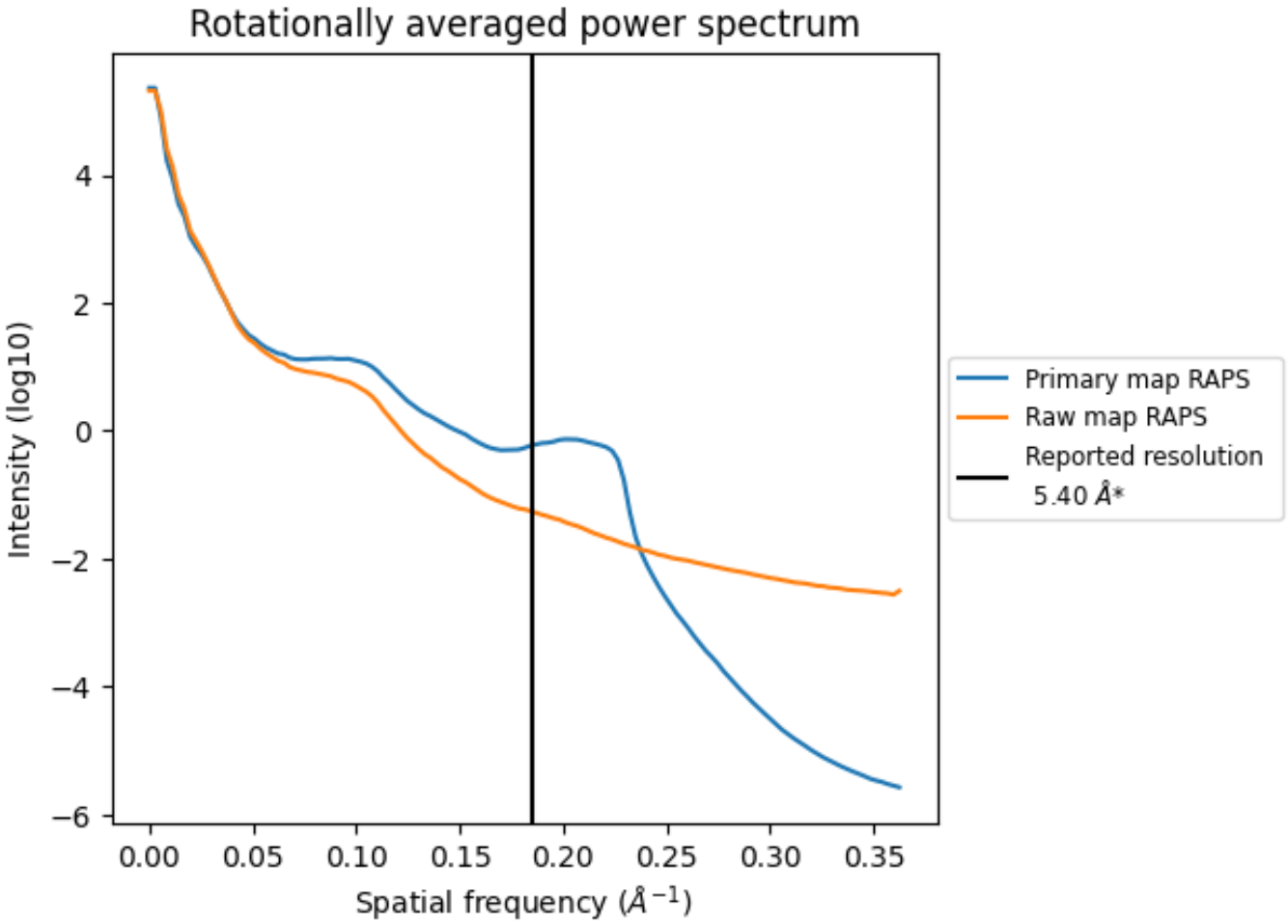
7.2 Volume estimate



The volume at the recommended contour level is 624 nm^3; this corresponds to an approximate mass of 564 kDa.

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

7.3 Rotationally averaged power spectrum (i)

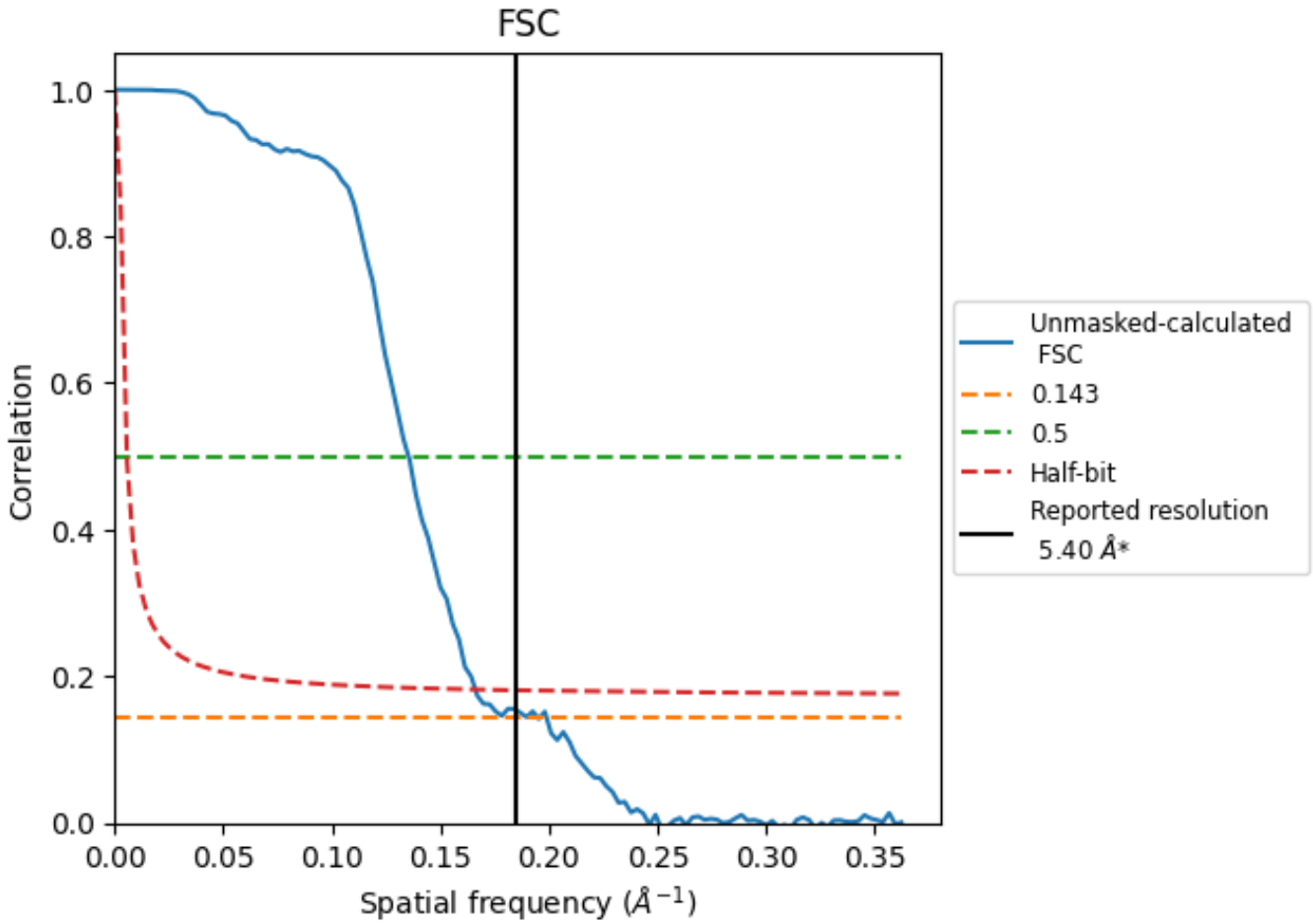


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8.2 Resolution estimates (i)

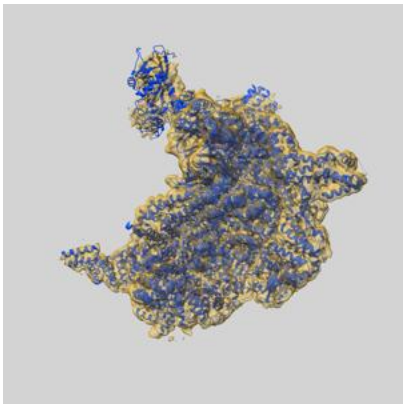
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.13	7.39	6.02

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

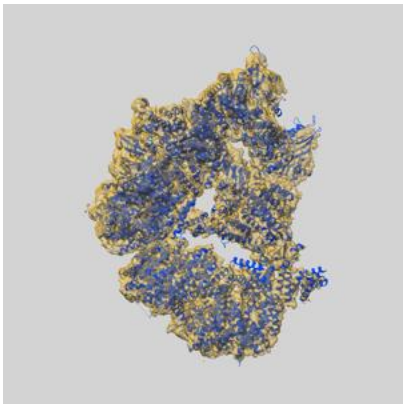
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15201 and PDB model 8A61. Per-residue inclusion information can be found in section 3 on page 7.

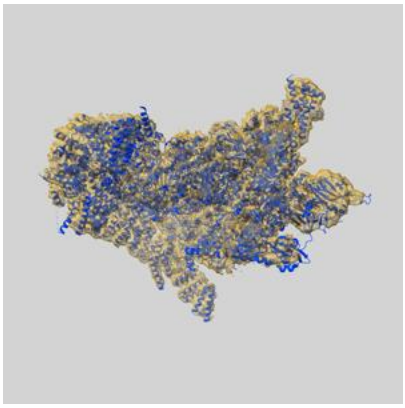
9.1 Map-model overlay



X



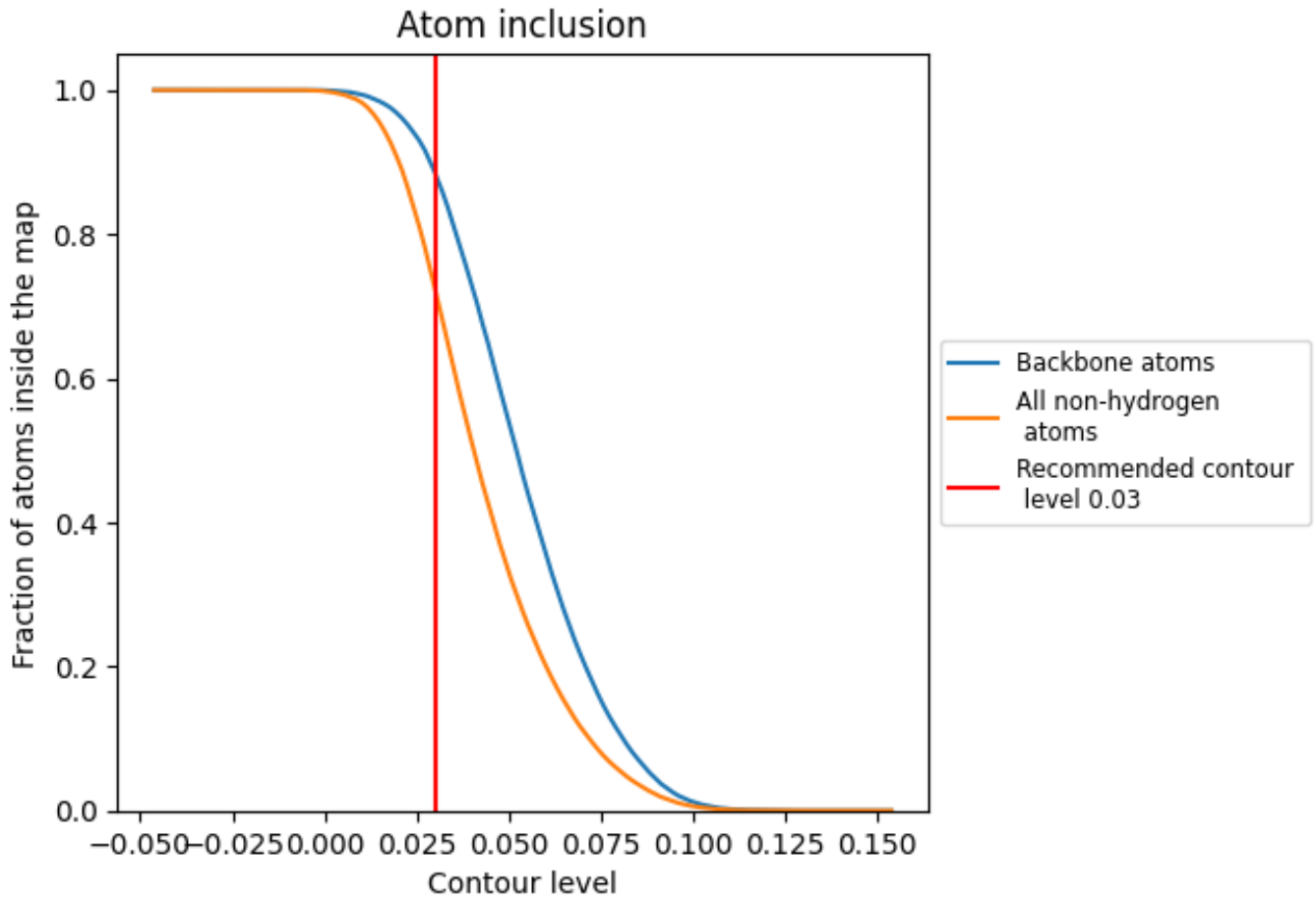
Y



Z

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

9.2 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.