



## Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 12:58 PM EDT

PDB ID : 7U4T / pdb\_00007u4t  
EMDB ID : EMD-26334  
Title : Human V-ATPase in state 2 with SidK and mEAK-7  
Authors : Wang, L.; Fu, T.M.  
Deposited on : 2022-03-01  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

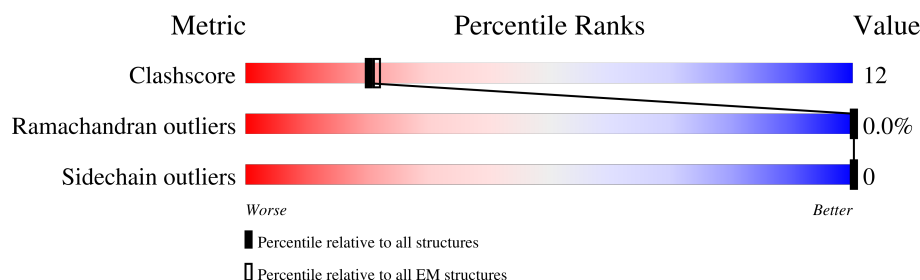
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	R	837	<div> <div>42%</div> <div>63%</div> <div>27%</div> <div>10%</div> </div>
2	O	382	<div> <div>57%</div> <div>93%</div> <div>•</div> <div>•</div> </div>
3	H	226	<div> <div>9%</div> <div>74%</div> <div>23%</div> <div>•</div> </div>
3	I	226	<div> <div>73%</div> <div>25%</div> <div>•</div> </div>
3	J	226	<div> <div>23%</div> <div>63%</div> <div>36%</div> </div>
4	K	118	<div> <div>15%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
4	L	118	<div> <div>14%</div> <div>77%</div> <div>19%</div> <div>•</div> </div>
4	M	118	<div> <div>27%</div> <div>64%</div> <div>33%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	S	81	
6	T	137	
7	U	470	
8	V	350	
9	0	205	
10	1	155	
10	2	155	
10	3	155	
10	4	155	
10	5	155	
10	6	155	
10	7	155	
10	8	155	
10	9	155	
11	Q	351	
12	A	617	
12	B	617	
12	C	617	
13	D	511	
13	E	511	
13	F	511	
14	X	573	
14	Y	573	
14	Z	573	
15	G	247	

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Mol	Chain	Length	Quality of chain
16	N	119	<div><div></div><div>9%</div><div>57%</div><div>35%</div><div>8%</div></div>
17	P	483	<div><div></div><div>53%</div><div>85%</div><div>12%</div></div>
18	W	456	<div><div></div><div>38%</div><div>69%</div><div>23%</div><div>8%</div></div>

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 71598 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 V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	753	Total	C	N	O	S	0	0
			5876	3827	982	1031	36		

- Molecule 2 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	365	Total	C	N	O	0	0
			1817	1087	365	365		

- Molecule 3 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	225	Total	C	N	O	S	0	0
			1774	1110	316	340	8		
3	I	221	Total	C	N	O	S	0	0
			1661	1040	302	311	8		
3	H	220	Total	C	N	O	S	0	0
			1611	1005	296	303	7		

- Molecule 4 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	114	Total	C	N	O	S	0	0
			889	544	170	172	3		
4	L	113	Total	C	N	O	S	0	0
			748	456	139	150	3		
4	K	114	Total	C	N	O	S	0	0
			735	448	136	148	3		

- Molecule 5 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 6 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	85	Total	C	N	O	S	0	0
			658	434	102	115	7		

- Molecule 7 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	204	Total	C	N	O	S	0	0
			1662	1086	267	299	10		

- Molecule 8 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	49	Total	C	N	O	S	0	0
			411	280	57	71	3		

- Molecule 9 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0	204	Total	C	N	O	S	0	0
			1498	990	238	259	11		

- Molecule 10 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	351	Total	C	N	O	S	0	0
			2844	1834	463	532	15		

- Molecule 12 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
12	A	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
12	B	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		

- Molecule 13 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
13	E	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
13	F	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		

- Molecule 14 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	262	Total	C	N	O	S	0	0
			2110	1339	353	408	10		
14	X	267	Total	C	N	O	S	0	0
			2136	1355	359	411	11		
14	Y	262	Total	C	N	O	S	0	0
			2111	1339	354	408	10		

- Molecule 15 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	213	Total	C	N	O	S	0	0
			1717	1090	310	312	5		

- Molecule 16 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	110	Total	C	N	O	S	0	0
			875	552	157	164	2		

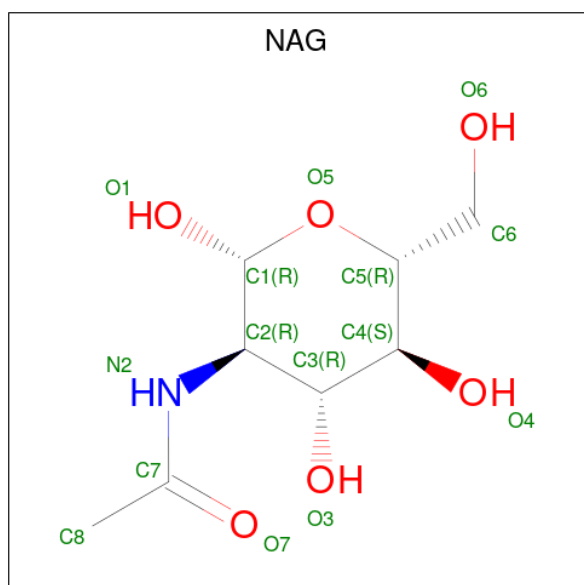
- Molecule 17 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	427	Total	C	N	O	S	0	0
			2121	1267	427	427			

- Molecule 18 is a protein called MTOR-associated protein MEAK7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	420	Total	C	N	O	S	0	0
			3023	1900	548	559	16		

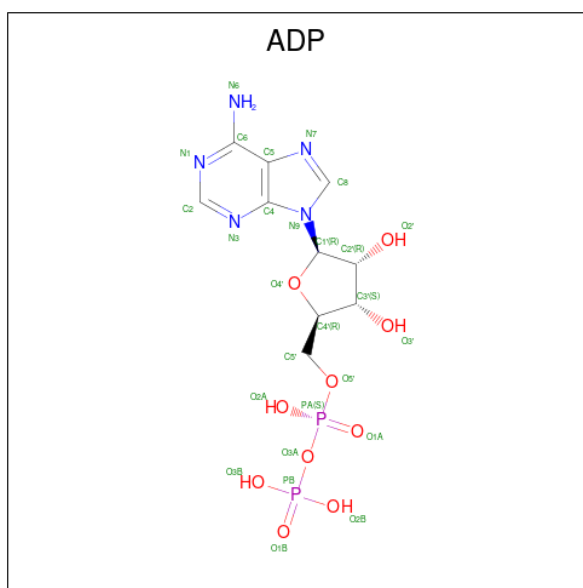
- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms				AltConf
19	R	1	Total	C	N	O	0
			14	8	1	5	
19	S	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

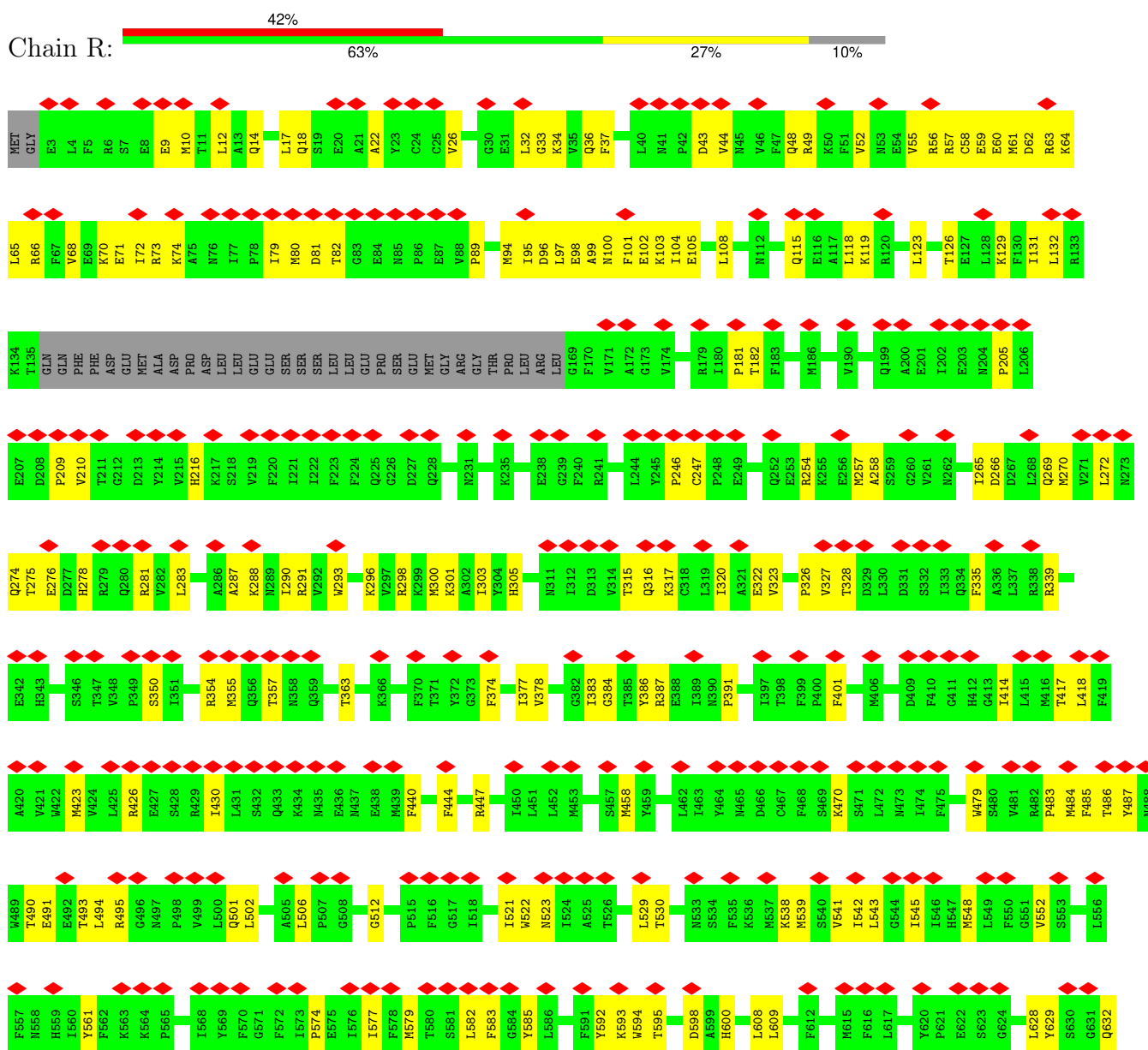


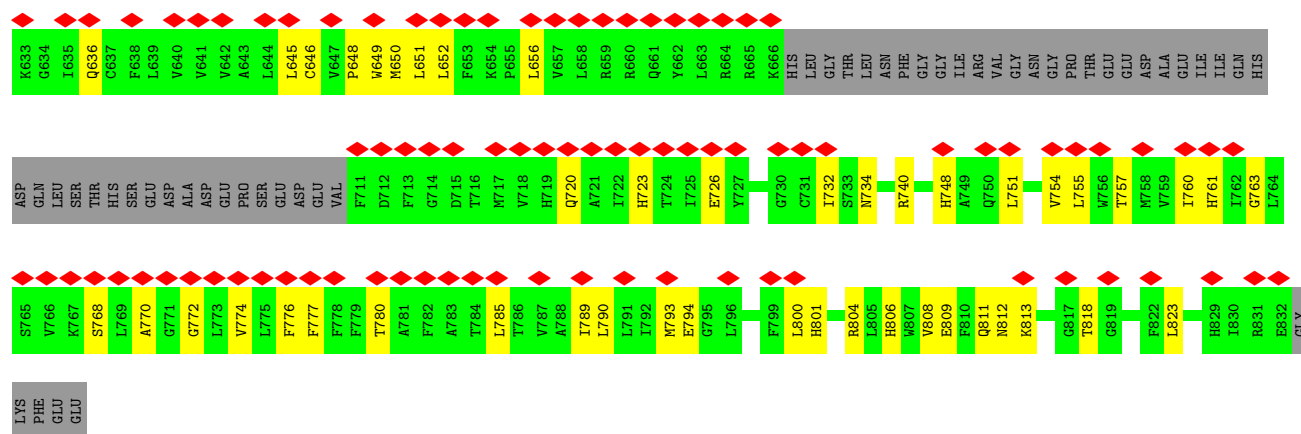
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

### 3 Residue-property plots

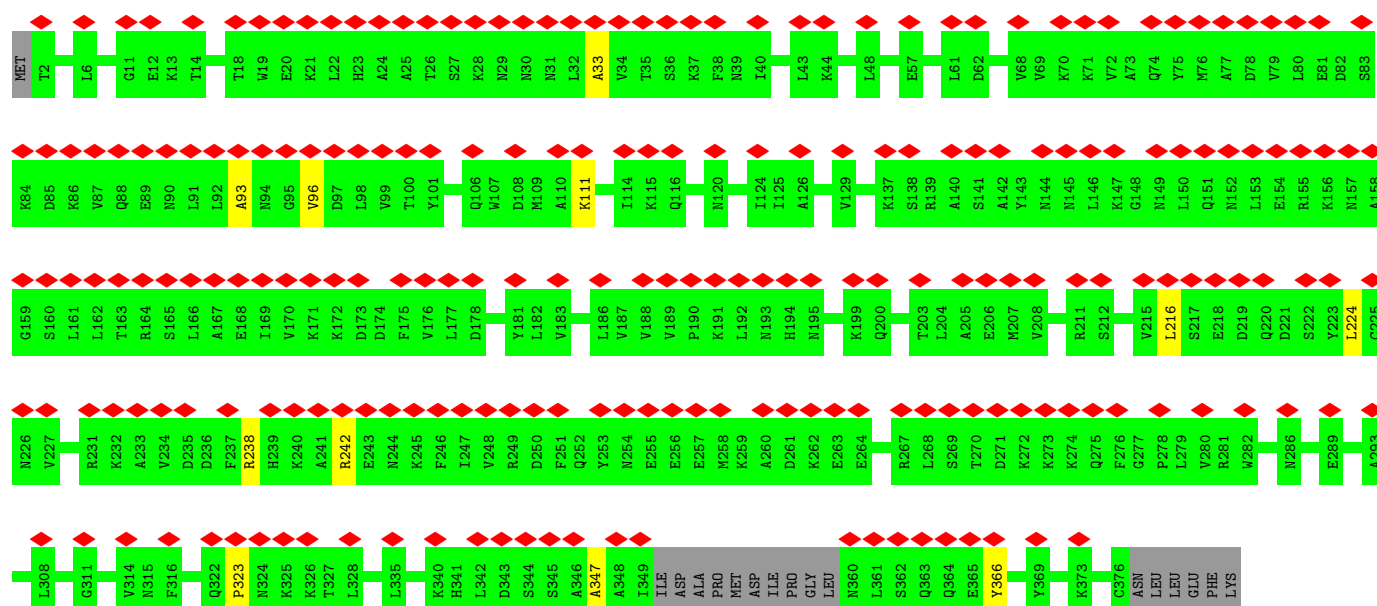
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: V-type proton ATPase 116 kDa subunit a isoform 1

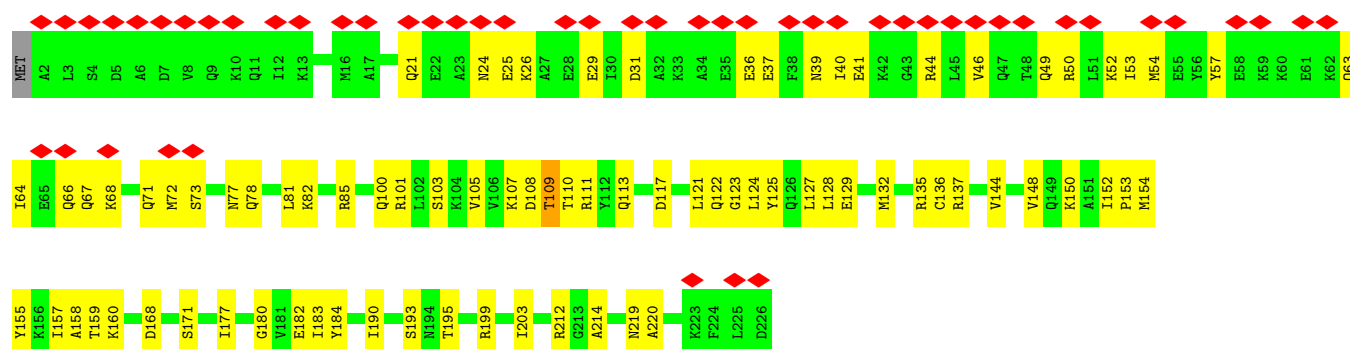




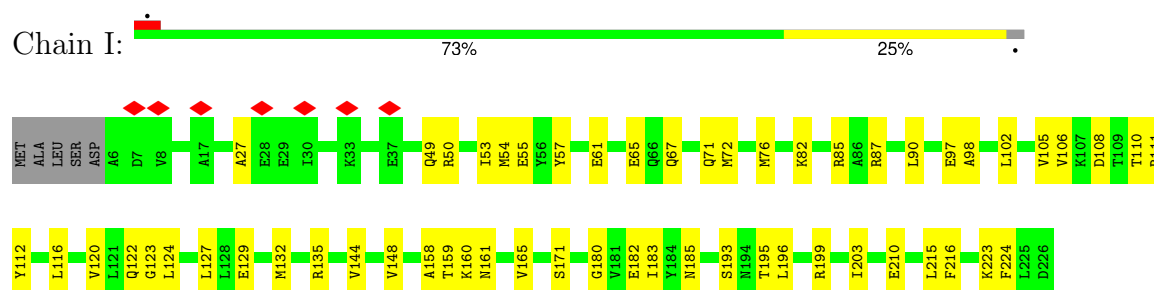
• Molecule 2: V-type proton ATPase subunit C 1



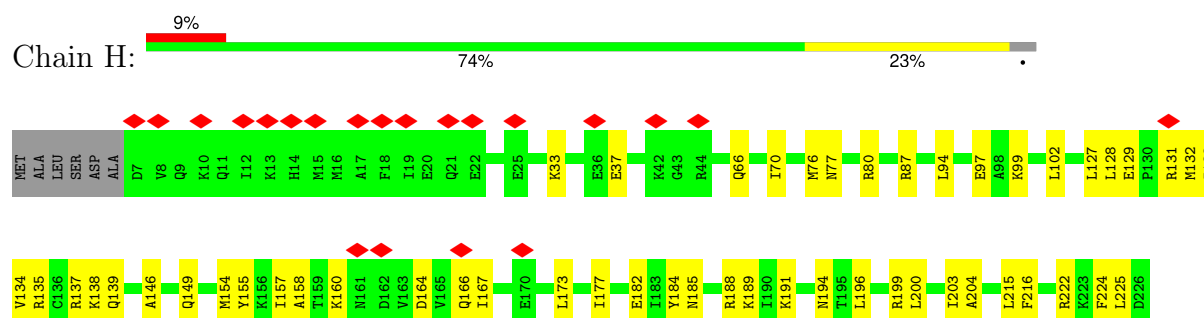
• Molecule 3: V-type proton ATPase subunit E 1



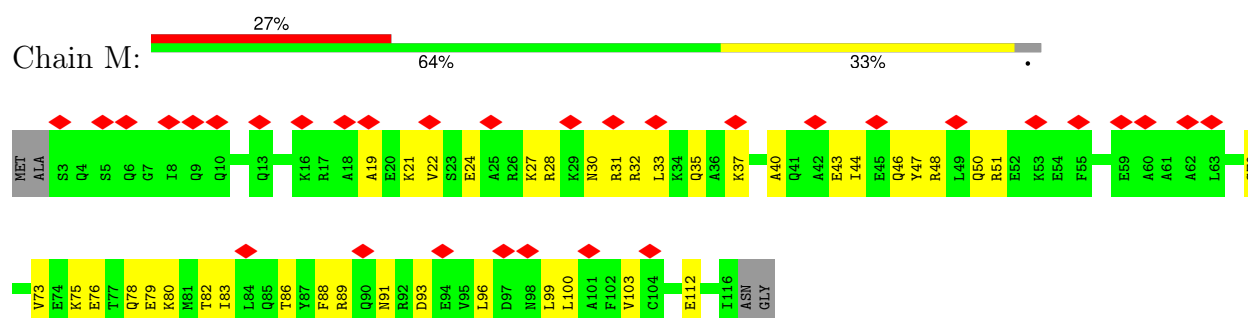
- Molecule 3: V-type proton ATPase subunit E 1



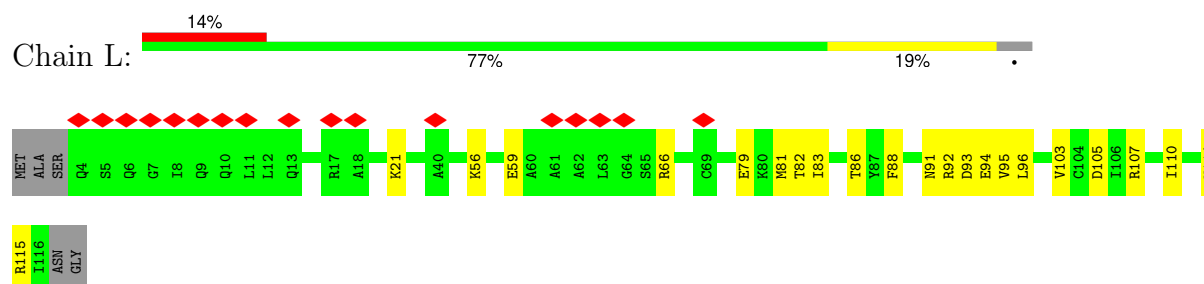
- Molecule 3: V-type proton ATPase subunit E 1



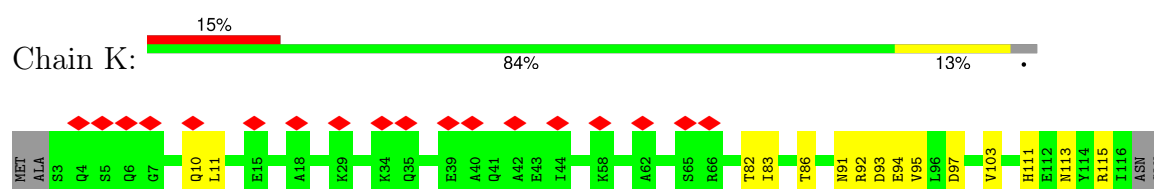
- Molecule 4: V-type proton ATPase subunit G 1



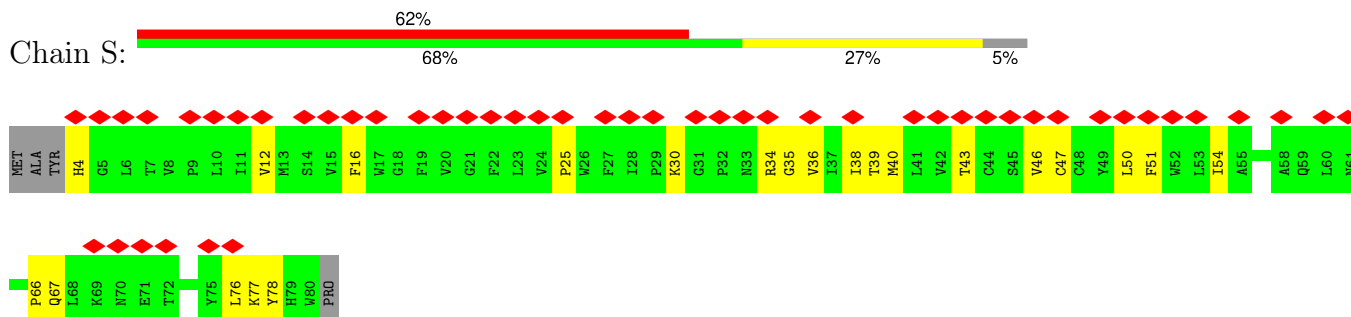
- Molecule 4: V-type proton ATPase subunit G 1



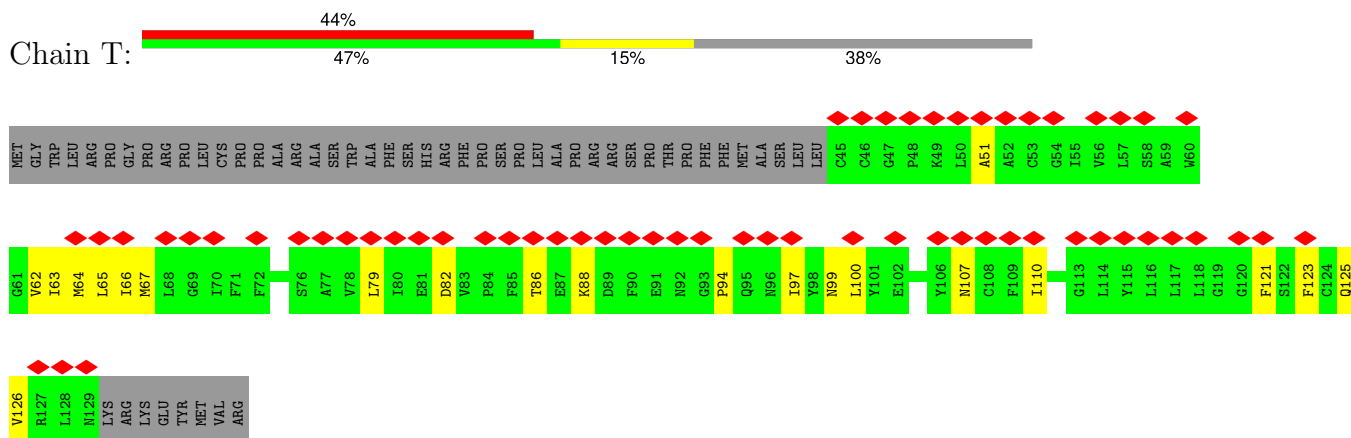
- Molecule 4: V-type proton ATPase subunit G 1



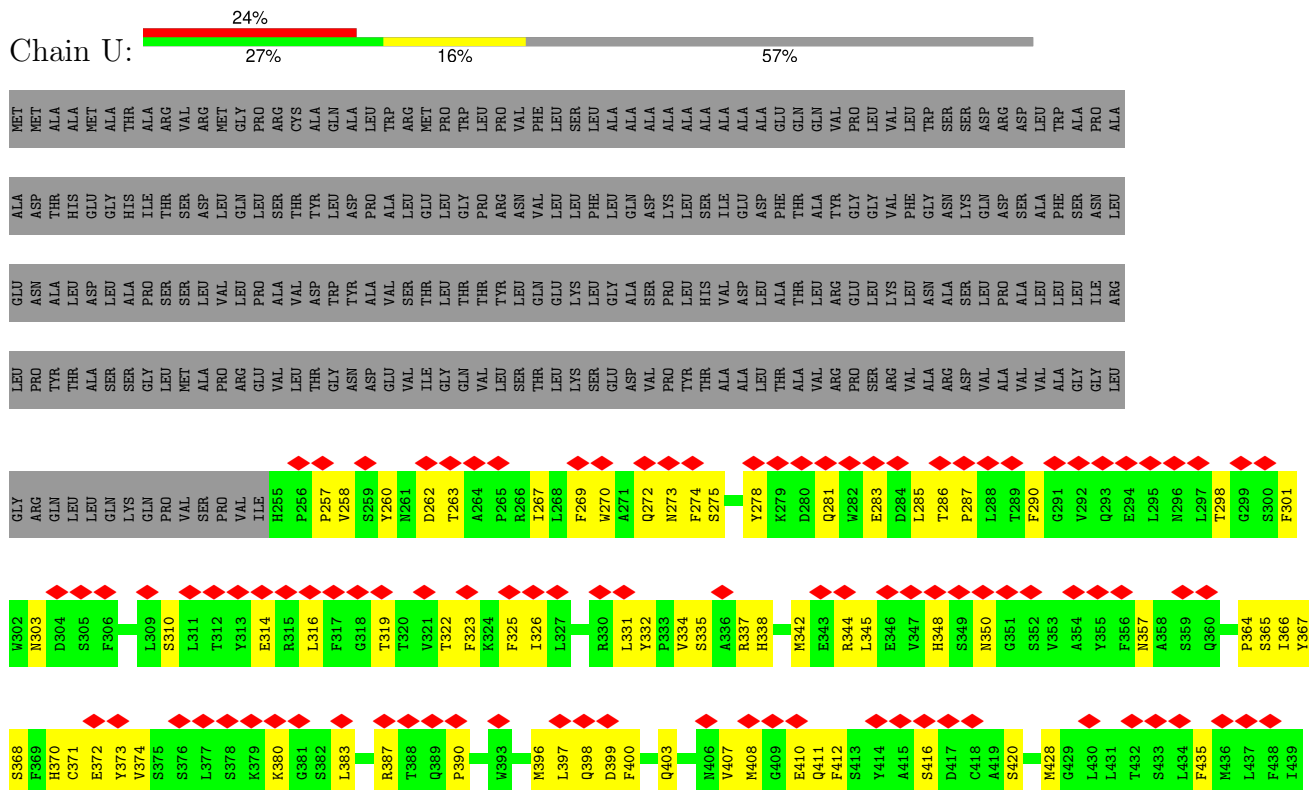
Chain S:



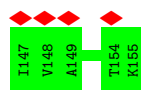
## Chain T:



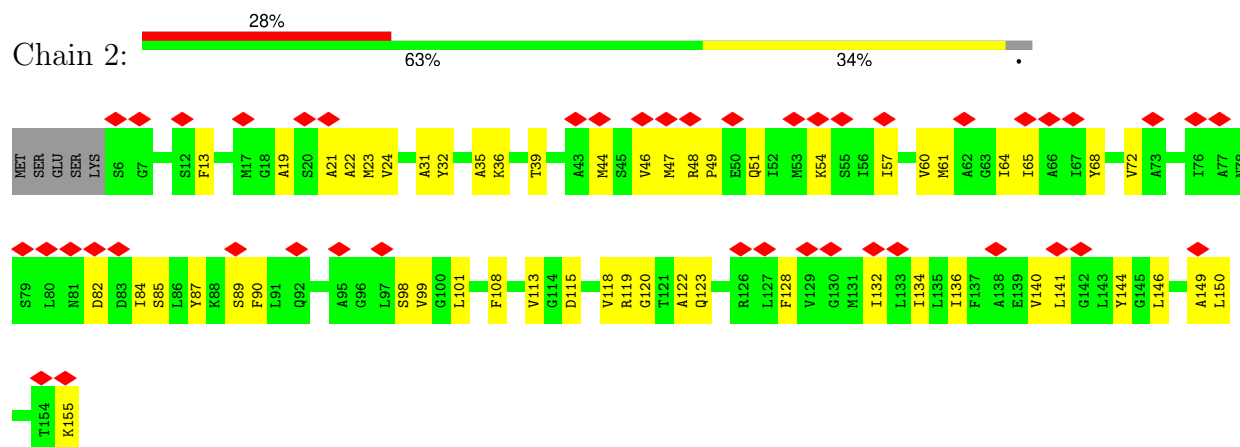
Chain U:



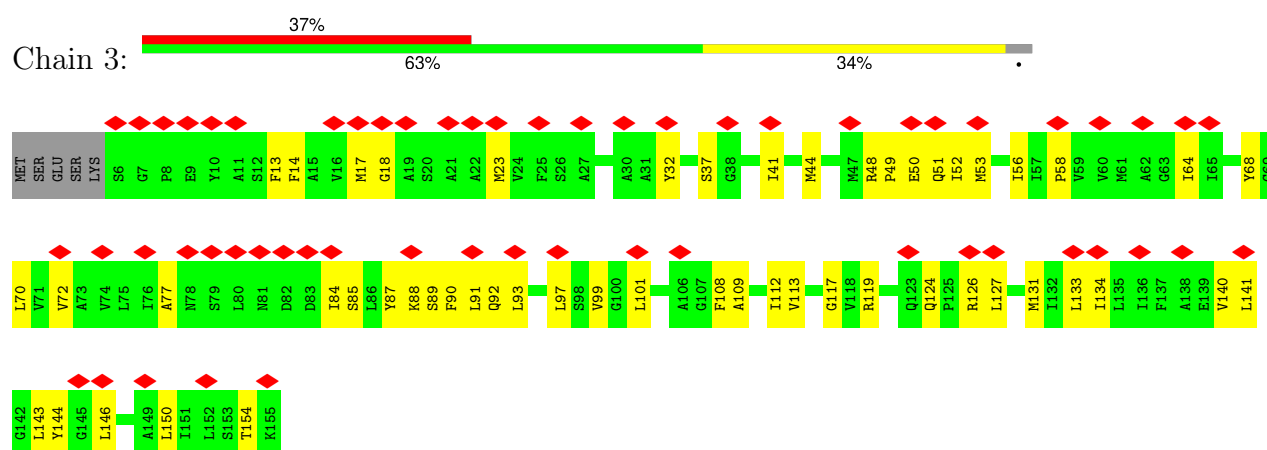




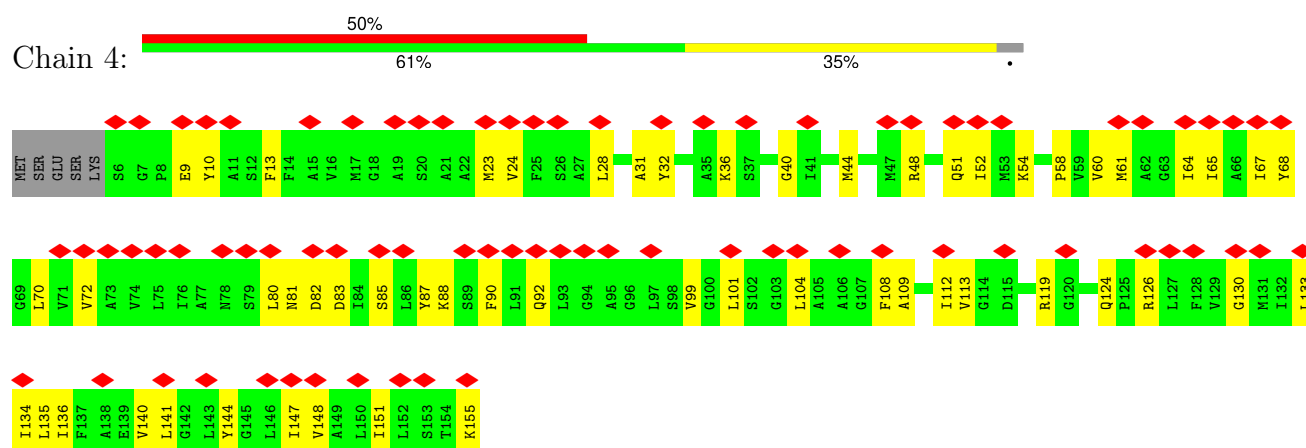
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



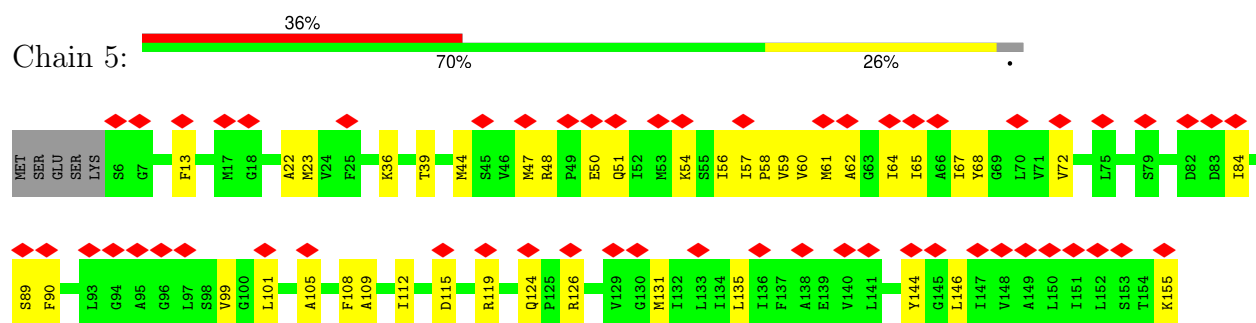
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



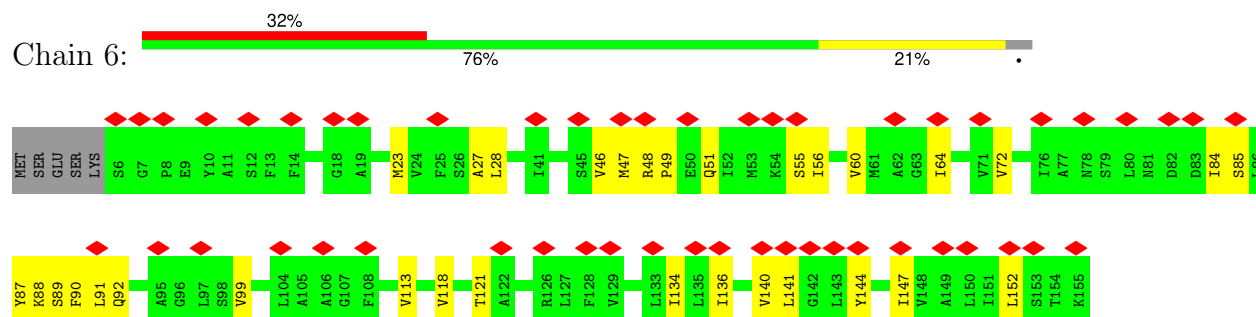
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



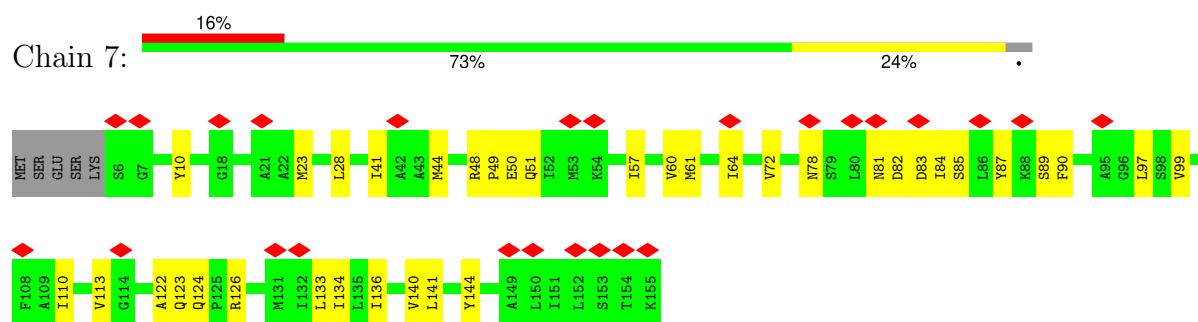
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



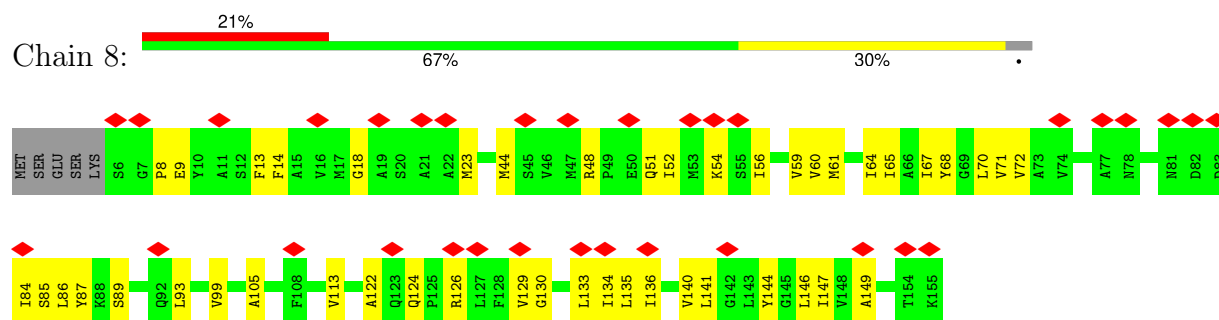
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



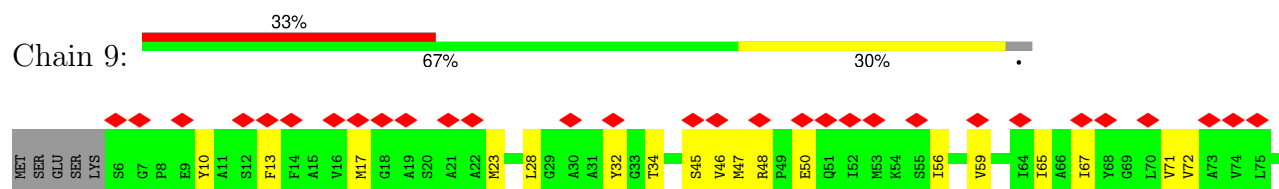
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



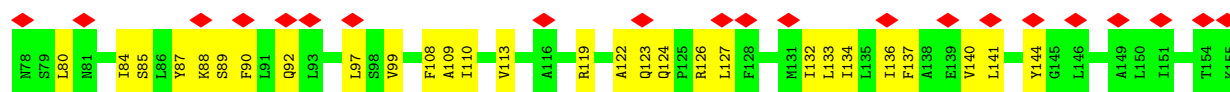
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



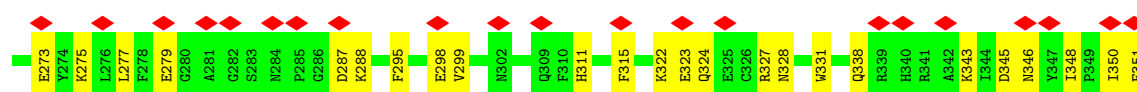
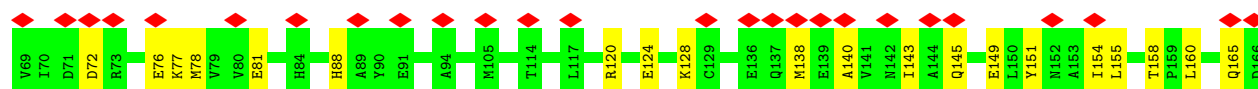
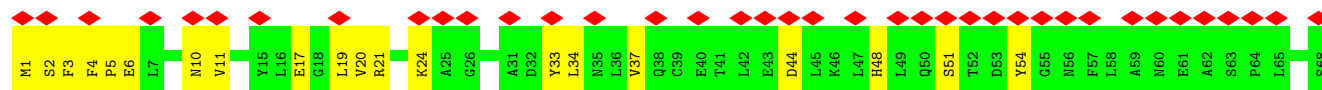
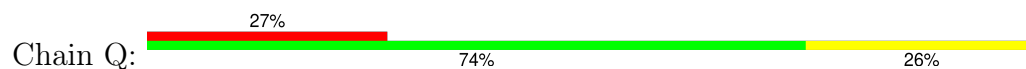
- Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



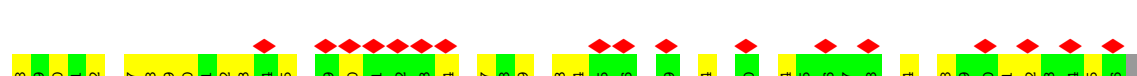
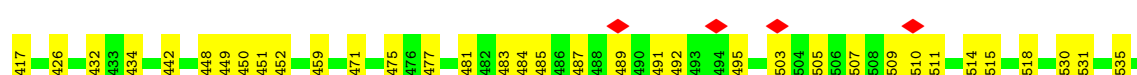
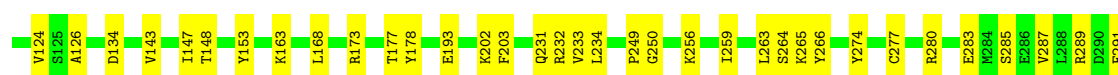




• Molecule 11: V-type proton ATPase subunit d 1

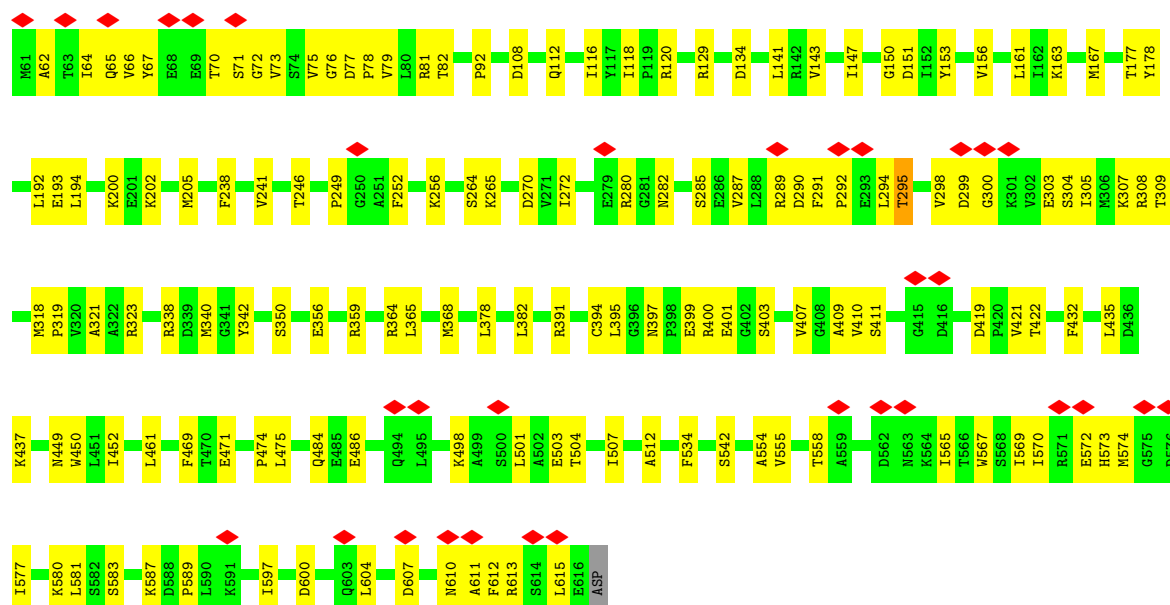


• Molecule 12: V-type proton ATPase catalytic subunit A



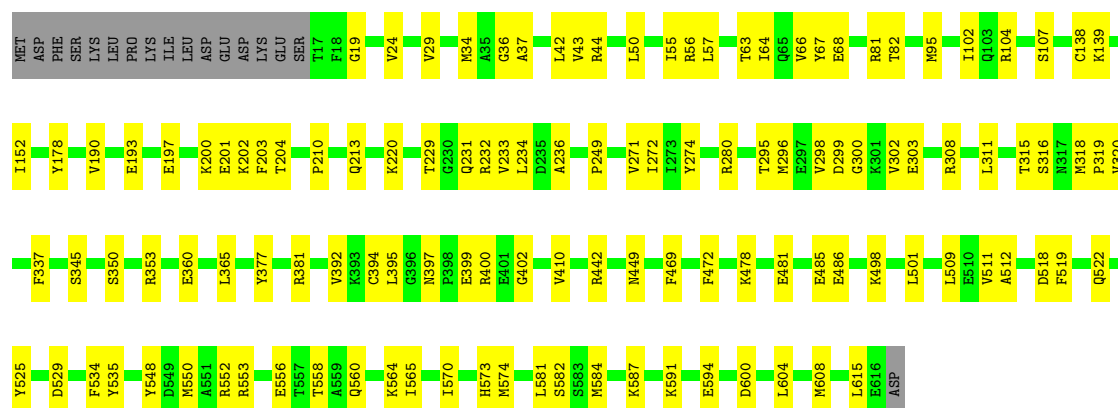
• Molecule 12: V-type proton ATPase catalytic subunit A





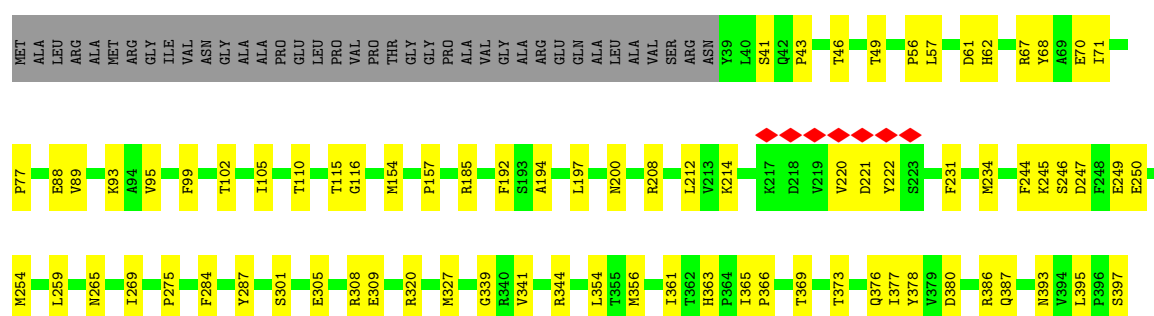
• Molecule 12: V-type proton ATPase catalytic subunit A

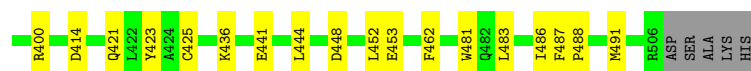
Chain B: 77% 20% .



• Molecule 13: V-type proton ATPase subunit B, brain isoform

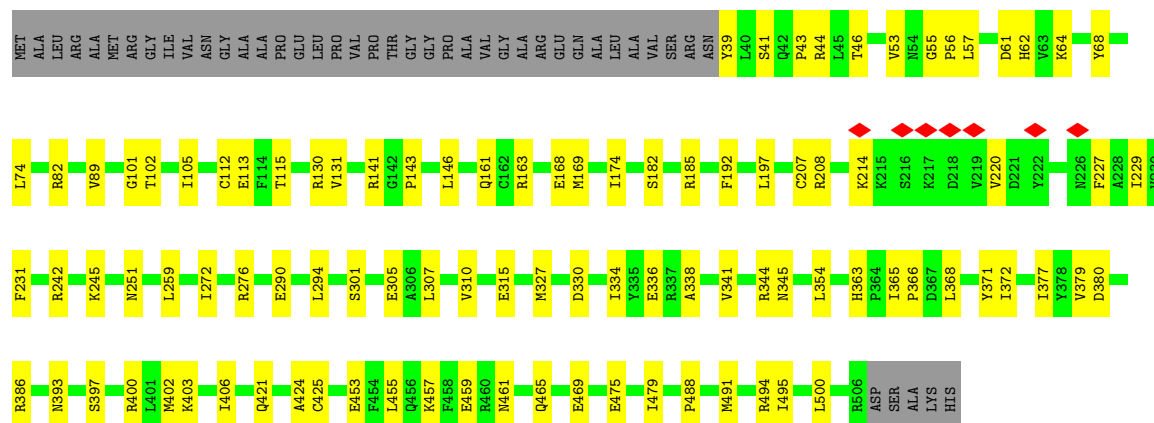
Chain D: 73% 19% 8%





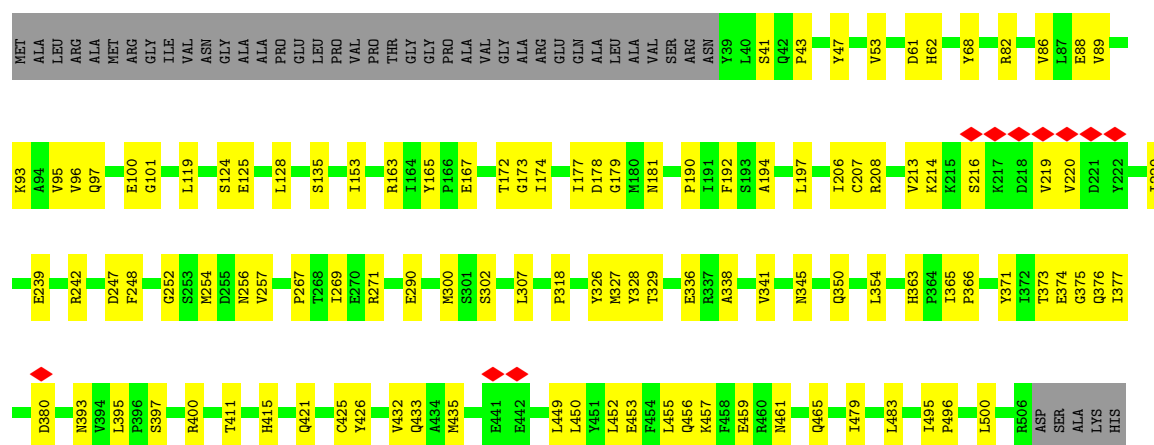
- Molecule 13: V-type proton ATPase subunit B, brain isoform

Chain E: 72% 19% 8%



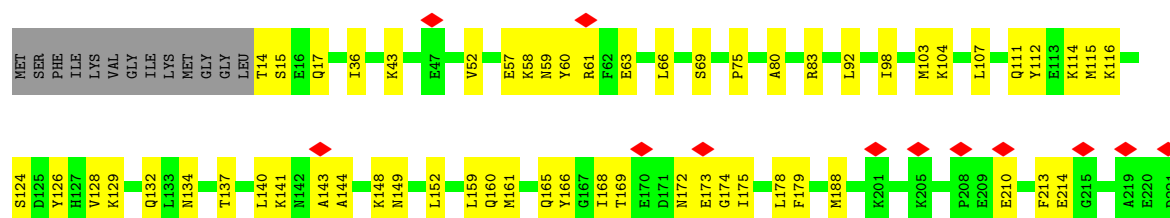
- Molecule 13: V-type proton ATPase subunit B, brain isoform

Chain F: 70% 21% 8%

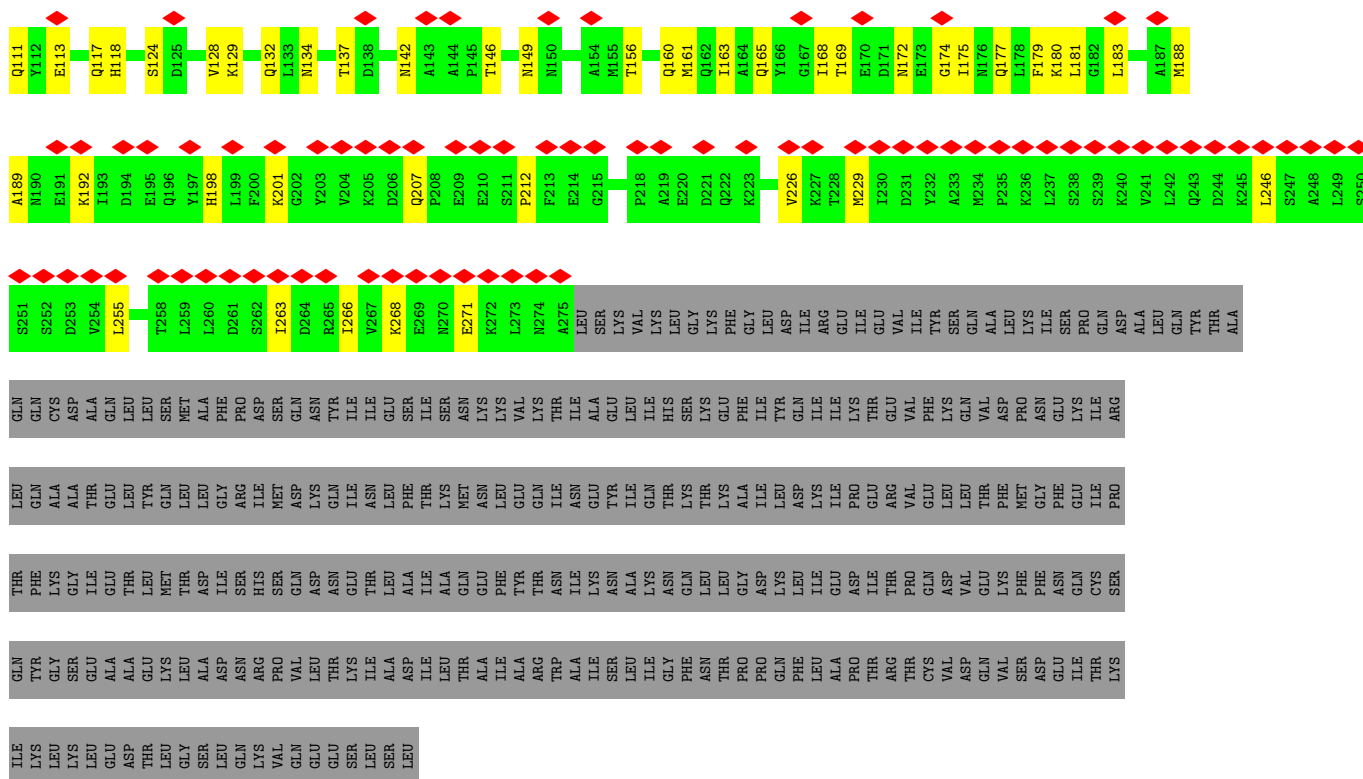


- Molecule 14: SidK

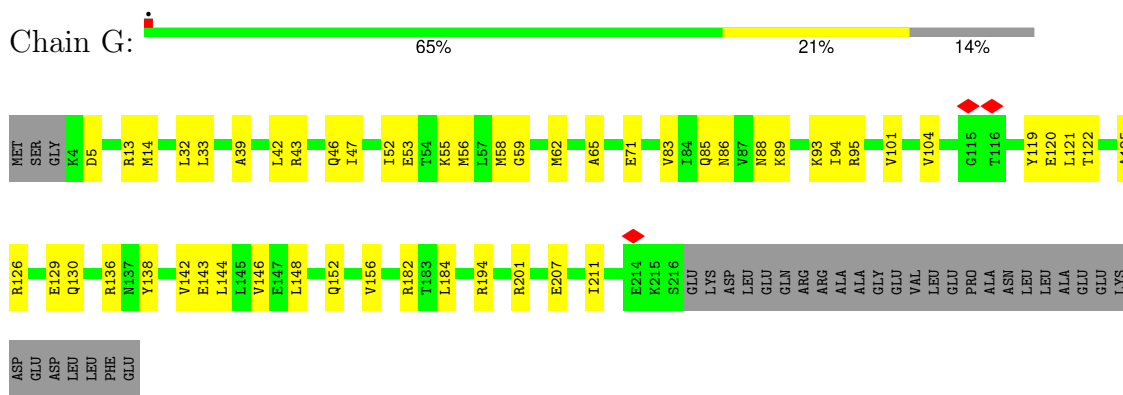
Chain Z: 6% 32% 14% 54%



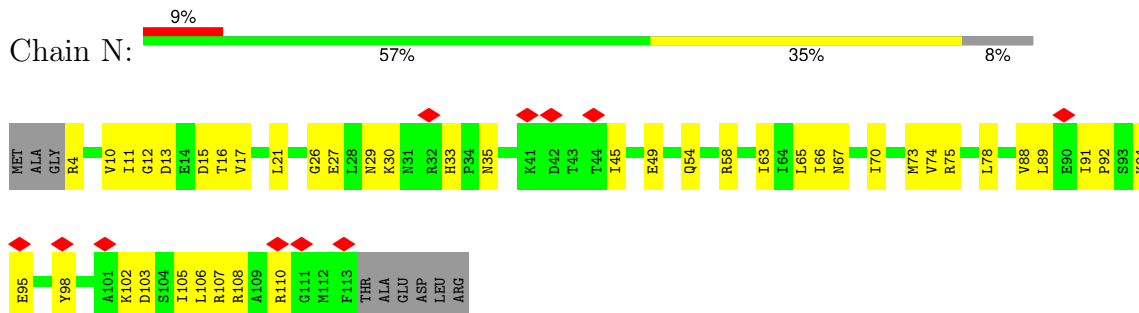





- Molecule 15: V-type proton ATPase subunit D

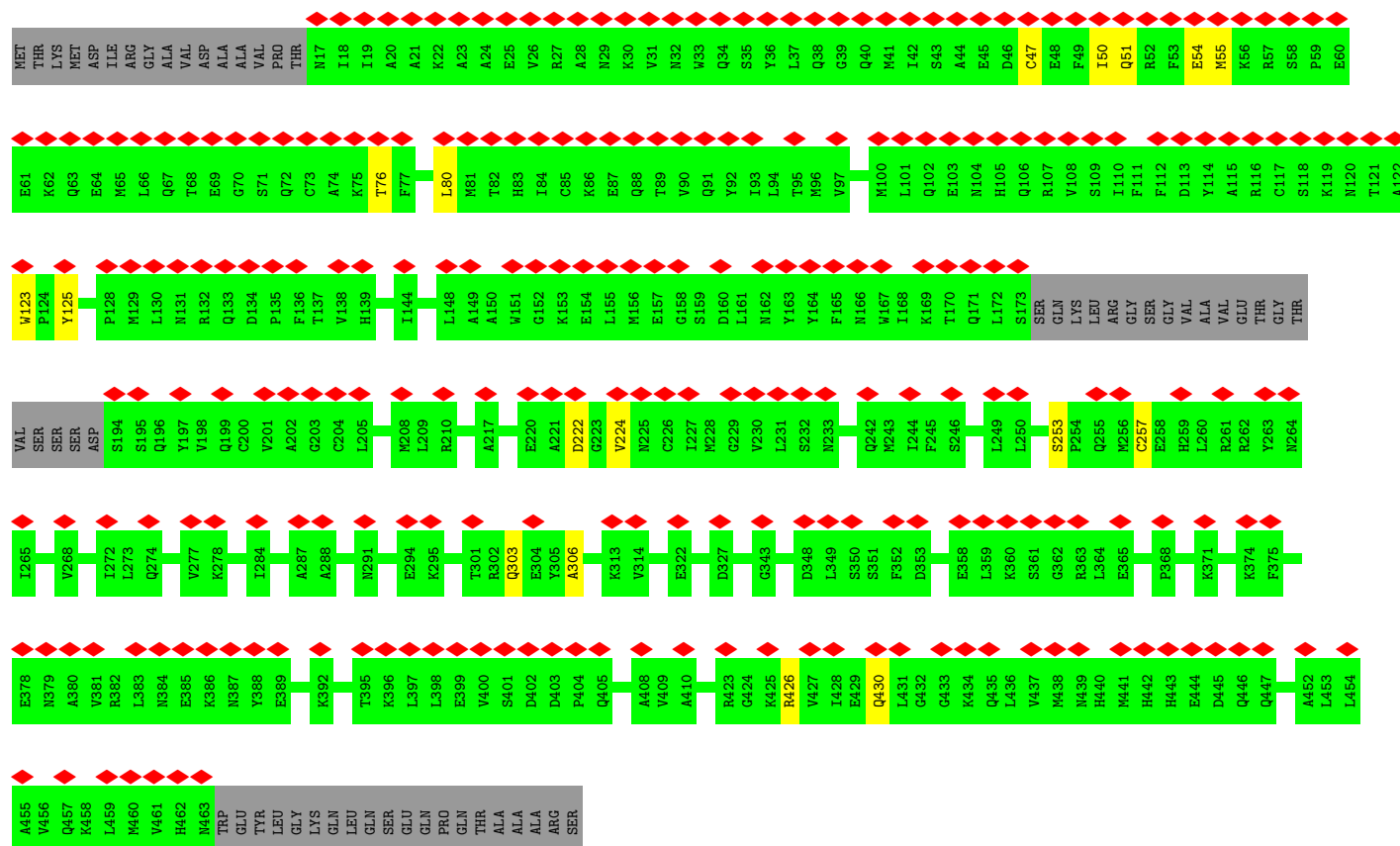


- Molecule 16: V-type proton ATPase subunit F




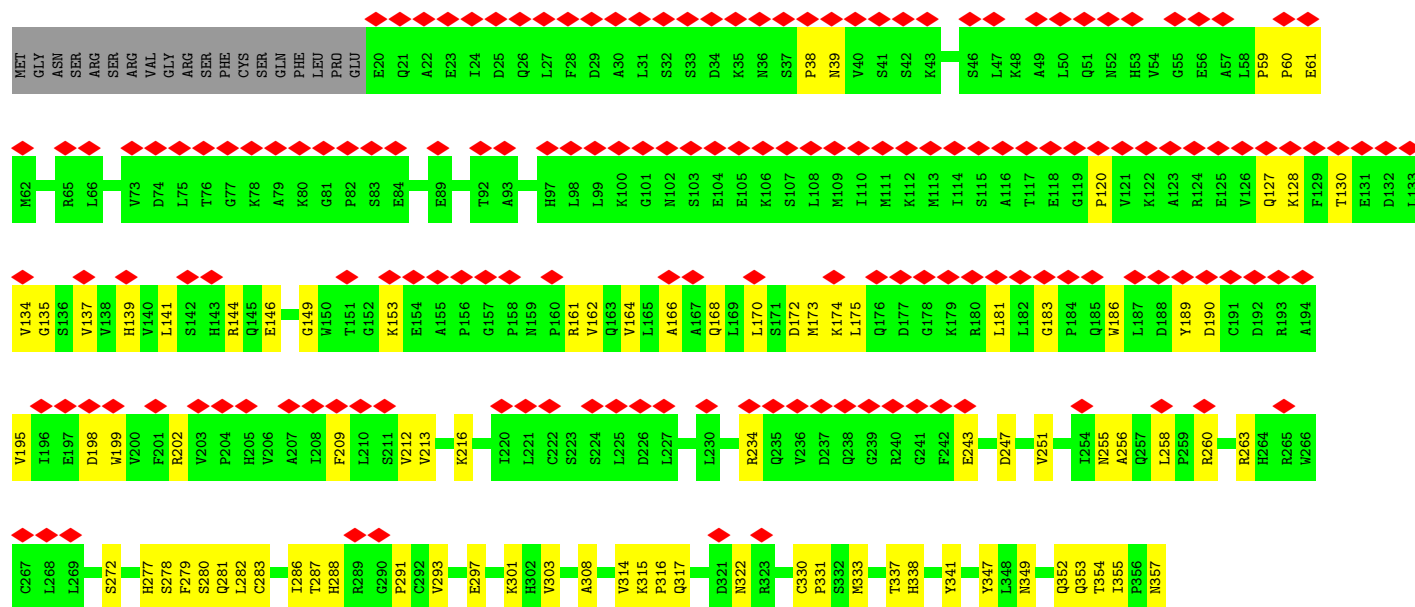
- Molecule 17: V-type proton ATPase subunit H

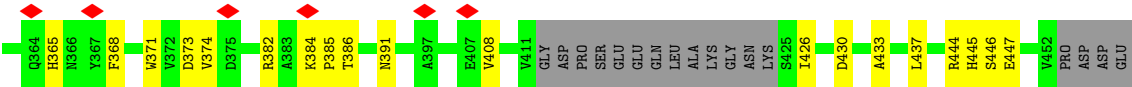
Chain P: 



• Molecule 18: MTOR-associated protein MEAK7

Chain W: 





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.354	Depositor
Minimum map value	-1.886	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.292	Depositor
Map size ( $\text{\AA}$ )	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	R	0.24	0/6023	0.45	0/8174
2	O	0.13	0/1816	0.31	1/2534 (0.0%)
3	H	0.22	0/1623	0.43	0/2190
3	I	0.22	0/1675	0.41	0/2256
3	J	0.24	0/1789	0.51	0/2401
4	K	0.25	0/740	0.39	0/1012
4	L	0.24	0/753	0.39	0/1026
4	M	0.23	0/896	0.53	0/1198
5	S	0.26	0/657	0.50	0/902
6	T	0.21	0/674	0.52	1/915 (0.1%)
7	U	0.23	0/1716	0.47	1/2333 (0.0%)
8	V	0.24	0/425	0.45	0/582
9	0	0.30	0/1532	0.46	0/2082
10	1	0.33	0/1080	0.51	0/1461
10	2	0.33	0/1080	0.53	0/1461
10	3	0.31	0/1080	0.53	0/1461
10	4	0.31	0/1080	0.53	0/1461
10	5	0.32	0/1080	0.53	0/1461
10	6	0.31	0/1080	0.45	0/1461
10	7	0.34	0/1080	0.50	0/1461
10	8	0.34	0/1080	0.50	0/1461
10	9	0.30	0/1080	0.44	0/1461
11	Q	0.27	0/2910	0.42	0/3940
12	A	0.32	0/4752	0.47	0/6435
12	B	0.33	0/4752	0.43	0/6435
12	C	0.29	0/4752	0.41	0/6435
13	D	0.33	0/3739	0.41	0/5067
13	E	0.32	0/3739	0.40	0/5067
13	F	0.31	0/3739	0.44	1/5067 (0.0%)
14	X	0.20	0/2170	0.40	0/2926
14	Y	0.16	0/2145	0.42	0/2893
14	Z	0.18	0/2143	0.39	0/2888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	G	0.22	0/1735	0.39	0/2320
16	N	0.15	0/889	0.34	0/1200
17	P	0.12	0/2119	0.31	0/2955
18	W	0.19	0/3095	0.37	0/4222
All	All	0.27	0/72718	0.44	4/98604 (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
3	I	0	1
12	A	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	496	PRO	CA-N-CD	-6.00	103.59	112.00
6	T	97	ILE	N-CA-C	-5.82	107.14	112.96
7	U	390	PRO	CA-N-CD	-5.43	104.40	112.00
2	O	111	LYS	N-CA-C	-5.21	107.58	114.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	295	THR	Peptide
3	I	224	PHE	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	5876	0	5678	166	0
2	O	1817	0	813	5	0
3	H	1611	0	1546	42	0
3	I	1661	0	1626	53	0
3	J	1774	0	1794	73	0
4	K	735	0	566	14	0
4	L	748	0	602	21	0
4	M	889	0	854	33	0
5	S	631	0	646	21	0
6	T	658	0	652	12	0
7	U	1662	0	1586	63	0
8	V	411	0	401	14	0
9	0	1498	0	1544	48	0
10	1	1065	0	1131	53	0
10	2	1065	0	1131	45	0
10	3	1065	0	1131	48	0
10	4	1065	0	1131	56	0
10	5	1065	0	1131	35	0
10	6	1065	0	1131	25	0
10	7	1065	0	1131	44	0
10	8	1065	0	1131	40	0
10	9	1065	0	1131	40	0
11	Q	2844	0	2782	67	0
12	A	4656	0	4642	145	0
12	B	4656	0	4642	90	0
12	C	4656	0	4642	112	0
13	D	3666	0	3665	76	0
13	E	3666	0	3665	68	0
13	F	3666	0	3665	82	0
14	X	2136	0	2158	44	0
14	Y	2111	0	2134	41	0
14	Z	2110	0	2132	58	0
15	G	1717	0	1829	51	0
16	N	875	0	878	35	0
17	P	2121	0	941	9	0
18	W	3023	0	2657	79	0
19	R	14	0	13	1	0
19	S	14	0	13	1	0
19	U	84	0	78	0	0
20	B	27	0	12	0	0
All	All	71598	0	69035	1688	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 12.

All (1688) 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)
14:Y:62:PHE:O	14:Y:66:LEU:HB2	1.60	1.00
3:J:122:GLN:HE21	13:F:43:PRO:HD3	1.25	0.98
10:3:48:ARG:HH12	10:3:51:GLN:HG2	1.28	0.97
10:5:124:GLN:HE22	10:5:126:ARG:HG2	1.29	0.96
14:Y:188:MET:HE3	14:Y:189:ALA:H	1.31	0.93
1:R:61:MET:HG3	1:R:98:GLU:HG2	1.53	0.90
12:C:489:LEU:HD11	12:C:509:LEU:HD21	1.55	0.87
7:U:428:MET:HE1	9:0:48:MET:HG2	1.56	0.87
10:2:113:VAL:HG21	10:2:134:ILE:HG21	1.57	0.87
3:H:133:ILE:HG12	3:H:166:GLN:HB2	1.57	0.86
3:J:155:TYR:O	3:J:158:ALA:O	1.92	0.86
15:G:59:GLY:HA2	15:G:62:MET:HE2	1.55	0.86
12:A:71:SER:O	12:A:120:ARG:NH1	2.10	0.83
13:F:421:GLN:NE2	13:F:425:CYS:SG	2.53	0.82
13:F:380:ASP:HB2	13:F:393:ASN:HB2	1.61	0.81
18:W:174:LYS:HB3	18:W:195:VAL:HG13	1.62	0.81
12:A:290:ASP:O	12:A:294:LEU:N	2.14	0.81
14:Y:113:GLU:OE2	14:Y:117:GLN:NE2	2.14	0.80
18:W:371:TRP:NE1	18:W:373:ASP:OD1	2.15	0.80
4:K:113:ASN:ND2	12:A:76:GLY:O	2.15	0.79
1:R:495:ARG:HG2	19:S:101:NAG:H3	1.63	0.79
8:V:331:MET:HE2	10:4:112:ILE:HD13	1.65	0.79
12:A:24:VAL:HG12	12:A:29:VAL:HA	1.64	0.78
12:B:178:TYR:HB3	12:B:193:GLU:HB3	1.64	0.78
12:A:45:VAL:HG13	12:A:79:VAL:HG22	1.65	0.77
10:4:44:MET:HE1	10:4:48:ARG:HE	1.48	0.77
12:A:391:ARG:NH1	12:A:401:GLU:OE2	2.18	0.77
12:A:39:MET:HB3	12:A:40:TYR:HD2	1.50	0.77
15:G:55:LYS:NZ	16:N:103:ASP:OD2	2.18	0.77
7:U:420:SER:OG	9:0:34:ARG:NH1	2.17	0.76
13:E:400:ARG:O	13:E:403:LYS:NZ	2.18	0.76
1:R:548:MET:HE1	1:R:813:LYS:HE2	1.65	0.76
12:A:51:VAL:HG23	12:A:67:TYR:HB2	1.67	0.76
3:J:36:GLU:HG2	18:W:385:PRO:HB2	1.66	0.76
7:U:428:MET:HG3	10:1:14:PHE:HZ	1.51	0.76
12:C:417:PHE:HE2	12:C:452:ILE:HD12	1.51	0.76
12:A:75:VAL:HG22	13:D:67:ARG:HA	1.66	0.75
7:U:428:MET:HG3	10:1:14:PHE:CZ	2.22	0.75
18:W:144:ARG:HD2	18:W:216:LYS:HG3	1.68	0.75
9:0:77:ILE:HG21	10:1:117:GLY:HA2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:289:ARG:NH1	12:A:290:ASP:OD1	2.19	0.75
1:R:444:PHE:O	1:R:447:ARG:NH1	2.19	0.75
12:C:391:ARG:NH1	12:C:401:GLU:OE2	2.20	0.75
1:R:748:HIS:ND1	1:R:794:GLU:OE1	2.17	0.74
12:A:610:ASN:OD1	12:A:613:ARG:NH1	2.20	0.74
1:R:12:LEU:HD23	1:R:357:THR:HG21	1.70	0.74
10:1:65:ILE:HA	10:1:68:TYR:HD2	1.53	0.73
10:1:48:ARG:HD2	10:1:122:ALA:HA	1.70	0.73
10:5:57:ILE:HG22	10:5:61:MET:HE2	1.71	0.73
10:6:72:VAL:HG11	10:6:99:VAL:HG11	1.68	0.73
12:B:560:GLN:HA	12:B:564:LYS:HE3	1.70	0.73
10:4:44:MET:SD	10:4:48:ARG:NH2	2.61	0.73
10:8:113:VAL:HG21	10:8:134:ILE:HG21	1.69	0.73
12:A:151:ASP:OD2	12:A:397:ASN:ND2	2.21	0.73
16:N:54:GLN:HG3	16:N:58:ARG:HH12	1.53	0.73
9:0:22:VAL:O	9:0:26:TYR:HB2	1.88	0.73
17:P:426:ARG:O	17:P:430:GLN:N	2.23	0.72
3:H:131:ARG:NH1	3:H:164:ASP:OD2	2.23	0.72
11:Q:218:ARG:NH1	11:Q:298:GLU:OE1	2.22	0.72
12:B:518:ASP:OD1	12:B:582:SER:HA	1.90	0.72
12:C:234:LEU:HD21	12:C:448:VAL:HG11	1.70	0.72
10:3:88:LYS:O	10:3:92:GLN:NE2	2.21	0.72
10:7:124:GLN:HE22	10:7:126:ARG:HB3	1.54	0.72
12:C:24:VAL:HG22	13:F:89:VAL:HG22	1.71	0.71
10:1:112:ILE:HD11	11:Q:11:VAL:HA	1.71	0.71
11:Q:44:ASP:O	11:Q:48:HIS:ND1	2.23	0.71
3:I:215:LEU:HD11	4:L:95:VAL:HG21	1.72	0.71
3:H:87:ARG:HD2	3:H:216:PHE:HE2	1.56	0.71
9:0:28:ILE:HD11	10:7:90:PHE:HZ	1.54	0.71
3:J:53:ILE:HD13	4:M:47:TYR:HE2	1.55	0.71
9:0:71:ILE:O	11:Q:10:ASN:ND2	2.24	0.71
13:E:168:GLU:OE1	13:E:185:ARG:NH2	2.23	0.71
1:R:115:GLN:NE2	1:R:276:GLU:OE2	2.23	0.71
13:E:82:ARG:NH1	13:E:101:GLY:O	2.24	0.71
12:B:525:TYR:CE1	13:E:403:LYS:HD2	2.26	0.70
14:Z:172:ASN:HB3	14:Z:175:ILE:HG12	1.71	0.70
10:8:65:ILE:HA	10:8:68:TYR:HD2	1.56	0.70
13:F:82:ARG:NH1	13:F:101:GLY:O	2.23	0.70
1:R:254:ARG:HA	1:R:257:MET:HE2	1.73	0.70
13:D:436:LYS:HG3	13:D:444:LEU:HD11	1.73	0.70
13:F:177:ILE:HA	13:F:181:ASN:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:50:LEU:HD23	12:C:68:GLU:HB2	1.74	0.70
12:A:178:TYR:HB3	12:A:193:GLU:HB3	1.71	0.70
9:0:107:MET:HG2	9:0:144:VAL:HG21	1.72	0.70
13:F:229:ILE:HB	13:F:257:VAL:HG12	1.71	0.70
10:1:61:MET:HE1	10:1:135:LEU:HB3	1.72	0.70
10:1:88:LYS:O	10:1:92:GLN:NE2	2.25	0.69
3:I:132:MET:HB2	3:I:165:VAL:HG12	1.74	0.69
11:Q:338:GLN:HE21	16:N:94:LYS:HE2	1.55	0.69
15:G:62:MET:HE1	16:N:92:PRO:HG2	1.72	0.69
10:6:113:VAL:HG21	10:6:134:ILE:HG21	1.75	0.69
10:3:70:LEU:HD22	10:4:144:TYR:HD2	1.58	0.69
14:Z:129:LYS:HD2	14:Z:168:ILE:HG23	1.73	0.69
10:1:70:LEU:HD12	10:2:144:TYR:HD2	1.56	0.69
10:8:44:MET:HG3	10:8:122:ALA:HB2	1.74	0.69
11:Q:120:ARG:NH2	15:G:85:GLN:O	2.26	0.69
12:A:507:ILE:HD11	12:A:555:VAL:HG21	1.75	0.69
18:W:135:GLY:O	18:W:139:HIS:ND1	2.23	0.69
1:R:58:CYS:HA	1:R:61:MET:HE2	1.74	0.69
12:B:397:ASN:O	12:B:399:GLU:N	2.26	0.69
12:C:43:VAL:HG21	12:C:64:ILE:HD13	1.75	0.68
14:X:165:GLN:HG3	14:X:166:TYR:HD1	1.57	0.68
3:H:97:GLU:OE1	4:K:92:ARG:NE	2.24	0.68
7:U:373:TYR:CD2	7:U:380:LYS:HD2	2.29	0.68
12:B:552:ARG:O	12:B:556:GLU:HG2	1.94	0.68
14:Z:213:PHE:O	14:Z:222:GLN:NE2	2.26	0.68
12:A:20:TYR:HE1	12:A:76:GLY:HA2	1.58	0.68
14:X:165:GLN:HG3	14:X:166:TYR:CD1	2.29	0.68
11:Q:328:ASN:ND2	11:Q:348:ILE:O	2.27	0.68
12:C:316:SER:OG	13:F:336:GLU:OE2	2.12	0.68
7:U:298:THR:O	7:U:310:SER:OG	2.12	0.68
18:W:255:ASN:HA	18:W:258:LEU:HD12	1.76	0.68
12:B:553:ARG:HA	18:W:354:THR:HG21	1.76	0.68
14:X:111:GLN:HE22	14:X:168:ILE:H	1.42	0.68
13:F:426:TYR:OH	13:F:459:GLU:OE2	2.09	0.68
1:R:71:GLU:HG2	1:R:108:LEU:HD11	1.76	0.68
1:R:131:ILE:HG13	1:R:246:PRO:HG2	1.76	0.68
10:5:65:ILE:HA	10:5:68:TYR:HD2	1.58	0.68
3:J:24:ASN:HA	4:M:21:LYS:HE3	1.74	0.67
10:4:72:VAL:HG11	10:4:99:VAL:HG11	1.76	0.67
10:5:124:GLN:NE2	10:5:126:ARG:HG2	2.07	0.67
12:A:298:VAL:O	12:A:300:GLY:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:305:GLU:OE1	13:D:308:ARG:NH2	2.28	0.67
14:Y:61:ARG:HG3	14:Y:63:GLU:OE1	1.95	0.67
12:A:161:LEU:HD12	12:A:307:LYS:HB2	1.75	0.67
1:R:755:LEU:HD11	1:R:785:LEU:HB3	1.76	0.67
12:B:296:MET:HE1	12:B:308:ARG:HE	1.59	0.67
14:X:242:LEU:HD23	14:X:245:LYS:HD2	1.76	0.67
10:4:64:ILE:HA	10:4:67:ILE:HD12	1.75	0.67
11:Q:54:TYR:OH	11:Q:322:LYS:NZ	2.26	0.67
1:R:423:MET:HE3	1:R:444:PHE:HD1	1.58	0.67
3:J:155:TYR:O	3:J:158:ALA:C	2.37	0.67
10:3:84:ILE:HG21	10:3:89:SER:HB3	1.77	0.67
1:R:793:MET:HG3	10:8:140:VAL:HG21	1.76	0.66
14:Y:113:GLU:O	14:Y:117:GLN:NE2	2.26	0.66
1:R:10:MET:HE1	1:R:326:PRO:HB3	1.78	0.66
1:R:181:PRO:HD2	1:R:182:THR:H	1.60	0.66
4:M:88:PHE:HD2	4:M:89:ARG:HH12	1.41	0.66
12:A:264:SER:O	12:A:308:ARG:NH2	2.28	0.66
7:U:412:PHE:O	8:V:294:ASN:ND2	2.29	0.66
10:1:88:LYS:HA	10:1:91:LEU:HD12	1.77	0.66
10:9:113:VAL:HG21	10:9:134:ILE:HG21	1.76	0.66
3:H:154:MET:O	3:H:157:ILE:HG12	1.95	0.66
6:T:121:PHE:O	6:T:125:GLN:NE2	2.29	0.66
3:H:224:PHE:CE2	13:D:344:ARG:HG3	2.30	0.66
10:3:48:ARG:HH12	10:3:51:GLN:CG	2.07	0.66
1:R:768:SER:O	6:T:107:ASN:ND2	2.26	0.66
3:J:50:ARG:NH1	4:M:47:TYR:OH	2.29	0.66
9:0:193:VAL:HG21	10:9:23:MET:HE3	1.76	0.66
10:3:77:ALA:O	10:4:155:LYS:NZ	2.26	0.66
16:N:78:LEU:HD11	16:N:88:VAL:HG11	1.78	0.66
17:P:76:THR:O	17:P:80:LEU:N	2.28	0.65
1:R:96:ASP:O	1:R:99:ALA:HB3	1.96	0.65
12:A:256:LYS:HG2	12:A:435:LEU:HD12	1.77	0.65
10:9:124:GLN:HE22	10:9:126:ARG:HB2	1.60	0.65
3:H:203:ILE:HD11	4:K:103:VAL:HA	1.77	0.65
12:A:573:HIS:CE1	12:A:615:LEU:HB2	2.32	0.65
12:A:587:LYS:HE3	12:A:600:ASP:HB3	1.78	0.65
10:4:80:LEU:HB3	10:5:155:LYS:HE2	1.79	0.65
12:B:316:SER:OG	13:E:336:GLU:OE2	2.14	0.65
3:I:210:GLU:OE2	13:E:39:TYR:OH	2.15	0.65
13:D:436:LYS:HD2	13:D:452:LEU:HD21	1.76	0.65
1:R:14:GLN:NE2	1:R:355:MET:SD	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:23:MET:HG2	10:4:148:VAL:HG11	1.79	0.64
12:C:298:VAL:HG22	12:C:299:ASP:H	1.62	0.64
12:A:29:VAL:HB	12:A:66:VAL:HG21	1.79	0.64
12:A:42:LEU:O	12:A:82:THR:OG1	2.14	0.64
14:Y:111:GLN:HE22	14:Y:168:ILE:H	1.45	0.64
15:G:43:ARG:NH1	15:G:46:GLN:OE1	2.30	0.64
10:4:140:VAL:HG12	10:4:144:TYR:CE1	2.32	0.64
13:D:421:GLN:NE2	13:D:425:CYS:SG	2.68	0.64
6:T:63:ILE:HG22	6:T:67:MET:HE2	1.79	0.64
7:U:273:ASN:HB3	7:U:398:GLN:HG3	1.78	0.64
1:R:209:PRO:HD2	1:R:210:VAL:H	1.63	0.64
3:H:77:ASN:OD1	3:H:80:ARG:NH2	2.31	0.64
12:C:450:TRP:CD1	12:C:483:LEU:HD23	2.33	0.64
12:A:252:PHE:O	12:A:437:LYS:NZ	2.27	0.64
12:A:300:GLY:HA3	14:X:139:TYR:CE1	2.33	0.64
10:2:115:ASP:O	10:2:119:ARG:HG3	1.97	0.64
13:F:61:ASP:OD1	13:F:62:HIS:N	2.30	0.63
1:R:552:VAL:HG21	1:R:579:MET:HE3	1.79	0.63
12:A:21:VAL:HA	12:A:31:ALA:HA	1.79	0.63
15:G:53:GLU:HA	15:G:56:MET:HE3	1.81	0.63
1:R:804:ARG:NH1	1:R:809:GLU:OE1	2.32	0.63
7:U:372:GLU:OE2	8:V:301:PHE:N	2.32	0.63
10:3:72:VAL:HG11	10:3:99:VAL:HG11	1.80	0.63
1:R:470:LYS:HA	1:R:523:ASN:HD21	1.62	0.63
3:J:113:GLN:NE2	3:J:117:ASP:OD1	2.32	0.63
18:W:256:ALA:O	18:W:263:ARG:NH2	2.31	0.63
12:B:560:GLN:NE2	18:W:314:VAL:O	2.32	0.62
12:A:163:LYS:O	12:A:342:TYR:OH	2.17	0.62
14:Y:33:MET:HG2	14:Y:53:LEU:HD11	1.82	0.62
16:N:26:GLY:HA2	16:N:35:ASN:HD21	1.63	0.62
3:J:36:GLU:HA	18:W:385:PRO:HG2	1.82	0.62
10:3:48:ARG:O	10:3:48:ARG:HD3	2.00	0.62
10:9:72:VAL:HG11	10:9:99:VAL:HG11	1.79	0.62
12:B:315:THR:H	12:B:318:MET:HE2	1.64	0.62
3:I:67:GLN:HE21	3:I:71:GLN:HE21	1.47	0.62
10:1:72:VAL:HG11	10:1:99:VAL:HG11	1.80	0.62
4:K:93:ASP:OD1	4:K:94:GLU:N	2.32	0.62
11:Q:177:ASN:HD22	15:G:121:LEU:HD12	1.64	0.62
12:C:274:TYR:HB3	12:C:311:LEU:HD23	1.81	0.62
13:D:61:ASP:OD2	13:D:93:LYS:NZ	2.32	0.62
10:4:148:VAL:HA	10:4:151:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:79:GLU:O	4:L:82:THR:OG1	2.17	0.62
10:2:140:VAL:HG12	10:2:144:TYR:CE1	2.34	0.62
10:8:23:MET:O	10:8:23:MET:HE3	2.00	0.62
12:A:249:PRO:HB3	12:A:410:VAL:HB	1.82	0.62
14:Z:236:LYS:O	14:Z:270:ASN:ND2	2.32	0.62
7:U:326:ILE:HD11	7:U:344:ARG:HB2	1.80	0.62
10:9:46:VAL:HG13	10:9:47:MET:HG3	1.82	0.62
13:D:102:THR:HA	13:D:105:ILE:HD12	1.81	0.62
18:W:303:VAL:HB	18:W:330:CYS:HB2	1.81	0.62
10:7:124:GLN:HE22	10:7:126:ARG:HE	1.47	0.61
1:R:648:PRO:HA	1:R:651:LEU:HB3	1.81	0.61
3:I:105:VAL:HG13	3:I:111:ARG:HE	1.65	0.61
1:R:574:PRO:HB2	1:R:650:MET:SD	2.40	0.61
14:Z:111:GLN:HE22	14:Z:169:THR:H	1.47	0.61
10:6:51:GLN:OE1	10:6:51:GLN:N	2.33	0.61
12:C:397:ASN:O	12:C:399:GLU:N	2.33	0.61
12:B:24:VAL:HG22	13:E:89:VAL:HG22	1.81	0.61
10:7:124:GLN:NE2	10:7:126:ARG:HB3	2.14	0.61
10:5:23:MET:HE1	10:6:144:TYR:HB3	1.82	0.61
13:F:248:PHE:HB3	13:F:254:MET:HE1	1.83	0.61
3:H:127:LEU:HD23	3:H:132:MET:HG2	1.83	0.61
12:A:574:MET:HB3	12:A:577:ILE:HB	1.83	0.61
3:H:199:ARG:NH1	13:D:41:SER:OG	2.33	0.61
8:V:309:MET:HA	8:V:309:MET:HE3	1.83	0.61
11:Q:299:VAL:HG11	11:Q:350:ILE:HG22	1.82	0.61
3:J:53:ILE:HG13	3:J:54:MET:N	2.16	0.60
12:B:591:LYS:HA	12:B:591:LYS:HE3	1.83	0.60
3:I:90:LEU:HD21	4:L:88:PHE:HB2	1.83	0.60
9:0:164:LEU:HD21	11:Q:21:ARG:HD2	1.83	0.60
14:Y:229:MET:HE3	14:Y:229:MET:O	2.02	0.60
15:G:83:VAL:HG13	15:G:119:TYR:HE2	1.65	0.60
15:G:83:VAL:O	15:G:119:TYR:OH	2.18	0.60
1:R:793:MET:HE2	10:8:140:VAL:HG11	1.83	0.60
10:3:68:TYR:HD2	10:3:146:LEU:HB2	1.66	0.60
3:J:46:VAL:HG22	3:J:50:ARG:HG2	1.82	0.60
12:C:574:MET:HG2	12:C:611:ALA:HB1	1.83	0.60
15:G:52:ILE:HD11	16:N:106:LEU:HD11	1.82	0.60
10:3:113:VAL:HG21	10:3:134:ILE:HG21	1.82	0.60
3:J:124:LEU:HD22	3:J:132:MET:SD	2.42	0.60
4:M:112:GLU:OE1	12:C:47:HIS:NE2	2.34	0.60
8:V:335:TYR:HD2	8:V:337:SER:H	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:48:ARG:NH1	10:3:51:GLN:HG2	2.10	0.60
10:7:61:MET:HB2	10:7:110:ILE:HD11	1.82	0.60
12:C:264:SER:O	12:C:308:ARG:NH2	2.34	0.60
12:C:277:CYS:SG	12:C:326:SER:OG	2.60	0.60
14:Z:43:LYS:HA	14:Z:43:LYS:HE3	1.82	0.60
18:W:120:PRO:HB2	18:W:190:ASP:HB2	1.83	0.60
10:7:23:MET:O	10:7:23:MET:HE3	2.01	0.60
7:U:281:GLN:OE1	7:U:281:GLN:N	2.26	0.60
12:C:395:LEU:O	12:C:400:ARG:NH2	2.35	0.60
12:A:62:ALA:O	12:A:64:ILE:HG13	2.02	0.60
12:A:298:VAL:HG22	12:A:299:ASP:H	1.67	0.60
12:B:193:GLU:OE1	12:B:202:LYS:HG2	2.01	0.60
1:R:71:GLU:HG3	1:R:283:LEU:HD11	1.84	0.60
10:4:136:ILE:O	10:4:140:VAL:HG23	2.02	0.60
12:C:560:GLN:HA	12:C:564:LYS:HE3	1.83	0.60
13:D:77:PRO:HD3	13:D:110:THR:HG22	1.83	0.60
13:D:246:SER:O	13:D:250:GLU:HB3	2.02	0.60
18:W:347:TYR:OH	18:W:349:ASN:ND2	2.25	0.60
3:J:39:ASN:HB3	18:W:384:LYS:HE2	1.83	0.59
8:V:339:ILE:O	10:4:119:ARG:NH2	2.35	0.59
10:7:113:VAL:HG21	10:7:134:ILE:HG21	1.84	0.59
3:H:70:ILE:HG23	13:D:250:GLU:HG3	1.84	0.59
12:C:280:ARG:NE	13:F:371:TYR:O	2.31	0.59
12:C:393:LYS:NZ	12:C:399:GLU:OE1	2.33	0.59
13:D:453:GLU:OE2	13:D:486:ILE:HD12	2.02	0.59
13:F:88:GLU:HB3	13:F:95:VAL:HB	1.84	0.59
13:F:365:ILE:HB	13:F:366:PRO:HD3	1.84	0.59
10:7:72:VAL:HG11	10:7:99:VAL:HG11	1.84	0.59
3:I:97:GLU:OE1	4:L:92:ARG:NH1	2.36	0.59
14:X:148:LYS:NZ	14:X:188:MET:O	2.35	0.59
13:F:377:ILE:O	13:F:397:SER:OG	2.19	0.59
1:R:18:GLN:O	1:R:22:ALA:N	2.33	0.59
10:5:44:MET:HA	10:5:47:MET:HE3	1.84	0.59
12:C:323:ARG:HH12	13:F:328:TYR:HE2	1.51	0.59
12:C:573:HIS:HB3	12:C:574:MET:HE2	1.84	0.59
12:B:395:LEU:O	12:B:400:ARG:NH2	2.36	0.59
12:B:511:VAL:HG21	12:B:548:TYR:HB2	1.84	0.59
4:M:47:TYR:O	4:M:50:GLN:HG3	2.03	0.59
13:E:207:CYS:SG	13:E:229:ILE:HD13	2.43	0.59
13:E:453:GLU:OE2	13:E:457:LYS:NZ	2.28	0.59
4:M:93:ASP:O	4:M:96:LEU:HG	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:55:ILE:HD12	12:B:365:LEU:HD11	1.83	0.59
3:I:199:ARG:HH12	13:E:41:SER:HB2	1.68	0.59
6:T:64:MET:SD	6:T:65:LEU:HD22	2.43	0.59
12:A:21:VAL:HB	12:A:75:VAL:HG11	1.85	0.59
12:B:274:TYR:HB3	12:B:311:LEU:HD23	1.85	0.59
14:Y:179:PHE:O	14:Y:183:LEU:HG	2.03	0.59
18:W:316:PRO:HG2	18:W:317:GLN:NE2	2.17	0.59
11:Q:324:GLN:OE1	11:Q:327:ARG:NH2	2.36	0.59
12:A:70:THR:O	12:A:72:GLY:N	2.35	0.59
10:1:44:MET:HG2	10:1:122:ALA:HB2	1.84	0.59
10:2:46:VAL:HG13	10:2:47:MET:SD	2.42	0.59
15:G:88:ASN:OD1	15:G:89:LYS:N	2.36	0.59
3:J:53:ILE:HD13	4:M:47:TYR:CE2	2.37	0.58
11:Q:158:THR:HG22	11:Q:160:LEU:H	1.69	0.58
16:N:75:ARG:HD2	16:N:107:ARG:HH12	1.68	0.58
11:Q:194:TYR:HH	11:Q:209:CYS:HG	1.51	0.58
10:2:48:ARG:HD2	10:2:122:ALA:HA	1.86	0.58
10:8:130:GLY:O	10:8:134:ILE:HD12	2.03	0.58
12:C:449:ASN:O	12:C:449:ASN:ND2	2.36	0.58
12:C:193:GLU:OE1	12:C:202:LYS:HG2	2.03	0.58
12:B:57:LEU:HB2	13:F:53:VAL:HG12	1.86	0.58
3:J:155:TYR:CZ	3:J:159:THR:HG21	2.38	0.58
3:I:135:ARG:NH1	3:I:171:SER:OG	2.36	0.58
3:H:200:LEU:O	3:H:204:ALA:HB3	2.04	0.58
13:E:231:PHE:HB3	13:E:259:LEU:HD23	1.85	0.58
14:Y:207:GLN:HE21	14:Y:212:PRO:HB3	1.67	0.58
1:R:804:ARG:HH12	1:R:808:VAL:HB	1.67	0.58
14:X:163:ILE:HD13	14:X:175:ILE:HD13	1.84	0.58
12:A:291:PHE:CD2	12:A:305:ILE:HG13	2.39	0.58
15:G:94:ILE:HD13	16:N:63:ILE:HD12	1.86	0.58
10:2:57:ILE:O	10:2:61:MET:HG3	2.03	0.58
16:N:29:ASN:N	16:N:33:HIS:O	2.31	0.58
18:W:281:GLN:HG2	13:F:450:LEU:HD21	1.84	0.58
1:R:485:PHE:HE2	1:R:494:LEU:HD11	1.69	0.58
3:H:215:LEU:HD12	4:K:91:ASN:HB2	1.85	0.58
13:D:488:PRO:HD2	13:D:491:MET:SD	2.44	0.58
1:R:502:LEU:HD12	5:S:66:PRO:HG2	1.85	0.57
4:M:96:LEU:O	4:M:99:LEU:HG	2.02	0.57
13:D:356:MET:HE1	13:D:361:ILE:HD13	1.84	0.57
14:Z:236:LYS:HE2	14:Z:267:VAL:HG21	1.85	0.57
14:X:51:ASP:CG	14:X:84:ARG:HH22	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:14:GLN:HB3	1:R:320:ILE:HD11	1.85	0.57
1:R:770:ALA:O	1:R:774:VAL:HG22	2.04	0.57
3:J:41:GLU:O	3:J:44:ARG:HG3	2.04	0.57
3:H:191:LYS:HB3	13:D:46:THR:OG1	2.03	0.57
12:A:116:ILE:HD12	13:D:341:VAL:HG11	1.86	0.57
12:A:118:ILE:HG23	13:D:157:PRO:HG2	1.86	0.57
14:X:37:ASP:HB2	14:X:42:LEU:HD12	1.85	0.57
4:M:50:GLN:NE2	4:M:51:ARG:HG2	2.18	0.57
3:I:85:ARG:NH1	13:E:141:ARG:O	2.36	0.57
9:O:46:PRO:HA	9:O:49:TRP:HD1	1.69	0.57
10:8:99:VAL:HB	10:8:149:ALA:HB2	1.85	0.57
12:A:574:MET:HG2	12:A:611:ALA:HB1	1.86	0.57
15:G:86:ASN:O	15:G:119:TYR:OH	2.13	0.57
15:G:126:ARG:HH11	15:G:126:ARG:HA	1.68	0.57
1:R:414:ILE:O	1:R:418:LEU:HG	2.05	0.57
3:J:100:GLN:O	3:J:103:SER:OG	2.18	0.57
10:2:68:TYR:HD1	10:2:146:LEU:HD13	1.70	0.57
12:C:259:ILE:O	12:C:263:LEU:HD12	2.04	0.57
13:D:214:LYS:HD3	13:D:220:VAL:HG22	1.86	0.57
7:U:374:VAL:HG23	7:U:397:LEU:HB2	1.86	0.57
10:4:64:ILE:HG22	10:4:68:TYR:HE2	1.68	0.57
11:Q:143:ILE:HB	11:Q:149:GLU:OE1	2.04	0.57
12:B:24:VAL:HG21	13:E:68:TYR:HB2	1.86	0.57
13:D:441:GLU:OE1	13:D:441:GLU:N	2.38	0.57
18:W:322:ASN:O	18:W:338:HIS:ND1	2.38	0.57
9:O:107:MET:HE3	9:O:194:ALA:HB3	1.87	0.57
10:8:124:GLN:HE22	10:8:126:ARG:HB2	1.68	0.57
18:W:354:THR:HG23	18:W:355:ILE:HG13	1.85	0.57
1:R:772:GLY:HA3	6:T:110:ILE:HD11	1.86	0.57
3:H:128:LEU:HA	3:H:155:TYR:OH	2.05	0.57
3:H:185:ASN:OD1	3:H:188:ARG:N	2.38	0.57
12:B:560:GLN:NE2	18:W:315:LYS:HA	2.20	0.57
1:R:205:PRO:HG3	1:R:216:HIS:HA	1.85	0.56
1:R:789:ILE:HG22	1:R:790:LEU:HD23	1.87	0.56
3:H:200:LEU:O	3:H:204:ALA:CB	2.54	0.56
12:A:22:HIS:O	13:D:68:TYR:OH	2.23	0.56
13:D:221:ASP:OD1	13:D:222:TYR:N	2.38	0.56
1:R:118:LEU:HD22	1:R:272:LEU:HD13	1.87	0.56
3:H:185:ASN:HD21	3:H:189:LYS:HB2	1.71	0.56
10:3:14:PHE:HD1	10:3:93:LEU:HD13	1.70	0.56
11:Q:20:VAL:HG21	11:Q:315:PHE:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:44:ASP:HB3	11:Q:48:HIS:HE1	1.70	0.56
12:A:21:VAL:HB	12:A:75:VAL:CG1	2.34	0.56
12:A:141:LEU:HD21	12:A:147:ILE:HD12	1.88	0.56
13:D:208:ARG:NH1	13:D:247:ASP:OD2	2.38	0.56
1:R:52:VAL:O	1:R:56:ARG:HG2	2.06	0.56
9:O:135:TYR:CD2	10:9:13:PHE:HB2	2.41	0.56
10:7:141:LEU:HA	10:7:144:TYR:HD2	1.69	0.56
12:C:306:MET:HA	12:C:309:THR:HG22	1.86	0.56
13:D:341:VAL:HG23	13:D:344:ARG:HB2	1.88	0.56
14:X:111:GLN:NE2	14:X:168:ILE:H	2.02	0.56
13:F:214:LYS:HD3	13:F:220:VAL:HG22	1.88	0.56
11:Q:72:ASP:O	11:Q:76:GLU:HG3	2.06	0.56
13:D:327:MET:HE1	13:D:365:ILE:HG12	1.88	0.56
14:Y:51:ASP:OD1	14:Y:84:ARG:NH2	2.38	0.56
10:4:23:MET:HE3	10:4:23:MET:O	2.05	0.56
13:D:67:ARG:HB2	13:D:70:GLU:HB2	1.88	0.56
14:Y:156:THR:O	14:Y:160:GLN:HG3	2.04	0.56
14:Y:246:LEU:HD21	14:Y:266:ILE:HG21	1.88	0.56
16:N:45:ILE:HD13	16:N:73:MET:HE3	1.87	0.56
1:R:414:ILE:HD13	1:R:458:MET:HE2	1.88	0.56
10:4:48:ARG:HH12	10:4:52:ILE:HA	1.69	0.56
13:D:365:ILE:HB	13:D:366:PRO:HD3	1.88	0.56
1:R:804:ARG:NH1	1:R:808:VAL:HB	2.21	0.56
4:M:76:GLU:O	4:M:80:LYS:HG2	2.06	0.56
11:Q:5:PRO:O	11:Q:6:GLU:HG2	2.05	0.56
14:X:56:ALA:O	14:X:58:LYS:HG2	2.06	0.56
10:5:84:ILE:HG21	10:5:89:SER:HB3	1.87	0.56
13:E:365:ILE:HB	13:E:366:PRO:HD3	1.88	0.56
1:R:101:PHE:O	1:R:104:ILE:HB	2.05	0.56
3:J:29:GLU:OE1	18:W:341:TYR:HE1	1.89	0.56
10:9:132:ILE:O	10:9:136:ILE:HD12	2.06	0.56
12:C:153:TYR:HH	12:C:203:PHE:HD2	1.54	0.56
12:C:376:ALA:HB1	13:D:309:GLU:HA	1.88	0.56
12:A:53:GLU:HG3	12:A:67:TYR:CE2	2.41	0.55
7:U:435:PHE:CZ	9:O:56:LEU:HD21	2.41	0.55
13:F:192:PHE:CE1	13:F:354:LEU:HD12	2.42	0.55
1:R:651:LEU:HD23	1:R:652:LEU:HD23	1.88	0.55
10:4:64:ILE:HG22	10:4:68:TYR:CE2	2.42	0.55
10:5:48:ARG:HB3	10:5:51:GLN:NE2	2.21	0.55
13:D:377:ILE:O	13:D:397:SER:OG	2.24	0.55
13:E:46:THR:HG22	13:E:113:GLU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:155:TYR:O	3:J:159:THR:HB	2.05	0.55
8:V:338:ILE:O	11:Q:165:GLN:NE2	2.40	0.55
10:2:60:VAL:O	10:2:64:ILE:HD12	2.05	0.55
10:4:48:ARG:HD2	10:4:48:ARG:O	2.07	0.55
10:4:109:ALA:O	10:4:113:VAL:HG12	2.06	0.55
12:C:503:GLU:OE1	12:C:567:TRP:N	2.39	0.55
3:J:81:LEU:HD21	3:J:85:ARG:HH21	1.70	0.55
3:I:129:GLU:H	3:I:132:MET:HE3	1.71	0.55
12:C:178:TYR:HB3	12:C:193:GLU:HB3	1.89	0.55
12:A:471:GLU:O	12:A:474:PRO:HD2	2.07	0.55
13:E:307:LEU:HD23	13:E:327:MET:HG3	1.88	0.55
3:J:73:SER:HB2	13:F:252:GLY:HA2	1.87	0.55
10:5:65:ILE:HA	10:5:68:TYR:CD2	2.41	0.55
18:W:60:PRO:HD2	18:W:61:GLU:H	1.70	0.55
1:R:800:LEU:HD11	10:7:57:ILE:HD13	1.87	0.55
12:A:55:ILE:HD12	12:A:365:LEU:HD11	1.88	0.55
13:E:380:ASP:HB2	13:E:393:ASN:HB2	1.89	0.55
12:A:291:PHE:CG	12:A:305:ILE:HG13	2.41	0.55
10:4:9:GLU:CD	10:4:10:TYR:H	2.15	0.55
12:A:394:CYS:HB2	12:A:400:ARG:HB2	1.87	0.55
14:Y:129:LYS:HD3	14:Y:179:PHE:HE2	1.71	0.55
18:W:161:ARG:HA	18:W:164:VAL:HG12	1.89	0.55
3:H:33:LYS:O	3:H:37:GLU:N	2.34	0.54
10:3:140:VAL:HG12	10:3:144:TYR:CE2	2.42	0.54
16:N:75:ARG:CZ	16:N:107:ARG:HH22	2.20	0.54
9:0:166:ASP:OD1	9:0:173:PHE:HB2	2.07	0.54
12:A:18:PHE:HB3	12:A:78:PRO:HA	1.88	0.54
18:W:127:GLN:HA	18:W:170:LEU:HD11	1.89	0.54
9:0:114:MET:HG3	9:0:137:MET:HE2	1.89	0.54
12:C:283:GLU:OE2	13:F:400:ARG:NH1	2.40	0.54
12:B:298:VAL:HG22	12:B:299:ASP:H	1.71	0.54
12:B:449:ASN:ND2	12:B:449:ASN:O	2.39	0.54
3:J:129:GLU:H	3:J:132:MET:HE2	1.73	0.54
9:0:60:LEU:HA	9:0:63:VAL:HG12	1.90	0.54
13:E:61:ASP:OD1	13:E:62:HIS:N	2.41	0.54
14:Z:172:ASN:OD1	14:Z:174:GLY:N	2.39	0.54
1:R:129:LYS:HZ2	1:R:265:ILE:HG21	1.73	0.54
4:L:105:ASP:OD2	4:L:107:ARG:NH2	2.40	0.54
10:1:113:VAL:HG21	10:1:134:ILE:HG21	1.88	0.54
12:A:46:GLY:HA2	12:A:77:ASP:HB3	1.90	0.54
15:G:94:ILE:O	15:G:95:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:247:CYS:O	1:R:254:ARG:NH1	2.40	0.54
1:R:632:GLN:NE2	1:R:636:GLN:OE1	2.23	0.54
10:2:64:ILE:HG22	10:2:68:TYR:CE2	2.42	0.54
12:C:231:GLN:HG3	12:C:234:LEU:HD12	1.88	0.54
16:N:70:ILE:HA	16:N:73:MET:HG2	1.88	0.54
1:R:316:GLN:HG3	1:R:317:LYS:H	1.73	0.54
10:1:23:MET:HA	10:1:23:MET:HE2	1.89	0.54
10:5:64:ILE:O	10:5:67:ILE:HB	2.08	0.54
18:W:278:SER:OG	13:F:453:GLU:OE1	2.24	0.54
1:R:26:VAL:HG12	1:R:303:ILE:HD11	1.90	0.54
12:A:75:VAL:HG21	13:D:89:VAL:HG21	1.90	0.54
1:R:315:THR:HG21	4:K:11:LEU:HA	1.90	0.53
10:1:119:ARG:HH21	11:Q:88:HIS:HB3	1.74	0.53
12:A:280:ARG:NH2	13:D:400:ARG:HH11	2.06	0.53
12:A:285:SER:O	12:A:289:ARG:HG2	2.08	0.53
14:Z:241:VAL:O	14:Z:245:LYS:HG3	2.08	0.53
1:R:574:PRO:HG3	1:R:649:TRP:HD1	1.73	0.53
3:I:123:GLY:HA3	3:I:183:ILE:HD13	1.90	0.53
12:A:44:ARG:HB3	12:A:49:GLU:HB3	1.90	0.53
13:E:197:LEU:HD23	13:E:379:VAL:HG12	1.90	0.53
1:R:542:ILE:HG13	1:R:543:LEU:N	2.24	0.53
12:C:24:VAL:HG21	13:F:68:TYR:HB2	1.90	0.53
11:Q:151:TYR:OH	11:Q:168:ILE:O	2.20	0.53
12:A:70:THR:HA	12:A:73:VAL:HG23	1.89	0.53
13:F:100:GLU:HA	13:F:267:PRO:HG2	1.90	0.53
3:I:27:ALA:HB2	4:L:21:LYS:HA	1.91	0.53
2:O:216:LEU:N	2:O:224:LEU:O	2.41	0.53
10:2:24:VAL:HG21	10:3:101:LEU:HB3	1.91	0.53
10:2:136:ILE:O	10:2:140:VAL:HG23	2.09	0.53
18:W:282:LEU:O	18:W:286:ILE:HG12	2.09	0.53
4:L:110:ILE:HD11	4:L:114:TYR:CD2	2.44	0.53
10:3:18:GLY:HA3	10:3:93:LEU:HA	1.91	0.53
10:5:48:ARG:HD3	10:5:51:GLN:HE22	1.73	0.53
12:A:18:PHE:CG	12:A:78:PRO:HB3	2.44	0.53
13:D:301:SER:O	13:D:305:GLU:HG2	2.08	0.53
4:L:56:LYS:O	4:L:59:GLU:HG3	2.09	0.53
3:H:102:LEU:HD21	3:H:196:LEU:HB3	1.91	0.53
7:U:274:PHE:HE1	7:U:285:LEU:HD12	1.73	0.53
10:1:84:ILE:HG21	10:1:89:SER:HB3	1.90	0.53
10:5:57:ILE:H	10:5:57:ILE:HD12	1.74	0.53
12:B:249:PRO:HB3	12:B:410:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:535:TYR:CZ	12:B:594:GLU:HG2	2.44	0.53
13:D:376:GLN:HG3	13:D:378:TYR:CE2	2.44	0.53
13:E:368:LEU:O	13:E:372:ILE:HD12	2.08	0.53
18:W:173:MET:HB2	18:W:181:LEU:HD11	1.91	0.53
13:F:173:GLY:O	13:F:465:GLN:NE2	2.37	0.53
1:R:808:VAL:O	1:R:812:ASN:ND2	2.42	0.53
9:O:51:ASN:HD21	10:1:91:LEU:HD23	1.74	0.53
10:4:58:PRO:HG3	10:4:135:LEU:HD21	1.91	0.53
12:C:350:SER:HB2	12:C:353:ARG:HG2	1.91	0.53
11:Q:138:MET:N	11:Q:138:MET:SD	2.82	0.52
11:Q:231:GLU:H	11:Q:231:GLU:CD	2.17	0.52
14:X:106:ASP:OD1	14:X:107:LEU:N	2.41	0.52
10:4:60:VAL:O	10:4:64:ILE:HG12	2.09	0.52
10:8:14:PHE:HD1	10:8:93:LEU:HD13	1.73	0.52
14:Y:161:MET:O	14:Y:165:GLN:HG2	2.09	0.52
1:R:100:ASN:OD1	1:R:101:PHE:N	2.42	0.52
10:2:48:ARG:CZ	10:2:51:GLN:HE22	2.22	0.52
10:4:48:ARG:NH1	10:4:51:GLN:O	2.42	0.52
18:W:38:PRO:HD2	18:W:39:ASN:H	1.74	0.52
18:W:337:THR:HG22	18:W:338:HIS:H	1.74	0.52
13:F:307:LEU:HD23	13:F:327:MET:HG3	1.91	0.52
3:J:37:GLU:O	3:J:41:GLU:N	2.37	0.52
3:J:121:LEU:HD11	3:J:125:TYR:CZ	2.45	0.52
10:8:56:ILE:HD13	10:9:133:LEU:HD23	1.92	0.52
11:Q:48:HIS:O	11:Q:51:SER:OG	2.22	0.52
12:B:236:ALA:HA	12:B:472:PHE:HZ	1.75	0.52
13:D:192:PHE:CE1	13:D:354:LEU:HD12	2.44	0.52
14:Z:140:LEU:HD21	14:Z:152:LEU:HB3	1.91	0.52
14:Y:134:ASN:HA	14:Y:137:THR:HG22	1.91	0.52
18:W:291:PRO:HA	18:W:308:ALA:O	2.09	0.52
1:R:129:LYS:NZ	1:R:265:ILE:HD13	2.24	0.52
11:Q:17:GLU:OE2	11:Q:21:ARG:NE	2.26	0.52
12:A:39:MET:HE1	13:E:53:VAL:HG11	1.90	0.52
14:X:23:VAL:HG22	14:X:65:ILE:HG12	1.91	0.52
14:X:207:GLN:HE21	14:X:212:PRO:HB3	1.74	0.52
14:Y:111:GLN:HE22	14:Y:169:THR:H	1.58	0.52
4:M:100:LEU:HA	4:M:103:VAL:HG22	1.91	0.52
9:O:49:TRP:HB3	9:O:138:PHE:HB2	1.90	0.52
10:1:118:VAL:HA	10:1:121:THR:HG22	1.92	0.52
18:W:426:ILE:HG21	13:F:432:VAL:HG13	1.92	0.52
1:R:17:LEU:HD23	1:R:350:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:13:PHE:HB2	10:3:90:PHE:CE2	2.45	0.52
12:C:250:GLY:HA2	12:C:256:LYS:HD2	1.91	0.52
12:A:34:MET:O	12:A:62:ALA:HB2	2.09	0.52
1:R:9:GLU:HG2	1:R:386:TYR:OH	2.10	0.52
1:R:542:ILE:HD13	5:S:54:ILE:HD13	1.92	0.52
1:R:777:PHE:O	1:R:780:THR:OG1	2.22	0.52
12:C:549:ASP:OD1	12:C:550:MET:N	2.42	0.52
12:A:498:LYS:HG3	12:A:501:LEU:HD12	1.92	0.52
13:D:483:LEU:O	13:D:486:ILE:HG12	2.09	0.52
1:R:487:TYR:HB3	19:R:901:NAG:HN2	1.75	0.52
3:J:199:ARG:NH1	13:F:41:SER:O	2.43	0.52
6:T:123:PHE:HA	6:T:126:VAL:HG12	1.92	0.52
9:O:30:ASP:OD1	10:7:10:TYR:OH	2.27	0.52
11:Q:177:ASN:HB3	11:Q:180:ILE:HG12	1.91	0.52
12:A:43:VAL:CG1	12:A:81:ARG:HG2	2.39	0.52
13:D:234:MET:HE2	13:D:275:PRO:HD3	1.92	0.52
1:R:81:ASP:H	1:R:291:ARG:HD3	1.75	0.52
4:M:19:ALA:HA	4:M:22:VAL:HG12	1.92	0.52
12:C:42:LEU:O	12:C:82:THR:OG1	2.26	0.52
12:A:75:VAL:CG2	13:D:67:ARG:HA	2.39	0.52
12:A:92:PRO:HG3	12:A:205:MET:HE2	1.92	0.52
13:E:272:ILE:HD11	13:E:310:VAL:HG21	1.90	0.52
18:W:280:SER:HB2	13:F:449:LEU:HB3	1.92	0.52
18:W:303:VAL:H	18:W:330:CYS:HB3	1.74	0.52
1:R:374:PHE:HA	1:R:377:ILE:HG12	1.91	0.51
3:J:128:LEU:HA	3:J:155:TYR:OH	2.09	0.51
12:A:45:VAL:HG22	12:A:79:VAL:HG13	1.92	0.51
3:J:78:GLN:OE1	3:J:78:GLN:HA	2.09	0.51
9:O:200:ARG:HH22	10:9:80:LEU:C	2.18	0.51
13:E:182:SER:OG	13:E:402:MET:HG3	2.10	0.51
18:W:172:ASP:OD1	18:W:199:TRP:NE1	2.37	0.51
1:R:44:VAL:HB	1:R:48:GLN:HB2	1.91	0.51
10:1:61:MET:HA	10:1:64:ILE:HG22	1.92	0.51
12:C:66:VAL:HG12	12:C:68:GLU:H	1.75	0.51
12:A:378:LEU:HD21	12:A:421:VAL:HG12	1.91	0.51
12:B:56:ARG:HE	12:B:365:LEU:HD22	1.75	0.51
15:G:129:GLU:OE2	15:G:130:GLN:HG2	2.10	0.51
13:F:61:ASP:OD1	13:F:62:HIS:ND1	2.43	0.51
3:J:101:ARG:HH21	4:M:100:LEU:HD21	1.75	0.51
10:1:13:PHE:HB2	10:2:90:PHE:CD2	2.46	0.51
12:C:265:LYS:HG3	12:C:296:MET:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:505:ASP:O	12:C:509:LEU:HD23	2.11	0.51
12:A:67:TYR:CD1	12:A:321:ALA:HB1	2.45	0.51
12:B:107:SER:OG	13:E:161:GLN:NE2	2.39	0.51
13:E:424:ALA:HB2	13:E:494:ARG:NH1	2.24	0.51
13:F:128:LEU:HD22	13:F:256:ASN:O	2.11	0.51
6:T:51:ALA:HB1	6:T:126:VAL:HB	1.92	0.51
12:C:24:VAL:HG12	12:C:29:VAL:HG22	1.93	0.51
12:C:115:SER:OG	12:C:116:ILE:N	2.44	0.51
13:E:55:GLY:O	13:E:102:THR:OG1	2.20	0.51
7:U:319:THR:HG21	7:U:350:ASN:HD21	1.75	0.51
9:O:92:VAL:HA	9:O:95:ILE:HD12	1.91	0.51
12:B:522:GLN:HG3	12:B:529:ASP:HB3	1.92	0.51
14:Y:146:THR:HG23	14:Y:149:ASN:H	1.75	0.51
1:R:301:LYS:NZ	1:R:305:HIS:HB2	2.25	0.51
1:R:490:THR:O	1:R:493:THR:OG1	2.26	0.51
2:O:33:ALA:HB1	2:O:323:PRO:HA	1.93	0.51
9:O:57:ALA:HB2	9:O:141:GLY:HA2	1.91	0.51
10:6:46:VAL:HG13	10:6:47:MET:SD	2.51	0.51
10:8:65:ILE:HA	10:8:68:TYR:CD2	2.42	0.51
12:C:134:ASP:OD1	12:C:134:ASP:N	2.43	0.51
12:C:507:ILE:HD11	12:C:555:VAL:HG21	1.93	0.51
14:X:52:VAL:HG12	14:X:75:PRO:HG2	1.91	0.51
13:F:300:MET:HB2	13:F:354:LEU:HD23	1.93	0.51
1:R:483:PRO:O	1:R:486:THR:HG22	2.10	0.51
10:3:141:LEU:HA	10:3:144:TYR:HD2	1.75	0.51
12:A:23:GLY:HA2	13:D:68:TYR:OH	2.11	0.51
12:B:280:ARG:NH1	13:E:371:TYR:O	2.40	0.51
14:Z:59:ASN:HB3	14:Z:61:ARG:HH22	1.76	0.51
18:W:146:GLU:OE2	18:W:216:LYS:HE3	2.11	0.51
10:6:23:MET:HE3	10:6:27:ALA:HB2	1.91	0.51
10:9:23:MET:HA	10:9:23:MET:HE2	1.93	0.51
10:9:32:TYR:HE2	10:9:108:PHE:HD1	1.58	0.51
12:B:68:GLU:OE2	12:B:104:ARG:NH1	2.43	0.51
14:X:37:ASP:OD2	14:X:42:LEU:N	2.37	0.51
14:X:256:THR:HG22	14:X:258:THR:H	1.74	0.51
1:R:401:PHE:CD1	5:S:47:CYS:SG	3.04	0.51
10:4:32:TYR:CE1	10:4:36:LYS:HE2	2.46	0.51
10:4:113:VAL:HG21	10:4:134:ILE:HG21	1.93	0.51
10:8:48:ARG:HH11	10:8:48:ARG:HG3	1.75	0.51
11:Q:154:ILE:O	11:Q:158:THR:HB	2.11	0.51
12:C:233:VAL:HG13	12:C:234:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:32:ARG:HD2	4:M:35:GLN:HE21	1.75	0.50
3:I:135:ARG:NH1	3:I:171:SER:O	2.43	0.50
12:A:18:PHE:CD1	12:A:78:PRO:HB3	2.46	0.50
12:B:138:CYS:O	12:B:139:LYS:HG2	2.11	0.50
18:W:146:GLU:OE1	18:W:146:GLU:N	2.44	0.50
1:R:37:PHE:HA	1:R:323:VAL:HG12	1.92	0.50
1:R:94:MET:SD	1:R:95:ILE:HG13	2.51	0.50
4:M:70:SER:O	4:M:73:VAL:HG22	2.11	0.50
3:I:203:ILE:HD11	4:L:103:VAL:HA	1.92	0.50
7:U:325:PHE:CD2	7:U:345:LEU:HD13	2.46	0.50
12:C:285:SER:O	12:C:289:ARG:HG2	2.12	0.50
18:W:330:CYS:HB3	18:W:331:PRO:HD3	1.92	0.50
3:J:199:ARG:O	3:J:203:ILE:HG12	2.11	0.50
3:H:129:GLU:OE1	3:H:185:ASN:HB2	2.12	0.50
9:O:116:GLU:OE2	9:O:117:PRO:HD2	2.11	0.50
10:1:50:GLU:HG2	10:1:51:GLN:OE1	2.12	0.50
10:8:13:PHE:HB2	10:9:90:PHE:CE2	2.47	0.50
10:8:60:VAL:HA	10:9:137:PHE:HE2	1.76	0.50
10:9:10:TYR:O	10:9:13:PHE:HB3	2.12	0.50
12:A:503:GLU:OE1	12:A:567:TRP:N	2.41	0.50
12:B:272:ILE:HD13	12:B:345:SER:HB3	1.93	0.50
1:R:65:LEU:HA	1:R:68:VAL:HG12	1.92	0.50
1:R:102:GLU:O	1:R:105:GLU:HG3	2.11	0.50
1:R:272:LEU:HA	1:R:275:THR:HG22	1.93	0.50
1:R:491:GLU:HA	1:R:494:LEU:HD12	1.93	0.50
3:J:78:GLN:O	3:J:82:LYS:HG2	2.12	0.50
7:U:257:PRO:HD3	8:V:293:TYR:CE2	2.47	0.50
10:8:8:PRO:HG2	10:8:86:LEU:HD22	1.92	0.50
18:W:137:VAL:O	18:W:141:LEU:HD23	2.12	0.50
10:1:82:ASP:OD1	10:1:83:ASP:N	2.44	0.50
10:1:112:ILE:CD1	11:Q:11:VAL:HA	2.38	0.50
12:C:510:GLU:HG2	12:C:567:TRP:HZ2	1.77	0.50
12:A:43:VAL:O	12:A:51:VAL:HA	2.11	0.50
14:Z:159:LEU:HD21	14:Z:179:PHE:HE1	1.77	0.50
14:Z:237:LEU:HA	14:Z:270:ASN:ND2	2.26	0.50
18:W:175:LEU:HD22	18:W:189:TYR:HD2	1.76	0.50
1:R:801:HIS:NE2	10:7:60:VAL:HG12	2.27	0.50
3:J:81:LEU:HD21	3:J:85:ARG:NH2	2.26	0.50
3:J:153:PRO:O	3:J:157:ILE:HG12	2.12	0.50
3:J:158:ALA:C	3:J:160:LYS:H	2.19	0.50
3:I:180:GLY:HA3	3:I:195:THR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:134:VAL:HG23	3:H:167:ILE:HG12	1.94	0.50
15:G:194:ARG:HH11	15:G:194:ARG:HG3	1.77	0.50
18:W:168:GLN:HG3	18:W:333:MET:HB2	1.93	0.50
4:M:30:ASN:O	4:M:33:LEU:HG	2.11	0.50
7:U:374:VAL:HG12	7:U:383:LEU:HD12	1.94	0.50
10:2:54:LYS:HB3	10:2:128:PHE:HE1	1.77	0.50
10:4:32:TYR:HE1	10:4:36:LYS:HE2	1.77	0.50
12:A:34:MET:SD	12:A:54:ILE:HG12	2.51	0.50
12:A:292:PRO:HA	12:A:304:SER:OG	2.12	0.50
12:B:511:VAL:HG11	12:B:548:TYR:CD1	2.46	0.50
14:Z:242:LEU:HD23	14:Z:245:LYS:HE2	1.93	0.50
14:Y:105:LEU:O	14:Y:109:GLU:HG3	2.12	0.50
14:Y:111:GLN:NE2	14:Y:168:ILE:H	2.09	0.50
1:R:522:TRP:CZ3	5:S:66:PRO:HB3	2.46	0.50
1:R:609:LEU:HD23	1:R:609:LEU:H	1.76	0.50
13:E:386:ARG:NH2	13:E:459:GLU:OE1	2.38	0.50
1:R:754:VAL:HA	1:R:757:THR:HG22	1.94	0.50
3:J:63:GLN:O	3:J:66:GLN:HB3	2.12	0.50
4:M:37:LYS:O	4:M:40:ALA:HB3	2.12	0.50
3:I:199:ARG:O	3:I:203:ILE:HG12	2.12	0.50
3:H:94:LEU:HD21	4:K:95:VAL:HG11	1.94	0.50
3:H:137:ARG:NH1	3:H:139:GLN:HE21	2.10	0.50
7:U:370:HIS:HA	7:U:400:PHE:O	2.12	0.50
10:1:65:ILE:HA	10:1:68:TYR:CD2	2.41	0.50
10:1:80:LEU:HB3	10:2:155:LYS:HE2	1.93	0.50
10:2:48:ARG:NE	10:2:51:GLN:HE22	2.08	0.50
10:5:72:VAL:HG11	10:5:99:VAL:HG11	1.93	0.50
11:Q:248:TYR:HA	11:Q:252:LEU:HD12	1.93	0.50
12:B:36:GLY:O	12:B:81:ARG:NH2	2.39	0.50
12:B:42:LEU:O	12:B:82:THR:OG1	2.29	0.50
18:W:283:CYS:O	18:W:287:THR:OG1	2.22	0.50
14:Z:159:LEU:HD21	14:Z:179:PHE:CE1	2.47	0.49
4:M:83:ILE:O	4:M:86:THR:OG1	2.20	0.49
8:V:338:ILE:HG13	11:Q:165:GLN:HG3	1.94	0.49
10:5:58:PRO:HA	10:5:61:MET:HE3	1.94	0.49
12:C:95:MET:HE2	12:C:308:ARG:HA	1.94	0.49
12:B:298:VAL:O	12:B:300:GLY:N	2.45	0.49
3:I:61:GLU:O	3:I:65:GLU:HG2	2.12	0.49
10:6:48:ARG:NH1	10:6:55:SER:OG	2.45	0.49
12:C:298:VAL:O	12:C:300:GLY:N	2.45	0.49
12:C:550:MET:SD	12:C:553:ARG:NH1	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:249:PRO:HA	12:B:410:VAL:O	2.11	0.49
13:D:192:PHE:HE1	13:D:354:LEU:HD12	1.77	0.49
14:X:172:ASN:OD1	14:X:174:GLY:N	2.46	0.49
15:G:93:LYS:HD3	16:N:4:ARG:HA	1.94	0.49
3:J:53:ILE:HB	3:J:57:TYR:CE1	2.46	0.49
10:4:70:LEU:HD22	10:5:144:TYR:HD1	1.77	0.49
12:A:569:ILE:HA	12:A:572:GLU:HG2	1.94	0.49
13:D:61:ASP:OD1	13:D:62:HIS:N	2.45	0.49
13:E:377:ILE:O	13:E:397:SER:OG	2.31	0.49
14:Z:36:ILE:HB	14:Z:92:LEU:HD12	1.94	0.49
1:R:316:GLN:HG3	1:R:317:LYS:N	2.28	0.49
10:9:84:ILE:HG21	10:9:89:SER:HB3	1.94	0.49
12:C:51:VAL:HG13	12:C:67:TYR:HD2	1.77	0.49
13:D:462:PHE:HB2	13:D:483:LEU:HD11	1.95	0.49
4:M:89:ARG:CZ	4:M:89:ARG:HA	2.43	0.49
4:K:83:ILE:O	4:K:86:THR:OG1	2.25	0.49
5:S:35:GLY:O	5:S:39:THR:HG23	2.13	0.49
8:V:339:ILE:O	8:V:339:ILE:HG13	2.12	0.49
12:C:55:ILE:HD12	12:C:365:LEU:HD11	1.93	0.49
12:C:451:LEU:HD11	12:C:487:GLU:HG3	1.94	0.49
12:A:21:VAL:HG22	12:A:31:ALA:HB2	1.93	0.49
14:Z:148:LYS:NZ	14:Z:188:MET:O	2.46	0.49
16:N:11:ILE:HB	16:N:66:ILE:HD13	1.95	0.49
1:R:32:LEU:HD13	1:R:34:LYS:NZ	2.28	0.49
5:S:51:PHE:O	5:S:54:ILE:HG22	2.13	0.49
9:O:81:VAL:HG11	11:Q:19:LEU:CD1	2.43	0.49
10:3:44:MET:HG2	10:3:119:ARG:HA	1.94	0.49
10:6:49:PRO:HB3	10:7:126:ARG:HH22	1.78	0.49
12:B:220:LYS:HG2	12:B:392:VAL:HG12	1.94	0.49
3:H:158:ALA:C	3:H:160:LYS:H	2.21	0.49
10:5:68:TYR:HD1	10:5:146:LEU:HD13	1.78	0.49
11:Q:78:MET:HE1	11:Q:323:GLU:HA	1.95	0.49
11:Q:275:LYS:O	11:Q:279:GLU:HG2	2.12	0.49
12:A:397:ASN:O	12:A:399:GLU:N	2.36	0.49
18:W:352:GLN:O	18:W:357:ASN:ND2	2.28	0.49
1:R:387:ARG:HE	1:R:561:TYR:HH	1.60	0.49
7:U:335:SER:O	7:U:337:ARG:N	2.43	0.49
10:4:130:GLY:O	10:4:134:ILE:HD12	2.13	0.49
12:C:481:GLU:O	12:C:485:GLU:HG3	2.13	0.49
3:J:64:ILE:O	3:J:67:GLN:HB2	2.13	0.49
10:1:61:MET:O	10:1:64:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:269:ASP:HA	11:Q:275:LYS:HB2	1.95	0.49
12:C:354:TRP:HZ3	12:C:382:LEU:HD23	1.78	0.49
12:C:471:GLU:O	12:C:475:LEU:HD23	2.13	0.49
12:B:229:THR:HG22	12:B:231:GLN:H	1.76	0.49
13:E:169:MET:HE3	13:E:182:SER:HB2	1.95	0.49
14:Z:52:VAL:HG12	14:Z:75:PRO:HG2	1.95	0.49
9:0:28:ILE:HD11	10:7:90:PHE:CZ	2.42	0.48
10:2:65:ILE:HA	10:2:68:TYR:HD2	1.78	0.48
12:C:249:PRO:HA	12:C:410:VAL:O	2.12	0.48
13:E:141:ARG:HA	14:X:9:LYS:HD2	1.95	0.48
13:F:194:ALA:H	13:F:197:LEU:HD12	1.78	0.48
13:F:338:ALA:HB2	13:F:350:GLN:HG3	1.94	0.48
4:L:66:ARG:HD2	4:L:66:ARG:C	2.38	0.48
12:C:495:LEU:HD23	15:G:32:LEU:HD13	1.95	0.48
12:A:19:GLY:HA3	12:A:33:ASP:HB3	1.96	0.48
1:R:70:LYS:NZ	1:R:74:LYS:HB3	2.27	0.48
4:M:43:GLU:O	4:M:46:GLN:HG3	2.13	0.48
9:0:81:VAL:HG13	9:0:82:LYS:HG2	1.95	0.48
10:1:72:VAL:HG21	10:1:99:VAL:HG21	1.95	0.48
10:4:124:GLN:HE22	10:4:126:ARG:HB2	1.78	0.48
10:5:50:GLU:H	10:5:50:GLU:CD	2.21	0.48
10:8:51:GLN:HB2	10:8:54:LYS:HB2	1.94	0.48
11:Q:138:MET:C	11:Q:140:ALA:H	2.21	0.48
14:Y:198:HIS:HA	14:Y:201:LYS:HG2	1.94	0.48
18:W:153:LYS:NZ	18:W:243:GLU:OE1	2.47	0.48
13:F:119:LEU:HD23	13:F:153:ILE:HD13	1.94	0.48
4:L:79:GLU:O	4:L:83:ILE:HD12	2.13	0.48
10:3:37:SER:OG	10:3:58:PRO:HB2	2.13	0.48
12:C:65:GLN:NE2	12:C:321:ALA:HB2	2.28	0.48
12:C:548:TYR:OH	12:C:552:ARG:NH1	2.46	0.48
12:B:37:ALA:O	12:B:57:LEU:HD21	2.13	0.48
12:B:63:THR:HG21	12:B:365:LEU:HD21	1.94	0.48
1:R:800:LEU:HD13	10:7:60:VAL:HG21	1.95	0.48
3:I:102:LEU:HD12	3:I:196:LEU:HD22	1.96	0.48
3:I:215:LEU:O	4:L:91:ASN:ND2	2.47	0.48
7:U:407:VAL:HG23	7:U:408:MET:H	1.78	0.48
10:3:53:MET:HE2	10:3:53:MET:HA	1.96	0.48
10:3:72:VAL:HG21	10:3:99:VAL:HG11	1.96	0.48
10:6:49:PRO:CA	10:7:126:ARG:HH22	2.27	0.48
10:9:134:ILE:H	10:9:134:ILE:HD12	1.78	0.48
12:C:45:VAL:HG12	12:C:79:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:457:LYS:O	13:E:461:ASN:HB2	2.13	0.48
14:Y:188:MET:HE2	14:Y:192:LYS:HD2	1.94	0.48
18:W:175:LEU:HD22	18:W:189:TYR:CD2	2.48	0.48
13:F:172:THR:HG22	13:F:178:ASP:OD1	2.13	0.48
3:J:73:SER:O	3:J:77:ASN:N	2.43	0.48
3:I:106:VAL:HA	3:I:112:TYR:HD2	1.79	0.48
4:L:110:ILE:HD11	4:L:114:TYR:HD2	1.78	0.48
17:P:222:ASP:O	17:P:224:VAL:N	2.47	0.48
1:R:278:HIS:HA	1:R:281:ARG:HG2	1.95	0.48
4:L:93:ASP:OD1	4:L:94:GLU:N	2.47	0.48
11:Q:211:ILE:O	11:Q:215:GLU:HG2	2.14	0.48
12:C:233:VAL:HG11	12:C:448:VAL:HG21	1.96	0.48
14:X:107:LEU:O	14:X:111:GLN:HG2	2.14	0.48
14:X:224:ILE:O	14:X:228:THR:HG23	2.14	0.48
14:Y:177:GLN:HA	14:Y:180:LYS:HG2	1.95	0.48
15:G:39:ALA:O	15:G:42:LEU:HG	2.13	0.48
9:O:51:ASN:ND2	10:1:91:LEU:HD23	2.29	0.48
10:5:36:LYS:O	10:5:39:THR:HG22	2.13	0.48
11:Q:197:CYS:SG	11:Q:208:MET:HB2	2.54	0.48
11:Q:343:LYS:HD2	11:Q:346:ASN:HD21	1.78	0.48
12:C:143:VAL:HG13	12:C:177:THR:HA	1.95	0.48
12:B:295:THR:HB	12:B:302:VAL:HG22	1.95	0.48
9:O:188:LEU:O	9:O:191:VAL:HG12	2.14	0.48
10:8:64:ILE:O	10:8:67:ILE:HB	2.14	0.48
12:B:67:TYR:HB3	12:B:102:ILE:HD11	1.96	0.48
13:E:242:ARG:HH11	13:E:242:ARG:HG3	1.79	0.48
1:R:57:ARG:NE	1:R:95:ILE:HG23	2.29	0.48
1:R:80:MET:HB3	1:R:82:THR:HG23	1.95	0.48
4:M:27:LYS:NZ	4:M:31:ARG:HB3	2.29	0.48
6:T:79:LEU:HB3	6:T:82:ASP:OD2	2.14	0.48
10:5:47:MET:HG3	10:5:48:ARG:HG2	1.96	0.48
11:Q:250:GLU:HG3	11:Q:251:GLY:H	1.79	0.48
12:A:193:GLU:OE1	12:A:202:LYS:HG2	2.14	0.48
14:Z:172:ASN:OD1	14:Z:173:GLU:N	2.47	0.48
18:W:279:PHE:CD2	18:W:374:VAL:HG23	2.49	0.48
1:R:266:ASP:O	1:R:269:GLN:HG3	2.14	0.47
10:2:128:PHE:O	10:2:132:ILE:HG12	2.14	0.47
11:Q:24:LYS:HD3	11:Q:351:PHE:CZ	2.48	0.47
12:A:241:VAL:HG12	12:A:461:LEU:HD21	1.96	0.47
10:1:137:PHE:O	10:1:140:VAL:HG12	2.13	0.47
10:6:134:ILE:H	10:6:134:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:34:MET:HE2	12:C:64:ILE:HD11	1.95	0.47
18:W:172:ASP:O	18:W:202:ARG:NH2	2.47	0.47
3:I:49:GLN:NE2	3:I:50:ARG:HG2	2.29	0.47
7:U:326:ILE:HD11	7:U:344:ARG:NE	2.30	0.47
10:8:136:ILE:O	10:8:140:VAL:HG23	2.14	0.47
13:D:71:ILE:O	13:D:115:THR:OG1	2.21	0.47
18:W:134:VAL:HG13	18:W:162:VAL:HG13	1.96	0.47
3:H:222:ARG:NH2	3:H:225:LEU:O	2.48	0.47
10:1:36:LYS:O	10:1:39:THR:HG22	2.14	0.47
10:2:61:MET:HA	10:2:64:ILE:HD13	1.96	0.47
10:5:131:MET:O	10:5:135:LEU:HD23	2.14	0.47
12:C:42:LEU:HD11	12:C:86:LEU:HD12	1.96	0.47
13:D:320:ARG:HH11	13:D:320:ARG:HG3	1.78	0.47
13:D:354:LEU:HD11	13:D:369:THR:HG21	1.96	0.47
13:E:301:SER:O	13:E:305:GLU:HG3	2.13	0.47
14:Z:256:THR:HG23	14:Z:258:THR:HG22	1.96	0.47
14:X:225:LEU:HB3	14:X:255:LEU:HD11	1.96	0.47
13:F:290:GLU:OE1	13:F:345:ASN:HB2	2.15	0.47
6:T:62:VAL:O	6:T:66:ILE:HG12	2.15	0.47
12:B:210:PRO:HB2	12:B:213:GLN:HG3	1.97	0.47
14:X:134:ASN:HA	14:X:137:THR:HG22	1.96	0.47
3:H:66:GLN:O	3:H:70:ILE:HG12	2.14	0.47
10:1:124:GLN:OE1	10:1:126:ARG:N	2.48	0.47
10:2:99:VAL:HB	10:2:149:ALA:HB2	1.97	0.47
12:B:50:LEU:HD23	12:B:68:GLU:HB2	1.97	0.47
12:B:498:LYS:HG3	12:B:501:LEU:HD12	1.97	0.47
14:Z:80:ALA:HA	14:Z:83:ARG:HE	1.79	0.47
13:F:208:ARG:NH2	13:F:247:ASP:OD2	2.45	0.47
9:O:28:ILE:HG23	9:O:29:PHE:HD1	1.78	0.47
10:3:41:ILE:HG23	10:3:52:ILE:HD11	1.97	0.47
10:6:84:ILE:HG21	10:6:89:SER:HB3	1.97	0.47
10:7:81:ASN:OD1	10:7:83:ASP:N	2.47	0.47
10:9:50:GLU:OE1	10:9:50:GLU:N	2.48	0.47
12:C:232:ARG:HD3	12:C:540:MET:HE1	1.97	0.47
12:A:486:GLU:HG3	12:A:512:ALA:HB3	1.97	0.47
15:G:58:MET:HB2	15:G:144:LEU:HD21	1.96	0.47
18:W:59:PRO:HG3	18:W:139:HIS:ND1	2.29	0.47
1:R:327:VAL:HG11	1:R:354:ARG:HH22	1.80	0.47
3:I:90:LEU:HD11	4:L:88:PHE:CD2	2.50	0.47
7:U:403:GLN:HG2	7:U:407:VAL:HG12	1.95	0.47
11:Q:208:MET:HE3	11:Q:208:MET:HB3	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:231:PHE:HB3	13:D:259:LEU:HD12	1.97	0.47
13:D:380:ASP:HB2	13:D:393:ASN:HB2	1.97	0.47
13:E:214:LYS:HE3	13:E:220:VAL:HA	1.96	0.47
13:F:172:THR:HG23	13:F:174:ILE:H	1.78	0.47
1:R:296:LYS:O	1:R:300:MET:HG2	2.15	0.47
2:O:238:ARG:O	2:O:242:ARG:N	2.42	0.47
3:J:122:GLN:NE2	13:F:43:PRO:HD3	2.10	0.47
3:I:182:GLU:HG2	3:I:193:SER:HA	1.95	0.47
14:Z:111:GLN:O	14:Z:115:MET:HG2	2.15	0.47
14:Z:111:GLN:OE1	14:Z:169:THR:HG23	2.15	0.47
3:I:72:MET:HE2	3:I:72:MET:HA	1.97	0.47
4:L:115:ARG:HH11	4:L:115:ARG:HG3	1.80	0.47
5:S:30:LYS:HA	5:S:30:LYS:HD2	1.79	0.47
10:4:61:MET:CE	10:4:135:LEU:HB3	2.45	0.47
10:7:28:LEU:HD23	10:8:105:ALA:HB2	1.97	0.47
11:Q:143:ILE:HG13	11:Q:145:GLN:H	1.79	0.47
12:A:143:VAL:HG13	12:A:177:THR:HA	1.97	0.47
12:A:192:LEU:HD23	12:A:193:GLU:N	2.30	0.47
14:Z:103:MET:HE3	14:Z:107:LEU:HD23	1.97	0.47
14:Y:268:LYS:HA	14:Y:271:GLU:OE1	2.15	0.47
18:W:181:LEU:HD13	18:W:186:TRP:CE3	2.50	0.47
13:F:163:ARG:NH2	13:F:338:ALA:O	2.48	0.47
1:R:43:ASP:OD1	1:R:44:VAL:N	2.48	0.46
3:I:223:LYS:HE3	13:E:290:GLU:HG3	1.96	0.46
7:U:260:TYR:HB3	7:U:267:ILE:HB	1.96	0.46
7:U:454:ASP:OD1	7:U:455:ARG:N	2.48	0.46
9:O:59:SER:OG	10:1:101:LEU:HB3	2.15	0.46
10:4:88:LYS:O	10:4:92:GLN:HG2	2.16	0.46
12:C:535:TYR:CZ	12:C:594:GLU:HG3	2.50	0.46
12:C:584:MET:HA	12:C:584:MET:HE2	1.96	0.46
12:A:73:VAL:O	13:D:68:TYR:HB2	2.15	0.46
12:B:320:VAL:HG11	12:B:360:GLU:OE1	2.15	0.46
14:Y:42:LEU:O	14:Y:46:ARG:HG3	2.15	0.46
14:Y:263:ILE:O	14:Y:266:ILE:HG22	2.15	0.46
16:N:12:GLY:HA3	16:N:67:ASN:OD1	2.14	0.46
16:N:45:ILE:O	16:N:49:GLU:HG2	2.16	0.46
18:W:130:THR:HG23	18:W:166:ALA:HB1	1.97	0.46
3:H:129:GLU:H	3:H:132:MET:HE3	1.80	0.46
7:U:334:VAL:HA	10:8:9:GLU:OE1	2.15	0.46
10:7:85:SER:C	10:7:87:TYR:H	2.23	0.46
12:A:27:PRO:O	12:A:66:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:395:LEU:HA	13:D:423:TYR:HE1	1.80	0.46
14:Z:61:ARG:HG3	14:Z:63:GLU:OE1	2.15	0.46
13:F:435:MET:HA	13:F:435:MET:HE3	1.96	0.46
1:R:479:TRP:CD1	1:R:521:ILE:HG21	2.51	0.46
3:J:105:VAL:HG22	3:J:111:ARG:NH2	2.30	0.46
3:J:108:ASP:O	3:J:110:THR:N	2.48	0.46
9:0:84:PRO:O	9:0:87:LYS:HG2	2.14	0.46
10:1:141:LEU:O	10:1:144:TYR:HB2	2.15	0.46
10:4:40:GLY:O	10:4:44:MET:HG3	2.15	0.46
10:9:72:VAL:HG21	10:9:99:VAL:HG11	1.97	0.46
12:C:477:THR:HG23	13:D:387:GLN:HG3	1.97	0.46
12:A:43:VAL:HG12	12:A:81:ARG:HG2	1.97	0.46
12:A:504:THR:HA	12:A:507:ILE:HD12	1.97	0.46
13:D:214:LYS:HD2	13:D:214:LYS:O	2.16	0.46
13:E:465:GLN:NE2	13:E:469:GLU:O	2.46	0.46
14:Z:134:ASN:HA	14:Z:137:THR:HG22	1.96	0.46
15:G:5:ASP:O	15:G:182:ARG:NH2	2.38	0.46
15:G:89:LYS:HA	16:N:27:GLU:HG2	1.96	0.46
1:R:593:LYS:HD3	1:R:608:LEU:HD23	1.96	0.46
10:9:48:ARG:HD3	10:9:122:ALA:O	2.15	0.46
12:A:39:MET:HE1	13:E:53:VAL:CG1	2.45	0.46
13:D:200:ASN:HB2	13:D:244:PHE:HZ	1.80	0.46
3:I:129:GLU:OE1	3:I:185:ASN:HB2	2.16	0.46
7:U:373:TYR:CE2	7:U:380:LYS:HD2	2.51	0.46
9:0:85:ARG:O	9:0:88:THR:HG22	2.15	0.46
10:3:48:ARG:N	10:3:49:PRO:HD3	2.31	0.46
10:7:113:VAL:HG21	10:7:134:ILE:CG2	2.44	0.46
10:8:141:LEU:HA	10:8:144:TYR:HD2	1.80	0.46
12:C:514:LEU:O	12:C:518:ASP:HB3	2.15	0.46
12:A:39:MET:HB3	12:A:40:TYR:CD2	2.39	0.46
12:A:246:THR:HG23	12:A:407:VAL:HG13	1.97	0.46
12:A:410:VAL:HG11	12:A:422:THR:HG23	1.96	0.46
12:A:554:ALA:HB2	12:A:612:PHE:CZ	2.50	0.46
12:A:577:ILE:HD11	12:A:607:ASP:HB3	1.96	0.46
12:B:232:ARG:HD2	12:B:519:PHE:O	2.15	0.46
14:Z:268:LYS:HA	14:Z:271:GLU:OE1	2.15	0.46
14:Y:118:HIS:CE1	14:Y:124:SER:HB3	2.51	0.46
18:W:198:ASP:O	18:W:202:ARG:HG3	2.15	0.46
13:F:433:GLN:OE1	13:F:455:LEU:HD22	2.14	0.46
1:R:36:GLN:OE1	1:R:823:LEU:N	2.47	0.46
1:R:529:LEU:HD23	1:R:529:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:0:154:CYS:SG	10:9:34:THR:HG23	2.55	0.46
9:0:172:LEU:HD13	10:9:45:SER:OG	2.15	0.46
10:4:48:ARG:HD3	10:4:51:GLN:HG2	1.98	0.46
10:7:126:ARG:O	10:7:126:ARG:HG2	2.16	0.46
12:C:397:ASN:C	12:C:399:GLU:H	2.24	0.46
12:A:42:LEU:HD21	12:A:67:TYR:HE2	1.80	0.46
14:X:237:LEU:HD23	14:X:270:ASN:HD22	1.80	0.46
3:J:182:GLU:HG2	3:J:193:SER:HA	1.97	0.46
3:I:67:GLN:NE2	3:I:71:GLN:HE21	2.12	0.46
7:U:331:LEU:HD12	7:U:338:HIS:NE2	2.31	0.46
10:2:72:VAL:HG21	10:2:99:VAL:HG11	1.97	0.46
10:7:82:ASP:HA	10:8:87:TYR:CE2	2.51	0.46
12:C:535:TYR:CE1	12:C:594:GLU:HG3	2.51	0.46
14:Y:57:GLU:HG2	14:Y:58:LYS:HD3	1.98	0.46
15:G:89:LYS:HE2	15:G:89:LYS:HB2	1.73	0.46
3:H:146:ALA:O	3:H:149:GLN:HG3	2.16	0.46
7:U:274:PHE:HD1	7:U:285:LEU:HB2	1.79	0.46
10:3:85:SER:C	10:3:87:TYR:H	2.24	0.46
12:A:319:PRO:O	12:A:323:ARG:HD3	2.15	0.46
12:A:411:SER:O	12:A:411:SER:OG	2.31	0.46
13:D:88:GLU:HB2	13:D:95:VAL:HB	1.97	0.46
13:F:271:ARG:NH1	13:F:302:SER:OG	2.48	0.46
3:J:21:GLN:O	3:J:25:GLU:HG2	2.16	0.46
10:4:82:ASP:OD2	10:4:83:ASP:N	2.49	0.46
10:9:141:LEU:O	10:9:144:TYR:HB2	2.15	0.46
13:D:363:HIS:HB3	13:D:366:PRO:HD2	1.96	0.46
14:Z:232:TYR:O	14:Z:235:PRO:HD2	2.16	0.46
13:F:86:VAL:HA	13:F:96:VAL:HA	1.96	0.46
1:R:290:ILE:HA	1:R:293:TRP:HD1	1.80	0.46
1:R:585:TYR:OH	1:R:629:TYR:OH	2.31	0.46
7:U:374:VAL:CG2	7:U:397:LEU:HB2	2.46	0.46
10:7:140:VAL:HG12	10:7:144:TYR:CE2	2.51	0.46
12:C:459:ARG:HB3	12:C:459:ARG:NH1	2.30	0.46
18:W:183:GLY:O	18:W:186:TRP:HD1	1.99	0.46
4:K:111:HIS:CE1	4:K:113:ASN:HB2	2.51	0.45
10:1:109:ALA:O	10:1:113:VAL:HG12	2.16	0.45
10:8:129:VAL:O	10:8:133:LEU:HD23	2.16	0.45
12:A:419:ASP:N	12:A:419:ASP:OD1	2.49	0.45
13:D:99:PHE:CD1	13:D:269:ILE:HG21	2.52	0.45
1:R:628:LEU:HB2	1:R:632:GLN:OE1	2.17	0.45
3:I:76:MET:HA	3:I:76:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:338:HIS:HB2	7:U:365:SER:OG	2.17	0.45
7:U:457:ASP:OD1	7:U:457:ASP:N	2.49	0.45
9:O:62:VAL:HG11	10:1:102:SER:HB2	1.97	0.45
10:3:133:LEU:HA	10:3:133:LEU:HD23	1.67	0.45
11:Q:151:TYR:O	11:Q:155:LEU:HD23	2.16	0.45
12:A:192:LEU:HD21	12:A:194:LEU:HD23	1.98	0.45
12:A:270:ASP:HB2	12:A:342:TYR:HB3	1.99	0.45
12:A:469:PHE:CZ	12:A:534:PHE:HD2	2.35	0.45
13:E:421:GLN:NE2	13:E:425:CYS:SG	2.84	0.45
1:R:55:VAL:HG13	1:R:56:ARG:HD3	1.98	0.45
1:R:63:ARG:HH21	1:R:66:ARG:HG3	1.81	0.45
3:J:214:ALA:O	4:M:91:ASN:HB2	2.16	0.45
10:7:44:MET:HE1	10:7:48:ARG:HD2	1.97	0.45
12:A:289:ARG:C	12:A:292:PRO:HD2	2.40	0.45
12:A:395:LEU:O	12:A:400:ARG:NH2	2.49	0.45
12:B:193:GLU:OE2	12:B:200:LYS:HB3	2.16	0.45
13:E:276:ARG:HH12	13:E:334:ILE:HD11	1.82	0.45
18:W:247:ASP:O	18:W:251:VAL:HG23	2.15	0.45
3:J:180:GLY:HA3	3:J:195:THR:HA	1.99	0.45
3:I:106:VAL:HG13	3:I:112:TYR:CE2	2.52	0.45
3:I:129:GLU:H	3:I:132:MET:CE	2.29	0.45
7:U:366:ILE:HG13	7:U:367:TYR:CD1	2.51	0.45
7:U:410:GLU:HG2	7:U:411:GLN:HG3	1.98	0.45
10:5:51:GLN:HB2	10:5:54:LYS:HB3	1.99	0.45
12:A:368:MET:HE2	12:A:368:MET:H	1.81	0.45
12:B:570:ILE:O	12:B:574:MET:HG2	2.17	0.45
14:Y:83:ARG:HA	14:Y:83:ARG:HD2	1.70	0.45
1:R:378:VAL:HG21	1:R:391:PRO:HG2	1.98	0.45
9:O:70:TYR:CD1	10:1:112:ILE:HG21	2.51	0.45
10:3:124:GLN:HE22	10:3:126:ARG:HB2	1.82	0.45
10:7:84:ILE:HG21	10:7:89:SER:HB3	1.99	0.45
12:C:287:VAL:HG13	12:C:291:PHE:CE2	2.51	0.45
12:A:368:MET:HE1	13:E:315:GLU:OE2	2.16	0.45
13:D:68:TYR:HD1	13:D:68:TYR:HA	1.57	0.45
13:E:341:VAL:HG23	13:E:344:ARG:HB2	1.97	0.45
13:E:402:MET:O	13:E:406:ILE:HG12	2.16	0.45
14:Z:126:TYR:HE2	14:Z:169:THR:HA	1.82	0.45
1:R:740:ARG:NH2	1:R:804:ARG:HE	2.14	0.45
5:S:30:LYS:HD2	5:S:34:ARG:HD3	1.99	0.45
10:2:32:TYR:CE2	10:2:108:PHE:HD1	2.35	0.45
10:8:48:ARG:HG3	10:8:48:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:65:ILE:HD11	10:9:110:ILE:HD12	1.99	0.45
11:Q:2:SER:C	11:Q:4:PHE:H	2.24	0.45
12:C:484:GLN:HG2	13:D:386:ARG:HG2	1.98	0.45
12:A:108:ASP:O	12:A:112:GLN:HG3	2.16	0.45
12:B:95:MET:HE1	12:B:271:VAL:CG1	2.46	0.45
12:B:95:MET:HE1	12:B:271:VAL:HG13	1.99	0.45
12:B:486:GLU:HG3	12:B:512:ALA:HB3	1.99	0.45
12:B:486:GLU:HG2	12:B:509:LEU:HD12	1.98	0.45
14:Z:114:LYS:HG2	14:Z:169:THR:HB	1.98	0.45
14:Z:126:TYR:CE2	14:Z:169:THR:HG22	2.52	0.45
14:Z:161:MET:O	14:Z:165:GLN:HG2	2.17	0.45
14:X:103:MET:HG3	14:X:107:LEU:HD23	1.98	0.45
1:R:541:VAL:O	1:R:545:ILE:HG12	2.16	0.45
3:J:53:ILE:HG22	4:M:48:ARG:NH1	2.31	0.45
5:S:34:ARG:O	5:S:38:ILE:HG12	2.17	0.45
10:8:84:ILE:HG21	10:8:89:SER:HB3	1.99	0.45
12:A:17:THR:HG23	12:A:18:PHE:CE1	2.52	0.45
12:A:449:ASN:HD22	12:A:452:ILE:HD11	1.81	0.45
14:X:172:ASN:OD1	14:X:173:GLU:N	2.49	0.45
18:W:297:GLU:HB2	18:W:303:VAL:HG22	1.99	0.45
3:J:137:ARG:HD3	3:J:177:ILE:HG22	1.99	0.45
10:5:47:MET:O	10:5:48:ARG:NE	2.43	0.45
10:8:52:ILE:HD13	10:9:127:LEU:HD12	1.98	0.45
12:C:163:LYS:O	12:C:342:TYR:OH	2.28	0.45
12:B:197:GLU:N	12:B:197:GLU:OE1	2.50	0.45
13:D:486:ILE:HG13	13:D:487:PHE:HD1	1.81	0.45
14:Z:237:LEU:HD23	14:Z:242:LEU:HB3	1.98	0.45
15:G:148:LEU:HD23	16:N:89:LEU:HD23	1.99	0.45
18:W:170:LEU:HB3	18:W:186:TRP:CH2	2.52	0.45
1:R:12:LEU:HD11	1:R:322:GLU:HB3	1.99	0.45
1:R:57:ARG:HG2	1:R:61:MET:HE1	1.97	0.45
5:S:25:PRO:HB3	5:S:38:ILE:HD12	1.98	0.45
7:U:332:TYR:HB3	7:U:334:VAL:HG22	1.99	0.45
7:U:364:PRO:HD2	7:U:367:TYR:HB2	1.98	0.45
10:1:20:SER:HB2	10:2:98:SER:HB3	1.97	0.45
10:3:87:TYR:O	10:3:91:LEU:HG	2.17	0.45
10:7:72:VAL:HG21	10:7:99:VAL:HG21	1.98	0.45
12:B:68:GLU:HA	12:B:319:PRO:HG2	1.99	0.45
13:D:194:ALA:H	13:D:197:LEU:HD12	1.82	0.45
13:E:131:VAL:HG22	13:E:259:LEU:HD12	1.99	0.45
14:Z:237:LEU:HD22	14:Z:246:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:417:THR:HG21	1:R:458:MET:HE3	1.99	0.45
3:J:127:LEU:HD23	3:J:132:MET:HG2	1.98	0.45
3:H:194:ASN:OD1	13:D:43:PRO:HG3	2.17	0.45
7:U:262:ASP:OD1	7:U:263:THR:N	2.50	0.45
10:1:70:LEU:HD23	10:1:70:LEU:O	2.17	0.45
10:2:141:LEU:HA	10:2:144:TYR:HD1	1.82	0.45
12:C:277:CYS:O	12:C:350:SER:OG	2.35	0.45
12:C:475:LEU:HD11	12:C:542:SER:HA	1.99	0.45
12:A:25:SER:O	12:A:28:VAL:HG12	2.17	0.45
13:F:207:CYS:SG	13:F:229:ILE:HG21	2.57	0.45
1:R:94:MET:O	1:R:97:LEU:HB2	2.17	0.44
3:J:148:VAL:O	3:J:152:ILE:HG13	2.17	0.44
4:M:28:ARG:NH2	4:M:31:ARG:HH22	2.15	0.44
10:2:19:ALA:O	10:2:22:ALA:HB3	2.17	0.44
10:2:31:ALA:HB1	10:3:109:ALA:HB2	1.99	0.44
10:6:136:ILE:O	10:6:140:VAL:HG23	2.17	0.44
10:6:147:ILE:H	10:6:147:ILE:HD12	1.83	0.44
12:C:116:ILE:HD11	13:F:341:VAL:HB	1.98	0.44
12:C:266:TYR:CD2	12:C:531:PHE:HB2	2.51	0.44
12:A:295:THR:HA	12:A:303:GLU:O	2.16	0.44
12:B:233:VAL:O	12:B:234:LEU:HB2	2.18	0.44
12:B:394:CYS:SG	12:B:402:GLY:N	2.89	0.44
14:Z:60:TYR:O	14:Z:61:ARG:HG2	2.17	0.44
14:Y:172:ASN:HB3	14:Y:175:ILE:HB	1.99	0.44
13:F:457:LYS:O	13:F:461:ASN:HB2	2.16	0.44
1:R:56:ARG:HA	1:R:59:GLU:CD	2.42	0.44
3:H:199:ARG:O	3:H:203:ILE:HG12	2.17	0.44
10:4:141:LEU:HA	10:4:144:TYR:HD1	1.81	0.44
12:A:46:GLY:HA2	12:A:77:ASP:CB	2.46	0.44
13:D:70:GLU:OE2	13:D:116:GLY:HA2	2.18	0.44
13:D:154:MET:HE3	13:D:154:MET:HB2	1.83	0.44
14:X:172:ASN:HB3	14:X:175:ILE:HB	1.99	0.44
14:Y:32:CYS:SG	14:Y:88:LEU:HG	2.57	0.44
18:W:149:GLY:O	18:W:234:ARG:NE	2.50	0.44
18:W:209:PHE:HA	18:W:212:VAL:HG12	1.99	0.44
10:4:104:LEU:HD21	10:4:108:PHE:HE1	1.81	0.44
10:9:137:PHE:O	10:9:140:VAL:HG22	2.18	0.44
12:C:100:ASP:OD1	12:C:100:ASP:N	2.47	0.44
12:A:567:TRP:CZ3	12:A:570:ILE:HG21	2.52	0.44
1:R:383:ILE:O	1:R:818:THR:HA	2.18	0.44
1:R:650:MET:O	1:R:720:GLN:NE2	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:135:ARG:HB2	3:H:182:GLU:HB3	1.99	0.44
10:3:84:ILE:CG2	10:3:89:SER:HB3	2.47	0.44
11:Q:223:ILE:HD11	15:G:125:ALA:HB2	2.00	0.44
13:F:300:MET:HB2	13:F:354:LEU:CD2	2.48	0.44
1:R:32:LEU:HD13	1:R:34:LYS:HG2	2.00	0.44
1:R:48:GLN:N	1:R:48:GLN:OE1	2.51	0.44
1:R:129:LYS:HZ3	1:R:265:ILE:HD13	1.83	0.44
1:R:757:THR:HA	1:R:761:HIS:HB2	1.99	0.44
3:J:39:ASN:HB3	18:W:384:LYS:CE	2.46	0.44
7:U:270:TRP:NE1	7:U:272:GLN:OE1	2.51	0.44
7:U:357:ASN:OD1	7:U:387:ARG:NH2	2.50	0.44
10:3:64:ILE:O	10:3:68:TYR:HD1	2.00	0.44
10:6:85:SER:C	10:6:87:TYR:H	2.25	0.44
12:A:134:ASP:OD1	12:A:134:ASP:N	2.43	0.44
12:B:272:ILE:HG13	12:B:308:ARG:NH1	2.32	0.44
12:B:558:THR:HA	18:W:317:GLN:HE21	1.83	0.44
13:D:56:PRO:HG2	13:D:57:LEU:HD12	2.00	0.44
18:W:144:ARG:HD3	18:W:216:LYS:HZ2	1.82	0.44
13:F:97:GLN:O	13:F:97:GLN:HG3	2.18	0.44
1:R:594:TRP:CH2	5:S:54:ILE:HD11	2.53	0.44
1:R:813:LYS:HA	1:R:813:LYS:HD3	1.82	0.44
3:I:49:GLN:HE22	3:I:50:ARG:HE	1.65	0.44
5:S:36:VAL:O	5:S:40:MET:HG2	2.18	0.44
10:6:141:LEU:O	10:6:144:TYR:HB2	2.18	0.44
11:Q:204:THR:HA	11:Q:311:HIS:HB2	2.00	0.44
12:B:201:GLU:OE2	12:B:203:PHE:HB2	2.18	0.44
13:E:163:ARG:NH2	13:E:338:ALA:O	2.51	0.44
13:E:363:HIS:HB3	13:E:366:PRO:HD2	1.98	0.44
14:Z:178:LEU:HD12	14:Z:178:LEU:HA	1.82	0.44
14:X:237:LEU:HA	14:X:270:ASN:ND2	2.32	0.44
15:G:95:ARG:NE	15:G:95:ARG:HA	2.32	0.44
17:P:51:GLN:O	17:P:55:MET:N	2.50	0.44
2:O:93:ALA:N	2:O:96:VAL:O	2.37	0.44
7:U:272:GLN:OE1	7:U:272:GLN:N	2.51	0.44
10:1:48:ARG:NE	10:1:51:GLN:HE21	2.16	0.44
10:2:22:ALA:O	10:2:23:MET:C	2.61	0.44
10:3:97:LEU:HA	10:3:97:LEU:HD23	1.70	0.44
12:C:249:PRO:HG2	12:C:434:GLY:HA2	1.99	0.44
12:C:426:LEU:HD21	12:C:432:PHE:CD1	2.52	0.44
12:A:475:LEU:HD21	12:A:542:SER:HA	2.00	0.44
14:X:41:ASN:HB3	14:X:105:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:108:ASP:C	3:J:110:THR:H	2.25	0.44
10:2:36:LYS:O	10:2:39:THR:HG22	2.18	0.44
10:2:48:ARG:NE	10:2:51:GLN:NE2	2.65	0.44
12:C:266:TYR:CE2	12:C:531:PHE:HB2	2.52	0.44
12:B:232:ARG:N	12:B:522:GLN:OE1	2.50	0.44
12:B:442:ARG:O	12:B:442:ARG:HG2	2.18	0.44
14:Y:128:VAL:O	14:Y:132:GLN:HG3	2.18	0.44
14:Y:142:ASN:OD1	14:Y:142:ASN:N	2.51	0.44
16:N:10:VAL:HG22	16:N:65:LEU:HD22	2.00	0.44
16:N:70:ILE:O	16:N:74:VAL:HG22	2.17	0.44
18:W:445:HIS:HD2	13:F:395:LEU:HD13	1.83	0.44
13:F:248:PHE:HB3	13:F:254:MET:CE	2.47	0.44
13:F:363:HIS:HB3	13:F:366:PRO:HD2	1.98	0.44
1:R:119:LYS:HD3	1:R:272:LEU:HD21	1.99	0.44
1:R:300:MET:HA	1:R:303:ILE:HG22	1.99	0.44
3:I:127:LEU:O	13:E:64:LYS:NZ	2.51	0.44
10:2:47:MET:C	10:2:49:PRO:HD3	2.43	0.44
10:5:115:ASP:OD1	10:5:119:ARG:NH2	2.50	0.44
10:6:118:VAL:HA	10:6:121:THR:HG22	2.00	0.44
10:8:61:MET:SD	10:8:135:LEU:HB3	2.58	0.44
10:8:65:ILE:H	10:8:65:ILE:HD12	1.82	0.44
10:9:85:SER:C	10:9:87:TYR:H	2.26	0.44
12:C:105:PRO:HD2	12:C:124:VAL:HG23	2.00	0.44
13:E:488:PRO:HD2	13:E:491:MET:SD	2.58	0.44
14:Z:104:LYS:HG3	14:Z:107:LEU:H	1.83	0.44
13:F:190:PRO:HD3	13:F:373:THR:HB	2.00	0.44
3:J:168:ASP:OD2	3:J:171:SER:OG	2.22	0.43
3:I:87:ARG:HH12	13:E:146:LEU:HD23	1.83	0.43
5:S:12:VAL:HG12	5:S:16:PHE:HE2	1.83	0.43
10:1:138:ALA:HA	10:1:141:LEU:HD13	2.00	0.43
10:2:82:ASP:HA	10:3:87:TYR:CE1	2.53	0.43
10:4:32:TYR:CE2	10:4:108:PHE:CD2	3.06	0.43
10:6:60:VAL:O	10:6:64:ILE:HG12	2.18	0.43
10:9:119:ARG:HG2	10:9:119:ARG:HH11	1.82	0.43
11:Q:273:GLU:O	11:Q:277:LEU:HD23	2.17	0.43
12:A:28:VAL:HB	12:A:364:ARG:HH11	1.83	0.43
12:A:304:SER:OG	12:A:305:ILE:N	2.51	0.43
16:N:102:LYS:O	16:N:107:ARG:NH2	2.51	0.43
18:W:272:SER:HB2	18:W:277:HIS:ND1	2.32	0.43
1:R:32:LEU:HD12	1:R:33:GLY:N	2.33	0.43
9:0:194:ALA:O	9:0:198:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:48:ARG:HD3	10:4:51:GLN:CD	2.43	0.43
11:Q:232:LEU:HD12	11:Q:232:LEU:HA	1.85	0.43
12:C:530:ARG:NH1	12:C:531:PHE:HB3	2.33	0.43
12:A:57:LEU:HB2	13:E:53:VAL:O	2.17	0.43
12:A:356:GLU:OE1	12:A:359:ARG:NH2	2.45	0.43
13:E:44:ARG:NH1	13:E:115:THR:HG22	2.34	0.43
14:Z:166:TYR:HD2	14:Z:172:ASN:HD22	1.64	0.43
14:X:42:LEU:HB3	14:X:45:ILE:CG1	2.48	0.43
16:N:107:ARG:HA	16:N:110:ARG:CZ	2.48	0.43
13:F:375:GLY:C	13:F:376:GLN:HG3	2.43	0.43
3:J:219:ASN:OD1	3:J:220:ALA:N	2.50	0.43
3:H:222:ARG:NH1	13:D:284:PHE:HE1	2.16	0.43
10:2:146:LEU:O	10:2:150:LEU:HD23	2.18	0.43
10:3:88:LYS:HA	10:3:91:LEU:HD12	1.99	0.43
10:3:113:VAL:HG21	10:3:134:ILE:CG2	2.48	0.43
13:E:56:PRO:HG2	13:E:57:LEU:HD12	2.00	0.43
13:E:208:ARG:HD3	13:E:251:ASN:HD21	1.82	0.43
13:E:276:ARG:NH2	13:E:330:ASP:OD1	2.45	0.43
14:Z:124:SER:HB2	14:Z:126:TYR:HD1	1.83	0.43
18:W:260:ARG:CZ	18:W:260:ARG:HB2	2.48	0.43
1:R:592:TYR:HA	1:R:595:THR:HG22	2.00	0.43
4:L:82:THR:O	4:L:86:THR:HG23	2.19	0.43
5:S:12:VAL:HG12	5:S:16:PHE:CE2	2.53	0.43
10:3:124:GLN:OE1	10:3:127:LEU:N	2.51	0.43
10:7:57:ILE:O	10:7:61:MET:HG2	2.19	0.43
12:A:153:TYR:CD1	12:A:192:LEU:HD12	2.53	0.43
12:A:272:ILE:O	12:A:309:THR:HA	2.19	0.43
14:Z:137:THR:O	14:Z:141:LYS:HG3	2.18	0.43
14:X:42:LEU:O	14:X:46:ARG:HG3	2.18	0.43
1:R:44:VAL:O	1:R:49:ARG:NH2	2.51	0.43
3:H:173:LEU:HB3	3:H:177:ILE:HG21	2.00	0.43
7:U:278:TYR:HB3	7:U:281:GLN:NE2	2.32	0.43
7:U:325:PHE:HD2	7:U:342:MET:HE2	1.84	0.43
10:3:117:GLY:HA3	10:3:131:MET:SD	2.58	0.43
12:C:287:VAL:HG13	12:C:291:PHE:HE2	1.84	0.43
12:A:150:GLY:O	12:A:400:ARG:NH2	2.28	0.43
12:A:292:PRO:HA	12:A:304:SER:HG	1.83	0.43
12:A:558:THR:OG1	12:A:565:ILE:HG22	2.18	0.43
12:B:19:GLY:HA3	12:B:34:MET:HE3	2.01	0.43
12:B:377:TYR:O	12:B:381:ARG:HG2	2.19	0.43
13:F:213:VAL:HG11	13:F:411:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:583:PHE:HZ	1:R:732:ILE:HD13	1.84	0.43
1:R:776:PHE:O	1:R:780:THR:HG23	2.17	0.43
3:J:158:ALA:O	3:J:160:LYS:N	2.50	0.43
3:I:120:VAL:O	3:I:124:LEU:HG	2.19	0.43
4:K:115:ARG:NH2	12:A:18:PHE:HB2	2.34	0.43
7:U:273:ASN:O	7:U:397:LEU:HA	2.19	0.43
7:U:456:PHE:CE2	10:2:120:GLY:HA2	2.53	0.43
9:0:60:LEU:O	9:0:63:VAL:HG12	2.18	0.43
9:0:122:ASP:HB3	9:0:125:ALA:HB3	2.01	0.43
10:1:23:MET:O	10:1:24:VAL:C	2.61	0.43
10:1:45:SER:HB3	10:1:52:ILE:HD11	2.01	0.43
10:4:13:PHE:HB2	10:5:90:PHE:CD2	2.54	0.43
10:4:32:TYR:HE2	10:4:108:PHE:CD2	2.37	0.43
12:C:323:ARG:NH1	13:F:328:TYR:HE2	2.15	0.43
12:C:569:ILE:HG12	12:C:615:LEU:HD11	1.99	0.43
12:A:238:PHE:CZ	12:A:450:TRP:HA	2.54	0.43
12:A:589:PRO:HA	12:A:597:ILE:HD11	2.00	0.43
14:Z:128:VAL:O	14:Z:132:GLN:HG3	2.19	0.43
14:X:44:LYS:HE2	14:X:44:LYS:HB2	1.83	0.43
14:Y:163:ILE:HD13	14:Y:175:ILE:HD13	2.00	0.43
13:F:165:TYR:O	13:F:167:GLU:HG3	2.19	0.43
1:R:538:LYS:HE3	1:R:608:LEU:HD21	2.01	0.43
1:R:809:GLU:OE1	1:R:809:GLU:N	2.51	0.43
3:J:36:GLU:O	3:J:40:ILE:HG13	2.19	0.43
3:H:189:LYS:HD3	13:D:49:THR:HG22	2.00	0.43
9:0:150:PHE:CZ	10:9:28:LEU:HD12	2.54	0.43
10:1:44:MET:HE1	10:1:52:ILE:HD13	2.00	0.43
10:3:150:LEU:O	10:3:154:THR:HG22	2.19	0.43
10:7:134:ILE:H	10:7:134:ILE:HD12	1.84	0.43
11:Q:224:THR:HA	11:Q:237:ARG:HD2	1.99	0.43
12:C:315:THR:H	12:C:318:MET:HE3	1.83	0.43
12:A:350:SER:H	12:A:409:ALA:HB3	1.82	0.43
14:X:105:LEU:O	14:X:109:GLU:HG3	2.18	0.43
15:G:65:ALA:HB1	15:G:138:TYR:CE1	2.54	0.43
1:R:68:VAL:O	1:R:72:ILE:HG13	2.19	0.43
3:H:99:LYS:HE3	3:H:99:LYS:HB2	1.75	0.43
10:1:68:TYR:HD1	10:1:146:LEU:CD1	2.32	0.43
10:3:13:PHE:CE1	10:3:17:MET:HE3	2.53	0.43
10:4:54:LYS:HA	10:4:54:LYS:HD3	1.75	0.43
12:C:147:ILE:HD12	12:C:168:LEU:HD22	2.01	0.43
12:C:442:ARG:HA	18:W:447:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:20:TYR:CE1	12:A:76:GLY:HA2	2.45	0.43
12:A:71:SER:OG	13:D:154:MET:HG3	2.19	0.43
13:E:102:THR:HA	13:E:105:ILE:HD12	2.00	0.43
15:G:94:ILE:HD13	16:N:63:ILE:CD1	2.49	0.43
3:J:129:GLU:H	3:J:132:MET:CE	2.32	0.43
3:I:108:ASP:O	3:I:110:THR:N	2.52	0.43
7:U:274:PHE:CE1	7:U:285:LEU:HD12	2.53	0.43
9:O:67:TRP:HA	9:O:70:TYR:CE2	2.54	0.43
10:3:13:PHE:HB2	10:4:90:PHE:CE2	2.54	0.43
10:9:132:ILE:HG22	10:9:136:ILE:HD11	2.01	0.43
12:A:338:ARG:HG3	12:A:403:SER:N	2.34	0.43
12:B:95:MET:HE2	12:B:337:PHE:CZ	2.53	0.43
12:B:190:VAL:HA	12:B:204:THR:HG22	2.00	0.43
13:D:444:LEU:HB3	13:D:448:ASP:HB2	2.00	0.43
13:D:486:ILE:HG13	13:D:487:PHE:CD1	2.54	0.43
15:G:126:ARG:HA	15:G:126:ARG:NH1	2.33	0.43
17:P:47:CYS:O	17:P:51:GLN:N	2.52	0.43
1:R:100:ASN:O	1:R:103:LYS:HB3	2.19	0.43
1:R:123:LEU:O	1:R:126:THR:OG1	2.17	0.43
3:I:144:VAL:O	3:I:148:VAL:HG23	2.19	0.43
3:I:159:THR:HG22	3:I:161:ASN:HB2	2.00	0.43
3:H:184:TYR:CE2	3:H:191:LYS:HG3	2.54	0.43
10:1:70:LEU:HD23	10:1:70:LEU:C	2.43	0.43
10:7:50:GLU:HG2	10:7:51:GLN:OE1	2.18	0.43
11:Q:252:LEU:HD23	11:Q:252:LEU:HA	1.85	0.43
12:B:44:ARG:HA	12:B:50:LEU:O	2.19	0.43
12:B:481:GLU:O	12:B:485:GLU:OE1	2.37	0.43
12:B:558:THR:OG1	12:B:565:ILE:HG22	2.18	0.43
14:X:114:LYS:HB3	14:X:169:THR:HG21	2.00	0.43
18:W:316:PRO:HA	18:W:349:ASN:ND2	2.34	0.43
18:W:337:THR:HG22	18:W:338:HIS:N	2.34	0.43
1:R:470:LYS:HA	1:R:523:ASN:ND2	2.30	0.42
1:R:645:LEU:O	1:R:648:PRO:HD2	2.18	0.42
3:J:46:VAL:HG22	3:J:50:ARG:CG	2.47	0.42
4:M:21:LYS:O	4:M:24:GLU:HB2	2.19	0.42
3:I:124:LEU:HD22	3:I:132:MET:SD	2.58	0.42
7:U:269:PHE:HE1	7:U:400:PHE:HE1	1.66	0.42
7:U:283:GLU:CD	7:U:316:LEU:HD11	2.43	0.42
10:1:24:VAL:HG13	10:2:101:LEU:HB3	2.01	0.42
10:4:141:LEU:HA	10:4:141:LEU:HD23	1.83	0.42
10:7:133:LEU:HD12	10:7:133:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:287:ASP:OD1	11:Q:288:LYS:N	2.50	0.42
12:C:530:ARG:HD3	12:C:530:ARG:H	1.84	0.42
12:A:53:GLU:O	12:A:64:ILE:HA	2.19	0.42
12:A:265:LYS:HD3	12:A:294:LEU:HD13	2.00	0.42
12:B:469:PHE:HE2	12:B:534:PHE:CD2	2.37	0.42
13:D:200:ASN:HB2	13:D:244:PHE:CZ	2.54	0.42
13:E:130:ARG:NH2	13:E:143:PRO:O	2.43	0.42
14:Z:214:GLU:OE2	14:Z:254:VAL:HG13	2.18	0.42
18:W:301:LYS:HA	18:W:301:LYS:HE3	2.01	0.42
18:W:430:ASP:HB3	18:W:433:ALA:HB3	2.01	0.42
13:F:179:GLY:HA2	13:F:415:HIS:NE2	2.34	0.42
4:M:75:LYS:HA	4:M:78:GLN:OE1	2.19	0.42
10:3:68:TYR:CE2	10:3:143:LEU:HA	2.54	0.42
10:4:65:ILE:HA	10:4:68:TYR:HD2	1.84	0.42
10:9:56:ILE:O	10:9:59:VAL:HG22	2.18	0.42
11:Q:254:GLN:HG2	11:Q:257:ARG:NH2	2.34	0.42
12:C:387:GLU:HB2	13:D:265:ASN:HD21	1.82	0.42
12:B:350:SER:HB2	12:B:353:ARG:HG2	2.00	0.42
12:B:478:LYS:HD2	12:B:478:LYS:HA	1.90	0.42
15:G:62:MET:HE1	16:N:92:PRO:CG	2.47	0.42
17:P:123:TRP:O	17:P:125:TYR:N	2.49	0.42
18:W:444:ARG:C	18:W:446:SER:H	2.26	0.42
1:R:73:ARG:NH2	1:R:79:ILE:HG22	2.34	0.42
10:4:28:LEU:HA	10:5:105:ALA:HB1	2.00	0.42
12:A:318:MET:HE3	12:A:318:MET:HB3	1.80	0.42
12:B:36:GLY:C	12:B:81:ARG:HH22	2.25	0.42
14:Z:98:ILE:HG23	14:Z:160:GLN:HB3	2.01	0.42
14:X:207:GLN:OE1	14:X:208:PRO:HD2	2.19	0.42
13:F:135:SER:O	13:F:135:SER:OG	2.33	0.42
13:F:174:ILE:HB	13:F:177:ILE:HG22	2.00	0.42
3:I:102:LEU:O	3:I:106:VAL:HG23	2.19	0.42
3:H:138:LYS:HA	3:H:138:LYS:HD2	1.86	0.42
7:U:310:SER:HA	7:U:323:PHE:O	2.19	0.42
7:U:411:GLN:CD	8:V:293:TYR:HA	2.44	0.42
10:1:14:PHE:O	10:1:18:GLY:N	2.51	0.42
10:7:97:LEU:HD12	10:7:97:LEU:HA	1.87	0.42
10:7:136:ILE:O	10:7:140:VAL:HG23	2.20	0.42
10:8:72:VAL:HG21	10:8:99:VAL:HG11	2.02	0.42
12:C:417:PHE:CE2	12:C:452:ILE:HD12	2.41	0.42
12:C:550:MET:HB3	12:C:612:PHE:CE2	2.54	0.42
12:A:205:MET:HE2	12:A:205:MET:HB3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:152:ILE:HD11	12:B:400:ARG:HD3	2.01	0.42
13:E:245:LYS:HE3	14:X:10:MET:HE1	2.02	0.42
14:X:178:LEU:HD12	14:X:178:LEU:HA	1.83	0.42
3:J:50:ARG:O	3:J:53:ILE:HG12	2.19	0.42
3:J:219:ASN:ND2	13:F:125:GLU:OE1	2.52	0.42
3:I:112:TYR:HE1	3:I:116:LEU:HD11	1.84	0.42
5:S:76:LEU:C	5:S:76:LEU:HD12	2.44	0.42
9:O:28:ILE:HG23	9:O:29:PHE:CD1	2.55	0.42
10:1:130:GLY:O	10:1:134:ILE:HD12	2.20	0.42
10:5:22:ALA:O	10:5:23:MET:C	2.62	0.42
10:6:140:VAL:HG12	10:6:144:TYR:CE1	2.54	0.42
10:8:85:SER:C	10:8:87:TYR:H	2.27	0.42
10:8:140:VAL:HG12	10:8:144:TYR:CE2	2.55	0.42
10:8:144:TYR:O	10:8:147:ILE:HB	2.20	0.42
11:Q:343:LYS:HB3	11:Q:346:ASN:ND2	2.34	0.42
12:C:61:MET:HE3	12:C:61:MET:HB3	1.94	0.42
12:C:547:PHE:N	12:C:608:MET:HE1	2.35	0.42
12:B:24:VAL:HG12	12:B:29:VAL:HG22	2.01	0.42
13:D:245:LYS:NZ	13:D:249:GLU:OE2	2.50	0.42
13:E:227:PHE:CE1	13:E:294:LEU:HB2	2.55	0.42
14:Y:180:LYS:HG3	14:Y:181:LEU:HD22	2.01	0.42
18:W:144:ARG:CD	18:W:216:LYS:HG3	2.45	0.42
18:W:279:PHE:CE1	18:W:282:LEU:HD23	2.55	0.42
13:F:326:TYR:O	13:F:329:THR:HG22	2.18	0.42
13:F:374:GLU:HB3	13:F:400:ARG:HD2	2.01	0.42
1:R:539:MET:HE2	1:R:539:MET:HB3	1.92	0.42
5:S:78:TYR:CD2	6:T:94:PRO:HD3	2.54	0.42
7:U:286:THR:N	7:U:287:PRO:HD2	2.35	0.42
10:3:56:ILE:O	10:3:56:ILE:HG13	2.19	0.42
12:C:148:THR:HA	12:C:173:ARG:HB2	2.02	0.42
14:Z:237:LEU:HA	14:Z:270:ASN:HD21	1.85	0.42
14:X:72:GLY:HA2	14:X:76:ASN:ND2	2.34	0.42
1:R:751:LEU:O	1:R:754:VAL:HG12	2.19	0.42
3:J:136:CYS:HB3	3:J:144:VAL:HG11	2.02	0.42
10:5:59:VAL:O	10:5:62:ALA:HB3	2.19	0.42
10:8:70:LEU:O	10:8:71:VAL:C	2.63	0.42
11:Q:238:ALA:HA	11:Q:241:PHE:CE2	2.55	0.42
12:C:233:VAL:HG22	12:C:234:LEU:H	1.84	0.42
12:A:280:ARG:C	12:A:282:ASN:H	2.27	0.42
13:E:500:LEU:HD23	13:E:500:LEU:HA	1.84	0.42
15:G:156:VAL:HA	16:N:108:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:13:ASP:O	16:N:17:VAL:HG23	2.19	0.42
1:R:52:VAL:O	1:R:55:VAL:HG12	2.19	0.42
5:S:39:THR:O	5:S:43:THR:HG22	2.20	0.42
10:6:49:PRO:HA	10:7:126:ARG:HH22	1.83	0.42
10:6:91:LEU:HB3	10:6:152:LEU:O	2.20	0.42
11:Q:219:ARG:O	11:Q:223:ILE:HG12	2.20	0.42
11:Q:331:TRP:HZ3	15:G:71:GLU:HA	1.84	0.42
12:B:43:VAL:HG21	12:B:64:ILE:HD13	2.00	0.42
12:B:236:ALA:HA	12:B:472:PHE:CZ	2.55	0.42
14:Z:210:GLU:O	14:Z:256:THR:OG1	2.32	0.42
14:X:225:LEU:HD23	14:X:225:LEU:HA	1.87	0.42
17:P:253:SER:O	17:P:257:CYS:N	2.47	0.42
1:R:270:MET:O	1:R:274:GLN:OE1	2.38	0.42
7:U:301:PHE:CE2	7:U:303:ASN:HB2	2.54	0.42
10:4:133:LEU:O	10:4:136:ILE:HG22	2.20	0.42
10:7:123:GLN:OE1	10:7:123:GLN:N	2.48	0.42
10:8:60:VAL:HA	10:9:137:PHE:CE2	2.55	0.42
10:9:17:MET:HE3	10:9:17:MET:HB3	1.89	0.42
12:C:483:LEU:HD11	12:C:515:ILE:HG21	2.02	0.42
12:A:249:PRO:CG	12:A:432:PHE:HE1	2.33	0.42
14:X:78:LEU:HD12	14:X:78:LEU:HA	1.84	0.42
16:N:95:GLU:OE2	16:N:95:GLU:N	2.45	0.42
18:W:365:HIS:HA	18:W:368:PHE:CE1	2.55	0.42
13:F:479:ILE:O	13:F:483:LEU:HD23	2.20	0.42
1:R:287:ALA:HA	1:R:290:ILE:HG22	2.02	0.42
3:J:190:ILE:HG12	13:F:47:TYR:HD1	1.85	0.42
3:I:54:MET:O	3:I:55:GLU:C	2.63	0.42
4:L:115:ARG:HG3	4:L:115:ARG:NH1	2.34	0.42
8:V:313:ILE:HG13	8:V:314:MET:N	2.33	0.42
10:2:21:ALA:O	10:2:22:ALA:C	2.61	0.42
10:2:85:SER:C	10:2:87:TYR:H	2.28	0.42
10:3:87:TYR:CE2	10:3:91:LEU:HD11	2.54	0.42
10:4:9:GLU:CG	10:4:10:TYR:H	2.33	0.42
10:4:144:TYR:HA	10:4:147:ILE:HD12	2.02	0.42
10:8:44:MET:O	10:8:44:MET:HG2	2.19	0.42
12:A:129:ARG:HA	12:A:129:ARG:HD3	1.93	0.42
12:A:156:VAL:HG21	12:A:205:MET:CE	2.49	0.42
13:E:475:GLU:O	13:E:479:ILE:HG12	2.20	0.42
14:Z:14:THR:HG23	14:Z:17:GLN:H	1.85	0.42
13:F:216:SER:HB3	13:F:219:VAL:HG23	2.01	0.42
1:R:62:ASP:O	1:R:65:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:326:ILE:HD11	7:U:344:ARG:HE	1.83	0.41
7:U:371:CYS:O	7:U:400:PHE:HB3	2.19	0.41
10:4:24:VAL:CG2	10:5:101:LEU:HB3	2.50	0.41
12:A:28:VAL:H	12:A:364:ARG:NH1	2.18	0.41
12:A:67:TYR:CE1	12:A:321:ALA:HB1	2.55	0.41
12:A:177:THR:OG1	12:A:200:LYS:NZ	2.38	0.41
12:B:66:VAL:HG12	12:B:68:GLU:H	1.84	0.41
12:B:581:LEU:HD23	12:B:584:MET:SD	2.59	0.41
13:E:290:GLU:OE1	13:E:345:ASN:N	2.50	0.41
14:Z:66:LEU:O	14:Z:69:SER:OG	2.31	0.41
14:X:45:ILE:CD1	14:X:112:TYR:HD2	2.34	0.41
15:G:85:GLN:NE2	15:G:86:ASN:HB2	2.34	0.41
16:N:67:ASN:HA	16:N:91:ILE:O	2.20	0.41
16:N:92:PRO:HG3	16:N:98:TYR:HA	2.02	0.41
13:F:229:ILE:O	13:F:257:VAL:HA	2.19	0.41
1:R:209:PRO:HD2	1:R:210:VAL:N	2.33	0.41
3:J:49:GLN:HG3	4:M:44:ILE:HD12	2.02	0.41
3:I:90:LEU:HD21	4:L:88:PHE:CB	2.50	0.41
3:H:128:LEU:HA	3:H:155:TYR:HH	1.84	0.41
3:H:185:ASN:CG	3:H:189:LYS:H	2.27	0.41
10:9:88:LYS:O	10:9:92:GLN:HG2	2.20	0.41
12:A:167:MET:HE2	12:A:340:MET:HG3	2.01	0.41
14:X:128:VAL:O	14:X:132:GLN:HG3	2.20	0.41
14:Y:63:GLU:O	14:Y:66:LEU:N	2.53	0.41
1:R:60:GLU:O	1:R:64:LYS:HG2	2.21	0.41
1:R:288:LYS:O	1:R:291:ARG:NH2	2.53	0.41
1:R:335:PHE:HB3	1:R:339:ARG:HH12	1.84	0.41
1:R:512:GLY:HA3	5:S:4:HIS:HB2	2.01	0.41
1:R:723:HIS:O	1:R:726:GLU:HG2	2.20	0.41
7:U:275:SER:O	7:U:396:MET:HB3	2.20	0.41
9:0:94:ILE:HG22	10:1:137:PHE:HD2	1.85	0.41
10:5:44:MET:SD	10:5:48:ARG:HB2	2.59	0.41
10:6:49:PRO:CB	10:7:126:ARG:HH22	2.33	0.41
10:8:59:VAL:HG12	10:9:137:PHE:CD2	2.56	0.41
10:9:67:ILE:O	10:9:71:VAL:HG23	2.19	0.41
11:Q:179:GLU:OE2	15:G:122:THR:HA	2.20	0.41
12:A:318:MET:HE3	12:A:319:PRO:HD2	2.02	0.41
12:B:552:ARG:HH12	18:W:353:GLN:CD	2.28	0.41
12:B:604:LEU:HD12	12:B:604:LEU:HA	1.84	0.41
14:Z:129:LYS:HD3	14:Z:179:PHE:HE2	1.85	0.41
1:R:734:ASN:OD1	1:R:809:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:94:GLU:HA	4:K:94:GLU:OE2	2.20	0.41
7:U:278:TYR:HB3	7:U:281:GLN:HE22	1.85	0.41
10:7:126:ARG:HB3	10:7:126:ARG:HE	1.55	0.41
10:8:18:GLY:HA3	10:8:93:LEU:HA	2.02	0.41
13:D:185:ARG:NH2	13:D:212:LEU:HD22	2.35	0.41
13:D:414:ASP:OD2	13:D:481:TRP:NE1	2.47	0.41
14:Z:143:ALA:HB1	14:Z:149:ASN:CG	2.46	0.41
14:Z:227:LYS:HA	14:Z:230:ILE:HG12	2.02	0.41
15:G:53:GLU:O	15:G:56:MET:HG2	2.20	0.41
15:G:152:GLN:CD	16:N:105:ILE:HG13	2.45	0.41
16:N:30:LYS:HA	16:N:30:LYS:HD3	1.80	0.41
13:F:93:LYS:HE3	13:F:93:LYS:HB3	1.75	0.41
13:F:452:LEU:O	13:F:456:GLN:HG2	2.19	0.41
1:R:315:THR:HG21	4:K:10:GLN:O	2.20	0.41
1:R:598:ASP:OD2	1:R:600:HIS:ND1	2.51	0.41
1:R:656:LEU:HD12	1:R:656:LEU:HA	1.91	0.41
4:M:79:GLU:HG2	4:M:80:LYS:N	2.36	0.41
4:M:89:ARG:HA	4:M:89:ARG:NE	2.36	0.41
3:I:71:GLN:OE1	3:I:71:GLN:HA	2.20	0.41
3:I:158:ALA:C	3:I:160:LYS:H	2.28	0.41
4:K:97:ASP:OD2	4:K:97:ASP:C	2.64	0.41
7:U:456:PHE:HD2	10:2:123:GLN:NE2	2.18	0.41
10:7:72:VAL:HG21	10:7:99:VAL:HG11	2.03	0.41
10:9:97:LEU:HA	10:9:97:LEU:HD23	1.81	0.41
11:Q:34:LEU:O	11:Q:37:VAL:HG22	2.20	0.41
12:C:105:PRO:HD3	12:C:126:ALA:HA	2.02	0.41
12:A:23:GLY:O	12:A:30:THR:N	2.54	0.41
13:E:74:LEU:HG	13:E:112:CYS:SG	2.60	0.41
13:E:174:ILE:HA	13:E:465:GLN:OE1	2.21	0.41
13:E:227:PHE:HE1	13:E:294:LEU:HD12	1.86	0.41
14:Z:112:TYR:CZ	14:Z:116:LYS:HD3	2.56	0.41
14:X:114:LYS:HG2	14:X:169:THR:HB	2.02	0.41
14:Y:226:VAL:HG12	14:Y:255:LEU:HB2	2.03	0.41
18:W:293:VAL:O	18:W:408:VAL:HA	2.20	0.41
1:R:32:LEU:HD13	1:R:34:LYS:HZ3	1.85	0.41
1:R:577:ILE:HG23	1:R:646:CYS:SG	2.61	0.41
1:R:806:HIS:O	1:R:811:GLN:HG3	2.21	0.41
3:J:40:ILE:HG23	18:W:382:ARG:HG2	2.02	0.41
3:I:98:ALA:O	3:I:102:LEU:HD23	2.21	0.41
5:S:76:LEU:HD12	5:S:77:LYS:N	2.36	0.41
7:U:322:THR:HG22	7:U:348:HIS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:48:ARG:NH1	10:4:52:ILE:HA	2.33	0.41
10:4:80:LEU:HD12	10:4:80:LEU:HA	1.88	0.41
10:4:85:SER:C	10:4:87:TYR:H	2.29	0.41
10:8:68:TYR:HD1	10:8:146:LEU:HD22	1.85	0.41
10:9:123:GLN:OE1	10:9:123:GLN:N	2.54	0.41
11:Q:77:LYS:O	11:Q:81:GLU:OE1	2.39	0.41
13:E:192:PHE:CE1	13:E:354:LEU:HD22	2.56	0.41
14:Z:59:ASN:HB3	14:Z:61:ARG:NH2	2.35	0.41
17:P:303:GLN:O	17:P:306:ALA:HB3	2.21	0.41
18:W:287:THR:HG22	18:W:288:HIS:ND1	2.35	0.41
13:F:254:MET:HE2	13:F:254:MET:HA	2.03	0.41
1:R:574:PRO:HA	1:R:577:ILE:HG22	2.03	0.41
3:J:31:ASP:OD1	4:M:28:ARG:HD3	2.20	0.41
3:J:107:LYS:C	3:J:109:THR:H	2.29	0.41
3:I:108:ASP:C	3:I:110:THR:H	2.28	0.41
10:4:101:LEU:HD23	10:4:101:LEU:HA	1.76	0.41
10:5:56:ILE:O	10:5:60:VAL:HG23	2.20	0.41
10:9:109:ALA:O	10:9:113:VAL:HG12	2.20	0.41
11:Q:120:ARG:HH22	15:G:85:GLN:HB2	1.86	0.41
12:C:274:TYR:HB3	12:C:311:LEU:CD2	2.50	0.41
12:A:382:LEU:HA	12:A:382:LEU:HD23	1.82	0.41
15:G:136:ARG:NE	15:G:136:ARG:HA	2.35	0.41
17:P:50:ILE:O	17:P:54:GLU:N	2.54	0.41
18:W:209:PHE:O	18:W:213:VAL:HG12	2.21	0.41
13:F:97:GLN:OE1	13:F:269:ILE:HD12	2.21	0.41
1:R:298:ARG:HD3	1:R:298:ARG:HA	1.84	0.41
1:R:530:THR:HB	10:7:78:ASN:ND2	2.35	0.41
3:J:123:GLY:HA3	3:J:183:ILE:HD13	2.03	0.41
3:J:154:MET:HE2	3:J:154:MET:HB3	1.96	0.41
3:I:215:LEU:HB3	3:I:216:PHE:CD1	2.56	0.41
7:U:372:GLU:HA	7:U:399:ASP:HA	2.03	0.41
10:2:146:LEU:HG	10:2:150:LEU:HD23	2.03	0.41
10:4:31:ALA:HB1	10:5:109:ALA:HB2	2.03	0.41
10:7:44:MET:HE2	10:7:122:ALA:HB2	2.01	0.41
11:Q:33:TYR:O	11:Q:37:VAL:HG13	2.20	0.41
12:C:426:LEU:HD11	12:C:432:PHE:CG	2.55	0.41
13:D:254:MET:HA	13:D:254:MET:HE2	2.02	0.41
13:E:421:GLN:HG2	13:E:495:ILE:HD11	2.03	0.41
14:Z:263:ILE:O	14:Z:266:ILE:HG22	2.21	0.41
14:Y:78:LEU:HD12	14:Y:78:LEU:HA	1.84	0.41
15:G:55:LYS:HE2	15:G:148:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:107:ARG:O	16:N:110:ARG:HD3	2.21	0.41
13:F:172:THR:OG1	13:F:206:ILE:HG23	2.20	0.41
1:R:423:MET:HE1	1:R:440:PHE:CZ	2.56	0.41
1:R:501:GLN:HA	5:S:67:GLN:HA	2.01	0.41
3:I:49:GLN:O	3:I:53:ILE:HG12	2.21	0.41
3:I:50:ARG:O	3:I:54:MET:HG2	2.21	0.41
3:I:82:LYS:HG3	4:L:81:MET:CE	2.51	0.41
3:I:122:GLN:NE2	13:E:43:PRO:HD3	2.35	0.41
4:K:82:THR:O	4:K:86:THR:HG23	2.21	0.41
5:S:46:VAL:O	5:S:50:LEU:HD23	2.20	0.41
6:T:99:ASN:OD1	6:T:100:LEU:N	2.54	0.41
7:U:314:GLU:H	7:U:314:GLU:CD	2.28	0.41
10:3:32:TYR:CD2	10:3:108:PHE:CD1	3.09	0.41
10:3:131:MET:HE2	10:3:131:MET:HB3	1.83	0.41
10:4:81:ASN:OD1	10:4:82:ASP:N	2.51	0.41
10:5:108:PHE:O	10:5:112:ILE:HG22	2.21	0.41
10:6:28:LEU:HD23	10:6:28:LEU:HA	1.85	0.41
10:9:133:LEU:HD12	10:9:133:LEU:HA	1.80	0.41
11:Q:1:MET:C	11:Q:3:PHE:H	2.29	0.41
12:C:535:TYR:HA	12:C:538:VAL:HG12	2.03	0.41
12:A:484:GLN:OE1	12:A:484:GLN:HA	2.21	0.41
12:A:581:LEU:HD23	12:A:604:LEU:HD21	2.03	0.41
12:B:573:HIS:ND1	12:B:615:LEU:HD13	2.36	0.41
14:X:181:LEU:CD2	14:X:203:TYR:HB2	2.51	0.41
14:Y:188:MET:HE3	14:Y:189:ALA:N	2.15	0.41
15:G:201:ARG:HD2	13:F:318:PRO:HG2	2.03	0.41
15:G:207:GLU:O	15:G:211:ILE:HG13	2.21	0.41
18:W:128:LYS:HB3	18:W:128:LYS:HE3	1.92	0.41
13:F:495:ILE:HG22	13:F:500:LEU:HG	2.03	0.41
1:R:426:ARG:O	1:R:430:ILE:HG12	2.20	0.41
1:R:760:ILE:O	1:R:763:GLY:N	2.52	0.41
1:R:801:HIS:CE1	10:7:64:ILE:HG13	2.56	0.41
4:M:78:GLN:O	4:M:82:THR:OG1	2.30	0.41
7:U:258:VAL:HG13	7:U:290:PHE:CD1	2.56	0.41
8:V:331:MET:SD	10:3:32:TYR:HE1	2.44	0.41
9:0:94:ILE:CG2	10:1:137:PHE:HD2	2.33	0.41
9:0:150:PHE:CE2	10:9:28:LEU:HB2	2.56	0.41
10:2:21:ALA:O	10:2:24:VAL:HG12	2.21	0.41
10:2:44:MET:HG2	10:2:118:VAL:HG12	2.03	0.41
12:A:287:VAL:O	12:A:291:PHE:HB2	2.21	0.41
12:A:580:LYS:HA	12:A:583:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:397:ASN:C	12:B:399:GLU:H	2.24	0.41
13:D:369:THR:O	13:D:373:THR:OG1	2.36	0.41
13:D:395:LEU:HD23	13:D:423:TYR:CE1	2.55	0.41
1:R:89:PRO:O	1:R:300:MET:HE1	2.21	0.40
1:R:132:LEU:HG	1:R:258:ALA:HB2	2.03	0.40
1:R:322:GLU:OE1	1:R:322:GLU:N	2.53	0.40
3:J:26:LYS:HA	3:J:29:GLU:HG3	2.02	0.40
4:L:92:ARG:O	4:L:96:LEU:HD23	2.20	0.40
9:O:54:ILE:O	9:O:58:ILE:HG22	2.21	0.40
9:O:63:VAL:HG23	10:1:105:ALA:HB2	2.03	0.40
12:C:491:GLU:OE2	12:C:492:ILE:HG13	2.21	0.40
12:C:511:VAL:HG11	12:C:548:TYR:HB2	2.03	0.40
12:C:604:LEU:HD12	12:C:604:LEU:HA	1.86	0.40
14:Z:103:MET:HE2	14:Z:103:MET:HB3	1.93	0.40
14:Z:111:GLN:HE22	14:Z:168:ILE:N	2.19	0.40
15:G:101:VAL:O	15:G:104:VAL:HG12	2.21	0.40
13:F:327:MET:HE2	13:F:327:MET:HB3	2.01	0.40
1:R:300:MET:O	1:R:303:ILE:HG22	2.21	0.40
1:R:582:LEU:HD23	1:R:582:LEU:HA	1.90	0.40
3:J:49:GLN:OE1	3:J:52:LYS:HD3	2.21	0.40
3:J:68:LYS:O	3:J:72:MET:HG2	2.22	0.40
3:J:135:ARG:HG3	3:J:184:TYR:CE1	2.56	0.40
3:J:212:ARG:NH1	13:F:124:SER:OG	2.53	0.40
3:I:57:TYR:O	3:I:61:GLU:HG2	2.21	0.40
3:H:137:ARG:HH12	3:H:139:GLN:HE21	1.68	0.40
10:1:48:ARG:HE	10:1:51:GLN:HE21	1.69	0.40
10:2:84:ILE:HG21	10:2:89:SER:HB3	2.03	0.40
10:4:24:VAL:HG23	10:5:101:LEU:HB3	2.03	0.40
10:5:13:PHE:HB2	10:6:90:PHE:CD2	2.56	0.40
11:Q:124:GLU:O	11:Q:128:LYS:NZ	2.48	0.40
12:C:94:ILE:HD13	12:C:333:LEU:HD22	2.04	0.40
12:A:55:ILE:HD13	12:A:65:GLN:HB2	2.04	0.40
12:B:102:ILE:HG22	12:B:102:ILE:O	2.21	0.40
12:B:550:MET:HE1	12:B:608:MET:HB3	2.02	0.40
15:G:13:ARG:HB2	15:G:14:MET:HE2	2.02	0.40
1:R:326:PRO:HB2	1:R:328:THR:HG22	2.03	0.40
1:R:484:MET:SD	1:R:506:LEU:HD21	2.61	0.40
3:J:71:GLN:O	3:J:72:MET:C	2.64	0.40
3:J:117:ASP:OD2	3:J:150:LYS:NZ	2.49	0.40
3:H:76:MET:HA	3:H:76:MET:HE3	2.03	0.40
6:T:86:THR:O	6:T:88:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:314:GLU:OE1	7:U:314:GLU:N	2.50	0.40
7:U:368:SER:O	7:U:416:SER:N	2.54	0.40
10:6:56:ILE:CD1	10:7:133:LEU:HD23	2.52	0.40
11:Q:295:PHE:HZ	15:G:126:ARG:HH22	1.67	0.40
12:C:60:ASP:OD1	12:C:60:ASP:N	2.53	0.40
12:A:577:ILE:HD13	12:A:577:ILE:HA	1.85	0.40
12:B:303:GLU:OE1	12:B:303:GLU:HA	2.22	0.40
12:B:573:HIS:ND1	12:B:615:LEU:HB2	2.36	0.40
12:B:587:LYS:HE3	12:B:600:ASP:HB3	2.03	0.40
13:D:287:TYR:OH	13:D:339:GLY:O	2.29	0.40
13:E:455:LEU:HD23	13:E:455:LEU:HA	1.75	0.40
14:Z:14:THR:OG1	14:Z:15:SER:N	2.55	0.40
15:G:47:ILE:HD13	15:G:47:ILE:HA	1.90	0.40
16:N:15:ASP:OD1	16:N:16:THR:N	2.54	0.40
18:W:386:THR:HB	18:W:391:ASN:HA	2.02	0.40
13:F:172:THR:HG21	13:F:177:ILE:HG23	2.04	0.40
4:M:96:LEU:HA	4:M:99:LEU:HG	2.04	0.40
7:U:257:PRO:HD3	8:V:293:TYR:HE2	1.85	0.40
10:1:48:ARG:CD	10:1:122:ALA:HA	2.45	0.40
10:2:23:MET:O	10:2:24:VAL:C	2.64	0.40
10:2:35:ALA:HB1	10:3:112:ILE:HG21	2.03	0.40
10:3:49:PRO:HD2	10:3:50:GLU:OE1	2.21	0.40
10:7:41:ILE:HA	10:7:44:MET:HG3	2.04	0.40
10:7:49:PRO:HB2	10:8:126:ARG:HH22	1.85	0.40
11:Q:221:PHE:HD1	11:Q:221:PHE:HA	1.77	0.40
11:Q:345:ASP:OD1	11:Q:345:ASP:N	2.50	0.40
12:C:295:THR:HG22	12:C:304:SER:HA	2.04	0.40
12:A:289:ARG:HG3	12:A:290:ASP:N	2.35	0.40
14:Z:57:GLU:C	14:Z:58:LYS:HD3	2.47	0.40
14:Y:174:GLY:O	14:Y:177:GLN:HG3	2.21	0.40
15:G:120:GLU:HG2	15:G:121:LEU:HG	2.04	0.40
15:G:138:TYR:O	15:G:142:VAL:HG23	2.21	0.40
15:G:143:GLU:O	15:G:146:VAL:HG12	2.22	0.40
15:G:184:LEU:HA	15:G:184:LEU:HD23	1.77	0.40
16:N:17:VAL:O	16:N:21:LEU:HD23	2.21	0.40
13:F:269:ILE:HD13	13:F:269:ILE:HA	1.93	0.40
1:R:71:GLU:O	1:R:74:LYS:HG3	2.21	0.40
1:R:303:ILE:HD12	1:R:303:ILE:HA	1.97	0.40
1:R:363:THR:HG21	1:R:384:GLY:O	2.22	0.40
2:O:347:ALA:HB1	2:O:366:TYR:HA	2.04	0.40
9:O:107:MET:HE1	9:O:195:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:88:LYS:O	10:6:92:GLN:HG2	2.21	0.40
10:7:61:MET:HG2	10:7:61:MET:H	1.70	0.40
12:C:324:GLU:HA	12:C:354:TRP:CD1	2.56	0.40
14:Z:144:ALA:O	14:Z:149:ASN:ND2	2.26	0.40
14:Y:25:LYS:HE2	14:Y:82:SER:HA	2.02	0.40
15:G:32:LEU:HD23	15:G:33:LEU:HD23	2.02	0.40
18:W:437:LEU:HD12	13:F:435:MET:SD	2.62	0.40
13:F:239:GLU:HG2	13:F:242:ARG:NH2	2.36	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	R	747/837 (89%)	708 (95%)	39 (5%)	0	100	100
2	O	361/382 (94%)	347 (96%)	14 (4%)	0	100	100
3	H	218/226 (96%)	204 (94%)	14 (6%)	0	100	100
3	I	219/226 (97%)	207 (94%)	12 (6%)	0	100	100
3	J	223/226 (99%)	205 (92%)	17 (8%)	1 (0%)	30	63
4	K	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
4	L	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
4	M	112/118 (95%)	101 (90%)	11 (10%)	0	100	100
5	S	75/81 (93%)	72 (96%)	3 (4%)	0	100	100
6	T	83/137 (61%)	79 (95%)	4 (5%)	0	100	100
7	U	202/470 (43%)	177 (88%)	25 (12%)	0	100	100
8	V	47/350 (13%)	43 (92%)	4 (8%)	0	100	100
9	0	202/205 (98%)	191 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	2	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	3	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
10	4	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
10	5	148/155 (96%)	136 (92%)	12 (8%)	0	100	100
10	6	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	7	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	8	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
10	9	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
11	Q	349/351 (99%)	322 (92%)	27 (8%)	0	100	100
12	A	598/617 (97%)	535 (90%)	63 (10%)	0	100	100
12	B	598/617 (97%)	555 (93%)	43 (7%)	0	100	100
12	C	598/617 (97%)	558 (93%)	40 (7%)	0	100	100
13	D	466/511 (91%)	441 (95%)	25 (5%)	0	100	100
13	E	466/511 (91%)	446 (96%)	20 (4%)	0	100	100
13	F	466/511 (91%)	442 (95%)	24 (5%)	0	100	100
14	X	265/573 (46%)	249 (94%)	16 (6%)	0	100	100
14	Y	260/573 (45%)	249 (96%)	11 (4%)	0	100	100
14	Z	258/573 (45%)	248 (96%)	10 (4%)	0	100	100
15	G	211/247 (85%)	205 (97%)	6 (3%)	0	100	100
16	N	108/119 (91%)	101 (94%)	7 (6%)	0	100	100
17	P	423/483 (88%)	370 (88%)	53 (12%)	0	100	100
18	W	416/456 (91%)	393 (94%)	23 (6%)	0	100	100
All	All	9526/11648 (82%)	8922 (94%)	603 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	109	THR

### 5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	602/746 (81%)	602 (100%)	0	100	100
2	O	1/344 (0%)	1 (100%)	0	100	100
3	H	149/199 (75%)	149 (100%)	0	100	100
3	I	159/199 (80%)	159 (100%)	0	100	100
3	J	184/199 (92%)	184 (100%)	0	100	100
4	K	48/101 (48%)	48 (100%)	0	100	100
4	L	53/101 (52%)	53 (100%)	0	100	100
4	M	85/101 (84%)	85 (100%)	0	100	100
5	S	69/72 (96%)	69 (100%)	0	100	100
6	T	71/116 (61%)	71 (100%)	0	100	100
7	U	182/397 (46%)	182 (100%)	0	100	100
8	V	44/308 (14%)	44 (100%)	0	100	100
9	0	154/155 (99%)	154 (100%)	0	100	100
10	1	107/112 (96%)	107 (100%)	0	100	100
10	2	107/112 (96%)	107 (100%)	0	100	100
10	3	107/112 (96%)	107 (100%)	0	100	100
10	4	107/112 (96%)	107 (100%)	0	100	100
10	5	107/112 (96%)	107 (100%)	0	100	100
10	6	107/112 (96%)	107 (100%)	0	100	100
10	7	107/112 (96%)	107 (100%)	0	100	100
10	8	107/112 (96%)	107 (100%)	0	100	100
10	9	107/112 (96%)	107 (100%)	0	100	100
11	Q	306/306 (100%)	306 (100%)	0	100	100
12	A	508/525 (97%)	508 (100%)	0	100	100
12	B	508/525 (97%)	508 (100%)	0	100	100
12	C	508/525 (97%)	508 (100%)	0	100	100
13	D	401/430 (93%)	401 (100%)	0	100	100
13	E	401/430 (93%)	401 (100%)	0	100	100
13	F	401/430 (93%)	401 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	X	239/519 (46%)	239 (100%)	0	100	100
14	Y	238/519 (46%)	238 (100%)	0	100	100
14	Z	237/519 (46%)	237 (100%)	0	100	100
15	G	184/212 (87%)	184 (100%)	0	100	100
16	N	94/100 (94%)	94 (100%)	0	100	100
18	W	276/396 (70%)	276 (100%)	0	100	100
All	All	7065/9482 (74%)	7065 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	106	ASN
1	R	356	GLN
1	R	359	GLN
1	R	375	GLN
1	R	523	ASN
1	R	604	ASN
3	J	39	ASN
3	J	122	GLN
3	J	166	GLN
3	J	169	GLN
4	M	30	ASN
3	I	49	GLN
3	I	71	GLN
3	I	206	GLN
4	L	78	GLN
3	H	122	GLN
3	H	139	GLN
7	U	394	GLN
7	U	411	GLN
9	0	51	ASN
10	2	51	GLN
10	3	92	GLN
10	5	51	GLN
10	5	124	GLN
10	7	78	ASN
10	7	124	GLN
11	Q	50	GLN

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Mol	Chain	Res	Type
11	Q	308	ASN
11	Q	346	ASN
12	C	261	GLN
12	A	22	HIS
12	A	317	ASN
12	A	441	GLN
12	A	468	HIS
13	D	205	GLN
13	D	209	GLN
13	D	421	GLN
13	E	251	ASN
13	E	363	HIS
13	E	415	HIS
14	Z	111	GLN
14	Z	162	GLN
14	Z	198	HIS
14	X	270	ASN
14	Y	111	GLN
14	Y	117	GLN
14	Y	270	ASN
18	W	281	GLN
18	W	366	ASN
18	W	400	ASN
13	F	42	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	NAG	U	503	7	14,14,15	0.19	0	17,19,21	0.46	0
19	NAG	S	101	5	14,14,15	0.46	0	17,19,21	0.55	0
19	NAG	R	901	1	14,14,15	0.34	0	17,19,21	0.51	0
19	NAG	U	502	-	14,14,15	0.23	0	17,19,21	0.40	0
19	NAG	U	505	-	14,14,15	0.22	0	17,19,21	0.43	0
20	ADP	B	701	-	24,29,29	0.85	0	29,45,45	1.25	3 (10%)
19	NAG	U	501	7	14,14,15	0.25	0	17,19,21	0.35	0
19	NAG	U	504	-	14,14,15	0.26	0	17,19,21	0.52	0
19	NAG	U	506	7	14,14,15	0.17	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	NAG	U	503	7	-	2/6/23/26	0/1/1/1
19	NAG	S	101	5	-	2/6/23/26	0/1/1/1
19	NAG	R	901	1	-	4/6/23/26	0/1/1/1
19	NAG	U	502	-	-	2/6/23/26	0/1/1/1
19	NAG	U	505	-	-	4/6/23/26	0/1/1/1
20	ADP	B	701	-	-	0/12/32/32	0/3/3/3
19	NAG	U	501	7	-	2/6/23/26	0/1/1/1
19	NAG	U	504	-	-	4/6/23/26	0/1/1/1
19	NAG	U	506	7	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	701	ADP	N3-C2-N1	-3.44	124.01	128.67
20	B	701	ADP	C4-C5-N7	-2.33	106.88	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	701	ADP	C4'-O4'-C1'	2.13	111.88	109.92

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	S	101	NAG	C4-C5-C6-O6
19	U	505	NAG	C4-C5-C6-O6
19	S	101	NAG	O5-C5-C6-O6
19	U	504	NAG	O5-C5-C6-O6
19	U	505	NAG	O5-C5-C6-O6
19	U	502	NAG	O5-C5-C6-O6
19	R	901	NAG	O5-C5-C6-O6
19	U	501	NAG	O5-C5-C6-O6
19	U	503	NAG	C4-C5-C6-O6
19	U	501	NAG	C4-C5-C6-O6
19	U	504	NAG	C4-C5-C6-O6
19	R	901	NAG	C4-C5-C6-O6
19	U	503	NAG	O5-C5-C6-O6
19	U	505	NAG	C8-C7-N2-C2
19	U	505	NAG	O7-C7-N2-C2
19	U	506	NAG	O5-C5-C6-O6
19	U	502	NAG	C4-C5-C6-O6
19	U	506	NAG	C4-C5-C6-O6
19	U	504	NAG	C1-C2-N2-C7
19	U	506	NAG	C1-C2-N2-C7
19	R	901	NAG	C3-C2-N2-C7
19	U	504	NAG	C3-C2-N2-C7
19	R	901	NAG	C1-C2-N2-C7
19	U	506	NAG	C3-C2-N2-C7

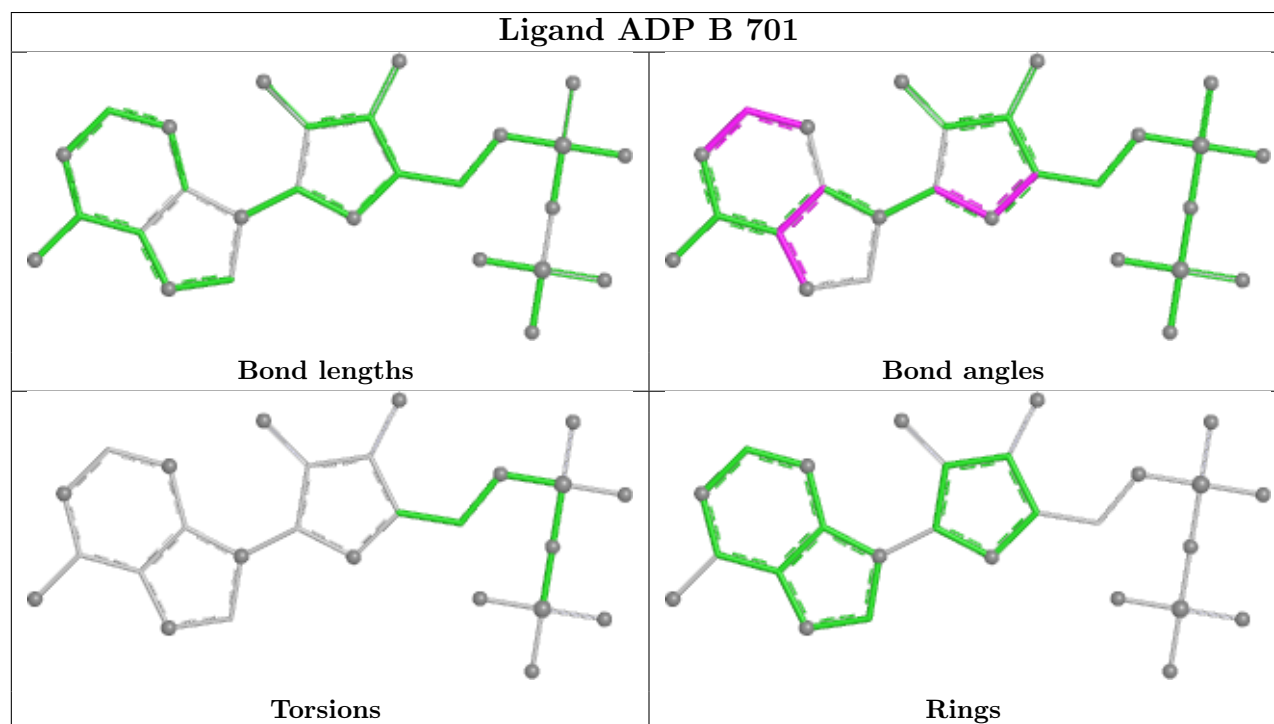
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S	101	NAG	1	0
19	R	901	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

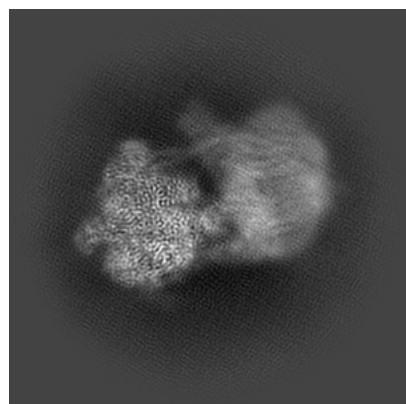
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26334. These allow visual inspection of the internal detail of the map and identification of artifacts.

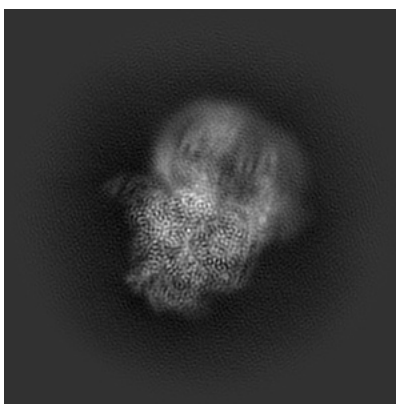
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

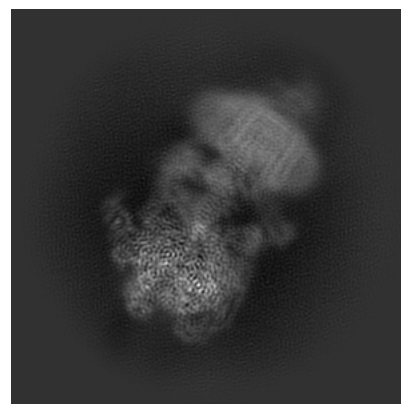
#### 6.1.1 Primary map



X

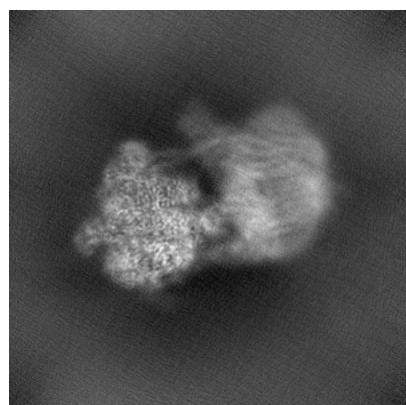


Y

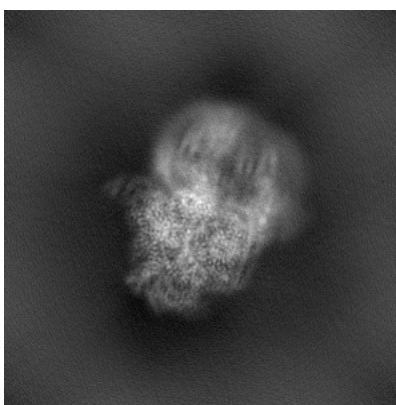


Z

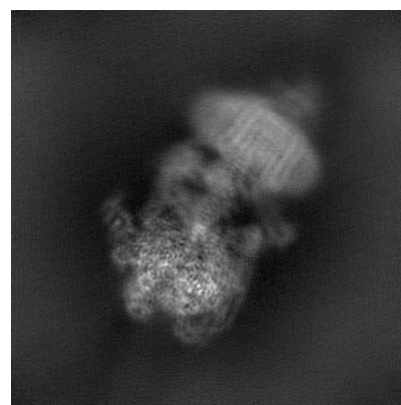
#### 6.1.2 Raw map



X



Y

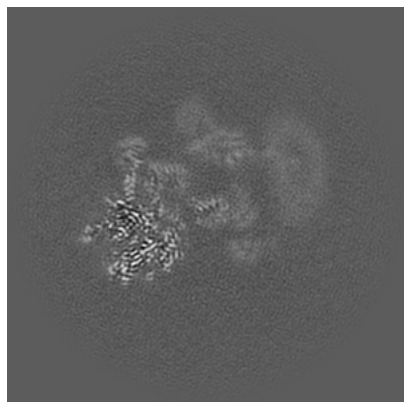


Z

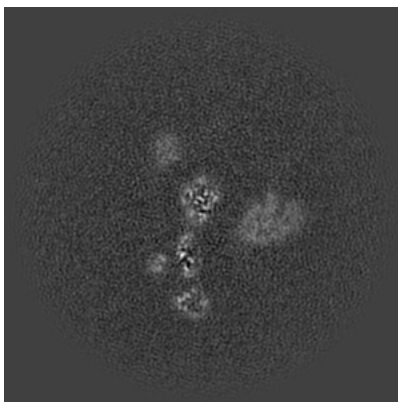
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

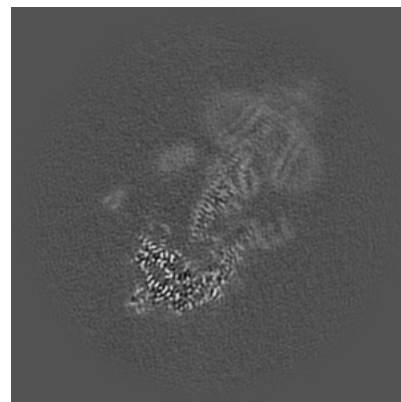
### 6.2.1 Primary map



X Index: 180



Y Index: 180

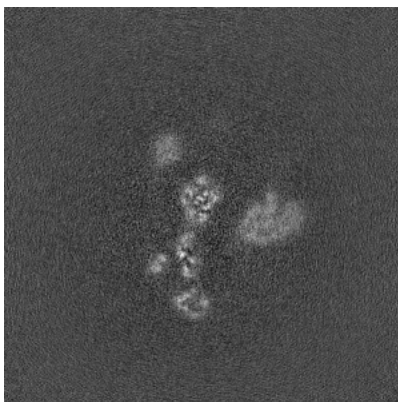


Z Index: 180

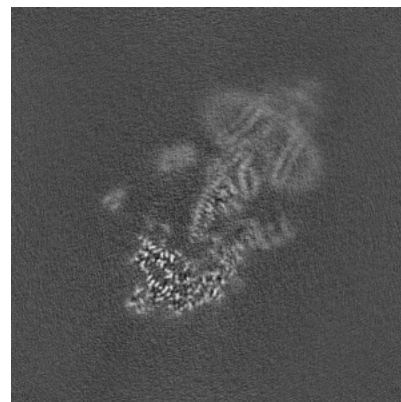
### 6.2.2 Raw map



X Index: 180



Y Index: 180



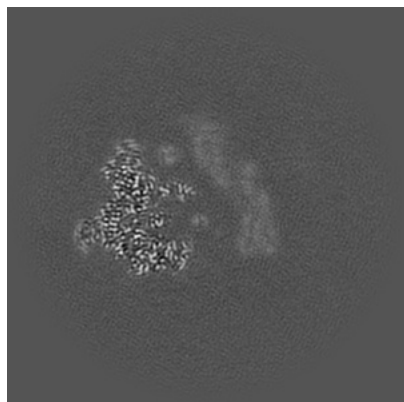
Z Index: 180

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

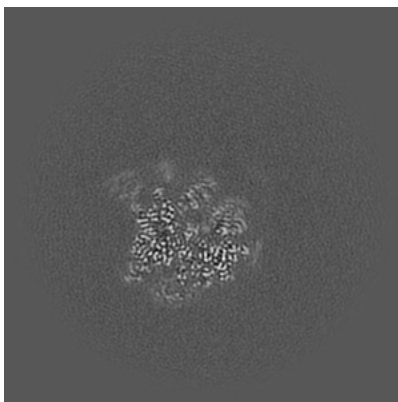


## 6.3 Largest variance slices [i](#)

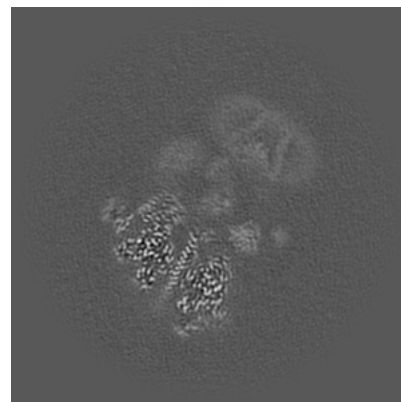
### 6.3.1 Primary map



X Index: 156

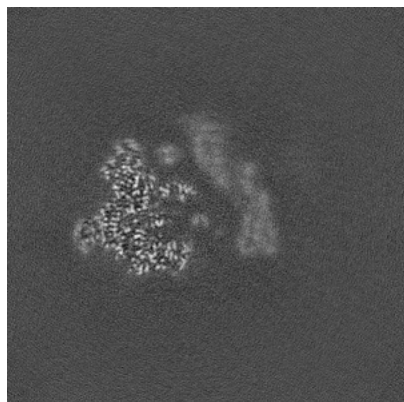


Y Index: 130

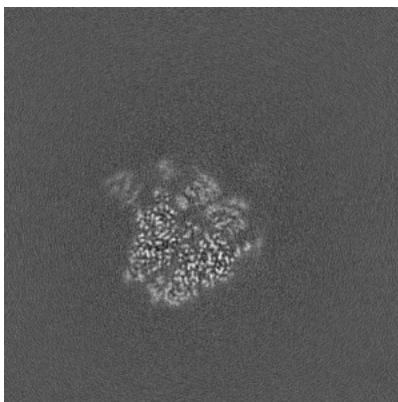


Z Index: 164

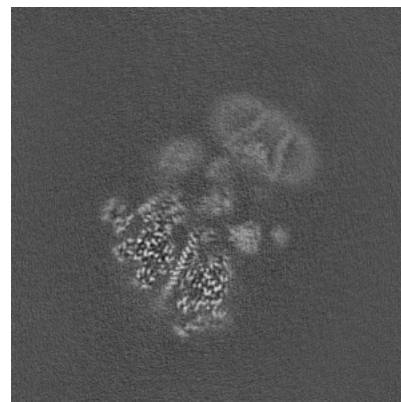
### 6.3.2 Raw map



X Index: 156



Y Index: 133

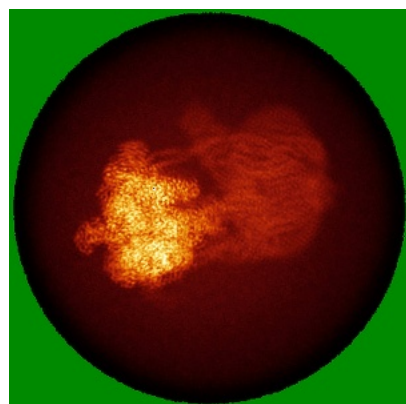


Z Index: 164

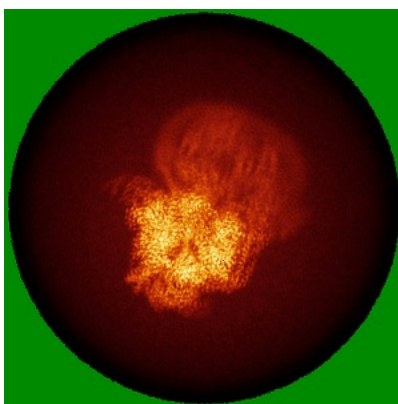
The images above show the largest variance slices of the map in three orthogonal directions.

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

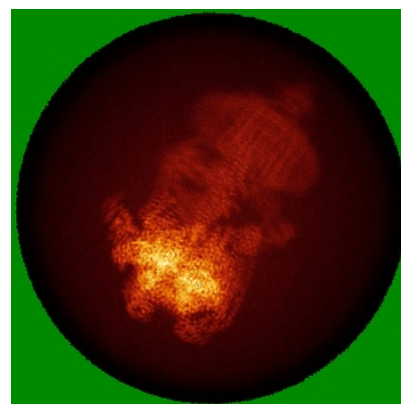
### 6.4.1 Primary map



X

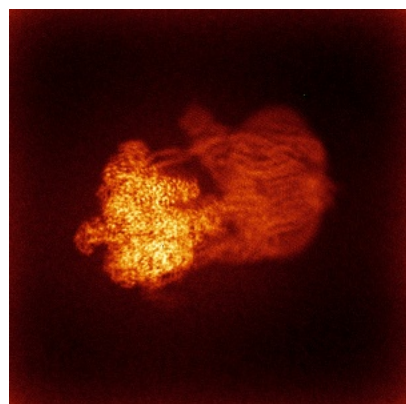


Y

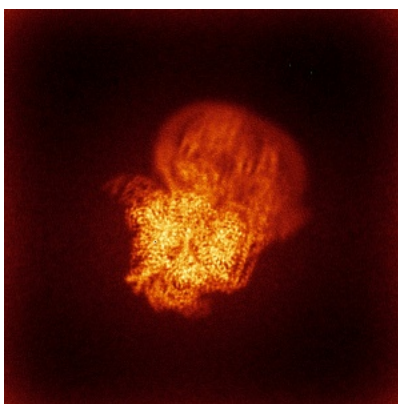


Z

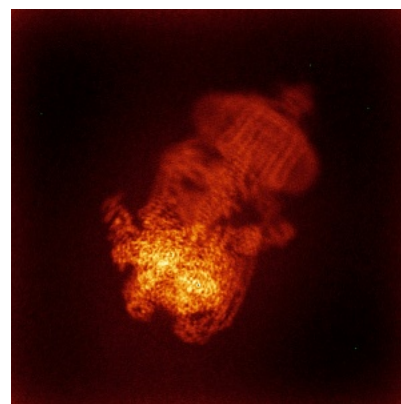
### 6.4.2 Raw map



X



Y



Z

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



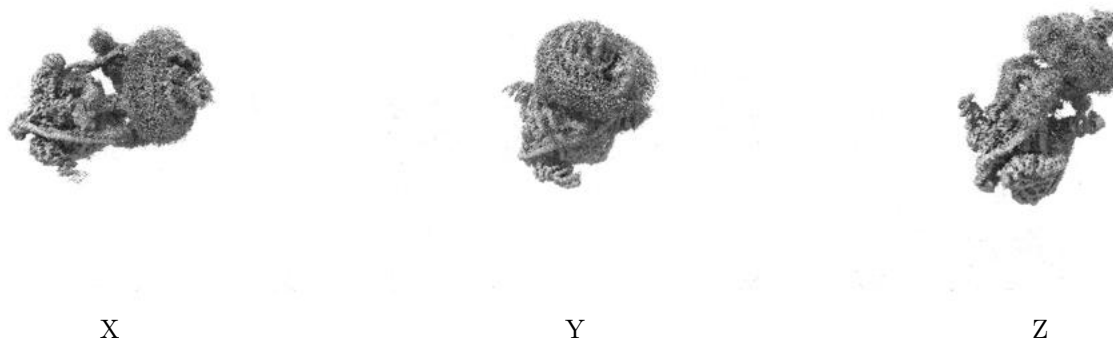
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

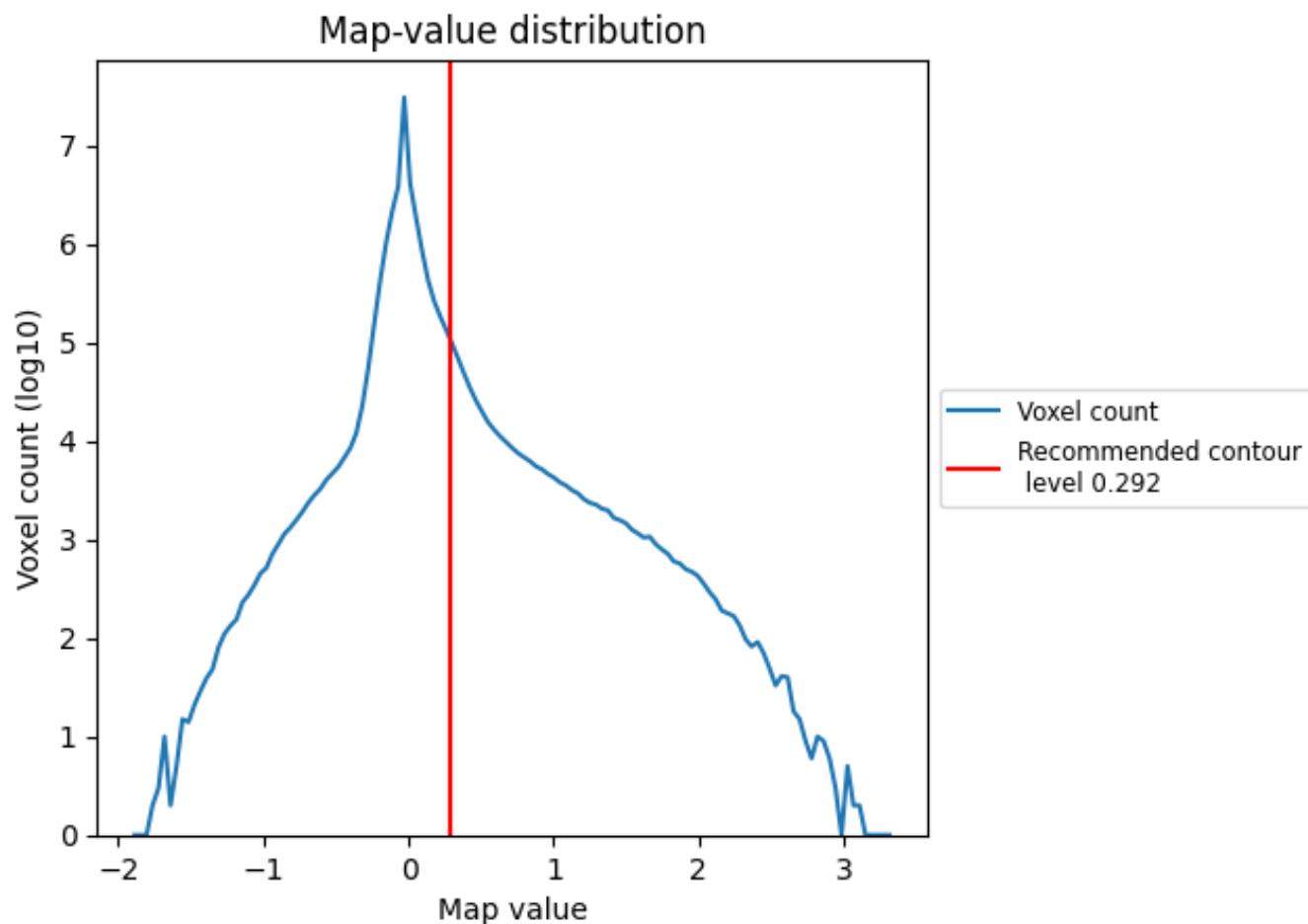
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

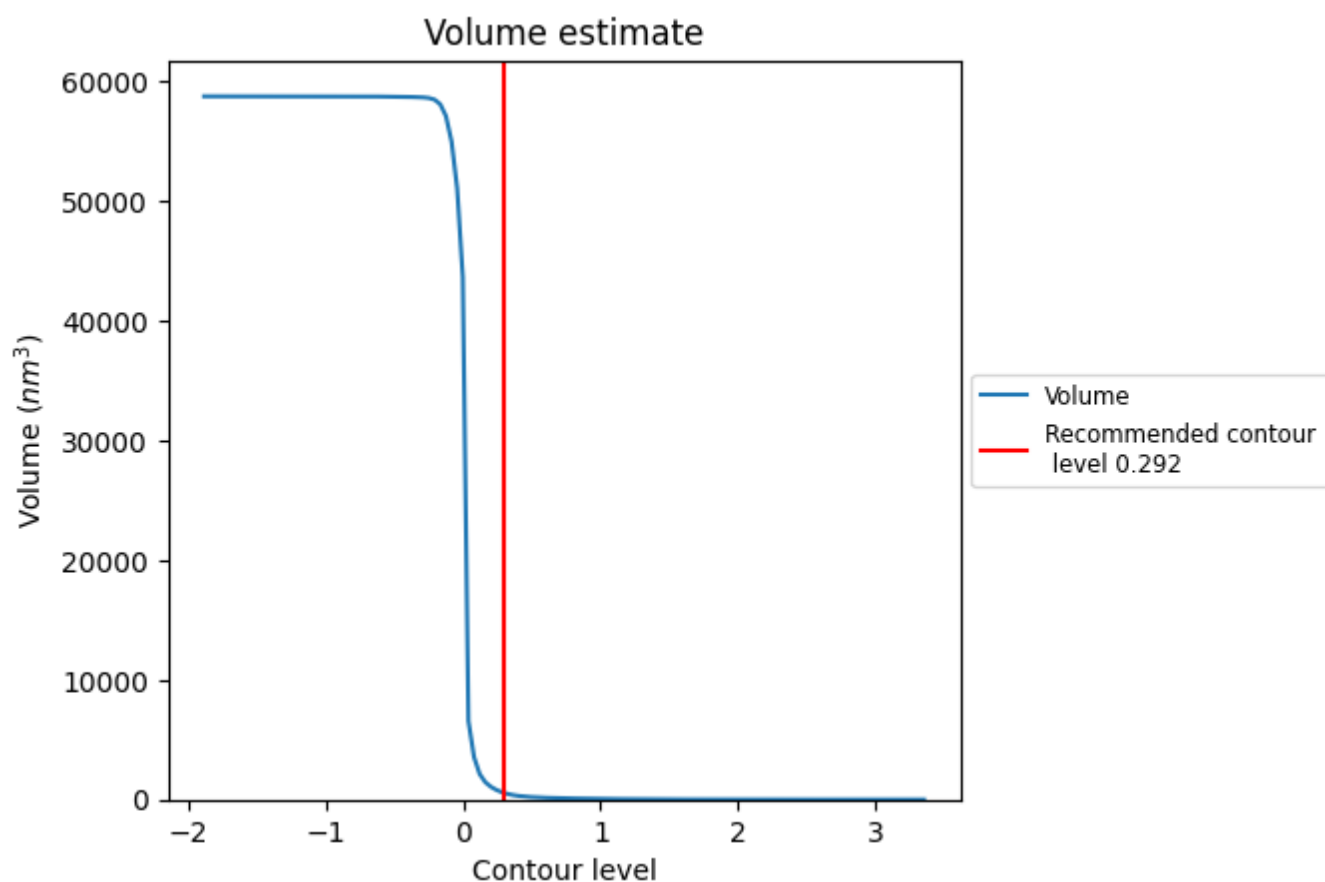
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

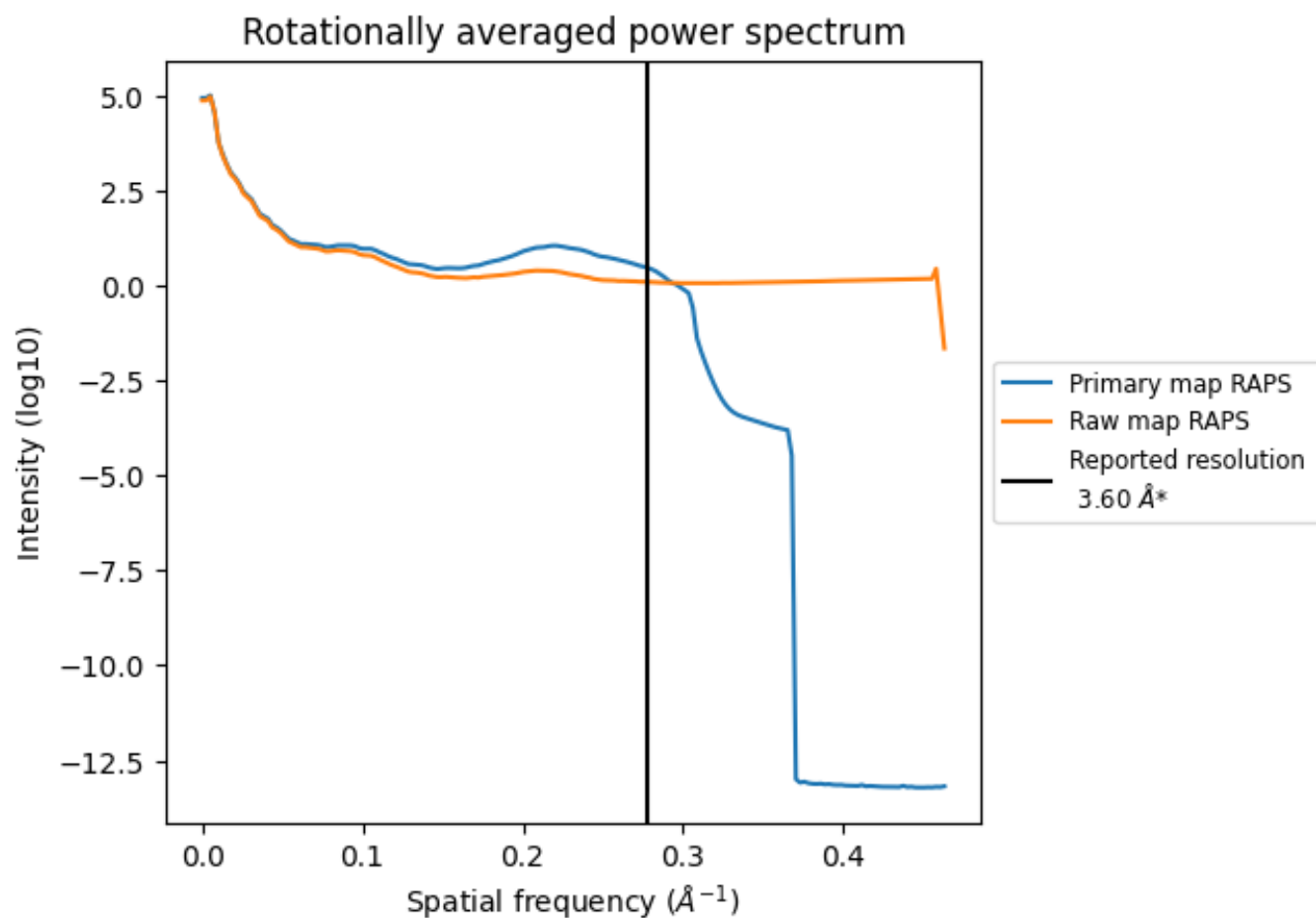
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 581 nm<sup>3</sup>; this corresponds to an approximate mass of 525 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

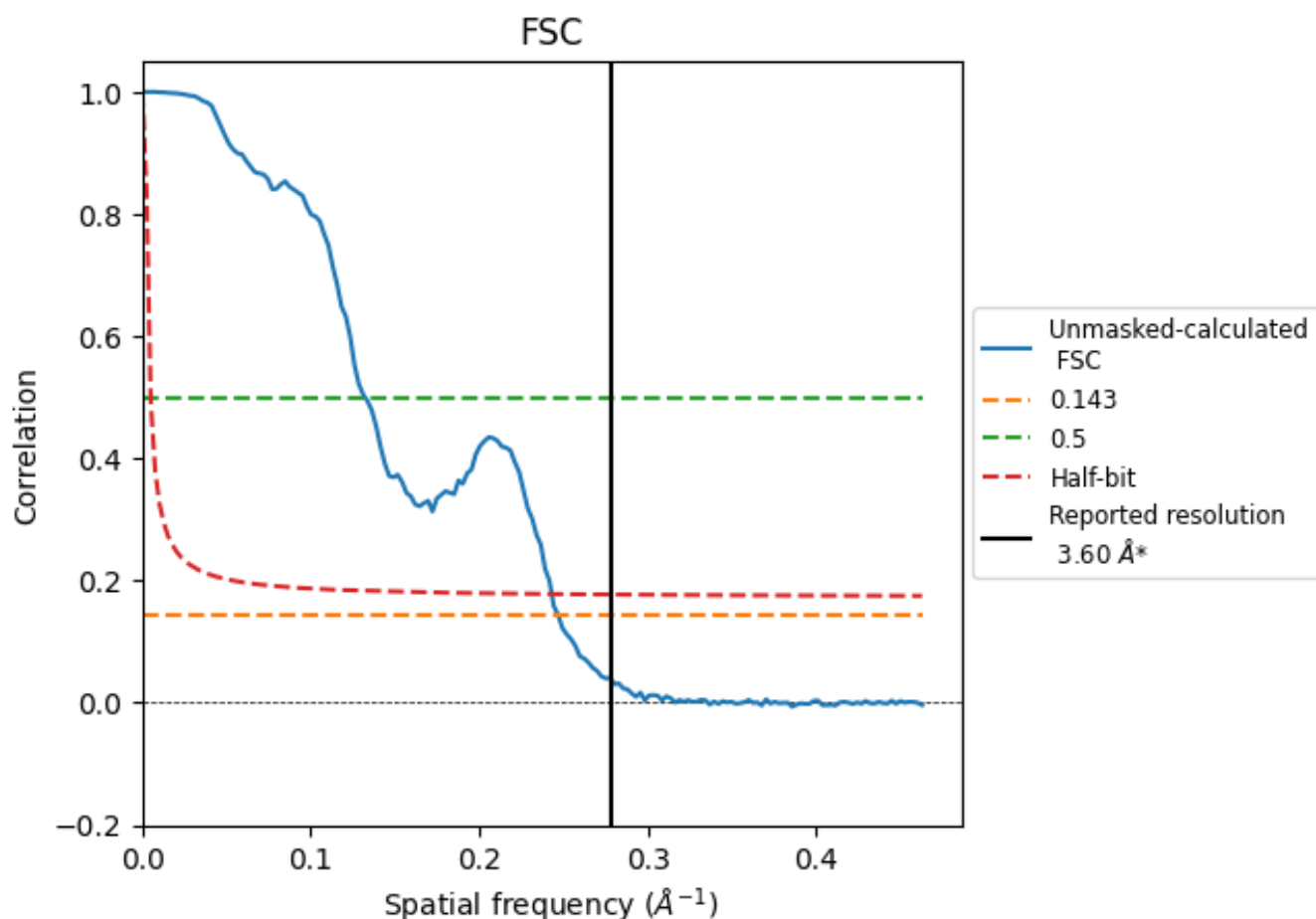


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

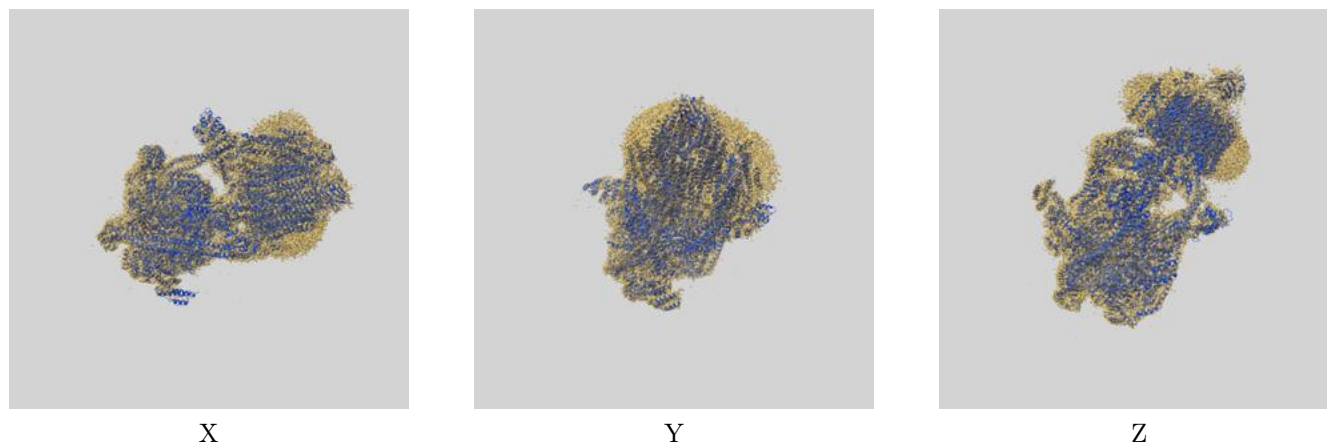
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	7.56	4.11

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.6 by more than 10 %

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

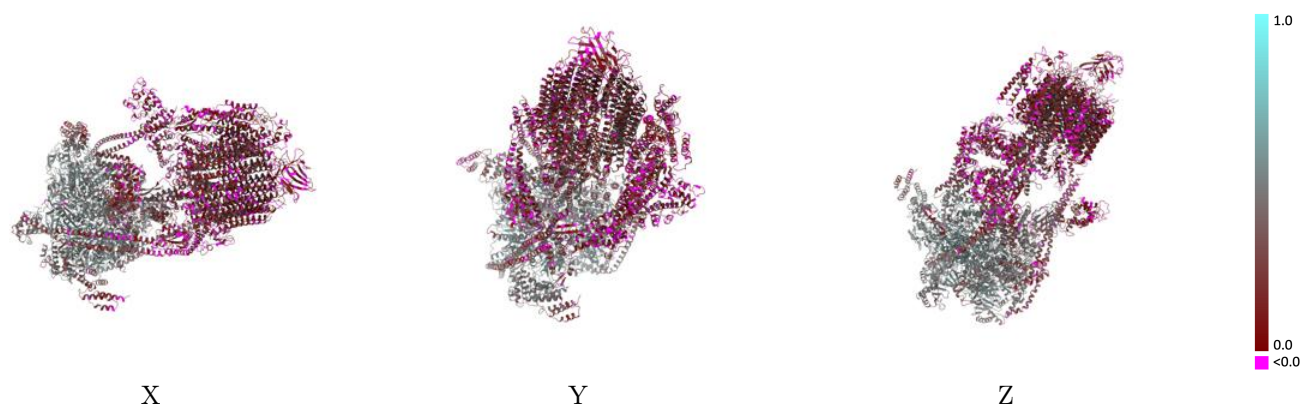
This section contains information regarding the fit between EMDB map EMD-26334 and PDB model 7U4T. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

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



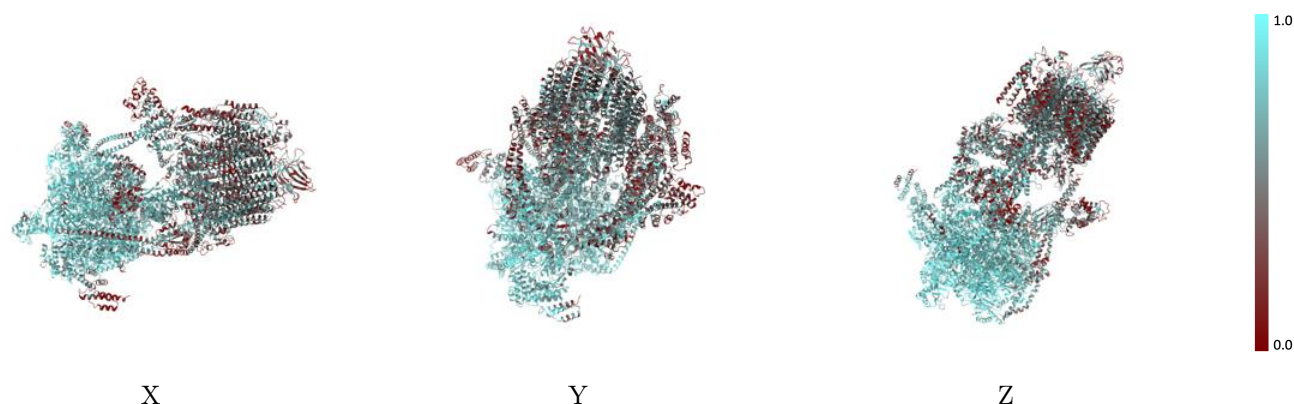
The images above show the 3D surface view of the map at the recommended contour level 0.292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

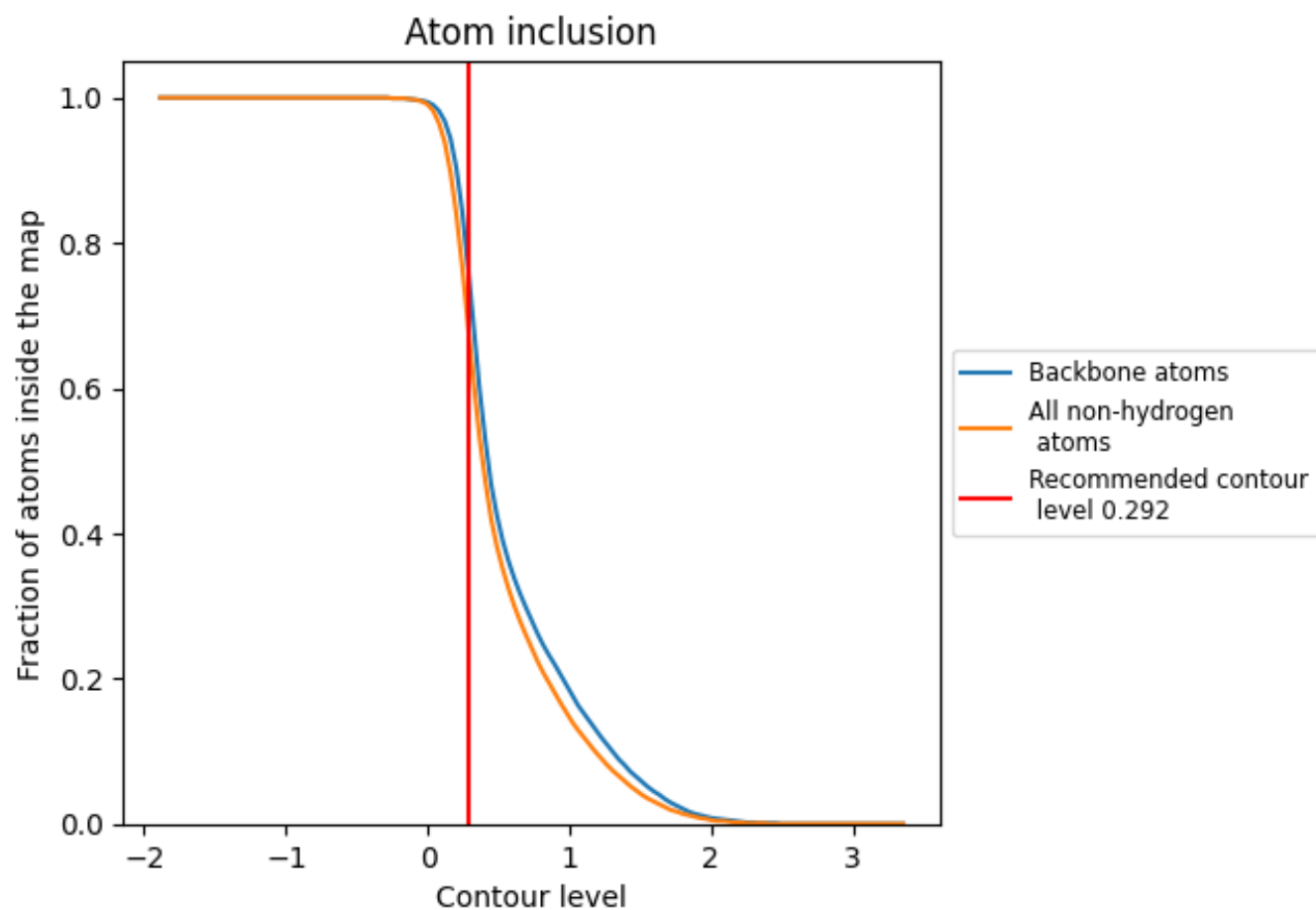
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.292).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.3310
0	 0.4640	 0.1820
1	 0.4800	 0.1840
2	 0.5380	 0.1860
3	 0.4720	 0.1400
4	 0.4240	 0.1500
5	 0.4720	 0.2010
6	 0.5090	 0.2190
7	 0.5800	 0.2630
8	 0.5590	 0.2630
9	 0.4740	 0.1810
A	 0.8310	 0.4480
B	 0.9130	 0.5180
C	 0.8600	 0.4720
D	 0.9090	 0.5270
E	 0.9110	 0.5290
F	 0.8770	 0.4980
G	 0.8310	 0.4220
H	 0.8100	 0.3710
I	 0.8480	 0.4240
J	 0.6830	 0.3320
K	 0.7700	 0.3380
L	 0.7740	 0.3290
M	 0.6280	 0.2790
N	 0.7040	 0.3110
O	 0.4110	 0.1100
P	 0.4060	 0.0860
Q	 0.5710	 0.2610
R	 0.4210	 0.1230
S	 0.3210	 0.1270
T	 0.3030	 0.0800
U	 0.3800	 0.1350
V	 0.4450	 0.1770
W	 0.5340	 0.2620
X	 0.7710	 0.4230



*Continued on next page...*

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Chain	Atom inclusion	Q-score
Y	 0.5210	 0.3310
Z	 0.7290	 0.3720