



## Full wwPDB EM Validation Report ⓘ

Sep 4, 2025 – 06:31 PM JST

PDB ID : 9UF8 / pdb\_00009uf8  
EMDB ID : EMD-64103  
Title : The cryo-EM structure of 26S proteasome-Midnolin complex in the MA state  
Authors : Wang, H.Y.; Xu, W.Q.; Wei, C.C.  
Deposited on : 2025-04-10  
Resolution : 4.32 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.dev126  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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) : 2.45.1

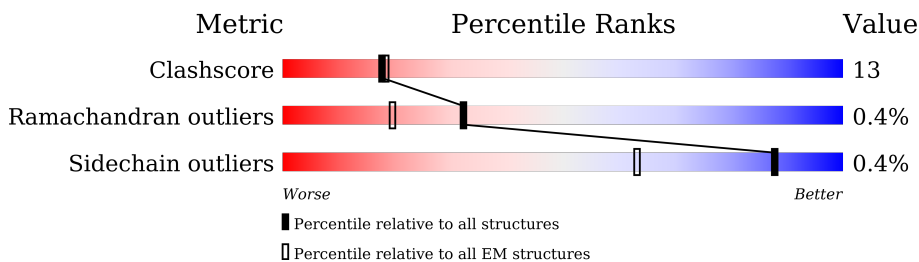
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.32 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.
















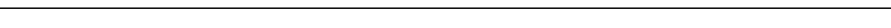











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	N	239	 65% 19% 16%
1	n	239	 70% 14% 16%
2	F	439	 59% 26% 15%
3	O	277	 59% 19% 21%
3	o	277	 57% 22% 21%
4	G	246	 70% 26%
4	g	246	 5% 75% 22%
5	P	205	 69% 30%

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Mol	Chain	Length	Quality of chain
5	p	205	
6	H	234	
6	h	234	
7	Q	201	
7	q	201	
8	I	261	
8	i	261	
9	R	263	
9	r	263	
10	J	248	
10	j	248	
11	S	241	
11	s	241	
12	K	241	
12	k	241	
13	T	264	
13	t	264	
14	L	263	
14	l	263	
15	M	255	
15	m	255	
16	U	953	
17	V	534	
18	W	456	
19	X	422	

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Mol	Chain	Length	Quality of chain
20	Y	389	
21	Z	324	
22	a	376	
23	b	377	
24	c	310	
25	d	350	
26	e	70	
27	f	908	
28	A	433	
29	u	491	
30	B	440	
31	C	406	
32	D	418	
33	E	389	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	ADP	F	501	-	-	X	-
35	ATP	D	501	-	-	X	-

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 103364 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 Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	201	Total	C	N	O	S	0	0
			1506	943	257	294	12		
1	n	201	Total	C	N	O	S	0	0
			1506	943	257	294	12		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	375	Total	C	N	O	S	0	0
			2826	1780	492	540	14		

- Molecule 3 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
3	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	238	Total	C	N	O	S	0	0
			1785	1135	303	335	12		
4	g	239	Total	C	N	O	S	0	0
			1865	1186	309	357	13		

- Molecule 5 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	226	Total	C	N	O	S	0	0
			1660	1057	285	314	4		
6	h	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

- Molecule 7 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
7	q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	249	Total	C	N	O	S	0	0
			1872	1179	321	364	8		
8	i	247	Total	C	N	O	S	0	0
			1945	1230	332	373	10		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		
9	r	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	241	Total	C	N	O	S	0	0
			1703	1066	309	323	5		
10	j	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
11	s	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	228	Total	C	N	O	S	0	0
			1681	1060	276	337	8		
12	k	237	Total	C	N	O	S	0	0
			1816	1139	301	365	11		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		
13	t	215	Total	C	N	O	S	0	0
			1681	1061	290	318	12		

- Molecule 14 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	240	Total	C	N	O	S	0	0
			1853	1164	337	342	10		
14	l	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

- Molecule 15 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	242	Total	C	N	O	S	0	0
			1851	1174	313	354	10		
15	m	241	Total	C	N	O	S	0	0
			1885	1195	322	357	11		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	812	Total	C	N	O	S	0	0
			6237	3948	1066	1181	42		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	508	Total	C	N	O	S	0	0
			3905	2462	705	728	10		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	456	Total	C	N	O	S	0	0
			3598	2264	613	697	24		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	380	Total	C	N	O	S	0	0
			2938	1865	502	562	9		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	378	Total	C	N	O	S	0	0
			3062	1952	524	572	14		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	286	Total	C	N	O	S	0	0
			2246	1429	390	422	5		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	373	Total	C	N	O	S	0	0
			2974	1898	503	558	15		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 4.



Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	191	Total	C	N	O	S	0	0
			1432	892	257	276	7		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	279	Total	C	N	O	S	0	0
			2139	1346	374	400	19		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	252	Total	C	N	O	S	0	0
			1990	1276	332	375	7		

- Molecule 26 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	39	Total	C	N	O	S	0	0
			313	188	52	71	2		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	889	Total	C	N	O	S	0	0
			6670	4171	1146	1311	42		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	393	Total	C	N	O	S	0	0
			3016	1896	526	577	17		

- Molecule 29 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	u	37	Total	C	N	O	S	0	0
			320	189	78	52	1		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	0	MET	-	initiating methionine	UNP Q504T8
u	469	GLY	-	expression tag	UNP Q504T8
u	470	SER	-	expression tag	UNP Q504T8
u	471	ASP	-	expression tag	UNP Q504T8
u	472	TYR	-	expression tag	UNP Q504T8
u	473	LYS	-	expression tag	UNP Q504T8
u	474	ASP	-	expression tag	UNP Q504T8
u	475	ASP	-	expression tag	UNP Q504T8
u	476	ASP	-	expression tag	UNP Q504T8
u	477	ASP	-	expression tag	UNP Q504T8
u	478	LYS	-	expression tag	UNP Q504T8
u	479	GLY	-	expression tag	UNP Q504T8
u	480	SER	-	expression tag	UNP Q504T8
u	481	HIS	-	expression tag	UNP Q504T8
u	482	HIS	-	expression tag	UNP Q504T8
u	483	HIS	-	expression tag	UNP Q504T8
u	484	HIS	-	expression tag	UNP Q504T8
u	485	HIS	-	expression tag	UNP Q504T8
u	486	HIS	-	expression tag	UNP Q504T8
u	487	HIS	-	expression tag	UNP Q504T8
u	488	HIS	-	expression tag	UNP Q504T8
u	489	HIS	-	expression tag	UNP Q504T8
u	490	HIS	-	expression tag	UNP Q504T8

- Molecule 30 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	384	Total	C	N	O	S	0	0
			2975	1870	510	581	14		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	C	363	Total	C	N	O	S	0	0
			2831	1784	507	525	15		

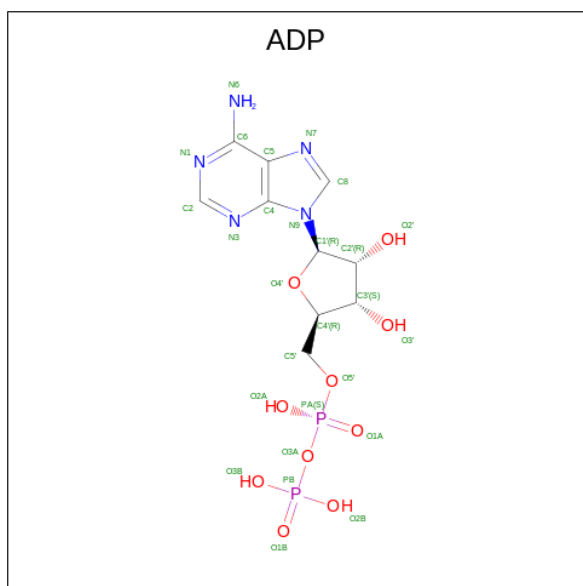
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	D	380	Total	C	N	O	S	0	0
			2991	1889	515	576	11		

- Molecule 33 is a protein called 26S proteasome regulatory subunit 10B.

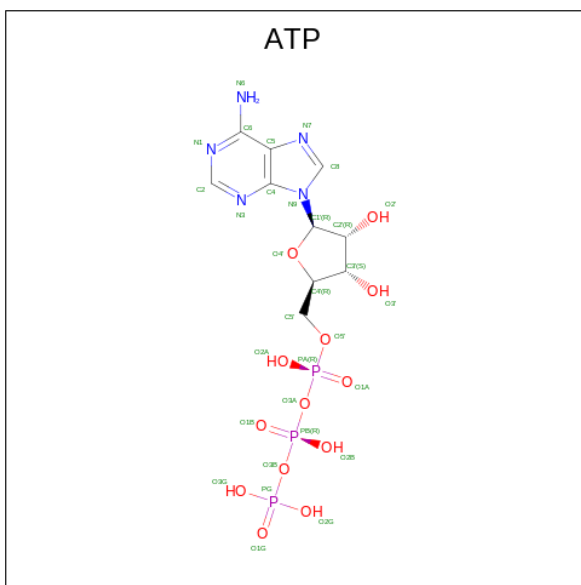
Mol	Chain	Residues	Atoms					AltConf	Trace
33	E	375	Total	C	N	O	S	0	0
			2828	1777	507	528	16		

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



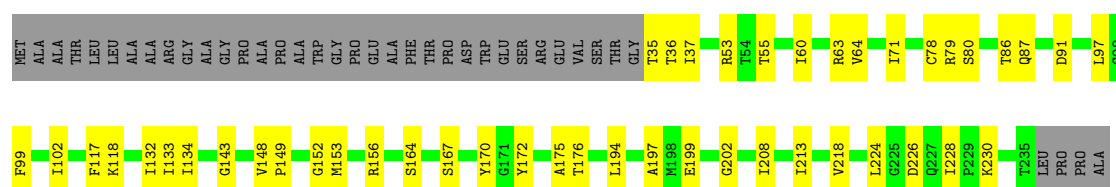
Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total 31	C 10	N 5	O 13	P 3	0
35	B	1	Total 31	C 10	N 5	O 13	P 3	0
35	D	1	Total 31	C 10	N 5	O 13	P 3	0
35	E	1	Total 31	C 10	N 5	O 13	P 3	0

### 3 Residue-property plots [i](#)

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

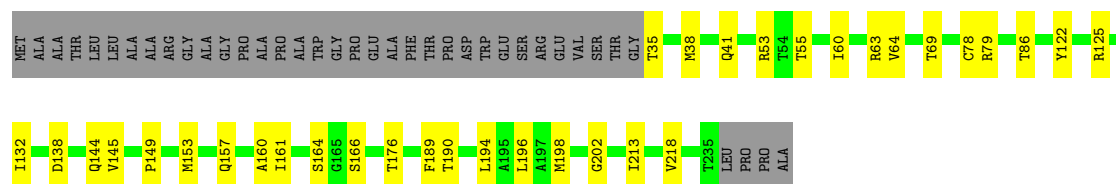
#### • Molecule 1: Proteasome subunit beta type-6

Chain N: 



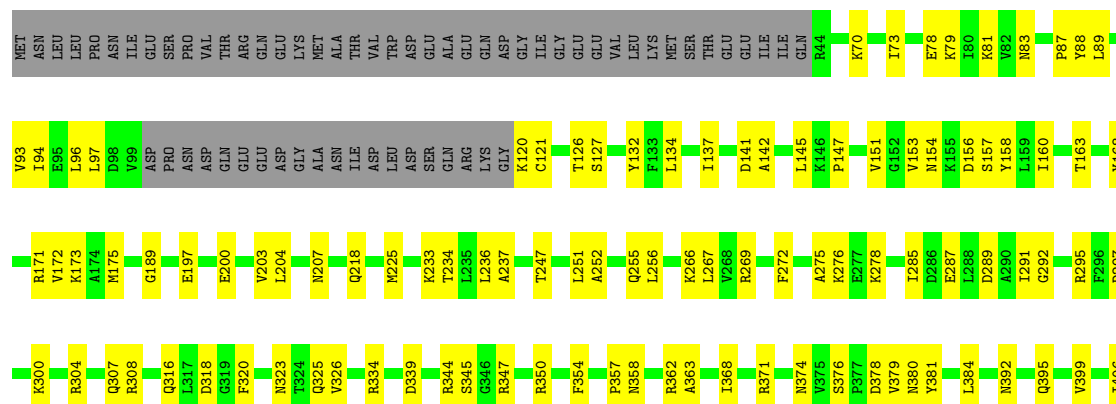
#### • Molecule 1: Proteasome subunit beta type-6

Chain n: 



#### • Molecule 2: 26S proteasome regulatory subunit 6A

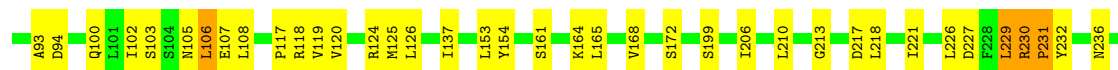
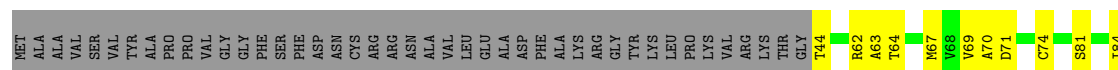
Chain F: 





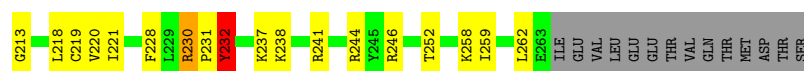
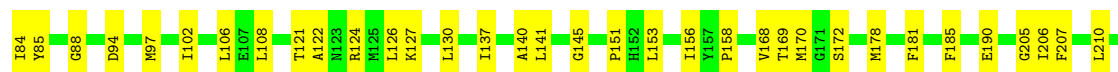
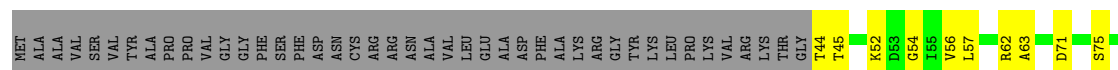
• Molecule 3: Proteasome subunit beta type-7

Chain O: 59% 19% 21%



• Molecule 3: Proteasome subunit beta type-7

Chain o: 57% 22% 21%



• Molecule 4: Proteasome subunit alpha type-6

Chain G: 70% 26% 4%



• Molecule 4: Proteasome subunit alpha type-6

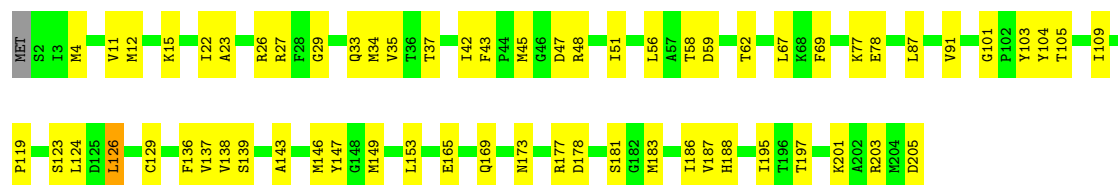
Chain g: 5% 75% 20%





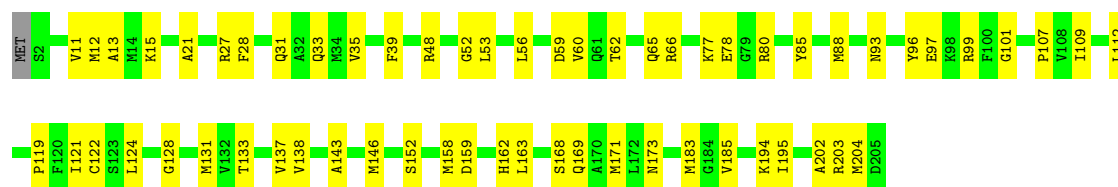
• Molecule 5: Proteasome subunit beta type-3

Chain P: 69% 30%



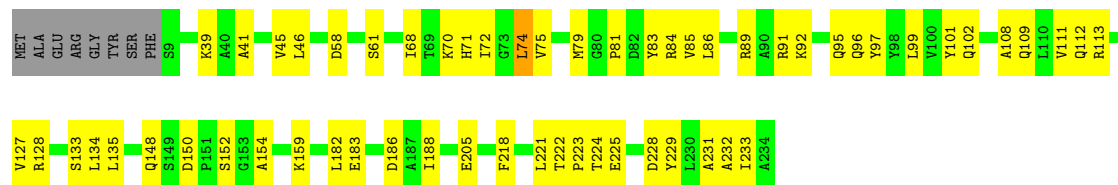
• Molecule 5: Proteasome subunit beta type-3

Chain p: 70% 29%



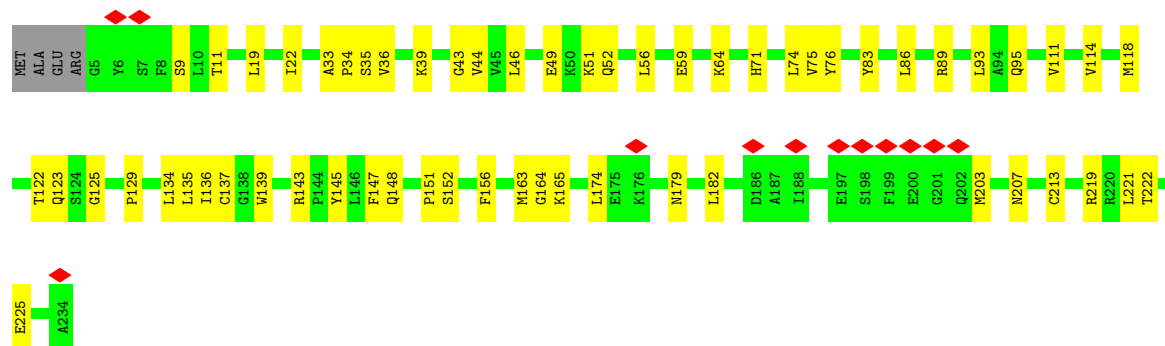
• Molecule 6: Proteasome subunit alpha type-2

Chain H: 72% 24%

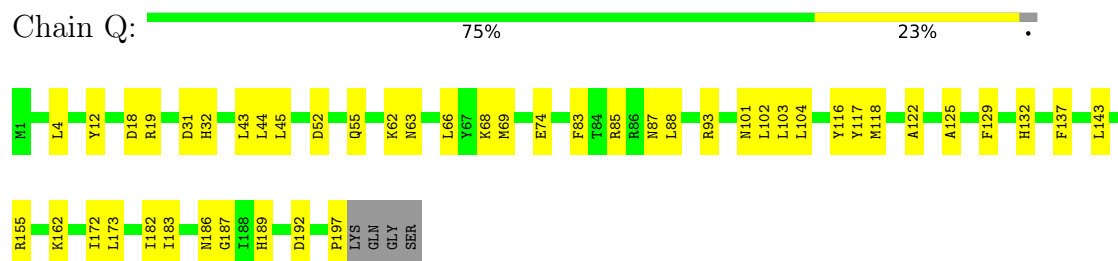


• Molecule 6: Proteasome subunit alpha type-2

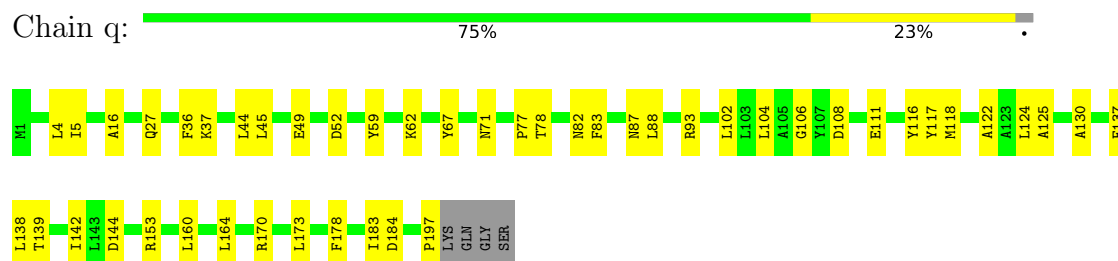
Chain h: 5% 73% 25%



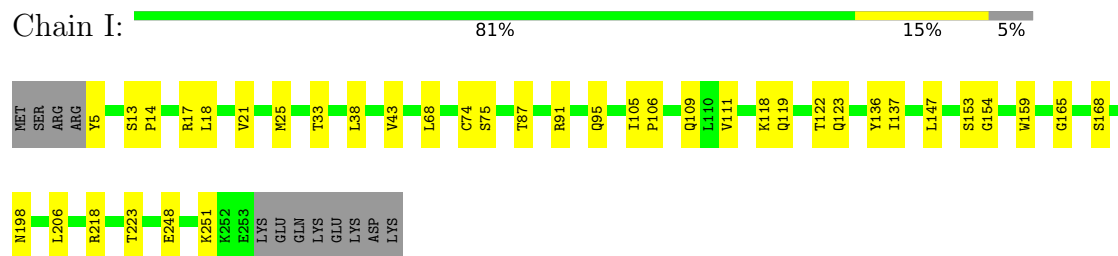
• Molecule 7: Proteasome subunit beta type-2



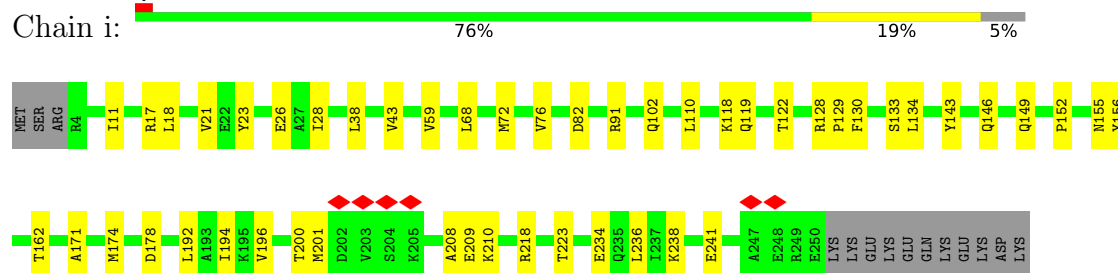
- Molecule 7: Proteasome subunit beta type-2



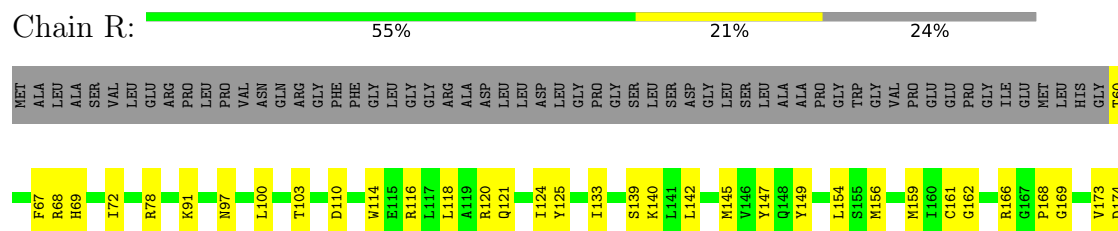
- Molecule 8: Proteasome subunit alpha type-4



- Molecule 8: Proteasome subunit alpha type-4

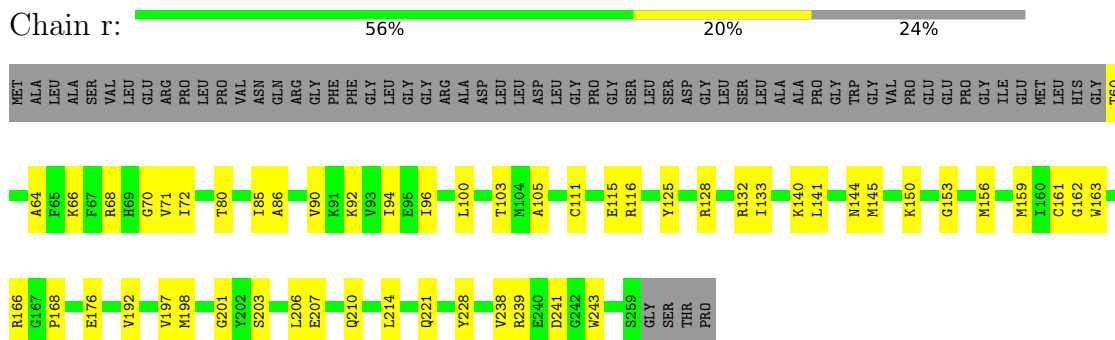


- Molecule 9: Proteasome subunit beta type-5

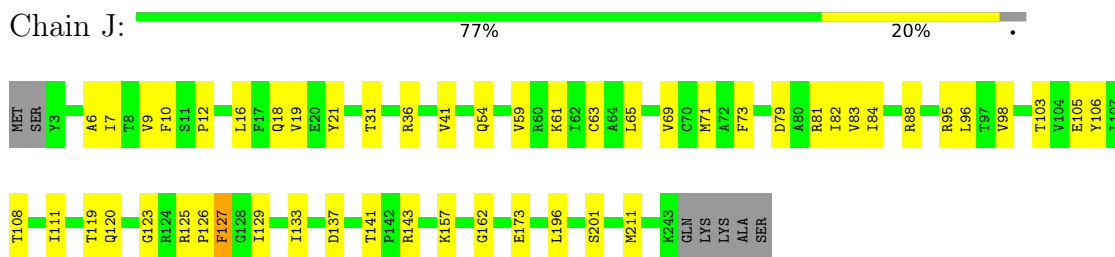




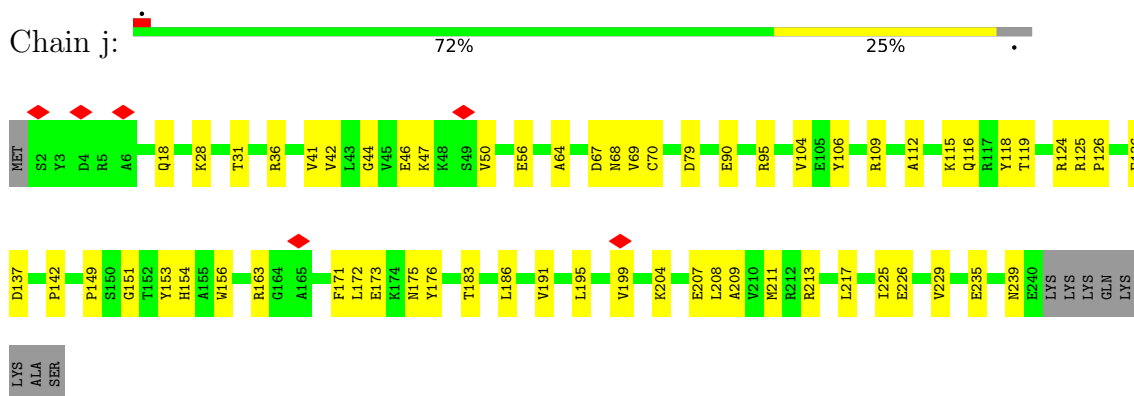
- Molecule 9: Proteasome subunit beta type-5



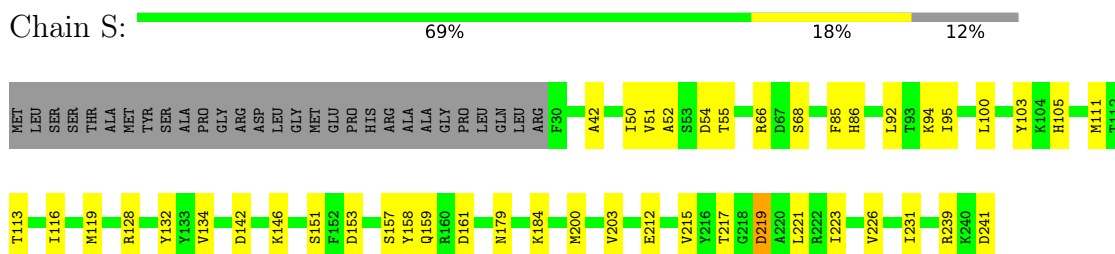
- Molecule 10: Proteasome subunit alpha type-7



- Molecule 10: Proteasome subunit alpha type-7

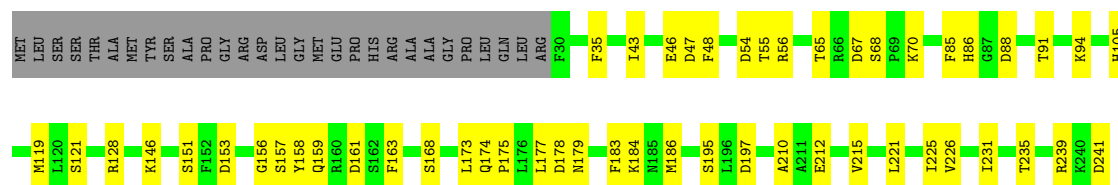


- Molecule 11: Proteasome subunit beta type-1



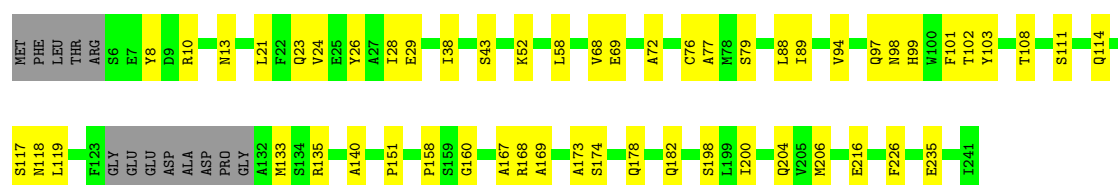
- Molecule 11: Proteasome subunit beta type-1

Chain s: 




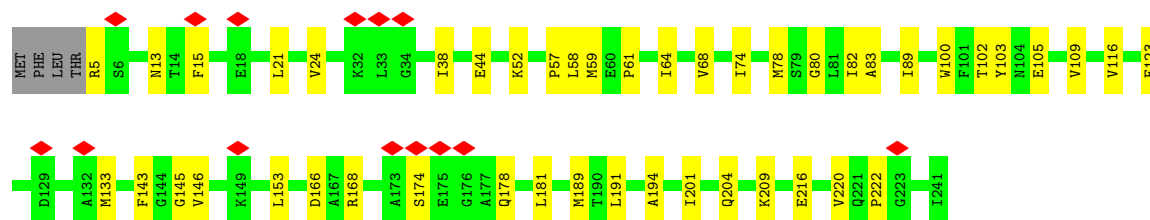
- Molecule 12: Proteasome subunit alpha type-5

Chain K: 



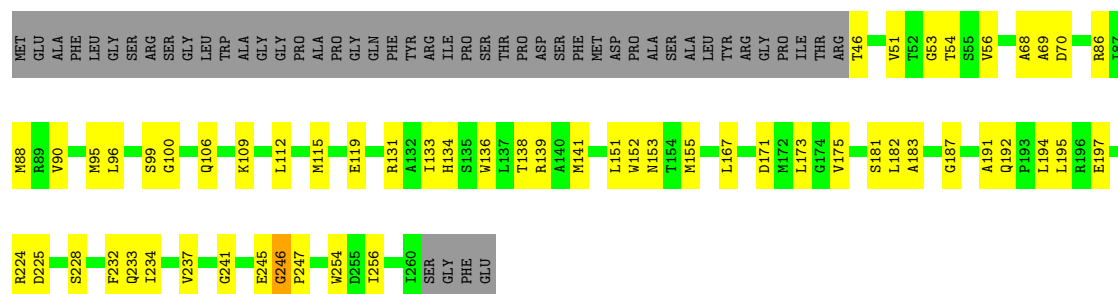
- Molecule 12: Proteasome subunit alpha type-5

Chain k: 



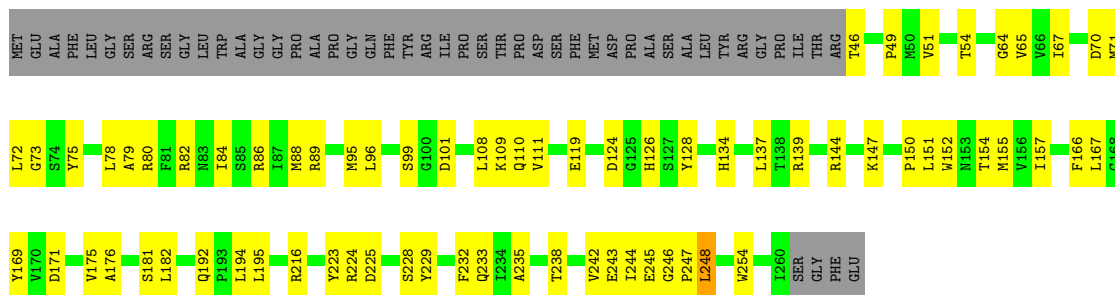
- Molecule 13: Proteasome subunit beta type-4

Chain T: 



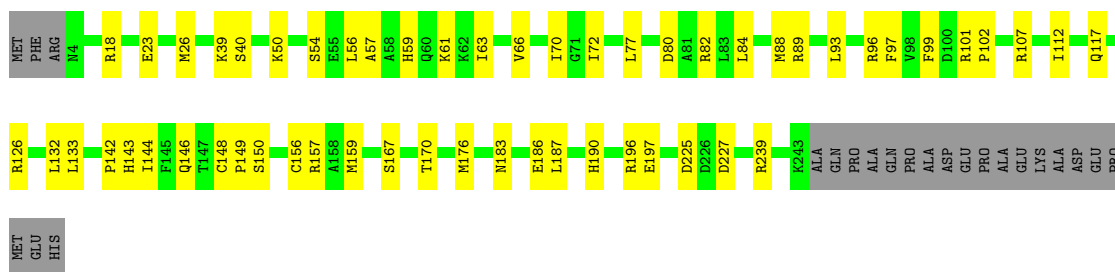
- Molecule 13: Proteasome subunit beta type-4

Chain t: 



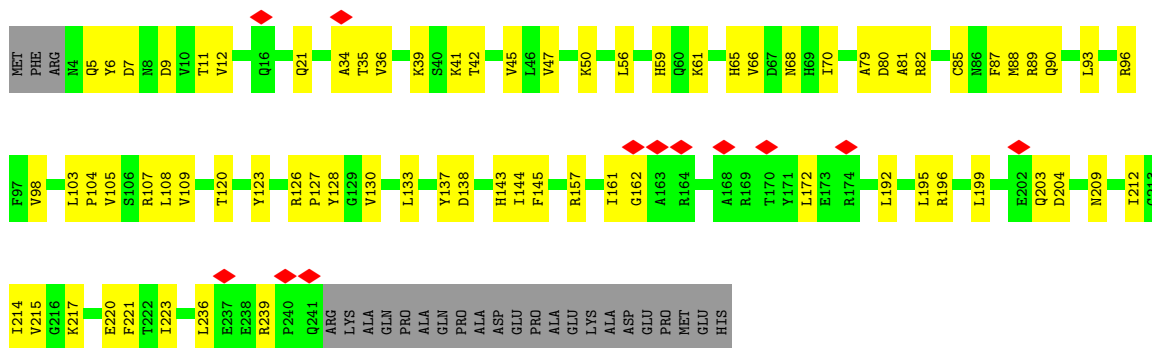
• Molecule 14: Proteasome subunit alpha type-1

Chain L: 70% 21% 9%



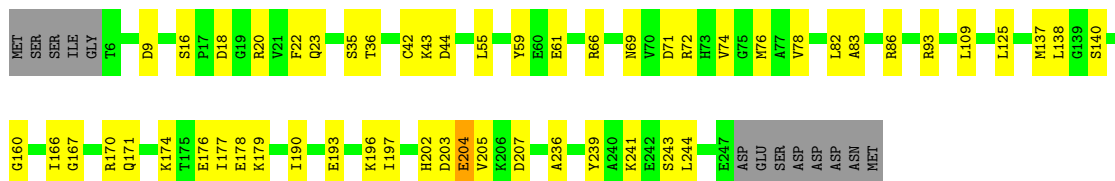
• Molecule 14: Proteasome subunit alpha type-1

Chain l: 5% 63% 28% 10%



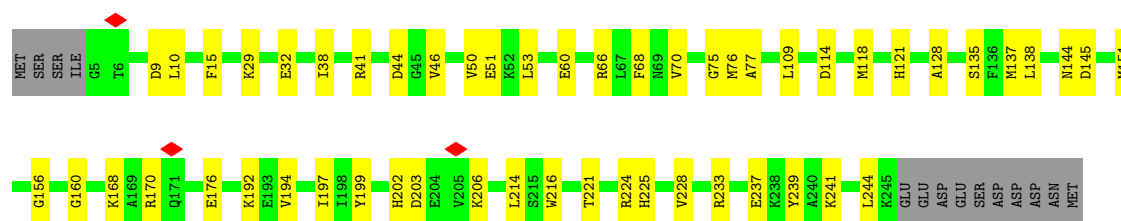
• Molecule 15: Proteasome subunit alpha type-3

Chain M: 74% 21% 5%



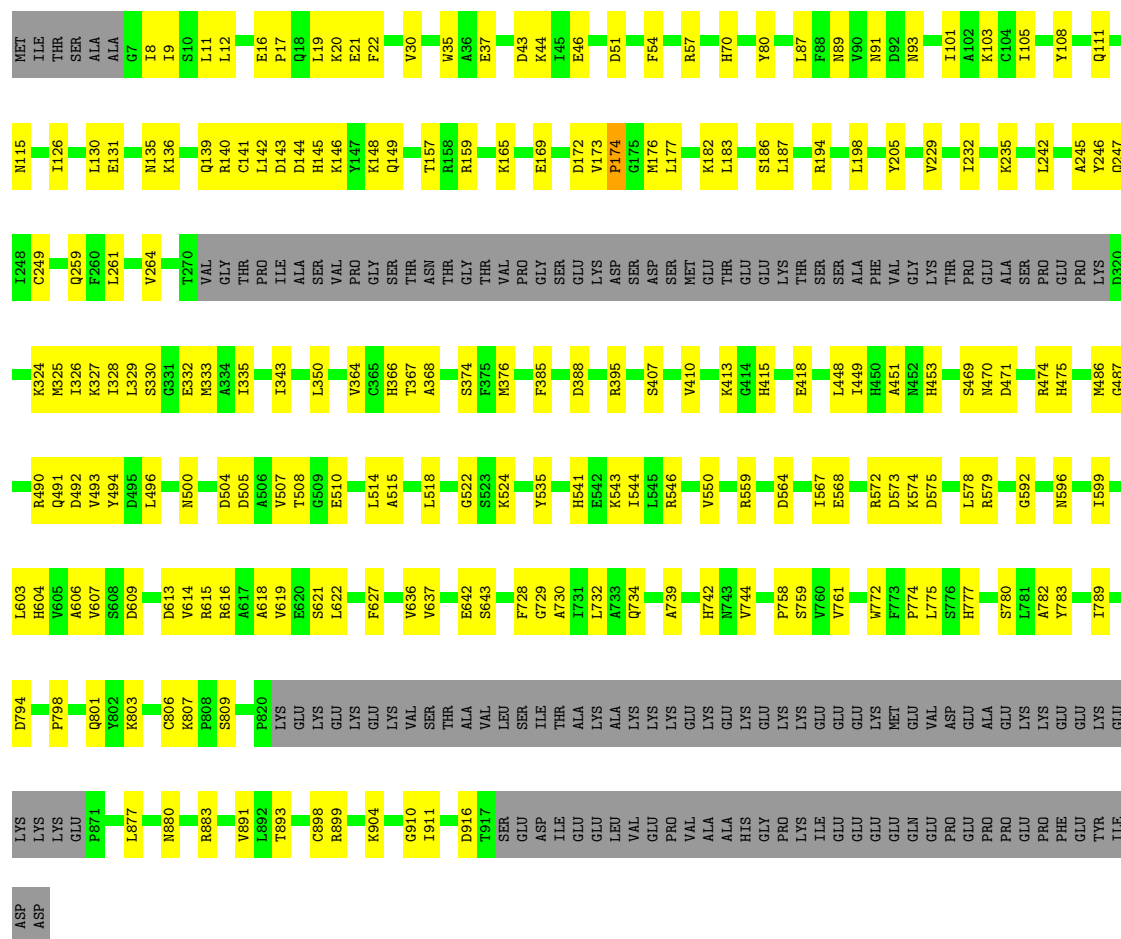
• Molecule 15: Proteasome subunit alpha type-3

Chain m: 74% 21% 5%



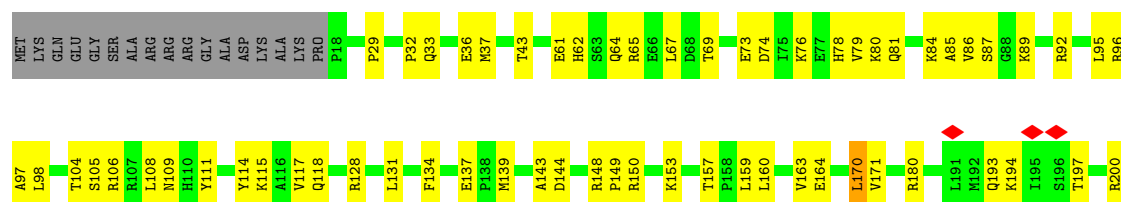
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 1

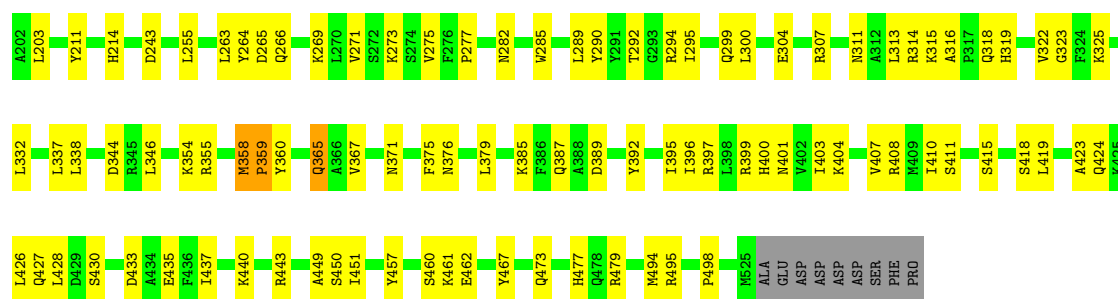
Chain U: 64% 21% 15%



• Molecule 17: 26S proteasome non-ATPase regulatory subunit 3

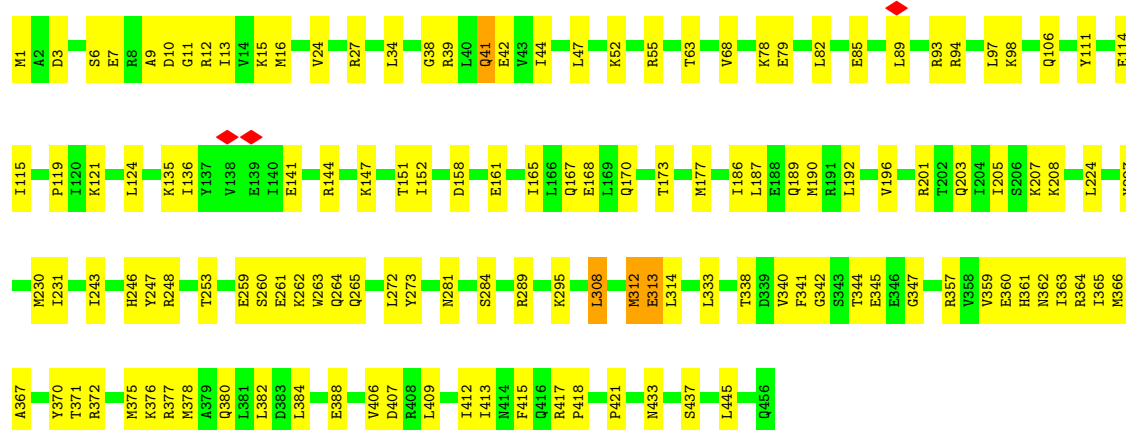
Chain V: 66% 29% 5%





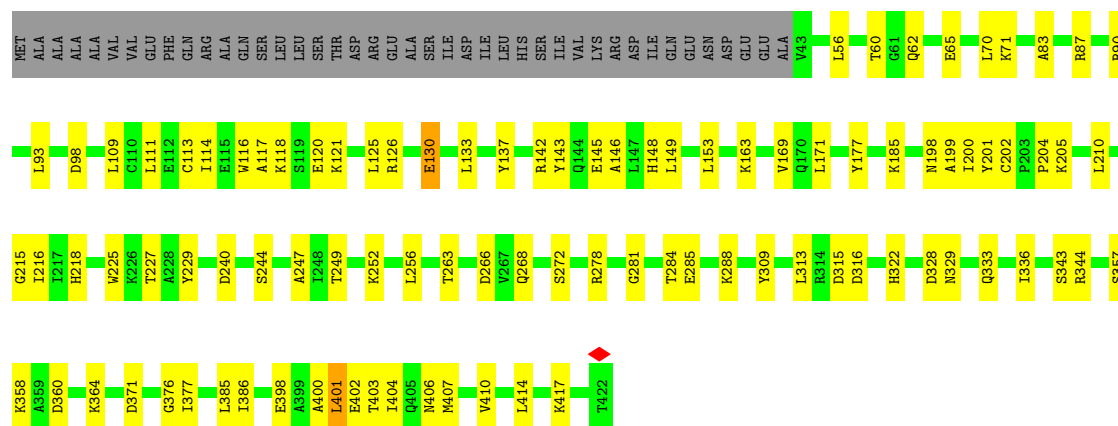
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 71% 28%



• Molecule 19: 26S proteasome non-ATPase regulatory subunit 11

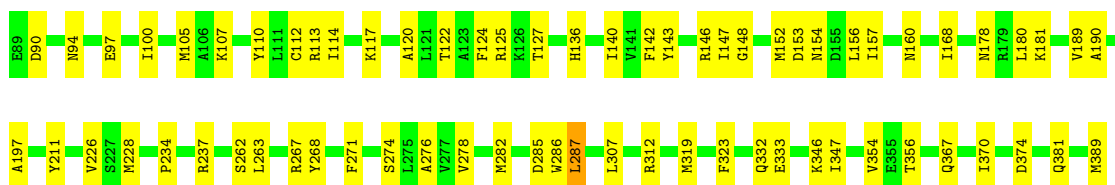
Chain X: 67% 23% 10%



• Molecule 20: 26S proteasome non-ATPase regulatory subunit 6

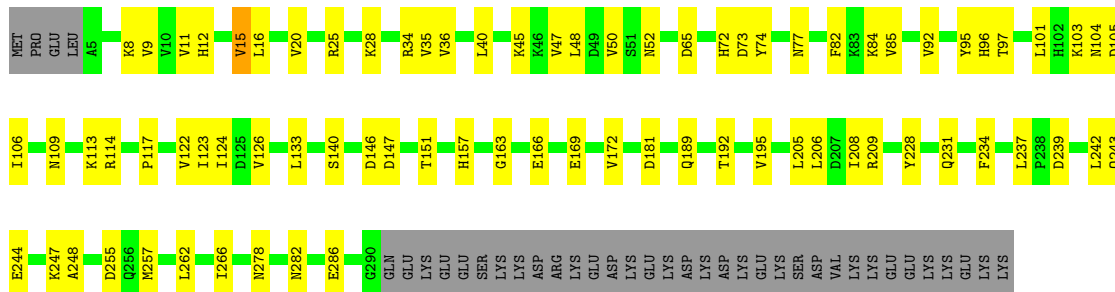
Chain Y: 72% 25%





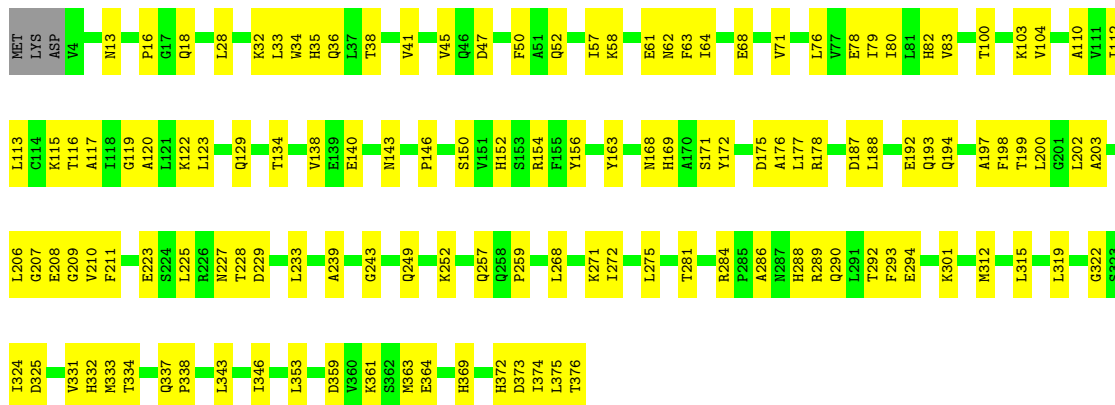
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 64% 24% 12%



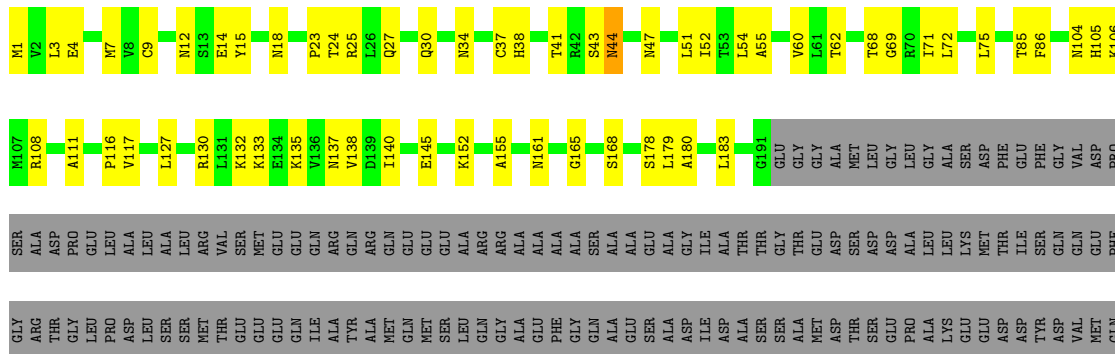
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 65% 34%

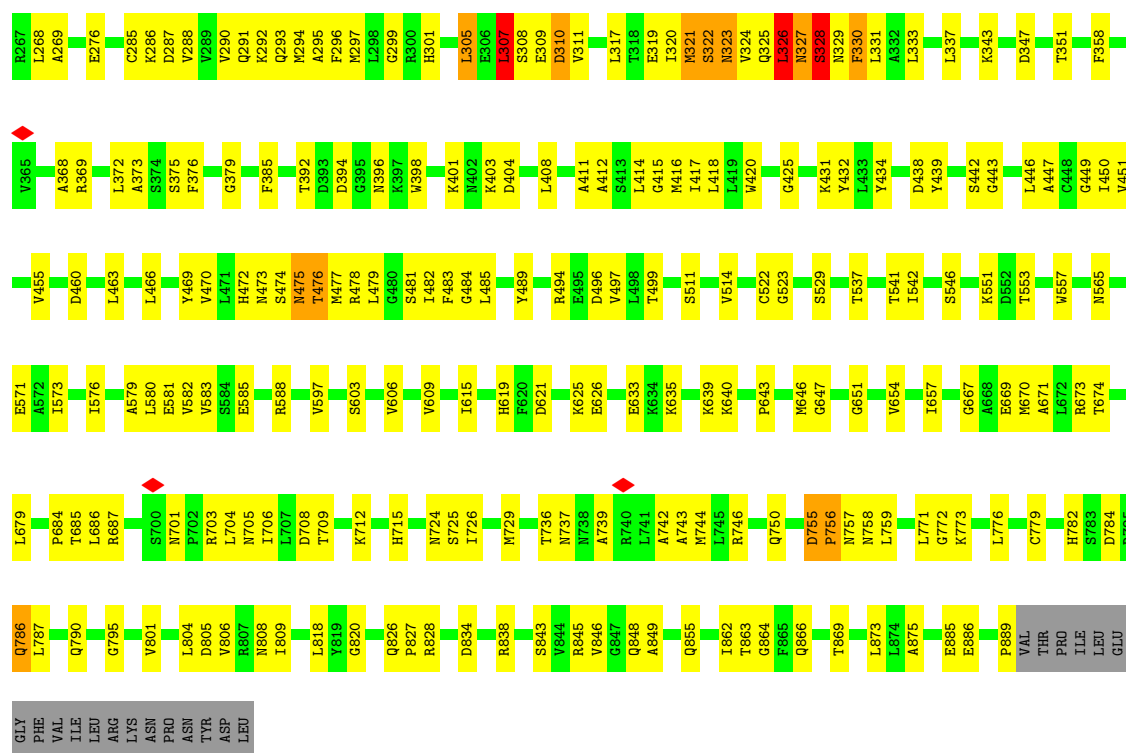


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 35% 15% 49%

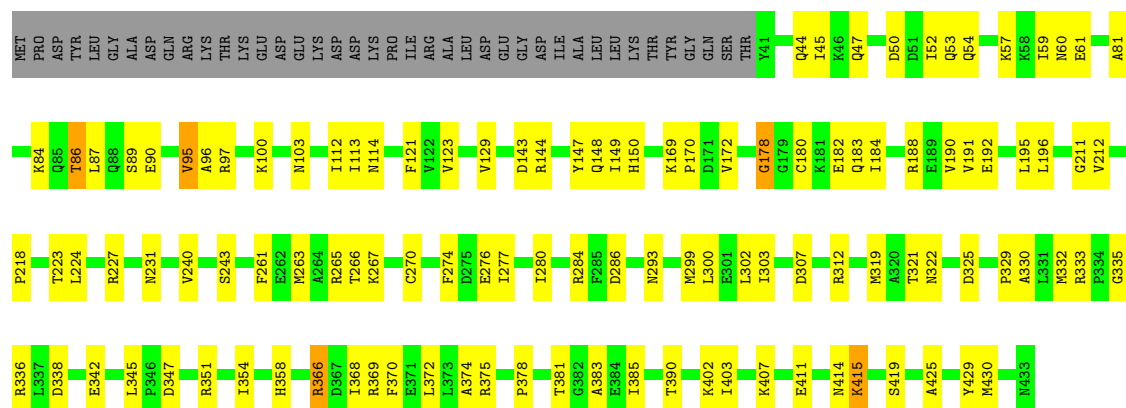






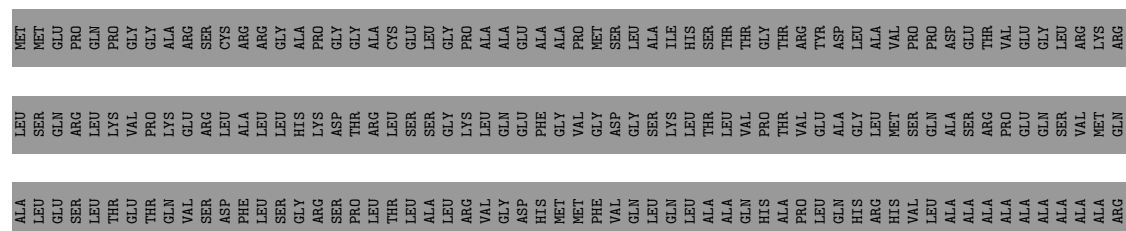
### • Molecule 28: 26S proteasome regulatory subunit 7

Chain A: 64% 25% 9%

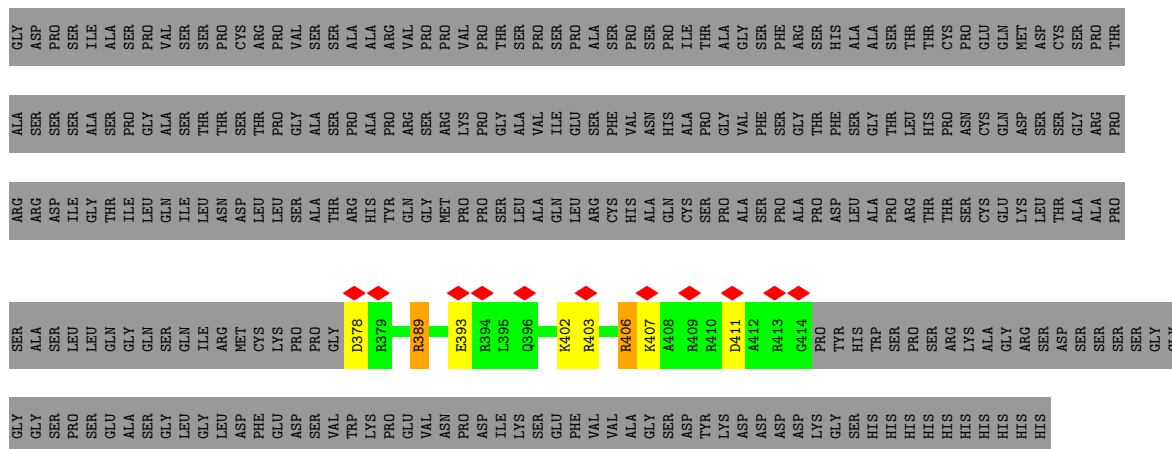


### • Molecule 29: Midnolin

Chain u: 6% 92% 2%

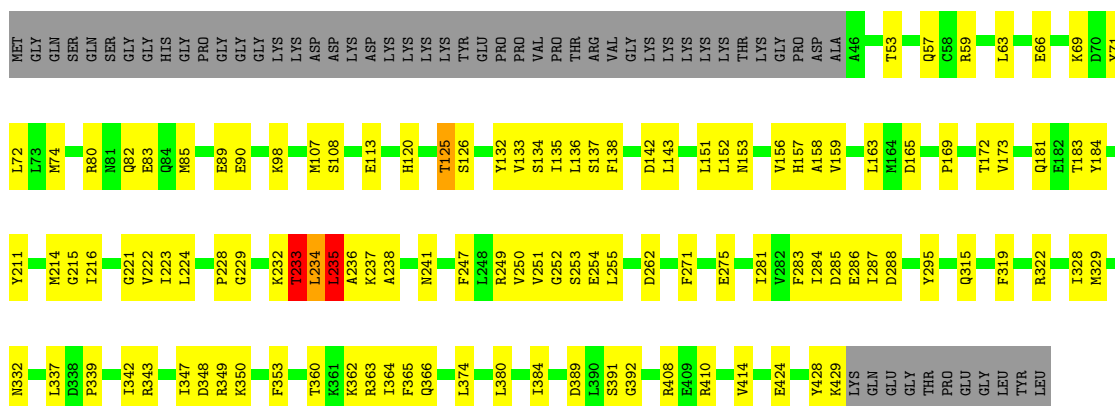






• Molecule 30: 26S proteasome regulatory subunit 4

Chain B: 61% 25% 13%



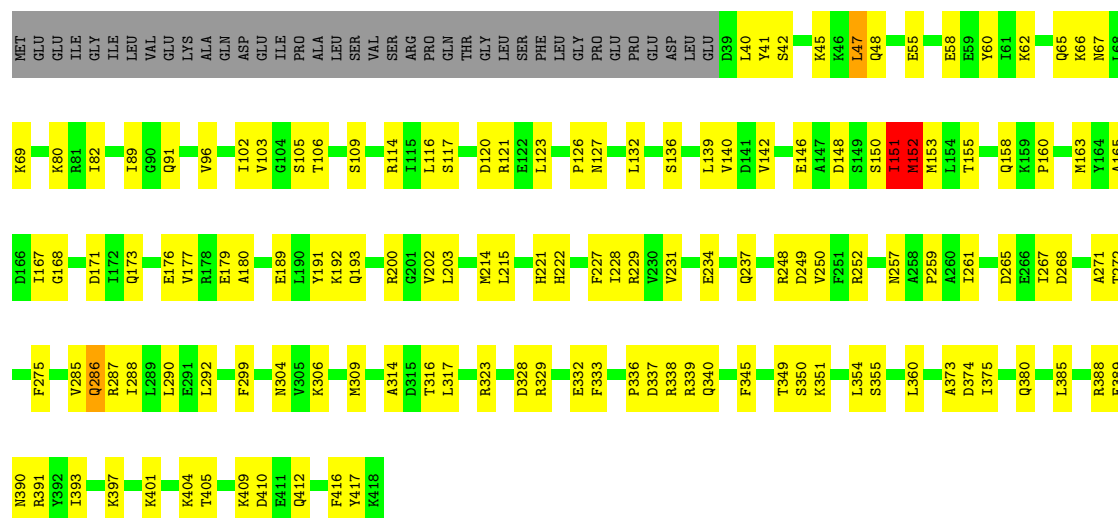
• Molecule 31: 26S proteasome regulatory subunit 8

Chain C: 63% 27% 11%



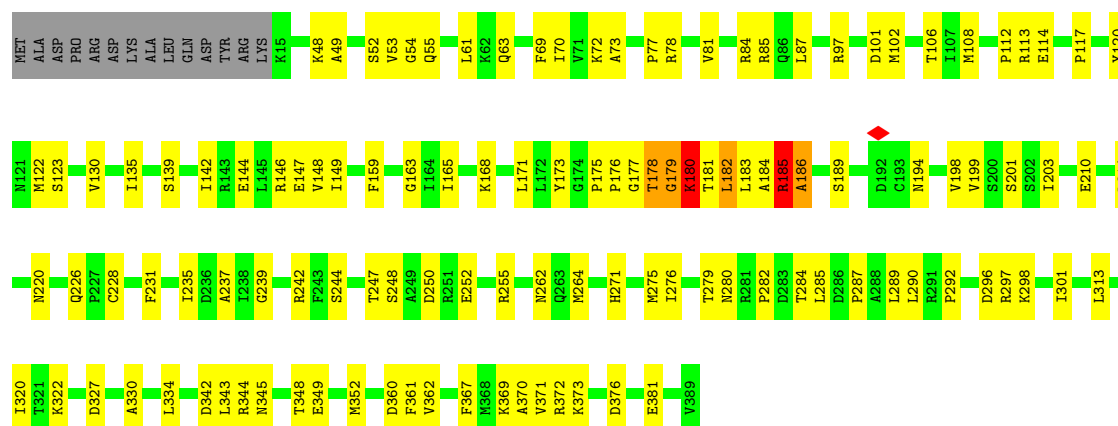
• Molecule 32: 26S proteasome regulatory subunit 6B

Chain D: 59% 31% 9%



### • Molecule 33: 26S proteasome regulatory subunit 10B

Chain E: 65% 30%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22328	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.397	Depositor
Minimum map value	-0.171	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.035	Depositor
Map size ( $\text{\AA}$ )	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	N	0.19	0/1532	0.47	0/2074
1	n	0.17	0/1532	0.42	0/2074
2	F	0.27	0/2864	0.59	0/3873
3	O	0.25	0/1686	0.52	1/2282 (0.0%)
3	o	0.19	0/1686	0.47	2/2282 (0.1%)
4	G	0.22	0/1818	0.55	0/2470
4	g	0.17	0/1899	0.42	0/2568
5	P	0.22	0/1620	0.49	0/2184
5	p	0.20	0/1620	0.48	0/2184
6	H	0.25	0/1695	0.57	1/2308 (0.0%)
6	h	0.16	0/1832	0.40	0/2481
7	Q	0.19	0/1611	0.50	0/2180
7	q	0.18	0/1611	0.49	0/2180
8	I	0.20	0/1900	0.53	0/2572
8	i	0.16	0/1975	0.43	0/2661
9	R	0.17	0/1586	0.41	0/2142
9	r	0.16	0/1586	0.40	0/2142
10	J	0.21	0/1727	0.55	1/2355 (0.0%)
10	j	0.14	0/1913	0.37	0/2581
11	S	0.19	0/1673	0.43	0/2254
11	s	0.17	0/1673	0.44	0/2254
12	K	0.19	0/1706	0.48	0/2314
12	k	0.16	0/1844	0.44	1/2489 (0.0%)
13	T	0.23	0/1714	0.55	0/2320
13	t	0.25	0/1714	0.58	1/2320 (0.0%)
14	L	0.20	0/1888	0.52	0/2555
14	l	0.18	0/1908	0.44	0/2579
15	M	0.19	0/1886	0.48	0/2550
15	m	0.17	0/1920	0.45	0/2585
16	U	0.22	0/6348	0.53	0/8603
17	V	0.30	0/3980	0.71	0/5394
18	W	0.26	0/3646	0.63	0/4916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	X	0.25	0/2979	0.62	3/4023 (0.1%)
20	Y	0.26	0/3120	0.63	2/4208 (0.0%)
21	Z	0.26	0/2287	0.63	3/3102 (0.1%)
22	a	0.25	0/3032	0.62	0/4107
23	b	0.31	0/1452	0.70	0/1968
24	c	0.27	0/2176	0.66	0/2939
25	d	0.31	0/2031	0.71	0/2751
26	e	0.26	0/317	0.69	0/425
27	f	0.36	0/6779	0.75	3/9183 (0.0%)
28	A	0.28	0/3065	0.68	3/4146 (0.1%)
29	u	0.84	0/319	1.44	0/419
30	B	0.26	0/3017	0.63	6/4076 (0.1%)
31	C	0.29	0/2868	0.66	2/3861 (0.1%)
32	D	0.31	0/3041	0.75	3/4111 (0.1%)
33	E	0.28	0/2871	0.70	4/3882 (0.1%)
All	All	0.25	0/104947	0.59	36/141927 (0.0%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	E	185	ARG	N-CA-C	-10.46	100.00	113.17
33	E	182	LEU	N-CA-C	-9.74	100.62	111.14
33	E	186	ALA	N-CA-C	-9.05	101.81	113.12
30	B	235	LEU	N-CA-C	-7.98	101.54	111.75
27	f	330	PHE	N-CA-C	-6.98	103.60	111.07
32	D	152	MET	CA-C-N	6.34	133.66	121.54
32	D	152	MET	C-N-CA	6.34	133.66	121.54
3	o	232	TYR	CA-C-N	-6.25	112.77	122.59
3	o	232	TYR	C-N-CA	-6.25	112.77	122.59
19	X	417	LYS	N-CA-C	-6.14	107.02	114.75
30	B	233	THR	N-CA-C	5.97	120.29	113.19
20	Y	16	ASP	CA-C-N	5.77	132.57	121.54
20	Y	16	ASP	C-N-CA	5.77	132.57	121.54
6	H	112	GLN	N-CA-CB	5.64	119.60	110.40
33	E	180	LYS	O-C-N	5.63	129.02	122.09
30	B	234	LEU	N-CA-C	-5.55	105.29	112.68
31	C	194	THR	CA-C-N	5.47	132.13	121.41
31	C	194	THR	C-N-CA	5.47	132.13	121.41
30	B	232	LYS	O-C-N	-5.41	116.40	122.03
21	Z	286	GLU	N-CA-CB	5.38	119.17	110.40
32	D	286	GLN	N-CA-CB	5.34	118.56	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	321	MET	CB-CA-C	5.28	119.31	110.92
28	A	178	GLY	N-CA-C	5.25	120.33	111.04
3	O	107	GLU	N-CA-CB	5.23	118.35	110.30
12	k	80	GLY	N-CA-C	5.20	116.81	111.56
19	X	130	GLU	N-CA-CB	5.20	118.87	110.40
10	J	59	VAL	N-CA-C	-5.16	107.31	111.91
19	X	205	LYS	N-CA-C	-5.13	108.04	114.56
30	B	233	THR	CA-C-N	5.09	132.17	122.60
30	B	233	THR	C-N-CA	5.09	132.17	122.60
13	t	110	GLN	N-CA-CB	5.07	118.14	110.28
21	Z	15	VAL	CA-C-N	5.07	131.23	121.54
21	Z	15	VAL	C-N-CA	5.07	131.23	121.54
27	f	328	SER	N-CA-C	-5.05	107.51	113.97
28	A	415	LYS	CA-C-N	-5.00	118.07	122.97
28	A	415	LYS	C-N-CA	-5.00	118.07	122.97

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1506	0	1473	37	0
1	n	1506	0	1473	22	0
2	F	2826	0	2786	100	0
3	O	1659	0	1678	64	0
3	o	1659	0	1678	59	0
4	G	1785	0	1736	46	0
4	g	1865	0	1872	41	0
5	P	1591	0	1609	57	0
5	p	1591	0	1609	41	0
6	H	1660	0	1577	53	0
6	h	1793	0	1787	39	0
7	Q	1578	0	1580	41	0
7	q	1578	0	1580	33	0
8	I	1872	0	1798	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	i	1945	0	1961	32	0
9	R	1555	0	1517	37	0
9	r	1555	0	1517	34	0
10	J	1703	0	1549	41	0
10	j	1887	0	1905	38	0
11	S	1643	0	1640	31	0
11	s	1643	0	1640	41	0
12	K	1681	0	1609	38	0
12	k	1816	0	1797	34	0
13	T	1681	0	1658	40	0
13	t	1681	0	1658	51	0
14	L	1853	0	1826	41	0
14	l	1873	0	1860	55	0
15	M	1851	0	1785	40	0
15	m	1885	0	1871	36	0
16	U	6237	0	6165	139	0
17	V	3905	0	3779	123	0
18	W	3598	0	3576	100	0
19	X	2938	0	2979	76	0
20	Y	3062	0	3008	74	0
21	Z	2246	0	2244	69	0
22	a	2974	0	2968	91	0
23	b	1432	0	1447	49	0
24	c	2139	0	2095	59	0
25	d	1990	0	1939	51	0
26	e	313	0	261	12	0
27	f	6670	0	6464	310	0
28	A	3016	0	2992	103	0
29	u	320	0	351	17	0
30	B	2975	0	2998	126	0
31	C	2831	0	2896	118	0
32	D	2991	0	2965	144	0
33	E	2828	0	2780	120	0
34	C	27	0	12	0	0
34	F	27	0	12	9	0
35	A	31	0	12	5	0
35	B	31	0	12	7	0
35	D	31	0	12	34	0
35	E	31	0	12	8	0
All	All	103364	0	102008	2715	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2715) 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)
27:f:404:ASP:HB3	27:f:439:TYR:CZ	1.50	1.44
27:f:414:LEU:HD12	27:f:417:ILE:CD1	1.49	1.40
19:X:256:LEU:HD21	19:X:322:HIS:NE2	1.42	1.31
27:f:404:ASP:HB3	27:f:439:TYR:CE2	1.69	1.28
30:B:233:THR:HG21	30:B:285:ASP:OD2	1.32	1.28
34:F:501:ADP:H4'	28:A:333:ARG:NH2	1.46	1.27
27:f:472:HIS:CE1	27:f:477:MET:HE3	1.69	1.27
27:f:418:LEU:HD12	27:f:425:GLY:CA	1.65	1.25
32:D:214:MET:HE1	35:D:501:ATP:C8	1.71	1.24
32:D:286:GLN:O	32:D:290:LEU:HG	1.37	1.23
27:f:418:LEU:CD1	27:f:425:GLY:HA3	1.68	1.22
27:f:418:LEU:HD21	27:f:451:VAL:CG2	1.69	1.22
30:B:234:LEU:CD1	30:B:237:LYS:HE2	1.69	1.20
32:D:214:MET:HE1	35:D:501:ATP:N9	1.55	1.18
27:f:477:MET:O	27:f:481:SER:HB2	1.42	1.18
2:F:320:PHE:CD1	33:E:185:ARG:HD2	1.79	1.17
27:f:416:MET:CE	27:f:804:LEU:HD11	1.74	1.17
27:f:416:MET:SD	27:f:804:LEU:HD11	1.86	1.16
27:f:404:ASP:CB	27:f:439:TYR:CE2	2.28	1.16
27:f:463:LEU:HD13	27:f:497:VAL:CG2	1.74	1.15
27:f:414:LEU:CD1	27:f:417:ILE:HD12	1.74	1.15
32:D:287:ARG:HA	32:D:290:LEU:HD12	1.23	1.15
29:u:402:LYS:HB3	29:u:406:ARG:NH2	1.62	1.12
27:f:404:ASP:CG	27:f:439:TYR:CE2	2.27	1.12
6:H:68:ILE:HD11	6:H:74:LEU:HD12	1.30	1.12
27:f:418:LEU:CD2	27:f:451:VAL:CG2	2.29	1.11
27:f:463:LEU:CD1	27:f:497:VAL:HG21	1.80	1.11
30:B:391:SER:CB	31:C:307:ARG:HH22	1.65	1.09
3:o:228:PHE:HE2	3:o:230:ARG:HD3	1.14	1.09
27:f:463:LEU:CD1	27:f:497:VAL:CG2	2.30	1.09
30:B:234:LEU:HD12	30:B:237:LYS:HE2	1.15	1.08
31:C:184:LYS:HD3	31:C:280:LEU:CG	1.83	1.08
30:B:233:THR:HG22	30:B:283:PHE:HZ	1.06	1.07
27:f:446:LEU:HD21	27:f:801:VAL:HG21	1.38	1.06
3:O:199:SER:HB2	3:O:232:TYR:HE2	1.19	1.05
30:B:233:THR:HG22	30:B:283:PHE:CZ	1.90	1.05
32:D:214:MET:HE1	35:D:501:ATP:C4	1.90	1.05
27:f:307:LEU:HD11	27:f:311:VAL:HG23	1.06	1.04
30:B:235:LEU:HD12	30:B:353:PHE:HZ	1.23	1.04
27:f:404:ASP:CB	27:f:439:TYR:CZ	2.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:88:ARG:NH1	15:m:118:MET:SD	2.31	1.03
2:F:233:LYS:O	2:F:236:LEU:HG	1.59	1.02
27:f:418:LEU:HG	27:f:451:VAL:HG22	1.37	1.02
3:o:75:SER:HB2	3:o:230:ARG:NH2	1.76	1.01
29:u:402:LYS:O	29:u:406:ARG:HG2	1.59	1.01
27:f:307:LEU:CD1	27:f:311:VAL:HG23	1.89	1.01
3:o:75:SER:HA	3:o:230:ARG:HH21	1.22	1.00
27:f:319:GLU:HG2	27:f:325:GLN:CB	1.91	1.00
6:H:74:LEU:O	6:H:74:LEU:HD22	1.60	1.00
2:F:320:PHE:HD1	33:E:185:ARG:HD2	1.13	1.00
32:D:214:MET:CE	35:D:501:ATP:C8	2.44	0.99
27:f:307:LEU:HD11	27:f:311:VAL:CG2	1.93	0.99
27:f:418:LEU:CG	27:f:451:VAL:CG2	2.40	0.99
31:C:184:LYS:HD3	31:C:280:LEU:HG	1.00	0.99
27:f:463:LEU:HD13	27:f:497:VAL:HG21	1.00	0.99
27:f:416:MET:HE1	27:f:804:LEU:HD11	1.40	0.99
17:V:263:LEU:HD13	25:d:83:PHE:HE2	1.27	0.98
27:f:418:LEU:CG	27:f:451:VAL:HG22	1.93	0.98
17:V:359:PRO:HG3	17:V:385:LYS:HG2	1.43	0.97
3:o:75:SER:CB	3:o:230:ARG:NH2	2.27	0.97
27:f:418:LEU:HD11	27:f:451:VAL:HG21	1.44	0.97
5:P:103:TYR:O	5:P:126:LEU:HD11	1.63	0.97
21:Z:36:VAL:HA	21:Z:95:TYR:O	1.63	0.97
32:D:214:MET:HE2	35:D:501:ATP:H2'	1.44	0.96
27:f:217:LEU:HD12	27:f:239:TYR:HE1	1.30	0.96
31:C:184:LYS:CD	31:C:280:LEU:HG	1.95	0.96
27:f:472:HIS:CE1	27:f:477:MET:CE	2.48	0.96
16:U:603:LEU:HD12	16:U:604:HIS:N	1.80	0.95
27:f:291:GLN:NE2	27:f:320:ILE:HD13	1.82	0.95
27:f:755:ASP:CB	27:f:756:PRO:HD3	1.97	0.95
34:F:501:ADP:C4'	28:A:333:ARG:NH2	2.28	0.95
17:V:263:LEU:CD1	25:d:83:PHE:HE2	1.80	0.94
27:f:463:LEU:HB2	27:f:489:TYR:HE2	1.33	0.94
30:B:224:LEU:HD21	30:B:235:LEU:HD13	1.50	0.94
3:o:228:PHE:CE2	3:o:230:ARG:HD3	2.03	0.94
18:W:308:LEU:CD2	18:W:312:MET:HE1	1.97	0.93
3:o:75:SER:HB2	3:o:230:ARG:HH22	1.33	0.93
27:f:418:LEU:CD1	27:f:425:GLY:CA	2.35	0.93
27:f:418:LEU:HD21	27:f:451:VAL:HG23	1.50	0.93
27:f:470:VAL:HG22	27:f:482:ILE:HG22	1.50	0.93
28:A:267:LYS:HG3	28:A:270:CYS:SG	2.09	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:416:MET:HE1	27:f:804:LEU:CD1	1.99	0.92
27:f:418:LEU:CD2	27:f:451:VAL:HG22	1.98	0.92
3:O:199:SER:HB2	3:O:232:TYR:CE2	2.05	0.91
30:B:234:LEU:CD1	30:B:237:LYS:CE	2.48	0.91
30:B:235:LEU:HD12	30:B:353:PHE:CZ	2.05	0.90
27:f:477:MET:O	27:f:481:SER:CB	2.20	0.90
31:C:230:MET:SD	31:C:233:GLU:OE2	2.30	0.89
32:D:373:ALA:CB	35:D:501:ATP:H5'2	2.01	0.89
18:W:308:LEU:HD21	18:W:361:HIS:CE1	2.07	0.89
27:f:414:LEU:CD1	27:f:417:ILE:CD1	2.40	0.89
32:D:151:ILE:HD13	32:D:151:ILE:H	1.36	0.89
27:f:463:LEU:HD11	27:f:497:VAL:HG23	1.52	0.89
27:f:418:LEU:HG	27:f:451:VAL:CG2	2.01	0.89
32:D:287:ARG:O	32:D:290:LEU:HB2	1.73	0.89
27:f:319:GLU:O	27:f:325:GLN:CB	2.22	0.88
27:f:295:ALA:HB2	27:f:323:ASN:HB2	1.53	0.88
33:E:181:THR:HA	33:E:184:ALA:HB3	1.55	0.88
27:f:756:PRO:HG2	27:f:758:ASN:O	1.73	0.87
33:E:175:PRO:O	33:E:178:THR:CG2	2.22	0.87
33:E:179:GLY:O	33:E:301:ILE:HD13	1.73	0.87
23:b:7:MET:HE2	23:b:52:ILE:CG1	2.02	0.87
27:f:411:ALA:HB3	27:f:443:GLY:HA3	1.54	0.87
31:C:189:TYR:C	31:C:196:LYS:HZ3	1.82	0.87
17:V:263:LEU:HD13	25:d:83:PHE:CE2	2.09	0.87
34:F:501:ADP:H4'	28:A:333:ARG:HH22	1.34	0.87
27:f:755:ASP:CB	27:f:756:PRO:CD	2.53	0.87
22:a:110:ALA:O	22:a:113:LEU:HB3	1.74	0.86
27:f:217:LEU:CD1	27:f:239:TYR:HE1	1.87	0.86
3:O:217:ASP:HB3	3:O:230:ARG:O	1.76	0.86
30:B:234:LEU:HD13	30:B:237:LYS:CE	2.06	0.86
27:f:404:ASP:CG	27:f:439:TYR:HE2	1.80	0.86
20:Y:17:LEU:HD11	20:Y:146:ARG:HG3	1.55	0.85
32:D:214:MET:SD	35:D:501:ATP:C8	2.69	0.85
23:b:7:MET:CE	23:b:60:VAL:CB	2.54	0.85
27:f:418:LEU:CD1	27:f:451:VAL:HG21	2.05	0.85
30:B:235:LEU:CD1	30:B:353:PHE:HZ	1.90	0.84
32:D:373:ALA:HB2	35:D:501:ATP:H5'2	1.57	0.84
30:B:391:SER:CB	31:C:307:ARG:NH2	2.41	0.84
21:Z:15:VAL:HG23	21:Z:16:LEU:CD1	2.08	0.84
27:f:301:HIS:O	27:f:305:LEU:HD21	1.78	0.84
5:P:103:TYR:O	5:P:126:LEU:CD1	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:256:LEU:CD2	19:X:322:HIS:NE2	2.36	0.84
30:B:233:THR:HG21	30:B:285:ASP:CG	2.04	0.83
32:D:214:MET:CE	35:D:501:ATP:N9	2.40	0.83
3:o:75:SER:CA	3:o:230:ARG:NH2	2.43	0.82
27:f:416:MET:SD	27:f:804:LEU:HD21	2.20	0.82
3:o:75:SER:HA	3:o:230:ARG:NH2	1.94	0.82
27:f:418:LEU:CG	27:f:451:VAL:HG21	2.09	0.81
27:f:463:LEU:HB2	27:f:489:TYR:CE2	2.15	0.81
27:f:291:GLN:NE2	27:f:320:ILE:HG21	1.94	0.81
27:f:294:MET:CB	27:f:321:MET:O	2.28	0.81
27:f:463:LEU:CD1	27:f:497:VAL:HG23	2.05	0.81
30:B:233:THR:CG2	30:B:285:ASP:OD2	2.23	0.81
3:O:230:ARG:HB3	3:O:231:PRO:HD3	1.63	0.81
28:A:97:ARG:HH12	28:A:144:ARG:HB3	1.45	0.81
18:W:308:LEU:HD21	18:W:312:MET:HE1	1.62	0.81
28:A:267:LYS:HB2	28:A:270:CYS:SG	2.22	0.80
32:D:214:MET:CE	35:D:501:ATP:H2'	2.12	0.80
3:o:230:ARG:HG2	3:o:230:ARG:HH11	1.47	0.80
30:B:234:LEU:CB	35:B:501:ATP:O1A	2.30	0.80
31:C:189:TYR:CA	31:C:196:LYS:NZ	2.44	0.80
33:E:135:ILE:HD13	33:E:182:LEU:CB	2.11	0.80
6:H:74:LEU:H	6:H:74:LEU:HD13	1.47	0.79
23:b:7:MET:HE2	23:b:52:ILE:HG12	1.65	0.79
27:f:217:LEU:CD1	27:f:239:TYR:CE1	2.65	0.79
27:f:290:VAL:HG21	27:f:317:LEU:HD22	1.64	0.79
21:Z:15:VAL:HG23	21:Z:16:LEU:HD13	1.63	0.79
27:f:217:LEU:HD12	27:f:239:TYR:CE1	2.17	0.79
34:F:501:ADP:C4'	28:A:333:ARG:HH22	1.92	0.79
29:u:403:ARG:HA	29:u:406:ARG:HD2	1.65	0.79
27:f:291:GLN:HE22	27:f:320:ILE:HD13	1.47	0.79
2:F:318:ASP:HB3	2:F:347:ARG:HG2	1.63	0.78
3:O:106:LEU:C	3:O:106:LEU:HD13	2.07	0.78
18:W:409:LEU:H	19:X:344:ARG:HH12	1.30	0.78
27:f:418:LEU:HD21	27:f:451:VAL:HG21	1.64	0.78
28:A:267:LYS:CB	28:A:270:CYS:SG	2.71	0.78
31:C:189:TYR:C	31:C:196:LYS:NZ	2.42	0.78
3:O:236:ASN:HD21	11:s:239:ARG:HB2	1.49	0.78
27:f:472:HIS:HE1	27:f:477:MET:HE3	1.42	0.78
20:Y:81:LEU:O	20:Y:84:LEU:HB3	1.83	0.78
32:D:214:MET:HE1	35:D:501:ATP:C5	2.19	0.78
17:V:359:PRO:CG	17:V:385:LYS:HG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:153:ASN:HD22	30:B:156:VAL:HG12	1.49	0.77
31:C:189:TYR:HA	31:C:196:LYS:NZ	1.97	0.77
16:U:603:LEU:HD13	32:D:60:TYR:CD1	2.19	0.77
22:a:271:LYS:O	22:a:275:LEU:HB2	1.83	0.77
27:f:411:ALA:CB	27:f:443:GLY:HA3	2.13	0.77
30:B:234:LEU:HA	30:B:237:LYS:HZ3	1.49	0.77
17:V:376:ASN:HA	17:V:379:LEU:HD12	1.66	0.77
32:D:214:MET:SD	35:D:501:ATP:O2'	2.42	0.77
31:C:228:ALA:HA	31:C:233:GLU:OE1	1.85	0.77
3:o:75:SER:CA	3:o:230:ARG:HH21	1.95	0.76
27:f:305:LEU:HD22	27:f:305:LEU:N	2.01	0.76
27:f:416:MET:SD	27:f:804:LEU:CD1	2.72	0.76
21:Z:35:VAL:H	21:Z:97:THR:HG22	1.51	0.76
18:W:190:MET:HE1	18:W:205:ILE:HG23	1.68	0.76
27:f:414:LEU:HD12	27:f:417:ILE:HD12	0.78	0.76
30:B:233:THR:CG2	30:B:283:PHE:HZ	1.95	0.76
33:E:181:THR:HG22	33:E:185:ARG:HG3	1.68	0.76
27:f:324:VAL:HG22	27:f:455:VAL:CG1	2.16	0.76
31:C:228:ALA:CB	31:C:233:GLU:OE1	2.34	0.76
16:U:599:ILE:O	16:U:603:LEU:HG	1.85	0.75
7:Q:62:LYS:O	7:Q:66:LEU:HG	1.87	0.75
30:B:234:LEU:HD13	30:B:237:LYS:HE2	1.61	0.75
27:f:438:ASP:HB3	27:f:476:THR:OG1	1.87	0.75
29:u:402:LYS:HB3	29:u:406:ARG:CZ	2.17	0.74
7:q:102:LEU:HB2	7:q:118:MET:HB2	1.68	0.74
2:F:233:LYS:CB	2:F:354:PHE:CZ	2.70	0.74
22:a:64:ILE:O	22:a:68:GLU:HB2	1.87	0.74
27:f:327:ASN:HD22	27:f:327:ASN:H	1.35	0.74
3:O:67:MET:SD	11:s:215:VAL:HG12	2.27	0.74
21:Z:16:LEU:HD23	21:Z:124:ILE:HD11	1.68	0.74
6:H:68:ILE:CD1	6:H:74:LEU:HD12	2.14	0.73
19:X:401:LEU:C	19:X:401:LEU:HD22	2.13	0.73
27:f:418:LEU:HD12	27:f:425:GLY:HA3	0.79	0.73
30:B:107:MET:HG2	30:B:151:LEU:HD13	1.70	0.73
28:A:267:LYS:CG	28:A:270:CYS:SG	2.76	0.73
17:V:401:ASN:O	17:V:404:LYS:HB3	1.89	0.73
32:D:261:ILE:HG12	32:D:306:LYS:HB2	1.70	0.73
28:A:178:GLY:C	35:A:501:ATP:HN62	1.97	0.72
16:U:141:CYS:HG	31:C:19:GLY:N	1.87	0.72
5:P:188:HIS:HD1	5:P:197:THR:HG1	1.35	0.72
30:B:234:LEU:HB3	35:B:501:ATP:O1A	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:44:THR:N	3:o:172:SER:HG	1.87	0.72
34:F:501:ADP:H4'	28:A:333:ARG:HH21	1.48	0.72
20:Y:97:GLU:HB3	31:C:162:LYS:HE2	1.72	0.72
33:E:181:THR:HG22	33:E:185:ARG:CG	2.20	0.72
22:a:210:VAL:O	22:a:210:VAL:HG12	1.89	0.71
3:O:199:SER:CB	3:O:232:TYR:HE2	2.00	0.71
6:h:219:ARG:HH12	6:h:221:LEU:HD23	1.55	0.71
27:f:446:LEU:CD1	27:f:483:PHE:HD2	2.03	0.71
18:W:308:LEU:HD23	18:W:312:MET:HE1	1.71	0.71
33:E:181:THR:HB	35:E:401:ATP:O2A	1.91	0.71
35:D:501:ATP:H3'	35:D:501:ATP:O1A	1.91	0.71
14:l:88:MET:HE2	14:l:108:LEU:HD21	1.73	0.71
3:O:106:LEU:HD11	3:O:117:PRO:HG3	1.71	0.71
29:u:403:ARG:O	29:u:406:ARG:HG3	1.90	0.71
27:f:138:GLU:HB3	27:f:189:LYS:HB3	1.73	0.70
3:O:229:LEU:N	3:O:229:LEU:HD23	2.06	0.70
6:H:74:LEU:N	6:H:74:LEU:CD1	2.54	0.70
15:M:42:CYS:SG	15:M:43:LYS:N	2.64	0.70
3:O:103:SER:O	3:O:106:LEU:HB3	1.90	0.70
4:G:118:ILE:HD11	4:G:138:MET:HE2	1.73	0.70
27:f:404:ASP:HB3	27:f:439:TYR:CE1	2.23	0.70
23:b:180:ALA:HA	23:b:183:LEU:HB2	1.74	0.70
32:D:373:ALA:CB	35:D:501:ATP:C5'	2.69	0.70
31:C:230:MET:SD	31:C:233:GLU:CD	2.75	0.70
6:H:74:LEU:HD13	6:H:74:LEU:N	2.05	0.70
19:X:398:GLU:O	19:X:401:LEU:HB3	1.91	0.70
32:D:373:ALA:HA	35:D:501:ATP:H5'1	1.74	0.70
18:W:308:LEU:O	18:W:308:LEU:HD22	1.90	0.70
31:C:161:ILE:HD12	31:C:199:LEU:HD21	1.74	0.70
11:S:94:LYS:HZ3	13:T:139:ARG:HD2	1.56	0.69
17:V:201:ARG:HH21	17:V:243:ASP:H	1.37	0.69
19:X:146:ALA:O	19:X:149:LEU:HB2	1.92	0.69
23:b:7:MET:HE1	23:b:60:VAL:CB	2.22	0.69
30:B:234:LEU:CA	30:B:237:LYS:HZ3	2.05	0.69
17:V:92:ARG:HE	17:V:114:TYR:HB3	1.57	0.69
27:f:889:PRO:HB2	28:A:366:ARG:HH12	1.57	0.69
18:W:115:ILE:HD12	18:W:119:PRO:HB2	1.73	0.69
32:D:173:GLN:HE22	32:D:333:PHE:HA	1.56	0.69
35:D:501:ATP:H3'	35:D:501:ATP:PA	2.32	0.69
30:B:59:ARG:O	30:B:63:LEU:HB2	1.92	0.69
27:f:291:GLN:CD	27:f:320:ILE:HG21	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:460:ASP:OD2	27:f:494:ARG:NH1	2.25	0.69
13:T:233:GLN:HG3	13:T:246:GLY:HA2	1.74	0.69
21:Z:16:LEU:HD23	21:Z:124:ILE:CD1	2.21	0.69
32:D:151:ILE:HD13	32:D:151:ILE:N	2.03	0.69
9:R:120:ARG:HA	12:K:97:GLN:HE21	1.57	0.68
4:g:228:ARG:HH12	4:g:230:LEU:HD23	1.58	0.68
12:k:78:MET:HE1	12:k:82:ILE:HA	1.74	0.68
11:S:103:TYR:HB3	11:S:111:MET:HE1	1.75	0.68
18:W:360:GLU:HG3	18:W:364:ARG:HH21	1.58	0.68
10:j:116:GLN:HG3	12:k:83:ALA:HB1	1.74	0.68
25:d:52:ARG:HH22	25:d:92:SER:HB3	1.58	0.68
25:d:131:VAL:HA	25:d:134:LYS:HB2	1.75	0.68
33:E:264:MET:HE2	33:E:275:MET:HE1	1.75	0.68
27:f:466:LEU:HB2	27:f:485:LEU:HD12	1.75	0.68
29:u:403:ARG:HA	29:u:406:ARG:CG	2.23	0.68
32:D:234:GLU:O	32:D:237:GLN:NE2	2.26	0.68
19:X:130:GLU:HG3	19:X:153:LEU:HD21	1.74	0.68
28:A:369:ARG:HG2	28:A:372:LEU:HB2	1.75	0.68
34:F:501:ADP:C3'	28:A:333:ARG:HH22	2.07	0.68
5:P:105:THR:H	5:P:126:LEU:HD21	1.56	0.68
27:f:756:PRO:C	27:f:758:ASN:H	2.02	0.68
2:F:347:ARG:NH2	35:E:401:ATP:PG	2.67	0.68
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.75	0.68
29:u:403:ARG:HA	29:u:406:ARG:HG3	1.75	0.67
3:O:230:ARG:CB	3:O:231:PRO:HD3	2.24	0.67
5:P:15:LYS:HE3	5:P:119:PRO:HB2	1.75	0.67
14:L:72:ILE:HD11	14:L:132:LEU:HB3	1.77	0.67
31:C:199:LEU:HD23	31:C:199:LEU:C	2.19	0.67
30:B:391:SER:HB2	31:C:307:ARG:HH22	1.57	0.67
33:E:181:THR:O	33:E:185:ARG:N	2.27	0.67
3:O:44:THR:N	3:O:172:SER:HG	1.92	0.67
27:f:418:LEU:H	27:f:418:LEU:HD23	1.58	0.67
7:q:139:THR:O	7:q:142:ILE:HB	1.95	0.67
27:f:217:LEU:HD11	27:f:239:TYR:CE1	2.30	0.67
31:C:194:THR:O	31:C:317:PHE:HD2	1.77	0.67
29:u:403:ARG:HA	29:u:406:ARG:CD	2.24	0.67
32:D:103:VAL:HG21	32:D:132:LEU:HD21	1.76	0.67
7:Q:129:PHE:HB2	7:Q:143:LEU:HD23	1.74	0.67
11:S:151:SER:O	11:S:158:TYR:HA	1.95	0.67
14:L:84:LEU:HD23	14:L:112:ILE:HD11	1.76	0.67
23:b:4:GLU:HA	23:b:106:LYS:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:415:GLY:O	27:f:450:ILE:HG22	1.95	0.67
1:N:213:ILE:HG12	1:N:218:VAL:HG22	1.77	0.67
16:U:636:VAL:HG23	16:U:637:VAL:HG23	1.75	0.67
1:n:55:THR:HG22	1:n:60:ILE:HA	1.77	0.67
27:f:828:ARG:NH2	27:f:863:THR:OG1	2.27	0.67
30:B:235:LEU:HD23	30:B:235:LEU:O	1.94	0.67
15:M:82:LEU:HD13	15:M:86:ARG:HH21	1.60	0.67
3:O:217:ASP:CB	3:O:230:ARG:O	2.42	0.66
7:Q:88:LEU:HG	7:Q:122:ALA:HB2	1.75	0.66
27:f:469:TYR:C	27:f:481:SER:OG	2.38	0.66
30:B:234:LEU:N	35:B:501:ATP:O1A	2.27	0.66
31:C:161:ILE:CD1	31:C:199:LEU:HD21	2.25	0.66
17:V:358:MET:HE2	17:V:358:MET:N	2.10	0.66
27:f:756:PRO:HG2	27:f:758:ASN:C	2.19	0.66
31:C:371:LEU:HD21	32:D:191:TYR:CZ	2.30	0.66
19:X:344:ARG:HA	19:X:385:LEU:O	1.95	0.66
27:f:551:LYS:HD3	27:f:553:THR:H	1.59	0.66
32:D:214:MET:CE	35:D:501:ATP:C2'	2.73	0.66
27:f:297:MET:HB2	27:f:772:GLY:HA3	1.77	0.66
32:D:148:ASP:HB3	33:E:61:LEU:HD12	1.76	0.66
18:W:371:THR:HG22	18:W:372:ARG:HG3	1.77	0.66
21:Z:40:LEU:HD12	21:Z:52:ASN:HB3	1.76	0.66
32:D:287:ARG:HA	32:D:290:LEU:CD1	2.15	0.66
10:j:137:ASP:O	10:j:213:ARG:NH2	2.29	0.66
14:l:81:ALA:HB2	14:l:130:VAL:HG21	1.78	0.66
24:c:287:HIS:O	24:c:291:LEU:N	2.27	0.66
7:Q:69:MET:SD	10:J:88:ARG:NH1	2.66	0.66
8:i:11:ILE:HG23	10:j:18:GLN:HE22	1.60	0.66
33:E:63:GLN:HG2	33:E:69:PHE:HE1	1.58	0.65
5:P:105:THR:N	5:P:126:LEU:HD21	2.11	0.65
10:J:65:LEU:HD13	10:J:88:ARG:HG3	1.79	0.65
23:b:47:ASN:HA	23:b:105:HIS:HE1	1.62	0.65
27:f:291:GLN:HE22	27:f:320:ILE:CD1	2.10	0.65
4:G:43:ARG:HG3	4:G:149:PRO:HB2	1.77	0.65
3:O:106:LEU:HD21	3:O:117:PRO:HB2	1.79	0.65
12:k:100:TRP:O	9:r:116:ARG:NH2	2.30	0.65
13:t:67:ILE:HB	13:t:95:MET:HE1	1.76	0.65
32:D:265:ASP:OD2	33:E:262:ASN:ND2	2.30	0.65
3:O:249:LYS:HA	5:P:165:GLU:HG3	1.79	0.65
5:P:45:MET:HE3	5:P:67:LEU:HD11	1.78	0.65
31:C:81:ASP:O	31:C:84:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:86:VAL:HA	17:V:89:LYS:HG3	1.78	0.65
17:V:495:ARG:NH2	17:V:498:PRO:O	2.30	0.65
2:F:392:ASN:H	2:F:395:GLN:HE21	1.43	0.65
17:V:263:LEU:CD1	25:d:83:PHE:CE2	2.71	0.65
20:Y:112:CYS:SG	20:Y:113:ARG:NH1	2.70	0.65
4:G:141:ILE:HG22	4:G:151:VAL:HG22	1.79	0.64
19:X:256:LEU:C	19:X:256:LEU:HD23	2.22	0.64
27:f:736:THR:HG22	27:f:737:ASN:N	2.12	0.64
28:A:218:PRO:HG3	28:A:429:TYR:HB3	1.79	0.64
5:P:51:ILE:HD11	5:P:87:LEU:HD21	1.78	0.64
18:W:52:LYS:HD3	18:W:55:ARG:HD3	1.78	0.64
30:B:391:SER:HB2	31:C:307:ARG:NH2	2.12	0.64
5:P:105:THR:H	5:P:126:LEU:CD2	2.11	0.64
11:s:163:PHE:HB2	11:s:177:LEU:HD13	1.79	0.64
14:l:214:ILE:O	14:l:221:PHE:HA	1.97	0.64
18:W:63:THR:HG22	18:W:68:VAL:HG13	1.79	0.64
27:f:673:ARG:HH22	27:f:709:THR:HA	1.63	0.64
31:C:228:ALA:CA	31:C:233:GLU:OE1	2.45	0.64
33:E:175:PRO:O	33:E:178:THR:HG23	1.98	0.64
11:s:179:ASN:HA	11:s:184:LYS:H	1.63	0.64
27:f:293:GLN:CG	27:f:321:MET:SD	2.85	0.64
7:Q:63:ASN:HA	7:Q:66:LEU:HD12	1.79	0.64
27:f:756:PRO:CG	27:f:758:ASN:O	2.46	0.64
29:u:402:LYS:HB3	29:u:406:ARG:HH21	1.57	0.64
29:u:402:LYS:CB	29:u:406:ARG:NH2	2.51	0.64
32:D:286:GLN:O	32:D:290:LEU:CG	2.31	0.64
33:E:84:ARG:HG2	33:E:87:LEU:HG	1.80	0.64
9:R:212:TYR:HB3	9:R:216:ARG:HH22	1.61	0.64
4:g:78:CYS:HB3	4:g:140:LEU:HD23	1.79	0.64
17:V:211:TYR:HA	17:V:214:HIS:HB3	1.80	0.64
21:Z:146:ASP:HB2	22:a:177:LEU:HD22	1.79	0.64
3:o:244:ARG:HH21	3:o:246:ARG:HD2	1.63	0.64
27:f:418:LEU:CD2	27:f:451:VAL:HG21	2.19	0.64
32:D:373:ALA:HB2	35:D:501:ATP:C5'	2.28	0.64
33:E:282:PRO:HA	33:E:285:LEU:HD23	1.79	0.64
27:f:475:ASN:O	27:f:479:LEU:N	2.31	0.64
30:B:82:GLN:NE2	30:B:83:GLU:OE1	2.31	0.64
13:T:95:MET:HE1	13:T:237:VAL:HB	1.79	0.63
33:E:175:PRO:O	33:E:178:THR:HG22	1.98	0.63
2:F:97:LEU:O	2:F:120:LYS:N	2.32	0.63
27:f:324:VAL:HG22	27:f:455:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:327:ASN:H	27:f:327:ASN:ND2	1.96	0.63
21:Z:228:TYR:HB2	22:a:338:PRO:HB2	1.81	0.63
31:C:147:THR:HG1	31:C:206:HIS:HE2	1.46	0.63
8:i:59:VAL:HG13	6:h:143:ARG:HH22	1.63	0.63
16:U:806:CYS:HB3	16:U:891:VAL:HG21	1.81	0.63
18:W:407:ASP:H	18:W:413:ILE:HG22	1.64	0.63
27:f:758:ASN:CG	27:f:855:GLN:HE22	2.06	0.63
27:f:773:LYS:HD3	27:f:776:LEU:HD13	1.81	0.63
3:O:102:ILE:HG13	3:O:126:LEU:HD23	1.81	0.63
27:f:322:SER:C	27:f:324:VAL:H	2.07	0.63
28:A:227:ARG:HG2	30:B:319:PHE:HB2	1.80	0.63
6:H:99:LEU:O	6:H:102:GLN:NE2	2.32	0.63
2:F:350:ARG:HH22	33:E:352:MET:HG2	1.63	0.62
3:o:106:LEU:HD11	3:o:122:ALA:HB2	1.80	0.62
13:t:167:LEU:HG	13:t:182:LEU:HD12	1.81	0.62
32:D:173:GLN:NE2	32:D:332:GLU:O	2.31	0.62
16:U:522:GLY:O	16:U:559:ARG:NH2	2.32	0.62
20:Y:78:GLU:HA	20:Y:81:LEU:HB2	1.79	0.62
4:G:127:GLN:HA	6:H:128:ARG:HH21	1.65	0.62
5:P:103:TYR:HA	7:Q:93:ARG:HH22	1.65	0.62
7:Q:43:LEU:HD12	7:Q:183:ILE:HD11	1.81	0.62
9:R:116:ARG:NH2	12:K:101:PHE:O	2.32	0.62
16:U:603:LEU:O	16:U:606:ALA:HB3	2.00	0.62
16:U:643:SER:O	31:C:57:ARG:NH2	2.31	0.62
12:k:52:LYS:HE2	12:k:216:GLU:HG3	1.81	0.62
23:b:130:ARG:O	23:b:133:LYS:NZ	2.32	0.62
27:f:368:ALA:O	27:f:403:LYS:NZ	2.32	0.62
4:g:76:ILE:HD11	4:g:140:LEU:HB3	1.79	0.62
21:Z:25:ARG:NH2	24:c:106:GLU:OE2	2.31	0.62
27:f:291:GLN:OE1	27:f:320:ILE:HG23	2.00	0.62
23:b:34:ASN:O	23:b:38:HIS:ND1	2.32	0.62
27:f:827:PRO:HD2	27:f:849:ALA:HA	1.82	0.62
31:C:141:GLU:O	32:D:323:ARG:NH1	2.32	0.62
15:M:137:MET:HE3	15:M:166:ILE:HG12	1.82	0.62
17:V:375:PHE:CE2	17:V:379:LEU:HD11	2.34	0.62
2:F:87:PRO:HA	28:A:123:VAL:HG12	1.82	0.62
3:O:206:ILE:HG23	3:O:213:GLY:HA2	1.82	0.62
7:Q:117:TYR:HB3	7:Q:125:ALA:HB3	1.80	0.62
8:i:143:TYR:HB2	8:i:146:GLN:HE21	1.64	0.62
6:h:118:MET:HE2	6:h:151:PRO:HA	1.81	0.62
21:Z:101:LEU:HD23	21:Z:123:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:13:LYS:HZ1	20:Y:142:PHE:HD2	1.46	0.62
31:C:134:LEU:HG	31:C:138:MET:HE1	1.82	0.62
27:f:291:GLN:CD	27:f:320:ILE:CG2	2.73	0.62
5:P:138:VAL:HB	5:P:146:MET:HE3	1.80	0.61
8:i:209:GLU:OE2	8:i:210:LYS:NZ	2.33	0.61
17:V:407:VAL:HA	17:V:410:ILE:HD12	1.81	0.61
24:c:288:VAL:O	24:c:291:LEU:HB2	2.00	0.61
27:f:293:GLN:HG3	27:f:321:MET:SD	2.39	0.61
27:f:333:LEU:HA	27:f:337:LEU:HD12	1.82	0.61
30:B:135:ILE:HA	30:B:159:VAL:HB	1.81	0.61
30:B:252:GLY:HA2	30:B:255:LEU:HD23	1.83	0.61
3:O:106:LEU:HD13	3:O:106:LEU:O	1.98	0.61
4:g:88:ARG:CZ	15:m:118:MET:SD	2.86	0.61
27:f:94:LYS:HD2	27:f:102:HIS:HE2	1.65	0.61
32:D:148:ASP:HB3	33:E:61:LEU:CD1	2.30	0.61
8:i:119:GLN:NE2	10:j:79:ASP:OD1	2.32	0.61
16:U:35:TRP:HE3	16:U:70:HIS:HB2	1.65	0.61
17:V:97:ALA:HB3	17:V:106:ARG:HH12	1.65	0.61
22:a:169:HIS:NE2	22:a:206:LEU:O	2.32	0.61
30:B:89:GLU:HG2	30:B:90:GLU:H	1.64	0.61
30:B:234:LEU:O	30:B:237:LYS:N	2.33	0.61
5:P:126:LEU:O	5:P:126:LEU:HD13	2.00	0.61
7:Q:4:LEU:HB2	7:Q:132:HIS:HB2	1.81	0.61
11:S:66:ARG:NH2	3:o:207:PHE:O	2.33	0.61
13:T:131:ARG:HH22	14:L:101:ARG:HB3	1.65	0.61
16:U:613:ASP:OD1	16:U:616:ARG:NH2	2.32	0.61
20:Y:43:ALA:O	20:Y:49:ASN:ND2	2.33	0.61
24:c:142:ALA:HB3	24:c:160:PHE:O	2.00	0.61
8:I:137:ILE:HG22	8:I:147:LEU:HG	1.82	0.61
6:h:74:LEU:HD11	6:h:134:LEU:HD22	1.82	0.61
12:k:168:ARG:HA	12:k:178:GLN:HE22	1.65	0.61
15:m:121:HIS:HB2	15:m:156:GLY:HA3	1.82	0.61
3:o:218:LEU:HD12	3:o:232:TYR:CE1	2.35	0.61
28:A:383:ALA:HB2	35:A:501:ATP:H4'	1.83	0.61
31:C:189:TYR:CA	31:C:196:LYS:HZ3	2.11	0.61
6:H:221:LEU:HD12	6:H:225:GLU:HG3	1.83	0.61
33:E:185:ARG:CG	33:E:185:ARG:HH11	2.13	0.61
13:T:88:MET:HE3	13:T:109:LYS:HG2	1.83	0.61
16:U:89:ASN:O	16:U:136:LYS:NZ	2.33	0.61
18:W:152:ILE:HD12	18:W:161:GLU:HB3	1.83	0.61
12:k:123:PHE:HB3	12:k:133:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:263:THR:HB	19:X:266:ASP:HB2	1.81	0.61
25:d:126:ASP:O	25:d:134:LYS:NZ	2.34	0.61
27:f:408:LEU:HD13	27:f:442:SER:OG	2.01	0.61
27:f:418:LEU:HG	27:f:418:LEU:O	1.99	0.61
13:t:134:HIS:HD1	13:t:166:PHE:HZ	1.46	0.61
2:F:172:VAL:HA	2:F:175:MET:HE2	1.83	0.61
2:F:233:LYS:N	34:F:501:ADP:O2A	2.31	0.61
9:R:184:THR:HB	9:R:198:MET:HE1	1.82	0.61
6:h:74:LEU:HD13	6:h:136:ILE:HG12	1.83	0.61
21:Z:11:VAL:O	21:Z:163:GLY:N	2.33	0.61
21:Z:65:ASP:HB2	21:Z:104:ASN:HB3	1.82	0.61
33:E:113:ARG:HH12	33:E:220:ASN:HB3	1.65	0.61
16:U:599:ILE:O	16:U:603:LEU:CG	2.49	0.61
17:V:375:PHE:O	17:V:379:LEU:HG	2.01	0.61
14:l:103:LEU:HD23	14:l:108:LEU:HD12	1.83	0.61
14:l:107:ARG:NH2	13:t:119:GLU:OE2	2.34	0.61
5:p:171:MET:HE1	5:p:185:VAL:HG13	1.82	0.61
11:s:86:HIS:HD2	13:t:175:VAL:HG13	1.65	0.61
33:E:194:ASN:HB3	33:E:228:CYS:HA	1.83	0.61
4:G:29:PHE:HA	4:G:32:ILE:HD12	1.81	0.60
16:U:568:GLU:OE1	16:U:572:ARG:NH1	2.31	0.60
25:d:45:LYS:HA	25:d:48:LEU:HB2	1.81	0.60
1:N:36:THR:HG21	1:N:197:ALA:HB1	1.82	0.60
6:H:74:LEU:HD23	6:H:134:LEU:HD12	1.82	0.60
15:M:9:ASP:O	15:M:23:GLN:NE2	2.34	0.60
17:V:33:GLN:NE2	17:V:84:LYS:O	2.33	0.60
15:m:51:GLU:OE2	15:m:202:HIS:ND1	2.34	0.60
21:Z:11:VAL:HA	21:Z:50:VAL:HB	1.82	0.60
22:a:194:GLN:NE2	22:a:225:LEU:O	2.32	0.60
22:a:373:ASP:O	22:a:376:THR:OG1	2.20	0.60
33:E:226:GLN:NE2	33:E:271:HIS:O	2.33	0.60
16:U:376:MET:HA	16:U:739:ALA:HA	1.82	0.60
17:V:73:GLU:HA	17:V:76:LYS:HB3	1.83	0.60
14:l:196:ARG:O	14:l:239:ARG:NH2	2.34	0.60
27:f:287:ASP:O	27:f:291:GLN:HG2	2.01	0.60
9:R:201:GLY:HA3	9:R:214:LEU:HD13	1.82	0.60
27:f:119:LYS:NZ	27:f:165:GLU:OE1	2.33	0.60
13:t:233:GLN:HA	13:t:248:LEU:HD12	1.83	0.60
28:A:211:GLY:O	28:A:338:ASP:N	2.34	0.60
30:B:424:GLU:HA	30:B:428:TYR:HB2	1.82	0.60
33:E:185:ARG:HG3	33:E:185:ARG:HH11	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:120:GLN:NE2	12:K:133:MET:O	2.35	0.60
17:V:304:GLU:OE2	17:V:307:ARG:NH2	2.35	0.60
23:b:24:THR:H	23:b:27:GLN:HE22	1.47	0.60
25:d:109:GLN:O	25:d:111:ARG:NH1	2.34	0.60
11:S:153:ASP:OD1	11:S:157:SER:N	2.34	0.60
16:U:242:LEU:O	16:U:246:TYR:N	2.35	0.60
17:V:494:MET:O	21:Z:278:ASN:ND2	2.35	0.60
24:c:46:ARG:HG3	33:E:85:ARG:HH12	1.66	0.60
24:c:70:ILE:HD11	24:c:106:GLU:HG3	1.83	0.60
22:a:172:TYR:O	22:a:176:ALA:HB2	2.01	0.60
16:U:603:LEU:HD12	16:U:603:LEU:C	2.27	0.60
17:V:92:ARG:HD3	17:V:111:TYR:HA	1.83	0.60
3:o:206:ILE:HG23	3:o:213:GLY:HA2	1.82	0.60
28:A:178:GLY:O	35:A:501:ATP:N6	2.35	0.60
29:u:389:ARG:NE	29:u:393:GLU:OE1	2.30	0.60
32:D:350:SER:OG	32:D:351:LYS:NZ	2.35	0.60
2:F:406:ILE:HD12	2:F:409:ARG:HD2	1.84	0.60
13:T:167:LEU:HG	13:T:182:LEU:HD12	1.84	0.60
20:Y:178:ASN:HA	20:Y:181:LYS:HE2	1.84	0.60
5:p:169:GLN:O	5:p:173:ASN:ND2	2.35	0.60
7:q:83:PHE:O	7:q:87:ASN:ND2	2.35	0.60
25:d:158:ILE:HG22	25:d:160:ALA:H	1.66	0.60
27:f:292:LYS:HG3	27:f:296:PHE:HD2	1.67	0.60
13:t:243:GLU:OE2	13:t:245:GLU:OE2	2.20	0.60
28:A:47:GLN:HG3	30:B:57:GLN:HE22	1.66	0.60
3:O:106:LEU:C	3:O:106:LEU:CD1	2.75	0.60
6:H:41:ALA:HB3	6:H:183:GLU:HA	1.83	0.60
7:Q:172:ILE:HA	7:q:27:GLN:HE22	1.66	0.60
17:V:98:LEU:HG	17:V:104:THR:HG22	1.82	0.59
20:Y:190:ALA:HA	20:Y:287:LEU:HD12	1.84	0.59
3:o:230:ARG:N	3:o:231:PRO:CD	2.65	0.59
27:f:472:HIS:HE1	27:f:477:MET:CE	2.05	0.59
30:B:365:PHE:HB3	30:B:380:LEU:HD13	1.83	0.59
5:P:104:TYR:HA	5:P:126:LEU:HD21	1.83	0.59
12:k:189:MET:HE2	12:k:194:ALA:HA	1.83	0.59
19:X:153:LEU:HG	19:X:169:VAL:HG21	1.83	0.59
19:X:407:MET:HA	19:X:410:VAL:HG22	1.84	0.59
20:Y:81:LEU:HD13	20:Y:84:LEU:HD13	1.83	0.59
28:A:191:VAL:O	28:A:191:VAL:HG12	2.02	0.59
32:D:380:GLN:NE2	33:E:165:ILE:O	2.31	0.59
2:F:428:GLN:HG3	2:F:430:LYS:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:230:ARG:CB	3:O:230:ARG:HH11	2.14	0.59
19:X:256:LEU:HD23	19:X:256:LEU:O	2.03	0.59
22:a:140:GLU:O	22:a:143:ASN:ND2	2.35	0.59
22:a:289:ARG:HB3	22:a:333:MET:HB2	1.83	0.59
23:b:127:LEU:HA	23:b:130:ARG:HG2	1.83	0.59
32:D:227:PHE:O	32:D:228:ILE:HG13	2.02	0.59
4:G:17:SER:OG	4:G:21:ARG:N	2.35	0.59
5:P:105:THR:O	5:P:126:LEU:HD22	2.02	0.59
10:J:63:CYS:HB2	10:J:88:ARG:HH21	1.67	0.59
16:U:177:LEU:O	16:U:205:TYR:OH	2.20	0.59
17:V:385:LYS:NZ	17:V:389:ASP:OD1	2.36	0.59
25:d:105:PHE:O	25:d:109:GLN:NE2	2.35	0.59
3:O:230:ARG:HB3	3:O:230:ARG:HH11	1.66	0.59
11:S:113:THR:HA	11:S:116:ILE:HD12	1.84	0.59
10:j:47:LYS:HE3	10:j:207:GLU:HB2	1.83	0.59
4:G:52:THR:HG21	4:G:79:VAL:HG21	1.84	0.59
12:K:167:ALA:HB3	14:L:56:LEU:HD13	1.85	0.59
18:W:124:LEU:HD22	18:W:151:THR:HG22	1.83	0.59
20:Y:34:ASP:O	20:Y:38:ARG:NH1	2.35	0.59
21:Z:231:GLN:HA	21:Z:234:PHE:HB2	1.83	0.59
32:D:167:ILE:HD12	35:D:501:ATP:HN61	1.68	0.59
2:F:275:ALA:HB1	2:F:326:VAL:HG11	1.84	0.59
5:P:178:ASP:O	5:P:203:ARG:NH2	2.35	0.59
19:X:376:GLY:HA3	19:X:386:ILE:O	2.02	0.59
20:Y:189:VAL:HG13	20:Y:287:LEU:HD11	1.85	0.59
3:o:140:ALA:HB1	3:o:170:MET:HE1	1.85	0.59
27:f:446:LEU:HD11	27:f:483:PHE:HD2	1.66	0.59
6:h:86:LEU:HD13	6:h:134:LEU:HD11	1.85	0.59
17:V:266:GLN:HA	17:V:295:ILE:HD11	1.85	0.59
22:a:203:ALA:O	22:a:207:GLY:N	2.31	0.59
22:a:343:LEU:HA	22:a:346:ILE:HD12	1.84	0.59
24:c:236:GLU:HA	24:c:239:LYS:HG2	1.84	0.59
28:A:178:GLY:O	28:A:354:ILE:CG2	2.51	0.59
32:D:373:ALA:HA	35:D:501:ATP:C5'	2.32	0.59
3:O:100:GLN:HE22	6:H:99:LEU:HA	1.68	0.59
12:K:117:SER:OG	14:L:82:ARG:NH2	2.35	0.59
3:o:230:ARG:HH11	3:o:230:ARG:CG	2.13	0.59
23:b:18:ASN:OD1	23:b:25:ARG:NE	2.35	0.59
31:C:99:VAL:HA	31:C:123:LEU:HB2	1.85	0.59
33:E:179:GLY:O	33:E:301:ILE:CD1	2.48	0.59
2:F:308:ARG:HG3	33:E:237:ALA:HB1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:263:LEU:HB3	17:V:265:ASP:CG	2.27	0.59
20:Y:49:ASN:HB3	20:Y:52:PRO:HB2	1.85	0.59
1:n:213:ILE:HG12	1:n:218:VAL:HG22	1.85	0.59
27:f:615:ILE:O	27:f:619:HIS:NE2	2.36	0.59
30:B:136:LEU:HG	30:B:138:PHE:H	1.66	0.59
22:a:290:GLN:HA	22:a:332:HIS:HA	1.85	0.58
24:c:164:ASN:ND2	24:c:166:ASN:OD1	2.35	0.58
8:I:198:ASN:HA	8:I:206:LEU:HD21	1.86	0.58
9:R:198:MET:HA	9:R:214:LEU:HD11	1.85	0.58
4:g:33:ASN:HB2	4:g:170:VAL:HG22	1.85	0.58
4:g:146:GLU:HG3	4:g:147:GLN:HG3	1.84	0.58
16:U:247:GLN:NE2	16:U:911:ILE:O	2.36	0.58
20:Y:17:LEU:HD12	20:Y:211:TYR:CE1	2.38	0.58
3:o:228:PHE:CE2	3:o:230:ARG:CD	2.82	0.58
33:E:135:ILE:CD1	33:E:182:LEU:CB	2.81	0.58
2:F:344:ARG:HG3	33:E:176:PRO:HB2	1.85	0.58
9:R:60:THR:N	9:R:228:TYR:O	2.37	0.58
8:i:102:GLN:NE2	5:p:65:GLN:OE1	2.34	0.58
6:h:135:LEU:HG	6:h:163:MET:HE2	1.85	0.58
24:c:219:ASN:O	24:c:222:LYS:NZ	2.36	0.58
13:t:72:LEU:HD22	13:t:229:TYR:HB2	1.85	0.58
28:A:286:ASP:OD2	28:A:293:ASN:ND2	2.36	0.58
28:A:329:PRO:HA	28:A:332:MET:HB2	1.84	0.58
33:E:48:LYS:O	33:E:52:SER:N	2.36	0.58
1:N:55:THR:HG22	1:N:60:ILE:HA	1.84	0.58
16:U:173:VAL:HG13	16:U:177:LEU:HD13	1.85	0.58
28:A:45:ILE:HA	30:B:57:GLN:HG2	1.85	0.58
31:C:376:VAL:HA	32:D:193:GLN:HE22	1.68	0.58
32:D:167:ILE:CD1	35:D:501:ATP:N6	2.67	0.58
10:J:12:PRO:HG2	28:A:430:MET:HE3	1.83	0.58
13:T:119:GLU:OE2	14:L:107:ARG:NH2	2.37	0.58
17:V:322:VAL:HG12	17:V:325:LYS:HB2	1.85	0.58
18:W:186:ILE:HA	18:W:189:GLN:HE22	1.69	0.58
15:m:32:GLU:OE2	15:m:170:ARG:NH2	2.36	0.58
3:o:94:ASP:OD1	5:p:96:TYR:OH	2.21	0.58
27:f:470:VAL:HG22	27:f:482:ILE:CG2	2.28	0.58
16:U:541:HIS:HB2	16:U:544:ILE:HG22	1.85	0.58
22:a:78:GLU:O	22:a:82:HIS:ND1	2.29	0.58
23:b:108:ARG:HH12	23:b:137:ASN:H	1.51	0.58
9:r:66:LYS:HG2	9:r:71:VAL:HG22	1.85	0.58
27:f:415:GLY:HA3	27:f:447:ALA:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:233:THR:CG2	30:B:285:ASP:CG	2.75	0.58
31:C:369:TYR:HA	31:C:372:ARG:HE	1.67	0.58
2:F:89:LEU:O	2:F:153:VAL:HB	2.04	0.58
8:I:38:LEU:HD12	8:I:147:LEU:HD13	1.84	0.58
18:W:227:TYR:HA	18:W:230:MET:HE2	1.86	0.58
22:a:187:ASP:OD1	22:a:193:GLN:NE2	2.36	0.58
22:a:312:MET:HA	22:a:315:LEU:HD12	1.85	0.58
27:f:327:ASN:HD22	27:f:327:ASN:N	1.96	0.58
27:f:756:PRO:C	27:f:758:ASN:N	2.61	0.58
33:E:181:THR:HA	33:E:184:ALA:CB	2.32	0.58
5:P:169:GLN:O	5:P:173:ASN:ND2	2.37	0.58
17:V:74:ASP:O	17:V:78:HIS:NE2	2.36	0.58
18:W:248:ARG:HH22	18:W:289:ARG:HH11	1.50	0.58
19:X:333:GLN:HA	19:X:336:ILE:HG12	1.86	0.58
32:D:202:VAL:HG22	32:D:329:ARG:HB2	1.86	0.58
33:E:146:ARG:HA	33:E:149:ILE:HG22	1.86	0.58
2:F:344:ARG:HD2	33:E:177:GLY:HA3	1.86	0.58
6:H:70:LYS:HD2	6:H:71:HIS:HB3	1.86	0.58
10:J:31:THR:HA	10:J:162:GLY:HA3	1.84	0.58
18:W:7:GLU:O	18:W:10:ASP:HB2	2.04	0.58
25:d:200:PHE:C	25:d:203:PRO:HD3	2.29	0.58
11:s:91:THR:HA	11:s:94:LYS:HE2	1.86	0.58
27:f:276:GLU:O	27:f:286:LYS:NZ	2.36	0.58
8:i:171:ALA:HB2	8:i:200:THR:HG21	1.86	0.58
7:q:118:MET:HE1	7:q:124:LEU:HA	1.86	0.58
27:f:291:GLN:NE2	27:f:320:ILE:CG2	2.67	0.58
28:A:44:GLN:O	30:B:57:GLN:NE2	2.36	0.58
28:A:53:GLN:HE22	28:A:54:GLN:HE21	1.51	0.58
30:B:285:ASP:OD1	30:B:286:GLU:N	2.37	0.58
31:C:228:ALA:HB1	31:C:233:GLU:OE1	2.04	0.58
5:P:77:LYS:HZ1	6:H:113:ARG:HE	1.51	0.57
13:T:54:THR:O	13:T:86:ARG:NH1	2.36	0.57
10:j:208:LEU:HD12	10:j:225:ILE:HG12	1.86	0.57
27:f:373:ALA:HB2	27:f:744:MET:HA	1.86	0.57
23:b:51:LEU:HD23	23:b:71:ILE:HG23	1.85	0.57
23:b:106:LYS:HE3	23:b:135:LYS:HG3	1.86	0.57
24:c:75:MET:SD	24:c:75:MET:N	2.77	0.57
4:G:158:GLY:O	6:H:84:ARG:NH1	2.33	0.57
6:H:68:ILE:HD13	6:H:72:ILE:HG22	1.86	0.57
11:S:52:ALA:HB1	11:S:221:LEU:HD11	1.85	0.57
16:U:51:ASP:O	16:U:57:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:798:PRO:O	16:U:880:ASN:ND2	2.31	0.57
21:Z:25:ARG:O	21:Z:28:LYS:NZ	2.35	0.57
27:f:295:ALA:CB	27:f:323:ASN:HB2	2.31	0.57
13:t:88:MET:HE3	13:t:109:LYS:HD3	1.86	0.57
35:D:501:ATP:PA	35:D:501:ATP:C3'	2.92	0.57
24:c:269:GLN:O	24:c:273:LYS:NZ	2.37	0.57
27:f:55:GLU:HA	27:f:59:LEU:HD12	1.85	0.57
33:E:168:LYS:N	33:E:296:ASP:OD2	2.36	0.57
33:E:322:LYS:HA	33:E:361:PHE:HB2	1.85	0.57
5:P:58:THR:O	7:Q:85:ARG:NH2	2.38	0.57
14:L:77:LEU:HD23	14:L:80:ASP:HB2	1.84	0.57
4:g:72:ILE:HB	4:g:76:ILE:HG23	1.85	0.57
16:U:111:GLN:O	16:U:115:ASN:ND2	2.37	0.57
16:U:574:LYS:O	16:U:579:ARG:NH2	2.38	0.57
16:U:592:GLY:HA3	16:U:627:PHE:HD2	1.68	0.57
10:j:50:VAL:HG11	10:j:56:GLU:HG2	1.87	0.57
22:a:223:GLU:O	22:a:227:ASN:ND2	2.38	0.57
23:b:7:MET:HE2	23:b:52:ILE:HG13	1.84	0.57
16:U:333:MET:SD	16:U:333:MET:N	2.75	0.57
14:l:98:VAL:HA	13:t:139:ARG:HG3	1.85	0.57
20:Y:94:ASN:HD22	30:B:410:ARG:HD2	1.69	0.57
26:e:53:SER:HA	26:e:57:ARG:HH22	1.69	0.57
13:t:144:ARG:HB3	13:t:150:PRO:HA	1.87	0.57
32:D:373:ALA:HB1	35:D:501:ATP:H5'2	1.87	0.57
3:O:84:ILE:HG12	3:O:119:VAL:HG22	1.86	0.57
12:K:168:ARG:HA	12:K:178:GLN:HE22	1.69	0.57
16:U:898:CYS:SG	16:U:899:ARG:N	2.77	0.57
17:V:148:ARG:HH22	17:V:197:THR:HB	1.69	0.57
17:V:337:LEU:HD13	17:V:367:VAL:HG21	1.87	0.57
18:W:114:GLU:HG3	18:W:115:ILE:HG23	1.87	0.57
15:m:176:GLU:HB3	15:m:197:ILE:HG12	1.87	0.57
28:A:407:LYS:NZ	28:A:411:GLU:OE2	2.38	0.57
16:U:144:ASP:O	16:U:145:HIS:ND1	2.38	0.57
18:W:11:GLY:O	18:W:15:LYS:NZ	2.37	0.57
18:W:94:ARG:HA	18:W:98:LYS:HG3	1.86	0.57
32:D:349:THR:HB	32:D:354:LEU:HD11	1.86	0.57
7:Q:104:LEU:HB2	7:Q:116:TYR:HB2	1.87	0.57
14:L:146:GLN:HG3	14:L:159:MET:HG2	1.87	0.57
18:W:9:ALA:HA	18:W:12:ARG:HB2	1.87	0.57
27:f:412:ALA:HB2	27:f:446:LEU:HD23	1.86	0.57
31:C:190:GLY:N	31:C:196:LYS:HZ1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:79:MET:HE1	32:D:417:TYR:HA	1.87	0.57
23:b:7:MET:HE3	23:b:60:VAL:CB	2.35	0.57
9:r:80:THR:HA	9:r:86:ALA:H	1.70	0.57
27:f:79:ARG:HG2	27:f:82:ILE:HG12	1.86	0.57
28:A:100:LYS:HB3	28:A:114:ASN:HB3	1.87	0.57
33:E:49:ALA:HA	33:E:52:SER:HB2	1.87	0.57
33:E:122:MET:HE2	33:E:198:VAL:HG12	1.86	0.57
16:U:242:LEU:HG	16:U:245:ALA:HB3	1.87	0.56
17:V:159:LEU:O	17:V:163:VAL:N	2.38	0.56
14:l:107:ARG:NH2	13:t:124:ASP:OD2	2.38	0.56
32:D:314:ALA:HA	32:D:317:LEU:HD23	1.87	0.56
32:D:401:LYS:O	32:D:405:THR:OG1	2.22	0.56
2:F:435:LEU:HB3	2:F:438:TYR:HE2	1.70	0.56
5:P:62:THR:OG1	7:Q:85:ARG:NH2	2.37	0.56
17:V:311:ASN:O	17:V:315:LYS:HB2	2.04	0.56
19:X:133:LEU:HD11	19:X:149:LEU:HD11	1.87	0.56
21:Z:74:TYR:HE1	24:c:98:MET:HB3	1.70	0.56
3:O:230:ARG:HH11	3:O:230:ARG:C	2.14	0.56
10:J:103:THR:HG23	10:J:106:TYR:H	1.69	0.56
12:K:235:GLU:N	12:K:235:GLU:OE1	2.35	0.56
14:L:61:LYS:NZ	14:L:63:ILE:O	2.36	0.56
16:U:259:GLN:NE2	16:U:487:GLY:O	2.39	0.56
6:h:111:VAL:HG22	6:h:136:ILE:HD12	1.86	0.56
17:V:418:SER:HA	17:V:457:TYR:HA	1.86	0.56
19:X:285:GLU:HA	19:X:288:LYS:HG2	1.87	0.56
20:Y:17:LEU:HD12	20:Y:211:TYR:HE1	1.69	0.56
20:Y:22:LEU:HA	20:Y:25:LEU:HB2	1.87	0.56
21:Z:243:GLN:O	21:Z:247:LYS:NZ	2.36	0.56
1:n:53:ARG:NH1	1:n:202:GLY:O	2.37	0.56
5:p:158:MET:HE2	5:p:163:LEU:HA	1.87	0.56
9:r:103:THR:HG21	9:r:159:MET:HE3	1.87	0.56
11:s:173:LEU:HD11	11:s:210:ALA:HB2	1.87	0.56
27:f:414:LEU:HA	27:f:417:ILE:HD12	1.87	0.56
30:B:173:VAL:HG21	31:C:233:GLU:HG2	1.87	0.56
32:D:117:SER:HA	32:D:121:ARG:HH22	1.70	0.56
8:i:194:ILE:HG13	8:i:236:LEU:HB3	1.86	0.56
12:k:103:TYR:HB3	12:k:105:GLU:HG2	1.88	0.56
16:U:93:ASN:HB2	16:U:140:ARG:HH22	1.70	0.56
21:Z:206:LEU:HD22	21:Z:209:ARG:HH21	1.70	0.56
5:p:11:VAL:HG11	5:p:52:GLY:HA3	1.86	0.56
9:r:140:LYS:NZ	9:r:144:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:233:LYS:CB	2:F:354:PHE:CE2	2.89	0.56
2:F:252:ALA:HB3	2:F:255:GLN:HB2	1.88	0.56
15:M:66:ARG:HB3	15:M:78:VAL:HB	1.87	0.56
27:f:790:GLN:O	27:f:795:GLY:N	2.38	0.56
28:A:103:ASN:HB3	28:A:112:ILE:HD13	1.88	0.56
22:a:197:ALA:HA	22:a:200:LEU:HB2	1.86	0.56
5:p:15:LYS:HE3	5:p:119:PRO:HB2	1.86	0.56
25:d:95:MET:HA	25:d:98:LEU:HD12	1.88	0.56
25:d:122:LEU:HD13	25:d:125:LYS:H	1.70	0.56
27:f:347:ASP:O	27:f:351:THR:N	2.39	0.56
27:f:412:ALA:CB	27:f:446:LEU:HD23	2.36	0.56
2:F:289:ASP:OD1	2:F:289:ASP:N	2.38	0.56
9:R:78:ARG:NH1	9:R:227:ALA:O	2.39	0.56
14:L:148:CYS:SG	14:L:150:SER:OG	2.63	0.56
6:h:89:ARG:HE	6:h:93:LEU:HG	1.71	0.56
15:m:70:VAL:HG23	15:m:76:MET:HB2	1.88	0.56
27:f:743:ALA:HA	27:f:746:ARG:HH21	1.71	0.56
31:C:190:GLY:N	31:C:196:LYS:NZ	2.54	0.56
4:G:127:GLN:OE1	6:H:128:ARG:NH2	2.39	0.56
13:T:70:ASP:OD1	13:T:86:ARG:NH2	2.38	0.56
16:U:642:GLU:O	31:C:53:ASN:ND2	2.39	0.56
17:V:316:ALA:HB1	17:V:318:GLN:HE22	1.71	0.56
18:W:259:GLU:OE1	18:W:262:LYS:NZ	2.39	0.56
5:p:12:MET:HB2	5:p:138:VAL:HG12	1.88	0.56
3:O:218:LEU:HD11	3:O:232:TYR:CE2	2.40	0.56
13:t:154:THR:HG23	13:t:171:ASP:HA	1.88	0.56
28:A:415:LYS:HA	28:A:419:SER:HB3	1.87	0.56
30:B:165:ASP:OD1	30:B:165:ASP:N	2.39	0.56
5:P:149:MET:O	5:P:153:LEU:HB2	2.06	0.55
6:H:68:ILE:HD11	6:H:74:LEU:CD1	2.20	0.55
16:U:46:GLU:OE1	16:U:80:TYR:OH	2.24	0.55
11:s:56:ARG:NH1	11:s:215:VAL:O	2.36	0.55
32:D:152:MET:HE3	32:D:257:ASN:HD21	1.70	0.55
7:Q:55:GLN:OE1	9:R:140:LYS:NZ	2.40	0.55
18:W:144:ARG:HA	18:W:147:LYS:HE3	1.87	0.55
20:Y:68:ASP:N	20:Y:68:ASP:OD1	2.39	0.55
22:a:50:PHE:HB3	22:a:52:GLN:HB3	1.87	0.55
27:f:438:ASP:HB3	27:f:476:THR:HG21	1.88	0.55
27:f:828:ARG:HD2	27:f:843:SER:HB3	1.88	0.55
32:D:96:VAL:HG23	32:D:102:ILE:HD11	1.88	0.55
1:N:53:ARG:NH1	1:N:202:GLY:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:149:PRO:HD2	1:N:153:MET:HB2	1.88	0.55
2:F:380:ASN:H	2:F:417:HIS:CE1	2.25	0.55
20:Y:154:ASN:HA	20:Y:157:ILE:HG12	1.87	0.55
22:a:293:PHE:HE1	22:a:331:VAL:HG23	1.71	0.55
24:c:176:GLN:OE1	24:c:176:GLN:N	2.39	0.55
7:q:108:ASP:HB3	7:q:111:GLU:HG2	1.87	0.55
4:G:189:TRP:HZ3	4:G:197:THR:HG21	1.72	0.55
9:R:60:THR:O	9:R:189:SER:N	2.38	0.55
4:g:80:MET:HE2	4:g:87:SER:HA	1.88	0.55
18:W:344:THR:OG1	18:W:345:GLU:OE1	2.24	0.55
22:a:175:ASP:OD1	22:a:178:ARG:NE	2.38	0.55
22:a:286:ALA:HA	22:a:289:ARG:HG3	1.87	0.55
27:f:307:LEU:HD11	27:f:311:VAL:N	2.21	0.55
13:t:96:LEU:HD22	13:t:157:ILE:HG22	1.88	0.55
28:A:81:ALA:HB3	30:B:137:SER:HB2	1.87	0.55
33:E:313:LEU:HB3	33:E:343:LEU:HD23	1.89	0.55
1:N:224:LEU:HD13	13:t:254:TRP:HB2	1.88	0.55
3:O:62:ARG:NH1	3:O:210:LEU:O	2.40	0.55
16:U:126:ILE:HG23	16:U:130:LEU:HD23	1.87	0.55
17:V:400:HIS:ND1	25:d:144:MET:O	2.40	0.55
22:a:150:SER:HB2	22:a:154:ARG:HH21	1.71	0.55
11:s:212:GLU:HA	11:s:239:ARG:HH11	1.71	0.55
2:F:424:ILE:HD12	2:F:427:VAL:HB	1.88	0.55
8:I:68:LEU:HD23	8:I:91:ARG:HE	1.72	0.55
10:J:108:THR:HG22	10:J:133:ILE:HG13	1.88	0.55
17:V:437:ILE:HA	25:d:146:GLY:HA3	1.88	0.55
14:l:41:LYS:HG3	14:l:42:THR:HG23	1.88	0.55
27:f:83:ARG:O	27:f:87:THR:OG1	2.24	0.55
28:A:169:LYS:HB2	28:A:231:ASN:HA	1.87	0.55
28:A:172:VAL:O	28:A:231:ASN:ND2	2.38	0.55
32:D:267:ILE:O	32:D:271:ALA:N	2.39	0.55
6:H:68:ILE:HG23	6:H:91:ARG:HA	1.87	0.55
16:U:603:LEU:CD1	16:U:604:HIS:N	2.64	0.55
20:Y:156:LEU:O	20:Y:160:ASN:ND2	2.40	0.55
21:Z:234:PHE:HZ	22:a:353:LEU:HB3	1.72	0.55
1:n:63:ARG:HG3	1:n:64:VAL:HG13	1.88	0.55
5:p:48:ARG:HD3	5:p:112:LEU:HD12	1.89	0.55
9:r:100:LEU:HD12	9:r:162:GLY:HA3	1.89	0.55
32:D:163:MET:HA	32:D:222:HIS:HE1	1.72	0.55
1:N:118:LYS:NZ	13:T:106:GLN:OE1	2.39	0.55
10:J:10:PHE:O	12:K:10:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:66:VAL:HB	14:L:70:ILE:HG23	1.88	0.55
18:W:376:LYS:NZ	18:W:380:GLN:OE1	2.40	0.55
21:Z:82:PHE:HA	21:Z:85:VAL:HG12	1.88	0.55
33:E:231:PHE:HD1	33:E:276:ILE:HG23	1.72	0.55
4:G:132:ARG:HB3	15:M:125:LEU:HD12	1.89	0.55
4:g:88:ARG:NH1	15:m:118:MET:CE	2.70	0.55
6:h:71:HIS:ND1	6:h:139:TRP:O	2.39	0.55
14:l:68:ASN:OD1	14:l:96:ARG:NH2	2.40	0.55
24:c:46:ARG:NH1	24:c:46:ARG:O	2.40	0.55
7:q:4:LEU:HD22	7:q:45:LEU:HD22	1.88	0.55
27:f:343:LYS:NZ	27:f:385:PHE:O	2.36	0.55
33:E:97:ARG:NH2	33:E:112:PRO:O	2.34	0.55
33:E:182:LEU:O	33:E:186:ALA:N	2.39	0.55
1:N:228:ILE:O	1:N:230:LYS:NZ	2.38	0.55
8:I:119:GLN:NE2	10:J:79:ASP:OD1	2.39	0.55
13:T:56:VAL:HG23	13:T:69:ALA:HB2	1.89	0.55
15:M:9:ASP:N	15:M:9:ASP:OD1	2.40	0.55
12:k:74:ILE:HG12	12:k:109:VAL:HG22	1.89	0.55
19:X:249:THR:HA	19:X:252:LYS:HG2	1.89	0.55
14:l:65:HIS:NE2	14:l:220:GLU:OE2	2.40	0.55
20:Y:88:LEU:HB2	20:Y:100:ILE:HG23	1.87	0.55
24:c:226:MET:N	24:c:226:MET:SD	2.80	0.55
9:r:166:ARG:NH2	9:r:168:PRO:O	2.39	0.55
27:f:414:LEU:HA	27:f:417:ILE:CD1	2.36	0.55
33:E:61:LEU:HB2	33:E:70:ILE:HG23	1.88	0.55
2:F:168:TYR:HB2	2:F:173:LYS:HE2	1.90	0.54
3:O:93:ALA:HB2	5:P:129:CYS:HB2	1.88	0.54
19:X:357:SER:OG	19:X:358:LYS:N	2.41	0.54
27:f:305:LEU:HD22	27:f:305:LEU:H	1.73	0.54
33:E:144:GLU:OE2	33:E:297:ARG:NH1	2.40	0.54
2:F:151:VAL:HG12	2:F:163:THR:HA	1.90	0.54
2:F:357:PRO:O	2:F:362:ARG:NH1	2.40	0.54
5:P:123:SER:HB3	5:P:137:VAL:HB	1.89	0.54
6:H:74:LEU:HD22	6:H:74:LEU:C	2.31	0.54
16:U:415:HIS:CE1	16:U:418:GLU:HG2	2.42	0.54
17:V:114:TYR:HA	17:V:117:VAL:HG12	1.89	0.54
10:j:31:THR:OG1	10:j:163:ARG:O	2.24	0.54
18:W:3:ASP:HA	18:W:47:LEU:HD21	1.88	0.54
18:W:308:LEU:HD22	18:W:308:LEU:C	2.33	0.54
27:f:131:MET:N	27:f:131:MET:SD	2.80	0.54
27:f:438:ASP:HB3	27:f:476:THR:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:233:THR:C	30:B:236:ALA:HB3	2.33	0.54
32:D:214:MET:HE1	35:D:501:ATP:N7	2.13	0.54
8:i:201:MET:HE1	8:i:210:LYS:HB3	1.89	0.54
19:X:218:HIS:NE2	19:X:227:THR:OG1	2.40	0.54
1:N:87:GLN:HE22	3:O:161:SER:HA	1.72	0.54
16:U:350:LEU:HD12	16:U:385:PHE:HE1	1.72	0.54
16:U:609:ASP:O	16:U:615:ARG:NH1	2.39	0.54
12:k:52:LYS:NZ	12:k:61:PRO:O	2.35	0.54
1:n:138:ASP:OD2	1:n:144:GLN:NE2	2.39	0.54
3:o:44:THR:N	3:o:172:SER:OG	2.39	0.54
31:C:76:VAL:HG12	31:C:112:CYS:H	1.73	0.54
6:H:222:THR:HG22	6:H:224:THR:H	1.71	0.54
9:R:67:PHE:CE1	9:R:72:ILE:HG12	2.43	0.54
12:K:79:SER:OG	12:K:140:ALA:O	2.26	0.54
13:T:181:SER:HB2	13:T:195:LEU:HD13	1.89	0.54
4:g:21:ARG:HH12	4:g:25:VAL:HB	1.73	0.54
16:U:603:LEU:HD12	16:U:604:HIS:CA	2.38	0.54
21:Z:84:LYS:HG2	24:c:76:PRO:HG3	1.90	0.54
1:n:149:PRO:HG2	1:n:153:MET:HE2	1.88	0.54
24:c:151:VAL:HG21	32:D:80:LYS:HB3	1.89	0.54
27:f:92:VAL:HG13	27:f:129:LEU:HD12	1.89	0.54
29:u:402:LYS:O	29:u:406:ARG:CG	2.46	0.54
32:D:160:PRO:HD2	32:D:221:HIS:HB2	1.89	0.54
32:D:167:ILE:HD12	35:D:501:ATP:N6	2.22	0.54
33:E:101:ASP:HB2	33:E:106:THR:H	1.71	0.54
33:E:168:LYS:NZ	33:E:264:MET:O	2.38	0.54
4:G:161:CYS:SG	4:G:162:GLY:N	2.80	0.54
19:X:198:ASN:HB2	31:C:392:GLN:HG3	1.89	0.54
20:Y:83:ARG:HA	20:Y:86:GLU:HB3	1.90	0.54
27:f:91:SER:HB3	27:f:110:TYR:HD1	1.73	0.54
28:A:143:ASP:HB3	28:A:147:TYR:H	1.73	0.54
30:B:222:VAL:HG22	30:B:349:ARG:HB2	1.89	0.54
16:U:469:SER:OG	16:U:470:ASN:N	2.40	0.54
20:Y:76:ALA:O	20:Y:79:ASP:HB2	2.08	0.54
9:r:198:MET:HA	9:r:214:LEU:HD11	1.89	0.54
1:N:60:ILE:O	13:t:224:ARG:NH1	2.40	0.54
10:j:109:ARG:NH1	9:r:128:ARG:O	2.41	0.54
14:l:120:THR:HG22	14:l:127:PRO:HG3	1.88	0.54
14:l:215:VAL:HB	14:l:221:PHE:HD1	1.72	0.54
5:p:12:MET:N	5:p:12:MET:SD	2.80	0.54
26:e:53:SER:OG	26:e:61:GLU:OE2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:288:VAL:HA	27:f:291:GLN:HG2	1.89	0.54
30:B:229:GLY:HA3	31:C:307:ARG:NH2	2.23	0.54
31:C:185:GLY:N	31:C:312:ASP:OD2	2.36	0.54
2:F:318:ASP:CB	2:F:347:ARG:HG2	2.34	0.54
2:F:334:ARG:NH1	28:A:284:ARG:O	2.41	0.54
2:F:416:THR:OG1	2:F:419:ASP:OD2	2.26	0.54
8:i:118:LYS:HE2	8:i:152:PRO:HA	1.90	0.54
24:c:56:LEU:HD21	24:c:108:VAL:HG23	1.89	0.54
30:B:251:VAL:HG12	30:B:253:SER:H	1.72	0.54
32:D:345:PHE:HB3	32:D:360:LEU:HD23	1.89	0.54
4:G:165:ALA:HB3	4:G:179:LEU:HD21	1.89	0.54
13:T:256:ILE:HG23	1:n:64:VAL:HG11	1.90	0.54
4:g:141:ILE:HG22	4:g:151:VAL:HG22	1.90	0.54
6:h:22:ILE:HD13	6:h:152:SER:HA	1.89	0.54
20:Y:105:MET:HE2	20:Y:127:THR:HB	1.89	0.54
24:c:46:ARG:O	33:E:85:ARG:NH1	2.41	0.54
9:r:238:VAL:HA	9:r:243:TRP:HA	1.90	0.54
27:f:446:LEU:HD11	27:f:483:PHE:CD2	2.44	0.54
3:O:257:GLU:OE1	3:O:257:GLU:N	2.41	0.53
4:g:122:SER:HA	4:g:125:TYR:HD2	1.73	0.53
6:h:51:LYS:NZ	6:h:52:GLN:O	2.36	0.53
18:W:407:ASP:OD1	19:X:343:SER:N	2.35	0.53
12:k:5:ARG:HH12	14:l:5:GLN:HA	1.71	0.53
21:Z:16:LEU:N	21:Z:16:LEU:HD12	2.23	0.53
23:b:69:GLY:HA2	23:b:72:LEU:HD12	1.90	0.53
11:s:153:ASP:OD1	11:s:157:SER:N	2.41	0.53
11:s:159:GLN:NE2	11:s:161:ASP:OD1	2.41	0.53
1:N:102:ILE:HG23	4:G:95:ARG:HH11	1.73	0.53
2:F:320:PHE:CD1	33:E:185:ARG:CD	2.72	0.53
5:P:11:VAL:HB	5:P:139:SER:HB3	1.91	0.53
5:P:177:ARG:HH21	11:s:174:GLN:HG2	1.74	0.53
11:S:50:ILE:HD11	11:S:223:ILE:HG23	1.90	0.53
4:g:150:GLN:HB3	4:g:152:TYR:HE1	1.74	0.53
17:V:292:THR:HA	17:V:295:ILE:HG22	1.90	0.53
17:V:423:ALA:HA	17:V:426:LEU:HB2	1.90	0.53
22:a:363:MET:HE3	24:c:307:VAL:HG12	1.89	0.53
23:b:68:THR:HA	23:b:71:ILE:HD12	1.90	0.53
7:q:78:THR:O	7:q:82:ASN:ND2	2.40	0.53
25:d:49:ILE:HG12	25:d:52:ARG:HH21	1.73	0.53
27:f:258:LYS:NZ	27:f:771:LEU:O	2.41	0.53
28:A:330:ALA:O	28:A:336:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C:214:VAL:HG22	31:C:216:GLY:H	1.73	0.53
33:E:185:ARG:CB	33:E:185:ARG:CZ	2.85	0.53
2:F:345:SER:HB2	33:E:342:ASP:HB3	1.90	0.53
17:V:149:PRO:HA	17:V:203:LEU:HD21	1.90	0.53
22:a:176:ALA:HB1	22:a:200:LEU:HD22	1.91	0.53
27:f:307:LEU:HD21	27:f:311:VAL:CG2	2.37	0.53
27:f:434:TYR:CG	27:f:434:TYR:O	2.60	0.53
27:f:669:GLU:OE1	27:f:705:ASN:ND2	2.40	0.53
31:C:191:PRO:O	31:C:194:THR:HB	2.08	0.53
32:D:401:LYS:HA	32:D:404:LYS:HG2	1.89	0.53
3:O:64:THR:HG22	3:O:69:VAL:HG22	1.90	0.53
7:Q:52:ASP:OD1	9:R:147:TYR:OH	2.25	0.53
14:l:109:VAL:HG21	14:l:145:PHE:HD2	1.73	0.53
22:a:188:LEU:O	22:a:193:GLN:NE2	2.41	0.53
5:p:107:PRO:HG2	5:p:124:LEU:HB2	1.89	0.53
24:c:39:LEU:HD13	24:c:42:LEU:HD21	1.89	0.53
28:A:274:PHE:HB3	28:A:277:ILE:HD11	1.91	0.53
31:C:199:LEU:HD23	31:C:199:LEU:O	2.08	0.53
31:C:241:HIS:O	31:C:244:SER:OG	2.23	0.53
2:F:234:THR:OG1	34:F:501:ADP:O3A	2.24	0.53
13:T:237:VAL:HA	13:T:241:GLY:O	2.08	0.53
27:f:581:GLU:HG2	27:f:582:VAL:HG13	1.91	0.53
30:B:108:SER:OG	30:B:153:ASN:O	2.22	0.53
30:B:363:ARG:NH1	30:B:366:GLN:OE1	2.41	0.53
31:C:184:LYS:N	31:C:312:ASP:OD2	2.41	0.53
12:K:206:MET:O	28:A:369:ARG:NH2	2.42	0.53
16:U:730:ALA:O	16:U:734:GLN:NE2	2.42	0.53
14:l:203:GLN:NE2	14:l:204:ASP:O	2.41	0.53
22:a:198:PHE:HD1	22:a:233:LEU:HD21	1.73	0.53
27:f:398:TRP:HE1	27:f:403:LYS:HE3	1.73	0.53
27:f:885:GLU:CD	27:f:886:GLU:H	2.15	0.53
2:F:292:GLY:O	2:F:339:ASP:N	2.41	0.53
12:K:108:THR:HG23	12:K:111:SER:H	1.73	0.53
13:T:133:ILE:HA	13:T:136:TRP:CD1	2.44	0.53
14:L:50:LYS:HG2	14:L:59:HIS:HB3	1.90	0.53
16:U:413:LYS:NZ	16:U:780:SER:O	2.42	0.53
23:b:44:ASN:C	23:b:44:ASN:HD22	2.15	0.53
5:p:85:TYR:HA	5:p:88:MET:HG3	1.91	0.53
25:d:3:GLU:H	25:d:25:ARG:HH21	1.57	0.53
25:d:200:PHE:O	25:d:202:THR:N	2.42	0.53
27:f:138:GLU:HA	27:f:142:TYR:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:322:SER:C	27:f:324:VAL:N	2.67	0.53
27:f:446:LEU:HD13	27:f:483:PHE:HD2	1.72	0.53
32:D:89:ILE:HG21	33:E:78:ARG:HB2	1.91	0.53
15:M:196:LYS:NZ	15:M:243:SER:O	2.37	0.53
14:l:50:LYS:HB3	14:l:59:HIS:HB3	1.91	0.53
22:a:239:ALA:O	22:a:243:GLY:N	2.36	0.53
23:b:25:ARG:NH2	23:b:145:GLU:OE1	2.41	0.53
31:C:134:LEU:HD13	31:C:237:MET:HE1	1.90	0.53
10:J:65:LEU:HB2	10:J:69:VAL:HG13	1.91	0.53
12:K:21:LEU:HD22	12:K:23:GLN:HE22	1.72	0.53
17:V:479:ARG:NH1	20:Y:374:ASP:OD1	2.42	0.53
20:Y:17:LEU:HD21	20:Y:146:ARG:CG	2.39	0.53
24:c:151:VAL:HG13	24:c:154:LYS:H	1.74	0.53
27:f:169:GLU:HA	27:f:172:GLU:HG3	1.90	0.53
27:f:307:LEU:HD11	27:f:311:VAL:H	1.73	0.53
27:f:414:LEU:O	27:f:417:ILE:HB	2.08	0.53
28:A:180:CYS:HB3	28:A:183:GLN:HB2	1.91	0.53
31:C:246:ILE:HB	31:C:291:VAL:HA	1.91	0.53
32:D:163:MET:HG3	32:D:165:ALA:H	1.74	0.53
4:G:155:ASP:OD1	4:G:159:TYR:N	2.40	0.53
17:V:338:LEU:O	17:V:401:ASN:ND2	2.42	0.53
15:m:109:LEU:HD11	15:m:138:LEU:HB3	1.90	0.53
3:o:54:GLY:HA2	3:o:151:PRO:HB3	1.91	0.53
3:o:97:MET:HE2	5:p:99:ARG:HH21	1.74	0.53
9:r:60:THR:N	9:r:228:TYR:O	2.42	0.53
28:A:184:ILE:O	28:A:188:ARG:HG2	2.09	0.53
32:D:106:THR:HG23	33:E:77:PRO:HB3	1.91	0.53
32:D:336:PRO:HB3	32:D:340:GLN:HB2	1.90	0.53
32:D:397:LYS:O	32:D:401:LYS:NZ	2.32	0.53
2:F:78:GLU:HA	2:F:81:LYS:HG2	1.90	0.52
18:W:224:LEU:HD12	18:W:253:THR:HB	1.89	0.52
19:X:117:ALA:O	19:X:121:LYS:N	2.42	0.52
27:f:19:ALA:O	27:f:23:GLY:N	2.42	0.52
27:f:80:ARG:NH1	27:f:80:ARG:O	2.42	0.52
27:f:326:LEU:HB3	27:f:329:ASN:HB3	1.90	0.52
32:D:171:ASP:OD1	32:D:171:ASP:N	2.42	0.52
32:D:285:VAL:HA	32:D:288:ILE:HG22	1.91	0.52
6:H:71:HIS:HA	6:H:218:PHE:H	1.74	0.52
13:T:141:MET:HE1	13:T:151:LEU:H	1.73	0.52
8:i:174:MET:O	8:i:178:ASP:HB2	2.09	0.52
16:U:87:LEU:O	16:U:91:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:6:SER:O	18:W:9:ALA:HB3	2.09	0.52
18:W:362:ASN:HA	18:W:365:ILE:HG12	1.90	0.52
27:f:416:MET:HE1	27:f:804:LEU:HD13	1.88	0.52
32:D:151:ILE:H	32:D:151:ILE:CD1	2.06	0.52
4:G:138:MET:SD	4:G:140:LEU:HG	2.49	0.52
8:i:196:VAL:O	8:i:200:THR:OG1	2.28	0.52
6:h:134:LEU:O	6:h:148:GLN:HA	2.09	0.52
18:W:135:LYS:HG2	18:W:136:ILE:H	1.73	0.52
31:C:184:LYS:HB3	31:C:280:LEU:CD2	2.40	0.52
1:N:78:CYS:HB2	1:N:133:ILE:HB	1.91	0.52
9:R:225:ARG:HH21	7:q:144:ASP:HB2	1.75	0.52
6:h:11:THR:HG22	6:h:19:LEU:HD22	1.92	0.52
32:D:65:GLN:HG3	32:D:69:LYS:HZ2	1.75	0.52
1:N:37:ILE:HB	1:N:78:CYS:HB3	1.92	0.52
5:P:203:ARG:NH1	5:P:205:ASP:O	2.38	0.52
12:K:173:ALA:HB2	28:A:375:ARG:HD3	1.90	0.52
4:g:88:ARG:NH2	15:m:121:HIS:HB3	2.24	0.52
17:V:282:ASN:ND2	20:Y:389:MET:O	2.42	0.52
17:V:415:SER:HB2	20:Y:346:LYS:HG3	1.92	0.52
19:X:70:LEU:HD23	19:X:109:LEU:HD22	1.90	0.52
20:Y:122:THR:HA	20:Y:125:ARG:HE	1.74	0.52
3:o:94:ASP:HB3	3:o:137:ILE:HG23	1.91	0.52
23:b:24:THR:O	23:b:27:GLN:NE2	2.42	0.52
27:f:247:ALA:HB1	27:f:249:LEU:HD23	1.91	0.52
3:O:210:LEU:HD22	11:s:215:VAL:HG22	1.91	0.52
5:P:34:MET:HE2	5:P:37:THR:HG22	1.90	0.52
5:P:101:GLY:O	7:Q:93:ARG:NH1	2.42	0.52
6:H:133:SER:OG	6:H:148:GLN:NE2	2.43	0.52
10:j:67:ASP:OD2	10:j:95:ARG:NH2	2.43	0.52
25:d:125:LYS:O	25:d:129:THR:OG1	2.28	0.52
9:r:238:VAL:HG22	9:r:243:TRP:HB3	1.91	0.52
27:f:640:LYS:HD2	27:f:651:GLY:HA3	1.92	0.52
30:B:113:GLU:OE1	30:B:113:GLU:N	2.42	0.52
33:E:185:ARG:CB	33:E:185:ARG:NH1	2.73	0.52
2:F:141:ASP:OD1	2:F:141:ASP:N	2.43	0.52
10:j:171:PHE:O	10:j:175:ASN:HB2	2.09	0.52
20:Y:17:LEU:CD1	20:Y:146:ARG:HG3	2.33	0.52
15:m:50:VAL:HG11	15:m:66:ARG:HB2	1.92	0.52
28:A:372:LEU:HD13	28:A:375:ARG:HD2	1.91	0.52
30:B:234:LEU:HB2	35:B:501:ATP:O1A	2.09	0.52
16:U:229:VAL:HA	16:U:232:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:179:ASN:HB3	6:h:182:LEU:HG	1.91	0.52
28:A:89:SER:OG	28:A:90:GLU:OE2	2.28	0.52
4:G:62:ASP:O	4:G:65:THR:OG1	2.26	0.52
16:U:505:ASP:HB3	16:U:508:THR:HG22	1.92	0.52
3:o:181:PHE:O	3:o:185:PHE:N	2.42	0.52
9:r:68:ARG:NH1	9:r:207:GLU:OE2	2.42	0.52
27:f:39:LYS:NZ	27:f:84:SER:O	2.42	0.52
27:f:418:LEU:CD2	27:f:418:LEU:H	2.23	0.52
27:f:472:HIS:ND1	27:f:477:MET:HE3	2.19	0.52
27:f:701:ASN:HB2	27:f:705:ASN:HD21	1.75	0.52
27:f:866:GLN:O	28:A:366:ARG:NH1	2.43	0.52
33:E:173:TYR:HA	33:E:180:LYS:HZ1	1.75	0.52
5:P:181:SER:O	5:P:203:ARG:NH2	2.42	0.52
6:H:81:PRO:HA	6:H:84:ARG:HG2	1.92	0.52
19:X:360:ASP:N	19:X:360:ASP:OD1	2.42	0.52
19:X:401:LEU:HD22	19:X:401:LEU:O	2.08	0.52
27:f:218:GLU:HA	27:f:221:ILE:HG12	1.91	0.52
27:f:862:ILE:H	27:f:862:ILE:HD12	1.75	0.52
30:B:211:TYR:HA	30:B:214:MET:HB2	1.92	0.52
30:B:285:ASP:CG	30:B:286:GLU:CD	2.77	0.52
31:C:83:LYS:HB2	31:C:99:VAL:HG12	1.91	0.52
2:F:79:LYS:O	2:F:83:ASN:HB2	2.10	0.51
21:Z:242:LEU:HG	21:Z:244:GLU:H	1.75	0.51
5:p:143:ALA:HA	5:p:146:MET:HE2	1.92	0.51
25:d:91:GLU:HG2	25:d:92:SER:H	1.75	0.51
11:s:195:SER:OG	11:s:197:ASP:OD1	2.26	0.51
29:u:403:ARG:C	29:u:406:ARG:HG3	2.35	0.51
29:u:403:ARG:CA	29:u:406:ARG:HG3	2.41	0.51
17:V:419:LEU:HD22	17:V:435:GLU:HA	1.92	0.51
21:Z:25:ARG:HE	24:c:104:ARG:H	1.57	0.51
22:a:249:GLN:HA	22:a:252:LYS:HB3	1.92	0.51
27:f:679:LEU:O	27:f:715:HIS:ND1	2.43	0.51
31:C:65:LEU:O	32:D:114:ARG:NH2	2.38	0.51
2:F:347:ARG:HH21	35:E:401:ATP:PG	2.34	0.51
12:k:68:VAL:HG21	12:k:89:ILE:HG13	1.91	0.51
20:Y:17:LEU:HD21	20:Y:146:ARG:HG3	1.92	0.51
22:a:16:PRO:HG2	22:a:47:ASP:HB2	1.91	0.51
22:a:100:THR:HA	22:a:103:LYS:HG2	1.92	0.51
27:f:307:LEU:HD13	27:f:310:ASP:OD1	2.10	0.51
30:B:107:MET:HG3	31:C:96:VAL:H	1.75	0.51
3:O:230:ARG:HB3	3:O:231:PRO:CD	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:63:ASN:O	7:Q:66:LEU:HB2	2.11	0.51
13:T:187:GLY:O	13:T:191:ALA:N	2.43	0.51
14:L:39:LYS:HE3	14:L:142:PRO:HB2	1.91	0.51
16:U:490:ARG:HB2	16:U:493:VAL:HG12	1.92	0.51
17:V:410:ILE:HD11	17:V:426:LEU:HD21	1.91	0.51
10:j:209:ALA:HB1	10:j:217:LEU:HD11	1.91	0.51
19:X:268:GLN:O	19:X:272:SER:OG	2.26	0.51
22:a:13:ASN:HA	22:a:18:GLN:HG2	1.93	0.51
22:a:80:ILE:HA	22:a:83:VAL:HG22	1.91	0.51
28:A:50:ASP:OD1	28:A:50:ASP:N	2.43	0.51
28:A:351:ARG:NH1	28:A:378:PRO:O	2.43	0.51
31:C:163:GLU:HA	31:C:167:LEU:HD12	1.91	0.51
4:G:221:THR:HG22	4:G:223:GLU:H	1.76	0.51
11:S:142:ASP:OD1	11:S:146:LYS:N	2.44	0.51
8:i:18:LEU:HD22	8:i:21:VAL:HG23	1.91	0.51
15:M:176:GLU:HA	15:M:179:LYS:HE3	1.93	0.51
14:l:5:GLN:HG2	15:m:10:LEU:HD21	1.92	0.51
20:Y:39:ASP:OD1	20:Y:39:ASP:N	2.42	0.51
27:f:420:TRP:HZ2	27:f:806:VAL:O	1.92	0.51
28:A:129:VAL:HG12	28:A:149:ILE:HD13	1.91	0.51
30:B:221:GLY:O	30:B:348:ASP:N	2.35	0.51
17:V:450:SER:OG	17:V:451:ILE:N	2.43	0.51
20:Y:18:ARG:NH1	20:Y:21:GLN:OE1	2.40	0.51
20:Y:347:ILE:HG22	20:Y:354:VAL:HG22	1.93	0.51
21:Z:166:GLU:OE2	33:E:85:ARG:NH2	2.43	0.51
23:b:30:GLN:NE2	23:b:34:ASN:OD1	2.43	0.51
5:p:28:PHE:HB2	5:p:39:PHE:HB2	1.91	0.51
27:f:415:GLY:O	27:f:450:ILE:CG2	2.57	0.51
27:f:670:MET:N	27:f:670:MET:SD	2.83	0.51
32:D:373:ALA:CA	35:D:501:ATP:H5'1	2.40	0.51
16:U:328:ILE:HG23	16:U:329:LEU:HG	1.93	0.51
16:U:592:GLY:HA3	16:U:627:PHE:CD2	2.44	0.51
14:l:35:THR:HG23	14:l:133:LEU:HD12	1.92	0.51
22:a:168:ASN:ND2	22:a:171:SER:OG	2.43	0.51
33:E:148:VAL:HB	33:E:297:ARG:HH21	1.74	0.51
3:O:44:THR:N	3:O:172:SER:OG	2.43	0.51
3:O:67:MET:SD	3:O:67:MET:C	2.94	0.51
11:S:86:HIS:HB3	13:T:175:VAL:HG22	1.92	0.51
4:g:43:ARG:HG3	4:g:149:PRO:HB2	1.93	0.51
16:U:54:PHE:HD2	16:U:57:ARG:HE	1.58	0.51
6:h:34:PRO:HA	6:h:163:MET:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:89:LEU:HD21	32:D:389:GLU:HB2	1.92	0.51
12:k:102:THR:HG22	11:s:119:MET:HE1	1.92	0.51
3:o:62:ARG:NH1	3:o:210:LEU:O	2.44	0.51
24:c:279:ASP:OD2	24:c:283:HIS:NE2	2.36	0.51
25:d:191:PHE:O	25:d:195:THR:OG1	2.28	0.51
25:d:195:THR:HA	25:d:205:LYS:HG2	1.93	0.51
11:s:121:SER:OG	11:s:156:GLY:O	2.25	0.51
27:f:307:LEU:CD1	27:f:311:VAL:H	2.24	0.51
27:f:808:ASN:OD1	27:f:809:ILE:N	2.44	0.51
28:A:223:THR:OG1	35:A:501:ATP:O3G	2.29	0.51
30:B:71:TYR:HA	30:B:74:MET:HE3	1.92	0.51
3:O:106:LEU:HD21	3:O:117:PRO:CB	2.41	0.51
4:G:71:LYS:HE2	4:G:74:GLU:HA	1.92	0.51
5:P:23:ALA:HA	5:P:186:ILE:O	2.10	0.51
7:Q:192:ASP:OD1	7:Q:192:ASP:N	2.44	0.51
8:I:5:TYR:O	12:K:8:TYR:OH	2.21	0.51
8:I:159:TRP:HA	10:J:54:GLN:HA	1.93	0.51
14:L:88:MET:HE3	14:L:112:ILE:HD12	1.92	0.51
8:i:208:ALA:HB2	8:i:234:GLU:HG3	1.93	0.51
21:Z:25:ARG:HD2	24:c:104:ARG:HD2	1.93	0.51
21:Z:73:ASP:O	21:Z:77:ASN:ND2	2.44	0.51
9:r:94:ILE:HG21	9:r:115:GLU:HB3	1.92	0.51
28:A:351:ARG:NH2	28:A:374:ALA:O	2.42	0.51
1:N:63:ARG:HG3	1:N:64:VAL:HG13	1.93	0.51
15:M:55:LEU:HB2	15:M:59:TYR:HE2	1.75	0.51
17:V:299:GLN:HB2	25:d:113:ALA:HB1	1.93	0.51
12:k:38:ILE:HG23	12:k:181:LEU:HD11	1.93	0.51
3:o:241:ARG:NH1	5:p:152:SER:O	2.44	0.51
28:A:192:GLU:O	28:A:196:LEU:N	2.38	0.51
31:C:141:GLU:OE2	32:D:323:ARG:NH1	2.44	0.51
32:D:275:PHE:HE1	32:D:285:VAL:HG13	1.75	0.51
6:H:228:ASP:OD1	19:X:87:ARG:NH1	2.44	0.50
17:V:264:TYR:O	17:V:266:GLN:N	2.44	0.50
14:l:39:LYS:HB3	14:l:144:ILE:HG12	1.93	0.50
11:s:65:THR:OG1	11:s:67:ASP:OD1	2.28	0.50
30:B:234:LEU:HA	30:B:237:LYS:NZ	2.24	0.50
4:G:159:TYR:HB2	32:D:416:PHE:HB3	1.92	0.50
10:J:36:ARG:HA	10:J:41:VAL:HG12	1.93	0.50
10:j:68:ASN:ND2	10:j:136:PHE:O	2.40	0.50
19:X:171:LEU:HD11	19:X:210:LEU:HD13	1.94	0.50
9:r:201:GLY:HA3	9:r:214:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:295:TYR:CE2	31:C:271:ARG:HD2	2.46	0.50
32:D:287:ARG:O	32:D:290:LEU:CB	2.54	0.50
33:E:178:THR:O	33:E:178:THR:OG1	2.28	0.50
2:F:266:LYS:HD3	2:F:269:ARG:HH11	1.77	0.50
7:Q:12:TYR:HB2	7:Q:182:ILE:HD11	1.92	0.50
14:l:6:TYR:OH	15:m:9:ASP:OD2	2.28	0.50
22:a:374:ILE:HG12	25:d:248:GLU:HA	1.93	0.50
5:p:13:ALA:HA	5:p:21:ALA:O	2.10	0.50
27:f:39:LYS:HD2	27:f:120:ARG:HH12	1.77	0.50
13:t:65:VAL:HG11	13:t:167:LEU:HD13	1.94	0.50
30:B:235:LEU:HD23	30:B:235:LEU:C	2.37	0.50
31:C:69:GLN:HG3	31:C:118:ASN:HD21	1.76	0.50
31:C:196:LYS:O	31:C:199:LEU:N	2.44	0.50
3:O:244:ARG:HH21	3:O:246:ARG:HE	1.57	0.50
9:R:100:LEU:HD13	9:R:162:GLY:HA3	1.94	0.50
9:R:156:MET:HE1	9:R:173:VAL:HG12	1.93	0.50
8:i:76:VAL:HG12	8:i:134:LEU:HG	1.93	0.50
22:a:119:GLY:O	22:a:123:LEU:N	2.44	0.50
22:a:272:ILE:HD13	22:a:275:LEU:HD23	1.94	0.50
9:r:70:GLY:HA2	9:r:163:TRP:HZ3	1.76	0.50
32:D:167:ILE:CD1	35:D:501:ATP:HN61	2.24	0.50
14:l:103:LEU:HD12	14:l:104:PRO:HD2	1.93	0.50
20:Y:143:TYR:HD1	20:Y:146:ARG:HH12	1.59	0.50
20:Y:285:ASP:OD1	20:Y:286:TRP:N	2.45	0.50
22:a:33:LEU:HA	23:b:18:ASN:HD22	1.76	0.50
22:a:113:LEU:O	22:a:116:THR:OG1	2.27	0.50
22:a:119:GLY:HA2	22:a:122:LYS:HB2	1.93	0.50
3:o:88:GLY:HA2	3:o:141:LEU:HD23	1.93	0.50
11:s:46:GLU:OE2	11:s:146:LYS:NZ	2.39	0.50
27:f:230:CYS:HA	27:f:233:LEU:HD12	1.92	0.50
27:f:726:ILE:O	27:f:750:GLN:NE2	2.45	0.50
9:R:110:ASP:OD2	11:S:128:ARG:NH2	2.44	0.50
13:T:232:PHE:O	13:T:246:GLY:O	2.30	0.50
17:V:358:MET:HB2	17:V:359:PRO:HD3	1.93	0.50
3:o:230:ARG:CG	3:o:230:ARG:NH1	2.73	0.50
13:t:70:ASP:HA	13:t:232:PHE:HA	1.93	0.50
30:B:233:THR:O	30:B:236:ALA:HB3	2.11	0.50
30:B:235:LEU:C	30:B:235:LEU:CD2	2.85	0.50
31:C:147:THR:HG23	31:C:149:GLU:H	1.77	0.50
31:C:147:THR:OG1	31:C:206:HIS:NE2	2.33	0.50
31:C:222:LYS:NZ	32:D:290:LEU:HD11	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:120:ASP:N	32:D:120:ASP:OD1	2.45	0.50
2:F:433:ALA:HB1	2:F:435:LEU:HD13	1.92	0.50
11:S:226:VAL:HG22	11:S:231:ILE:HG12	1.94	0.50
13:T:112:LEU:HA	13:T:115:MET:HG2	1.94	0.50
16:U:410:VAL:HG23	16:U:448:LEU:HD13	1.94	0.50
17:V:358:MET:H	17:V:358:MET:CE	2.25	0.50
22:a:194:GLN:NE2	22:a:228:THR:OG1	2.44	0.50
25:d:167:ILE:HA	25:d:170:LEU:HD12	1.94	0.50
27:f:724:ASN:OD1	27:f:725:SER:N	2.45	0.50
28:A:84:LYS:HA	28:A:87:LEU:HD13	1.94	0.50
28:A:321:THR:OG1	28:A:322:ASN:N	2.45	0.50
1:N:153:MET:HE3	13:T:51:VAL:HB	1.94	0.50
6:H:74:LEU:CD2	6:H:83:TYR:HE1	2.24	0.50
14:L:96:ARG:HH12	14:L:102:PRO:HD3	1.77	0.50
25:d:195:THR:O	25:d:199:PHE:O	2.30	0.50
27:f:736:THR:HG22	27:f:737:ASN:H	1.75	0.50
27:f:736:THR:CG2	27:f:737:ASN:N	2.74	0.50
31:C:268:GLU:HA	31:C:271:ARG:HG2	1.93	0.50
33:E:199:VAL:HG23	33:E:201:SER:H	1.76	0.50
2:F:137:ILE:HD13	2:F:142:ALA:HB2	1.94	0.50
2:F:251:LEU:HB2	2:F:285:ILE:HG13	1.93	0.50
2:F:376:SER:OG	2:F:378:ASP:OD1	2.28	0.50
5:P:26:ARG:HH21	5:P:186:ILE:HB	1.77	0.50
7:Q:62:LYS:HE3	10:J:95:ARG:HG2	1.94	0.50
11:S:100:LEU:HD22	11:S:111:MET:HG3	1.94	0.50
16:U:618:ALA:O	16:U:621:SER:OG	2.30	0.50
6:h:95:GLN:HG3	3:o:108:LEU:HG	1.94	0.50
17:V:449:ALA:HB2	17:V:461:LYS:H	1.76	0.50
17:V:477:HIS:O	25:d:245:GLN:NE2	2.44	0.50
19:X:402:GLU:O	19:X:406:ASN:ND2	2.44	0.50
14:l:157:ARG:HG3	15:m:60:GLU:HG2	1.94	0.50
20:Y:276:ALA:HB1	26:e:58:ALA:HB1	1.92	0.50
22:a:36:GLN:NE2	23:b:145:GLU:OE2	2.41	0.50
5:p:56:LEU:HB3	5:p:59:ASP:HB2	1.94	0.50
28:A:50:ASP:HA	28:A:53:GLN:HG3	1.93	0.50
2:F:156:ASP:OD1	2:F:157:SER:N	2.45	0.49
3:O:217:ASP:HA	3:O:230:ARG:O	2.11	0.49
4:G:127:GLN:HE21	6:H:127:VAL:HB	1.77	0.49
4:G:134:LEU:HD12	4:G:135:GLY:H	1.77	0.49
4:G:148:GLY:O	4:G:150:GLN:NE2	2.40	0.49
6:H:229:TYR:CZ	19:X:83:ALA:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:39:LYS:HB3	14:L:144:ILE:HG12	1.94	0.49
16:U:9:ILE:HB	16:U:11:LEU:HD23	1.94	0.49
5:p:124:LEU:HB3	5:p:128:GLY:HA2	1.93	0.49
11:s:85:PHE:HB3	11:s:88:ASP:HB2	1.93	0.49
27:f:49:ASP:H	27:f:126:ILE:HD13	1.76	0.49
30:B:120:HIS:HB3	30:B:134:SER:HA	1.93	0.49
31:C:371:LEU:CD2	32:D:191:TYR:CZ	2.95	0.49
33:E:322:LYS:HE2	33:E:362:VAL:HB	1.93	0.49
1:N:91:ASP:OD2	3:O:124:ARG:NH2	2.38	0.49
4:G:17:SER:H	4:G:20:GLY:HA2	1.77	0.49
8:I:14:PRO:HA	10:J:21:TYR:CZ	2.46	0.49
13:T:183:ALA:HB3	13:T:192:GLN:HB2	1.94	0.49
4:g:196:GLU:HG2	4:g:242:LEU:HG	1.94	0.49
16:U:131:GLU:O	16:U:135:ASN:ND2	2.45	0.49
17:V:33:GLN:HB3	17:V:115:LYS:HE3	1.94	0.49
18:W:260:SER:O	18:W:260:SER:OG	2.29	0.49
22:a:103:LYS:HG3	22:a:104:VAL:HG23	1.94	0.49
27:f:358:PHE:HE1	28:A:267:LYS:HA	1.77	0.49
6:H:96:GLN:HG3	6:H:99:LEU:HD12	1.94	0.49
7:Q:44:LEU:HD11	7:Q:102:LEU:HD11	1.95	0.49
9:R:125:TYR:HB3	9:R:133:ILE:HD11	1.94	0.49
12:K:38:ILE:HD12	12:K:198:SER:HB2	1.94	0.49
15:M:193:GLU:O	15:M:197:ILE:HG12	2.13	0.49
4:g:88:ARG:HA	4:g:91:VAL:HG12	1.95	0.49
16:U:475:HIS:NE2	16:U:507:VAL:O	2.45	0.49
16:U:789:ILE:N	16:U:910:GLY:O	2.44	0.49
17:V:462:GLU:OE1	20:Y:346:LYS:NZ	2.43	0.49
18:W:227:TYR:HB3	18:W:246:HIS:HE1	1.76	0.49
20:Y:15:PRO:HG2	20:Y:113:ARG:HE	1.77	0.49
15:m:221:THR:OG1	15:m:224:ARG:O	2.27	0.49
24:c:181:LEU:O	24:c:186:LYS:NZ	2.44	0.49
7:q:49:GLU:HB3	7:q:52:ASP:HB2	1.92	0.49
27:f:324:VAL:CG2	27:f:455:VAL:CG1	2.87	0.49
27:f:496:ASP:N	27:f:496:ASP:OD1	2.44	0.49
28:A:95:VAL:HG23	28:A:96:ALA:H	1.78	0.49
32:D:410:ASP:OD1	32:D:410:ASP:N	2.40	0.49
33:E:185:ARG:CZ	33:E:185:ARG:HB3	2.41	0.49
33:E:203:ILE:HG23	33:E:214:LEU:HD11	1.92	0.49
8:i:128:ARG:NE	6:h:123:GLN:OE1	2.46	0.49
22:a:187:ASP:OD1	22:a:187:ASP:N	2.42	0.49
27:f:250:ARG:NH2	27:f:285:CYS:SG	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:LEU:HD11	2:F:142:ALA:HB1	1.95	0.49
8:I:111:VAL:HG22	8:I:136:TYR:HD2	1.78	0.49
11:S:179:ASN:ND2	11:S:184:LYS:O	2.44	0.49
15:M:241:LYS:HA	15:M:244:LEU:HD23	1.93	0.49
16:U:324:LYS:HA	16:U:327:LYS:HE3	1.94	0.49
10:j:118:TYR:HA	10:j:124:ARG:HE	1.78	0.49
20:Y:124:PHE:HD1	20:Y:140:ILE:HG23	1.75	0.49
21:Z:25:ARG:NH2	24:c:104:ARG:O	2.42	0.49
22:a:172:TYR:O	22:a:176:ALA:CB	2.61	0.49
27:f:294:MET:HA	27:f:299:GLY:HA2	1.95	0.49
27:f:305:LEU:N	27:f:305:LEU:CD2	2.72	0.49
27:f:756:PRO:O	27:f:758:ASN:N	2.45	0.49
13:t:169:TYR:O	13:t:176:ALA:HA	2.12	0.49
31:C:31:LEU:CD2	32:D:47:LEU:HD13	2.42	0.49
33:E:72:LYS:NZ	33:E:73:ALA:O	2.45	0.49
4:g:21:ARG:NH1	4:g:22:LEU:O	2.44	0.49
16:U:801:GLN:HB3	16:U:877:LEU:HB3	1.94	0.49
25:d:234:ASP:OD1	25:d:235:THR:N	2.41	0.49
26:e:53:SER:OG	26:e:59:GLU:OE1	2.29	0.49
27:f:319:GLU:C	27:f:325:GLN:CB	2.84	0.49
27:f:369:ARG:HG3	27:f:372:LEU:HD12	1.94	0.49
27:f:418:LEU:CD1	27:f:425:GLY:C	2.86	0.49
27:f:834:ASP:HB2	30:B:53:THR:HG21	1.92	0.49
32:D:265:ASP:OD1	32:D:265:ASP:N	2.45	0.49
7:Q:101:ASN:HB3	7:Q:132:HIS:CE1	2.48	0.49
8:I:118:LYS:HD3	8:I:154:GLY:HA2	1.94	0.49
16:U:599:ILE:O	16:U:603:LEU:CD2	2.61	0.49
16:U:603:LEU:HD13	32:D:60:TYR:HD1	1.73	0.49
18:W:3:ASP:OD1	18:W:3:ASP:N	2.45	0.49
15:m:38:ILE:HD11	15:m:194:VAL:HG13	1.94	0.49
24:c:163:ILE:HD12	24:c:199:HIS:HA	1.93	0.49
7:q:153:ARG:NH1	7:q:184:ASP:OD2	2.41	0.49
11:s:67:ASP:OD1	11:s:67:ASP:N	2.43	0.49
27:f:375:SER:O	27:f:379:GLY:N	2.45	0.49
27:f:571:GLU:HG2	27:f:573:ILE:H	1.76	0.49
27:f:633:GLU:OE2	27:f:674:THR:OG1	2.26	0.49
28:A:243:SER:N	28:A:276:GLU:OE2	2.46	0.49
31:C:48:GLN:NE2	31:C:48:GLN:O	2.46	0.49
31:C:49:ARG:HH22	31:C:53:ASN:HD22	1.59	0.49
31:C:145:ASP:OD1	31:C:145:ASP:N	2.45	0.49
2:F:272:PHE:HD2	2:F:316:GLN:HG3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:81:SER:HB3	3:O:106:LEU:CD1	2.42	0.49
3:O:221:ILE:HG23	3:O:226:LEU:HD12	1.94	0.49
3:O:255:LEU:HG	5:P:201:LYS:HG2	1.95	0.49
10:J:105:GLU:OE2	10:J:143:ARG:NH1	2.46	0.49
16:U:174:PRO:HD2	16:U:176:MET:HG2	1.95	0.49
18:W:372:ARG:HB3	18:W:412:ILE:HD11	1.94	0.49
19:X:256:LEU:CD2	19:X:256:LEU:C	2.85	0.49
14:l:47:VAL:HG12	14:l:195:LEU:HD22	1.94	0.49
21:Z:239:ASP:HA	24:c:310:LYS:HG2	1.94	0.49
1:n:35:THR:N	1:n:164:SER:OG	2.46	0.49
9:r:207:GLU:H	9:r:210:GLN:NE2	2.10	0.49
27:f:103:TYR:O	27:f:141:LYS:NZ	2.44	0.49
32:D:116:LEU:HD23	32:D:140:VAL:HA	1.95	0.49
32:D:152:MET:HE3	32:D:257:ASN:ND2	2.28	0.49
14:L:26:MET:HE2	14:L:149:PRO:HG2	1.95	0.49
4:g:176:THR:HG23	6:h:56:LEU:HD12	1.94	0.49
19:X:240:ASP:OD1	19:X:278:ARG:NH1	2.46	0.49
19:X:315:ASP:N	19:X:315:ASP:OD1	2.46	0.49
19:X:316:ASP:N	19:X:316:ASP:OD1	2.45	0.49
27:f:621:ASP:OD2	27:f:625:LYS:N	2.44	0.49
33:E:349:GLU:HA	33:E:352:MET:HG3	1.95	0.49
10:j:125:ARG:NH1	10:j:126:PRO:O	2.46	0.49
20:Y:312:ARG:HA	20:Y:356:THR:HG22	1.95	0.49
21:Z:151:THR:HG21	22:a:146:PRO:HG3	1.94	0.49
22:a:34:TRP:O	22:a:38:THR:OG1	2.26	0.49
7:q:67:TYR:O	7:q:71:ASN:ND2	2.43	0.49
7:q:164:LEU:HD13	7:q:178:PHE:HD2	1.77	0.49
27:f:9:ALA:HA	27:f:13:PRO:HD2	1.95	0.49
27:f:416:MET:SD	27:f:804:LEU:CD2	2.97	0.49
13:t:194:LEU:HD22	13:t:216:ARG:HH21	1.78	0.49
31:C:384:GLU:HA	31:C:387:VAL:HG12	1.94	0.49
33:E:344:ARG:NH2	33:E:345:ASN:OD1	2.45	0.49
5:P:27:ARG:HG3	5:P:34:MET:HE1	1.95	0.48
7:Q:19:ARG:O	7:Q:32:HIS:N	2.42	0.48
9:R:233:VAL:HG23	9:R:251:VAL:HG22	1.94	0.48
17:V:139:MET:HA	17:V:143:ALA:HB2	1.94	0.48
1:n:122:TYR:O	1:n:125:ARG:NH1	2.34	0.48
3:o:218:LEU:HD12	3:o:232:TYR:CZ	2.48	0.48
7:q:139:THR:HA	7:q:142:ILE:HD12	1.95	0.48
1:N:199:GLU:O	13:t:82:ARG:NH2	2.47	0.48
2:F:154:ASN:ND2	2:F:156:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:21:VAL:HG13	8:i:152:PRO:HB2	1.95	0.48
15:M:36:THR:HA	15:M:166:ILE:O	2.12	0.48
16:U:510:GLU:OE2	16:U:546:ARG:NH2	2.36	0.48
27:f:293:GLN:HG2	27:f:321:MET:SD	2.53	0.48
28:A:263:MET:O	28:A:266:THR:OG1	2.27	0.48
30:B:152:LEU:HD23	30:B:159:VAL:HA	1.94	0.48
33:E:182:LEU:O	33:E:186:ALA:CB	2.61	0.48
6:H:89:ARG:HH21	6:H:92:LYS:NZ	2.11	0.48
6:H:150:ASP:OD1	6:H:154:ALA:N	2.46	0.48
13:T:96:LEU:HD11	13:T:155:MET:HB2	1.94	0.48
6:h:33:ALA:HA	6:h:165:LYS:HZ2	1.77	0.48
17:V:79:VAL:HG13	17:V:81:GLN:H	1.77	0.48
17:V:300:LEU:HA	17:V:397:ARG:HH22	1.77	0.48
17:V:428:LEU:HD12	17:V:430:SER:H	1.78	0.48
23:b:152:LYS:HA	23:b:155:ALA:HB3	1.95	0.48
24:c:224:SER:HB3	24:c:227:GLU:HB2	1.96	0.48
27:f:442:SER:HB2	27:f:476:THR:O	2.14	0.48
13:t:49:PRO:HB3	13:t:101:ASP:HB2	1.95	0.48
32:D:214:MET:SD	35:D:501:ATP:C2'	3.00	0.48
32:D:373:ALA:CA	35:D:501:ATP:C5'	2.90	0.48
33:E:185:ARG:CG	33:E:185:ARG:NH1	2.73	0.48
33:E:334:LEU:HB3	33:E:371:VAL:HG11	1.94	0.48
2:F:171:ARG:HH12	2:F:267:LEU:HD11	1.78	0.48
2:F:300:LYS:HG3	33:E:244:SER:HB2	1.94	0.48
7:Q:83:PHE:O	7:Q:87:ASN:ND2	2.32	0.48
9:R:174:ASP:OD1	9:R:178:ASN:N	2.43	0.48
4:g:70:PHE:HB3	4:g:91:VAL:HG21	1.95	0.48
19:X:177:TYR:CZ	19:X:185:LYS:HD3	2.47	0.48
21:Z:20:VAL:HG22	21:Z:126:VAL:HG12	1.95	0.48
22:a:68:GLU:OE2	22:a:71:VAL:HG23	2.13	0.48
24:c:279:ASP:HB2	24:c:282:ARG:HB2	1.94	0.48
27:f:174:ASP:N	27:f:174:ASP:OD1	2.46	0.48
27:f:606:VAL:HG13	30:B:74:MET:HE1	1.95	0.48
31:C:147:THR:HG22	31:C:150:MET:HE1	1.96	0.48
31:C:325:ARG:HD3	31:C:353:GLY:HA2	1.94	0.48
3:O:108:LEU:HD23	6:H:95:GLN:NE2	2.29	0.48
4:G:22:LEU:HD23	4:G:24:GLN:HE22	1.78	0.48
5:P:143:ALA:HA	5:P:146:MET:HE2	1.96	0.48
11:S:212:GLU:HG3	3:o:238:LYS:HE3	1.94	0.48
18:W:281:ASN:O	18:W:284:SER:OG	2.24	0.48
21:Z:74:TYR:OH	24:c:102:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:45:VAL:HG22	22:a:79:ILE:HD13	1.94	0.48
11:s:54:ASP:O	11:s:70:LYS:NZ	2.37	0.48
27:f:307:LEU:CG	27:f:311:VAL:HG23	2.42	0.48
27:f:416:MET:CE	27:f:804:LEU:CD1	2.61	0.48
28:A:192:GLU:O	28:A:195:LEU:N	2.46	0.48
2:F:347:ARG:NH2	35:E:401:ATP:O3G	2.46	0.48
8:I:165:GLY:O	8:I:168:SER:OG	2.24	0.48
11:S:159:GLN:NE2	11:S:161:ASP:OD1	2.47	0.48
8:i:238:LYS:HA	8:i:241:GLU:HG2	1.96	0.48
15:M:109:LEU:HD11	15:M:138:LEU:HB3	1.95	0.48
18:W:55:ARG:HH12	18:W:79:GLU:HB3	1.79	0.48
18:W:173:THR:HA	18:W:177:MET:HE3	1.94	0.48
21:Z:169:GLU:HA	21:Z:172:VAL:HG22	1.95	0.48
5:p:53:LEU:HB2	5:p:60:VAL:HG13	1.96	0.48
27:f:293:GLN:NE2	27:f:293:GLN:O	2.46	0.48
28:A:148:GLN:HB3	28:A:150:HIS:CE1	2.48	0.48
2:F:247:THR:HG21	2:F:278:LYS:HG3	1.96	0.48
3:O:94:ASP:HB3	3:O:137:ILE:HG23	1.96	0.48
5:P:43:PHE:HB2	5:P:45:MET:HE1	1.94	0.48
6:H:74:LEU:O	6:H:74:LEU:CD2	2.48	0.48
15:M:170:ARG:HD2	15:M:174:LYS:HZ2	1.79	0.48
6:h:34:PRO:HA	6:h:164:GLY:HA3	1.96	0.48
18:W:187:LEU:HA	18:W:190:MET:HG2	1.96	0.48
18:W:263:TRP:CZ2	18:W:295:LYS:HD2	2.48	0.48
27:f:326:LEU:HD23	27:f:330:PHE:CZ	2.49	0.48
27:f:418:LEU:HD13	27:f:425:GLY:CA	2.35	0.48
30:B:211:TYR:O	30:B:215:GLY:N	2.47	0.48
2:F:83:ASN:O	2:F:88:TYR:OH	2.30	0.48
11:S:200:MET:HA	11:S:203:VAL:HG12	1.96	0.48
13:T:234:ILE:HG22	13:T:245:GLU:HB2	1.96	0.48
15:M:20:ARG:HE	15:M:22:PHE:HE1	1.60	0.48
17:V:323:GLY:H	26:e:6:GLN:NE2	2.12	0.48
18:W:38:GLY:HA2	18:W:44:ILE:HG21	1.95	0.48
18:W:272:LEU:HD22	18:W:340:VAL:HG21	1.94	0.48
27:f:305:LEU:HG	27:f:321:MET:HE1	1.95	0.48
27:f:759:LEU:HD13	27:f:808:ASN:HA	1.96	0.48
27:f:869:THR:OG1	27:f:885:GLU:N	2.41	0.48
31:C:199:LEU:C	31:C:199:LEU:CD2	2.85	0.48
32:D:409:LYS:HE2	32:D:412:GLN:HB2	1.96	0.48
33:E:242:ARG:HD3	33:E:242:ARG:HA	1.72	0.48
7:Q:88:LEU:HD23	7:Q:122:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:104:LYS:O	3:o:124:ARG:NH1	2.47	0.48
4:g:115:CYS:HB3	4:g:140:LEU:HD12	1.94	0.48
16:U:146:LYS:HD3	32:D:40:LEU:HD13	1.96	0.48
17:V:64:GLN:HA	17:V:67:LEU:HB3	1.95	0.48
17:V:96:ARG:HH22	17:V:108:LEU:HA	1.79	0.48
10:j:36:ARG:HG3	10:j:142:PRO:HB2	1.96	0.48
19:X:403:THR:HA	19:X:406:ASN:HD22	1.78	0.48
9:r:150:LYS:NZ	9:r:176:GLU:O	2.47	0.48
27:f:327:ASN:ND2	27:f:327:ASN:N	2.60	0.48
30:B:234:LEU:C	30:B:236:ALA:N	2.69	0.48
30:B:362:LYS:HB3	30:B:384:ILE:HD11	1.96	0.48
30:B:374:LEU:HA	30:B:414:VAL:HG12	1.94	0.48
1:N:132:ILE:HG22	1:N:148:VAL:HB	1.96	0.48
1:N:172:TYR:O	1:N:176:THR:OG1	2.29	0.48
7:Q:45:LEU:HB2	7:Q:103:LEU:HB2	1.96	0.48
8:I:123:GLN:HA	10:J:125:ARG:HD2	1.95	0.48
8:i:91:ARG:HH11	5:p:77:LYS:HZ3	1.62	0.48
16:U:194:ARG:O	16:U:198:LEU:HB2	2.14	0.48
16:U:899:ARG:NE	16:U:916:ASP:OD2	2.47	0.48
17:V:170:LEU:HG	17:V:170:LEU:O	2.14	0.48
18:W:205:ILE:HD12	18:W:208:LYS:HD3	1.95	0.48
3:o:57:LEU:HB2	3:o:219:CYS:HB3	1.95	0.48
3:o:124:ARG:HG2	3:o:127:LYS:HZ1	1.79	0.48
23:b:37:CYS:O	23:b:41:THR:OG1	2.23	0.48
24:c:273:LYS:O	24:c:278:GLN:NE2	2.46	0.48
27:f:670:MET:HB2	27:f:673:ARG:HG3	1.95	0.48
31:C:188:LEU:HD13	31:C:315:ILE:HB	1.96	0.48
33:E:376:ASP:OD1	33:E:376:ASP:N	2.46	0.48
16:U:182:LYS:O	16:U:186:SER:HB2	2.14	0.47
19:X:62:GLN:HG3	19:X:65:GLU:HB2	1.96	0.47
20:Y:79:ASP:HA	20:Y:82:LYS:HE3	1.95	0.47
1:n:78:CYS:O	1:n:132:ILE:HA	2.14	0.47
11:s:239:ARG:NH2	11:s:241:ASP:OD2	2.47	0.47
28:A:190:VAL:HG11	28:A:212:VAL:HG21	1.96	0.47
31:C:161:ILE:HA	31:C:164:VAL:HG12	1.96	0.47
31:C:344:LEU:HA	31:C:347:ILE:HD12	1.95	0.47
2:F:233:LYS:O	2:F:236:LEU:CG	2.46	0.47
18:W:1:MET:SD	18:W:39:ARG:NH1	2.88	0.47
14:l:192:LEU:HD13	14:l:236:LEU:HD11	1.94	0.47
20:Y:82:LYS:O	20:Y:86:GLU:N	2.45	0.47
22:a:58:LYS:HA	22:a:61:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:56:VAL:HG22	3:o:220:VAL:HG13	1.96	0.47
30:B:133:VAL:HB	30:B:158:ALA:HA	1.95	0.47
30:B:234:LEU:C	30:B:237:LYS:H	2.22	0.47
31:C:189:TYR:HA	31:C:196:LYS:HZ1	1.75	0.47
2:F:256:LEU:HD21	2:F:291:ILE:HG13	1.95	0.47
16:U:491:GLN:HE22	16:U:494:TYR:HD2	1.61	0.47
17:V:371:ASN:HA	17:V:427:GLN:NE2	2.29	0.47
20:Y:62:ASP:HB2	20:Y:64:GLN:HG2	1.95	0.47
20:Y:66:ASP:O	20:Y:70:LEU:N	2.39	0.47
1:n:69:THR:OG1	1:n:79:ARG:NE	2.44	0.47
13:t:46:THR:O	13:t:152:TRP:NE1	2.40	0.47
28:A:59:ILE:HG22	30:B:72:LEU:HD12	1.95	0.47
30:B:234:LEU:O	30:B:238:ALA:N	2.44	0.47
31:C:274:LEU:O	31:C:278:ASN:ND2	2.47	0.47
2:F:93:VAL:HG13	2:F:147:PRO:HA	1.96	0.47
6:H:182:LEU:HD23	6:H:186:ASP:HB3	1.96	0.47
9:R:118:LEU:HD22	9:R:142:LEU:HD11	1.96	0.47
12:K:76:CYS:SG	12:K:77:ALA:N	2.87	0.47
18:W:94:ARG:NH2	32:D:390:ASN:OD1	2.46	0.47
18:W:121:LYS:HA	18:W:124:LEU:HG	1.95	0.47
15:m:237:GLU:OE2	15:m:241:LYS:NZ	2.43	0.47
21:Z:181:ASP:OD1	21:Z:181:ASP:N	2.45	0.47
23:b:54:LEU:O	23:b:85:THR:OG1	2.33	0.47
27:f:307:LEU:HD21	27:f:311:VAL:HG22	1.96	0.47
27:f:529:SER:O	27:f:529:SER:OG	2.31	0.47
13:t:75:TYR:HB2	13:t:80:ARG:HB2	1.96	0.47
2:F:218:GLN:NE2	33:E:348:THR:OG1	2.47	0.47
14:L:40:SER:HB3	14:L:187:LEU:HD22	1.97	0.47
16:U:139:GLN:HA	16:U:142:LEU:HG	1.97	0.47
16:U:143:ASP:OD1	16:U:143:ASP:N	2.45	0.47
6:h:9:SER:HA	6:h:125:GLY:HA2	1.97	0.47
17:V:358:MET:HE2	17:V:358:MET:H	1.79	0.47
19:X:130:GLU:HA	19:X:133:LEU:HG	1.97	0.47
20:Y:197:ALA:HB3	20:Y:226:VAL:HG21	1.95	0.47
1:n:194:LEU:O	1:n:198:MET:HG2	2.14	0.47
27:f:258:LYS:HB3	27:f:258:LYS:HE2	1.60	0.47
27:f:736:THR:CG2	27:f:737:ASN:H	2.28	0.47
27:f:758:ASN:CG	27:f:759:LEU:H	2.23	0.47
27:f:828:ARG:HD3	27:f:846:VAL:HG23	1.95	0.47
5:P:78:GLU:OE2	6:H:109:GLN:NE2	2.48	0.47
6:H:231:ALA:O	6:H:233:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:35:SER:OG	15:M:66:ARG:NH1	2.48	0.47
16:U:451:ALA:O	16:U:453:HIS:ND1	2.44	0.47
17:V:81:GLN:HB3	17:V:85:ALA:HB3	1.95	0.47
17:V:395:ILE:HG13	17:V:396:ILE:HD12	1.96	0.47
10:j:226:GLU:HA	10:j:229:VAL:HG22	1.96	0.47
19:X:371:ASP:HA	20:Y:237:ARG:HH22	1.78	0.47
9:r:153:GLY:O	11:s:128:ARG:NH2	2.45	0.47
11:s:151:SER:O	11:s:158:TYR:HA	2.13	0.47
27:f:326:LEU:HD22	27:f:326:LEU:H	1.79	0.47
33:E:159:PHE:O	33:E:163:GLY:N	2.47	0.47
2:F:70:LYS:HA	2:F:73:ILE:HD12	1.97	0.47
4:G:19:GLU:O	32:D:417:TYR:OH	2.33	0.47
9:R:139:SER:OG	9:R:179:ARG:NE	2.46	0.47
9:R:166:ARG:NH1	9:R:168:PRO:O	2.48	0.47
11:S:85:PHE:HZ	13:T:173:LEU:HB3	1.79	0.47
12:K:99:HIS:O	12:K:103:TYR:HB2	2.15	0.47
14:L:142:PRO:O	14:L:143:HIS:ND1	2.48	0.47
16:U:803:LYS:H	16:U:893:THR:HB	1.79	0.47
17:V:271:VAL:HA	17:V:273:LYS:HE2	1.96	0.47
18:W:24:VAL:HA	18:W:27:ARG:HG2	1.97	0.47
12:k:52:LYS:HD3	12:k:64:ILE:HB	1.97	0.47
21:Z:105:ASP:O	21:Z:109:ASN:N	2.46	0.47
27:f:496:ASP:O	27:f:499:THR:OG1	2.31	0.47
28:A:84:LYS:O	28:A:86:THR:N	2.48	0.47
30:B:408:ARG:NE	31:C:163:GLU:OE2	2.48	0.47
1:N:143:GLY:O	1:N:156:ARG:NH2	2.48	0.47
5:P:69:PHE:CD1	8:I:95:GLN:HG3	2.49	0.47
6:H:68:ILE:HA	6:H:91:ARG:HG2	1.97	0.47
10:J:71:MET:HG2	10:J:133:ILE:HD13	1.95	0.47
16:U:146:LYS:O	16:U:149:GLN:NE2	2.40	0.47
17:V:289:LEU:HA	17:V:292:THR:HG22	1.96	0.47
18:W:227:TYR:HB3	18:W:246:HIS:CE1	2.49	0.47
14:l:34:ALA:HA	14:l:161:ILE:O	2.15	0.47
24:c:289:ASP:OD1	24:c:290:VAL:N	2.47	0.47
32:D:374:ASP:HB3	33:E:292:PRO:HG2	1.97	0.47
7:Q:68:LYS:HG3	7:Q:74:GLU:HG2	1.97	0.47
19:X:344:ARG:HB2	19:X:386:ILE:HD13	1.97	0.47
20:Y:87:GLU:O	20:Y:90:ASP:HB2	2.15	0.47
25:d:168:ASP:HA	25:d:171:LEU:HD12	1.97	0.47
26:e:7:PRO:O	26:e:9:ASP:N	2.47	0.47
31:C:156:LYS:HA	31:C:159:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:177:VAL:HG11	32:D:215:LEU:HD11	1.96	0.47
33:E:250:ASP:OD1	33:E:250:ASP:N	2.46	0.47
3:O:230:ARG:HD2	3:O:230:ARG:HA	1.57	0.47
3:O:258:LYS:HG3	5:P:197:THR:HB	1.97	0.47
6:H:97:TYR:O	6:H:101:TYR:HB2	2.15	0.47
10:J:120:GLN:OE1	12:K:135:ARG:NE	2.48	0.47
10:J:196:LEU:HD12	10:J:201:SER:HB3	1.97	0.47
6:h:43:GLY:CA	6:h:213:CYS:O	2.63	0.47
20:Y:84:LEU:HD11	20:Y:107:LYS:HD3	1.96	0.47
1:n:35:THR:N	1:n:164:SER:HG	2.12	0.47
22:a:112:ILE:O	22:a:115:LYS:HB2	2.14	0.47
9:r:96:ILE:HG21	9:r:100:LEU:HD23	1.97	0.47
27:f:873:LEU:HG	27:f:875:ALA:H	1.80	0.47
28:A:183:GLN:NE2	28:A:342:GLU:O	2.39	0.47
28:A:218:PRO:HB2	30:B:343:ARG:NH2	2.30	0.47
31:C:145:ASP:HA	31:C:201:ARG:HG2	1.97	0.47
32:D:345:PHE:HE1	32:D:375:ILE:HD12	1.79	0.47
2:F:320:PHE:HA	33:E:185:ARG:HD3	1.96	0.46
3:O:230:ARG:CB	3:O:231:PRO:CD	2.92	0.46
16:U:599:ILE:O	16:U:603:LEU:HD23	2.15	0.46
16:U:729:GLY:HA2	16:U:732:LEU:HG	1.96	0.46
17:V:403:ILE:HD11	17:V:426:LEU:HD12	1.97	0.46
18:W:41:GLN:HG2	18:W:42:GLU:HG2	1.96	0.46
19:X:401:LEU:C	19:X:401:LEU:CD2	2.85	0.46
14:l:9:ASP:OD2	14:l:11:THR:OG1	2.26	0.46
22:a:322:GLY:HA2	22:a:334:THR:HG23	1.95	0.46
27:f:307:LEU:CD1	27:f:311:VAL:N	2.78	0.46
27:f:511:SER:HB3	27:f:514:VAL:HB	1.96	0.46
32:D:139:LEU:HD12	32:D:139:LEU:HA	1.71	0.46
33:E:360:ASP:N	33:E:360:ASP:OD1	2.48	0.46
33:E:369:LYS:O	33:E:373:LYS:N	2.43	0.46
11:S:92:LEU:HD23	11:S:95:ILE:HD11	1.97	0.46
11:S:105:HIS:ND1	14:L:89:ARG:HD3	2.29	0.46
13:T:53:GLY:N	13:T:100:GLY:O	2.47	0.46
8:i:174:MET:SD	8:i:196:VAL:HG22	2.55	0.46
16:U:744:VAL:HB	16:U:783:TYR:HB3	1.98	0.46
17:V:194:LYS:HB2	17:V:200:ARG:NH2	2.31	0.46
17:V:498:PRO:HD3	21:Z:278:ASN:HD21	1.80	0.46
18:W:201:ARG:O	18:W:205:ILE:HG22	2.15	0.46
22:a:284:ARG:NH1	22:a:288:HIS:O	2.49	0.46
3:o:237:LYS:NZ	3:o:238:LYS:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:64:ALA:HA	9:r:72:ILE:O	2.16	0.46
27:f:449:GLY:HA3	27:f:484:GLY:HA3	1.97	0.46
13:t:108:LEU:HD21	13:t:151:LEU:HD13	1.98	0.46
28:A:224:LEU:HA	28:A:227:ARG:HG3	1.95	0.46
30:B:285:ASP:OD1	30:B:286:GLU:CD	2.58	0.46
31:C:158:ILE:HA	31:C:161:ILE:HG12	1.97	0.46
5:P:103:TYR:O	5:P:126:LEU:HD13	2.14	0.46
7:Q:45:LEU:O	7:Q:102:LEU:HA	2.14	0.46
10:J:18:GLN:HB3	10:J:126:PRO:HG2	1.97	0.46
10:J:103:THR:OG1	10:J:105:GLU:OE1	2.34	0.46
10:J:137:ASP:OD1	10:J:141:THR:N	2.48	0.46
12:K:200:ILE:HG23	12:K:204:GLN:HE22	1.79	0.46
13:T:90:VAL:HG11	13:T:133:ILE:HD13	1.98	0.46
13:T:171:ASP:OD1	13:T:175:VAL:N	2.49	0.46
14:L:157:ARG:NH1	15:M:59:TYR:O	2.49	0.46
16:U:575:ASP:HB3	16:U:578:LEU:HB3	1.97	0.46
19:X:56:LEU:O	19:X:60:THR:OG1	2.33	0.46
21:Z:104:ASN:N	21:Z:104:ASN:OD1	2.49	0.46
13:t:51:VAL:HG22	13:t:75:TYR:HA	1.98	0.46
30:B:223:ILE:HG12	30:B:347:ILE:HG21	1.97	0.46
33:E:235:ILE:O	33:E:239:GLY:N	2.47	0.46
33:E:287:PRO:HA	33:E:290:LEU:HB3	1.97	0.46
2:F:189:GLY:H	34:F:501:ADP:HN62	1.63	0.46
10:J:65:LEU:HD21	10:J:71:MET:HE2	1.98	0.46
16:U:492:ASP:N	16:U:492:ASP:OD1	2.47	0.46
3:o:85:TYR:HB2	3:o:221:ILE:HD11	1.97	0.46
23:b:178:SER:OG	23:b:179:LEU:N	2.49	0.46
7:q:36:PHE:N	7:q:44:LEU:O	2.48	0.46
26:e:45:ASP:OD1	26:e:46:ASP:N	2.48	0.46
28:A:60:ASN:OD1	28:A:61:GLU:N	2.48	0.46
30:B:235:LEU:CD1	30:B:353:PHE:CZ	2.81	0.46
31:C:295:THR:OG1	31:C:296:ASN:N	2.49	0.46
33:E:182:LEU:O	33:E:186:ALA:HB2	2.15	0.46
3:O:118:ARG:HH12	3:O:120:VAL:HG12	1.81	0.46
10:J:7:ILE:HG22	10:J:9:VAL:H	1.80	0.46
16:U:541:HIS:ND1	24:c:63:ASP:OD2	2.45	0.46
12:k:201:ILE:HA	12:k:204:GLN:HG2	1.98	0.46
15:m:216:TRP:CE3	15:m:228:VAL:HG22	2.51	0.46
3:o:130:LEU:HD13	3:o:158:PRO:HA	1.98	0.46
5:p:101:GLY:O	7:q:93:ARG:NH1	2.48	0.46
24:c:303:MET:HE3	25:d:236:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:104:LEU:HB3	7:q:116:TYR:HB2	1.97	0.46
7:q:117:TYR:HD2	7:q:130:ALA:HB1	1.80	0.46
27:f:202:HIS:ND1	27:f:242:GLU:OE2	2.48	0.46
30:B:247:PHE:HD1	30:B:281:ILE:HG23	1.80	0.46
31:C:235:PHE:HA	31:C:238:ALA:HB3	1.98	0.46
32:D:231:VAL:HG23	33:E:262:ASN:HD22	1.79	0.46
33:E:175:PRO:C	33:E:178:THR:CG2	2.89	0.46
13:T:68:ALA:HB2	13:T:234:ILE:HD12	1.97	0.46
14:L:225:ASP:OD1	14:L:225:ASP:N	2.48	0.46
19:X:401:LEU:O	19:X:404:ILE:N	2.48	0.46
7:q:117:TYR:HB3	7:q:125:ALA:HB3	1.97	0.46
31:C:84:LYS:HB3	31:C:96:VAL:HG13	1.97	0.46
31:C:299:ASP:OD1	31:C:299:ASP:N	2.48	0.46
32:D:268:ASP:N	32:D:268:ASP:OD1	2.48	0.46
32:D:391:ARG:HH12	32:D:397:LYS:HE3	1.81	0.46
33:E:54:GLY:HA3	33:E:108:MET:HE1	1.98	0.46
16:U:148:LYS:HE3	32:D:40:LEU:HB3	1.96	0.46
16:U:794:ASP:N	16:U:794:ASP:OD1	2.48	0.46
17:V:95:LEU:HA	17:V:137:GLU:HB3	1.98	0.46
21:Z:147:ASP:N	21:Z:147:ASP:OD1	2.49	0.46
22:a:271:LYS:O	22:a:275:LEU:CB	2.60	0.46
3:o:230:ARG:N	3:o:231:PRO:HD3	2.29	0.46
5:p:159:ASP:O	5:p:163:LEU:N	2.41	0.46
1:N:79:ARG:HH12	1:N:87:GLN:HA	1.81	0.46
2:F:304:ARG:HB3	2:F:308:ARG:HH12	1.81	0.46
8:I:74:CYS:SG	8:I:75:SER:N	2.89	0.46
16:U:471:ASP:HB2	16:U:507:VAL:HG23	1.97	0.46
16:U:486:MET:SD	16:U:487:GLY:N	2.88	0.46
16:U:504:ASP:OD1	16:U:535:TYR:OH	2.21	0.46
17:V:144:ASP:O	17:V:150:ARG:NH2	2.49	0.46
17:V:313:LEU:HD22	17:V:332:LEU:HD22	1.97	0.46
18:W:259:GLU:HG2	18:W:261:GLU:H	1.79	0.46
19:X:400:ALA:O	19:X:404:ILE:HG12	2.16	0.46
20:Y:17:LEU:CD1	20:Y:211:TYR:HE1	2.28	0.46
22:a:117:ALA:O	22:a:120:ALA:HB3	2.15	0.46
22:a:156:TYR:HD1	22:a:175:ASP:HB3	1.80	0.46
24:c:124:GLY:HA2	24:c:127:ILE:HG22	1.98	0.46
24:c:178:THR:HG23	24:c:183:HIS:CE1	2.51	0.46
7:q:45:LEU:O	7:q:102:LEU:HA	2.16	0.46
25:d:12:LYS:HG2	25:d:13:SER:H	1.81	0.46
27:f:305:LEU:CG	27:f:321:MET:HE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:704:LEU:O	27:f:708:ASP:N	2.40	0.46
30:B:125:THR:OG1	30:B:126:SER:N	2.48	0.46
31:C:31:LEU:HD22	32:D:47:LEU:CD1	2.45	0.46
2:F:381:TYR:HA	2:F:384:LEU:HD12	1.98	0.46
8:I:159:TRP:CD1	10:J:54:GLN:HB3	2.50	0.46
10:J:36:ARG:O	10:J:157:LYS:NZ	2.49	0.46
13:T:70:ASP:HA	13:T:232:PHE:HA	1.98	0.46
14:L:93:LEU:O	14:L:97:PHE:HB2	2.15	0.46
16:U:247:GLN:HG3	16:U:904:LYS:HD3	1.98	0.46
18:W:260:SER:OG	18:W:264:GLN:OE1	2.28	0.46
12:k:166:ASP:OD1	12:k:166:ASP:N	2.49	0.46
12:k:178:GLN:HE21	14:l:56:LEU:HD12	1.81	0.46
15:m:44:ASP:OD1	15:m:44:ASP:N	2.49	0.46
9:r:203:SER:HB3	9:r:206:LEU:HG	1.97	0.46
11:s:146:LYS:HE2	11:s:146:LYS:HB2	1.72	0.46
27:f:291:GLN:OE1	27:f:320:ILE:CG2	2.64	0.46
28:A:325:ASP:OD1	28:A:325:ASP:N	2.48	0.46
31:C:142:LYS:HE3	32:D:323:ARG:HG2	1.98	0.46
3:O:218:LEU:HB2	3:O:229:LEU:HD12	1.97	0.46
7:Q:102:LEU:O	7:Q:118:MET:HB3	2.16	0.46
15:M:44:ASP:OD1	15:M:44:ASP:N	2.48	0.46
18:W:63:THR:HA	18:W:68:VAL:HG22	1.97	0.46
12:k:13:ASN:HB2	14:l:126:ARG:HD3	1.98	0.46
23:b:161:ASN:HB2	23:b:165:GLY:HA3	1.98	0.46
24:c:118:PHE:HB3	24:c:121:TRP:HE1	1.81	0.46
27:f:494:ARG:NH2	27:f:496:ASP:OD2	2.47	0.46
13:t:108:LEU:HA	13:t:111:VAL:HG12	1.98	0.46
13:t:119:GLU:HB2	13:t:128:TYR:CE2	2.51	0.46
28:A:84:LYS:O	28:A:87:LEU:N	2.49	0.46
33:E:181:THR:O	33:E:185:ARG:CG	2.64	0.46
4:G:101:TRP:CD2	4:G:109:ILE:HD12	2.50	0.45
5:P:51:ILE:HD12	5:P:109:ILE:HG12	1.97	0.45
6:H:85:VAL:O	6:H:89:ARG:HG2	2.16	0.45
8:i:28:ILE:HD13	8:i:133:SER:HB2	1.98	0.45
16:U:165:LYS:O	16:U:169:GLU:N	2.48	0.45
17:V:43:THR:HA	17:V:62:HIS:HE1	1.81	0.45
18:W:152:ILE:HG23	18:W:161:GLU:HB3	1.97	0.45
14:l:85:CYS:SG	14:l:89:ARG:NH1	2.88	0.45
22:a:35:HIS:ND1	23:b:14:GLU:OE2	2.39	0.45
23:b:138:VAL:HG12	23:b:140:ILE:HG13	1.98	0.45
27:f:667:GLY:HA2	27:f:671:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:144:ARG:HA	13:t:147:LYS:HZ3	1.81	0.45
29:u:403:ARG:CA	29:u:406:ARG:CG	2.94	0.45
32:D:167:ILE:HD12	35:D:501:ATP:N7	2.30	0.45
32:D:189:GLU:HA	32:D:192:LYS:HG2	1.98	0.45
1:N:167:SER:HA	1:N:170:TYR:CE2	2.51	0.45
5:P:205:ASP:N	5:P:205:ASP:OD1	2.48	0.45
7:Q:137:PHE:HB3	9:r:192:VAL:HG21	1.98	0.45
8:I:25:MET:HE3	8:I:153:SER:HB3	1.98	0.45
17:V:314:ARG:NH1	20:Y:381:GLN:OE1	2.49	0.45
15:m:144:ASN:OD1	15:m:145:ASP:N	2.49	0.45
23:b:7:MET:HB3	23:b:52:ILE:HG13	1.98	0.45
23:b:51:LEU:N	23:b:62:THR:OG1	2.49	0.45
5:p:27:ARG:NH2	5:p:31:GLN:O	2.47	0.45
27:f:39:LYS:HE3	27:f:120:ARG:HH22	1.81	0.45
33:E:320:ILE:HB	33:E:322:LYS:HE3	1.98	0.45
2:F:415:LEU:HB3	2:F:419:ASP:HB2	1.98	0.45
3:O:71:ASP:HB3	3:O:74:CYS:HB2	1.97	0.45
4:G:180:GLU:HA	4:G:183:VAL:HG12	1.98	0.45
12:K:43:SER:HA	12:K:151:PRO:HG3	1.99	0.45
15:M:16:SER:OG	15:M:18:ASP:OD1	2.21	0.45
15:M:69:ASN:O	15:M:93:ARG:NH1	2.48	0.45
3:o:75:SER:CB	3:o:230:ARG:HH22	2.08	0.45
24:c:46:ARG:HA	24:c:46:ARG:HD2	1.82	0.45
24:c:241:ASN:O	24:c:245:VAL:HG23	2.16	0.45
30:B:80:ARG:NH2	30:B:83:GLU:OE2	2.50	0.45
11:S:132:TYR:HB3	11:S:134:VAL:HG22	1.99	0.45
4:g:37:LEU:HD21	4:g:82:GLY:H	1.81	0.45
17:V:277:PRO:HG2	17:V:285:TRP:HZ3	1.82	0.45
18:W:407:ASP:HB3	19:X:344:ARG:NH1	2.31	0.45
18:W:421:PRO:HB3	21:Z:248:ALA:HA	1.98	0.45
21:Z:113:LYS:NZ	21:Z:117:PRO:O	2.42	0.45
25:d:217:LEU:HD13	25:d:222:TYR:HE1	1.81	0.45
11:s:175:PRO:HA	11:s:178:ASP:HB2	1.97	0.45
11:s:183:PHE:HB3	11:s:186:MET:HG2	1.97	0.45
27:f:522:CYS:SG	27:f:523:GLY:N	2.90	0.45
32:D:227:PHE:C	32:D:228:ILE:HG13	2.42	0.45
5:P:47:ASP:OD2	5:P:48:ARG:NH1	2.49	0.45
5:P:105:THR:N	5:P:126:LEU:CD2	2.77	0.45
6:H:46:LEU:HD23	6:H:75:VAL:HG13	1.98	0.45
12:K:26:TYR:HA	12:K:29:GLU:HG3	1.98	0.45
15:M:42:CYS:HB2	15:M:190:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:207:ASP:OD1	15:M:207:ASP:N	2.50	0.45
6:h:43:GLY:HA3	6:h:213:CYS:O	2.17	0.45
17:V:344:ASP:HB2	26:e:42:ASN:HA	1.97	0.45
17:V:460:SER:O	17:V:460:SER:OG	2.31	0.45
14:l:7:ASP:O	14:l:21:GLN:NE2	2.35	0.45
21:Z:11:VAL:HG23	21:Z:50:VAL:HG11	1.98	0.45
3:o:244:ARG:HE	3:o:246:ARG:HB3	1.81	0.45
7:q:59:TYR:O	7:q:62:LYS:HG3	2.17	0.45
25:d:190:LEU:HB3	25:d:193:GLU:OE1	2.16	0.45
27:f:287:ASP:OD1	27:f:317:LEU:HD21	2.16	0.45
27:f:288:VAL:HG11	27:f:873:LEU:HD22	1.97	0.45
13:t:71:MET:N	13:t:71:MET:SD	2.90	0.45
28:A:224:LEU:HD13	35:A:501:ATP:H2'	1.98	0.45
30:B:315:GLN:O	30:B:322:ARG:NH1	2.49	0.45
30:B:391:SER:HB3	31:C:307:ARG:NH2	2.27	0.45
31:C:88:LYS:HB3	31:C:94:LYS:HG3	1.98	0.45
33:E:178:THR:O	33:E:301:ILE:HG21	2.17	0.45
33:E:179:GLY:N	35:E:401:ATP:O2B	2.50	0.45
3:O:108:LEU:HD11	6:H:91:ARG:HB3	1.98	0.45
10:J:6:ALA:HB3	10:J:123:GLY:HA3	1.97	0.45
13:T:225:ASP:HB3	13:T:228:SER:HB3	1.97	0.45
10:j:46:GLU:HG3	10:j:199:VAL:HG22	1.99	0.45
10:j:116:GLN:HB2	10:j:151:GLY:HA3	1.99	0.45
19:X:177:TYR:CE2	19:X:185:LYS:HB3	2.51	0.45
21:Z:48:LEU:HD11	21:Z:92:VAL:HG21	1.99	0.45
27:f:469:TYR:HB3	27:f:481:SER:HB2	1.99	0.45
30:B:224:LEU:CD2	30:B:235:LEU:HD13	2.33	0.45
2:F:374:ASN:N	2:F:414:GLU:HG3	2.32	0.45
4:G:191:PHE:O	4:G:194:THR:OG1	2.29	0.45
12:K:28:ILE:HD13	12:K:158:PRO:HG2	1.99	0.45
16:U:364:VAL:O	16:U:367:THR:OG1	2.30	0.45
10:j:156:TRP:HZ3	12:k:58:LEU:HB3	1.82	0.45
18:W:93:ARG:HA	18:W:97:LEU:HD13	1.98	0.45
18:W:445:LEU:HB3	21:Z:157:HIS:CE1	2.51	0.45
20:Y:148:GLY:O	20:Y:152:MET:N	2.48	0.45
20:Y:234:PRO:HA	20:Y:237:ARG:NE	2.31	0.45
1:n:79:ARG:HD2	1:n:86:THR:HB	1.99	0.45
22:a:199:THR:HA	22:a:202:LEU:HB2	1.98	0.45
25:d:204:LYS:O	25:d:207:THR:OG1	2.33	0.45
28:A:178:GLY:O	28:A:354:ILE:HG22	2.16	0.45
30:B:288:ASP:OD1	30:B:288:ASP:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:45:LYS:O	32:D:48:GLN:HG2	2.17	0.45
32:D:176:GLU:O	32:D:180:ALA:HB2	2.17	0.45
33:E:130:VAL:O	33:E:189:SER:OG	2.24	0.45
33:E:176:PRO:HG3	33:E:280:ASN:HD21	1.82	0.45
2:F:134:LEU:HB3	33:E:55:GLN:HE22	1.81	0.45
2:F:158:TYR:HD2	33:E:55:GLN:HG2	1.82	0.45
2:F:344:ARG:NH1	35:E:401:ATP:O3G	2.49	0.45
2:F:358:ASN:O	2:F:362:ARG:NH1	2.47	0.45
4:g:79:VAL:HG12	4:g:139:ILE:HB	1.99	0.45
16:U:515:ALA:HA	16:U:518:LEU:HB2	1.99	0.45
14:l:66:VAL:O	11:s:105:HIS:NE2	2.50	0.45
14:l:104:PRO:HB3	13:t:126:HIS:NE2	2.32	0.45
23:b:1:MET:N	23:b:43:SER:OG	2.50	0.45
24:c:59:GLY:HA3	24:c:69:VAL:HA	1.98	0.45
27:f:463:LEU:HD11	27:f:497:VAL:CG2	2.15	0.45
28:A:218:PRO:HG2	30:B:343:ARG:NH2	2.31	0.45
31:C:339:THR:OG1	31:C:378:VAL:O	2.28	0.45
14:L:227:ASP:OD1	14:L:227:ASP:N	2.49	0.45
8:i:72:MET:SD	8:i:110:LEU:HD21	2.57	0.45
6:h:52:GLN:HG3	6:h:59:GLU:HG2	1.99	0.45
6:h:203:MET:HA	6:h:207:ASN:HD21	1.82	0.45
17:V:467:TYR:OH	21:Z:255:ASP:OD1	2.32	0.45
18:W:384:LEU:HD13	18:W:388:GLU:HG3	1.98	0.45
5:p:203:ARG:NH1	5:p:204:MET:H	2.13	0.45
11:s:35:PHE:HZ	11:s:168:SER:HB3	1.82	0.45
27:f:470:VAL:HG13	27:f:482:ILE:HG21	1.98	0.45
30:B:262:ASP:OD1	30:B:262:ASP:N	2.47	0.45
33:E:120:TYR:HA	33:E:123:SER:HB3	1.99	0.45
1:N:63:ARG:HD3	13:t:254:TRP:HZ3	1.82	0.45
1:N:99:PHE:HE2	4:G:96:TYR:HA	1.82	0.45
7:Q:162:LYS:HD2	7:Q:162:LYS:HA	1.73	0.45
12:K:117:SER:OG	12:K:160:GLY:O	2.24	0.45
8:i:82:ASP:HB3	8:i:130:PHE:HB3	1.99	0.45
15:M:74:VAL:HG22	15:M:140:SER:HB2	1.99	0.45
15:M:76:MET:HA	15:M:137:MET:O	2.17	0.45
16:U:603:LEU:CD1	32:D:60:TYR:CD1	2.97	0.45
10:j:112:ALA:HB3	10:j:153:TYR:HD2	1.82	0.45
18:W:357:ARG:HD3	18:W:357:ARG:HA	1.76	0.45
18:W:382:LEU:HB3	18:W:384:LEU:HG	1.99	0.45
19:X:225:TRP:O	19:X:229:TYR:N	2.45	0.45
19:X:256:LEU:HD21	19:X:322:HIS:CD2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:138:ASP:OD1	14:l:143:HIS:NE2	2.45	0.45
1:n:176:THR:HB	1:n:189:PHE:HE1	1.82	0.45
22:a:369:HIS:HA	22:a:372:HIS:NE2	2.33	0.45
23:b:12:ASN:HB3	23:b:55:ALA:HB2	1.99	0.45
28:A:113:ILE:HD13	28:A:123:VAL:HG22	1.99	0.45
30:B:151:LEU:HB2	30:B:163:LEU:HD21	1.98	0.45
33:E:139:SER:HA	33:E:142:ILE:HD12	1.98	0.45
2:F:234:THR:O	2:F:237:ALA:N	2.50	0.44
5:P:177:ARG:HG3	11:s:175:PRO:HG3	1.99	0.44
16:U:149:GLN:HB3	32:D:40:LEU:HD21	1.99	0.44
16:U:603:LEU:CD1	32:D:60:TYR:HD1	2.30	0.44
17:V:355:ARG:C	17:V:358:MET:HE3	2.42	0.44
10:j:173:GLU:HG2	12:k:57:PRO:HG2	1.99	0.44
20:Y:153:ASP:N	20:Y:153:ASP:OD1	2.41	0.44
25:d:52:ARG:NH2	25:d:91:GLU:O	2.50	0.44
30:B:275:GLU:OE2	30:B:322:ARG:NE	2.46	0.44
31:C:19:GLY:HA3	31:C:22:GLN:NE2	2.33	0.44
2:F:97:LEU:N	2:F:121:CYS:O	2.50	0.44
3:O:227:ASP:OD1	3:O:227:ASP:N	2.49	0.44
4:G:65:THR:HG21	15:M:160:GLY:HA3	1.99	0.44
4:g:13:ILE:HG13	4:g:15:ILE:HG12	1.98	0.44
16:U:249:CYS:HB2	16:U:328:ILE:HA	1.99	0.44
6:h:35:SER:OG	6:h:76:TYR:O	2.34	0.44
17:V:32:PRO:O	17:V:36:GLU:HB3	2.18	0.44
18:W:203:GLN:O	18:W:207:LYS:HG3	2.17	0.44
18:W:231:ILE:HG22	18:W:243:ILE:HG22	1.99	0.44
19:X:285:GLU:HA	19:X:288:LYS:HZ2	1.82	0.44
20:Y:262:SER:OG	20:Y:267:ARG:O	2.36	0.44
9:r:239:ARG:NH2	9:r:241:ASP:OD2	2.49	0.44
30:B:284:ILE:HG12	30:B:329:MET:HE1	1.99	0.44
31:C:19:GLY:HA3	31:C:22:GLN:HE21	1.82	0.44
32:D:150:SER:OG	32:D:229:ARG:O	2.31	0.44
32:D:168:GLY:H	35:D:501:ATP:HN61	1.65	0.44
2:F:276:LYS:NZ	2:F:325:GLN:OE1	2.50	0.44
2:F:418:GLU:O	2:F:421:MET:HG2	2.17	0.44
6:H:92:LYS:HG2	6:H:96:GLN:HE22	1.82	0.44
16:U:374:SER:HB3	16:U:407:SER:HB3	1.99	0.44
18:W:78:LYS:HA	18:W:78:LYS:HD2	1.74	0.44
18:W:313:GLU:OE1	18:W:314:LEU:N	2.49	0.44
19:X:252:LYS:O	19:X:256:LEU:HB2	2.17	0.44
20:Y:332:GLN:NE2	20:Y:333:GLU:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:16:LEU:HD23	21:Z:124:ILE:HD13	1.99	0.44
21:Z:72:HIS:CG	21:Z:114:ARG:HH22	2.36	0.44
25:d:91:GLU:HG2	25:d:92:SER:N	2.33	0.44
27:f:126:ILE:HA	27:f:173:LEU:HD11	1.98	0.44
27:f:261:ARG:HA	27:f:268:LEU:HB3	1.99	0.44
31:C:115:ALA:HB3	31:C:124:HIS:HB3	1.98	0.44
31:C:195:GLY:O	31:C:317:PHE:HE2	2.01	0.44
33:E:185:ARG:NH1	33:E:185:ARG:HB2	2.32	0.44
5:P:138:VAL:HG21	5:P:147:TYR:CE1	2.52	0.44
16:U:261:LEU:HA	16:U:264:VAL:HG12	1.98	0.44
16:U:772:TRP:HD1	16:U:775:LEU:HB2	1.82	0.44
18:W:192:LEU:O	18:W:196:VAL:HG23	2.18	0.44
18:W:359:VAL:O	18:W:363:ILE:HG12	2.18	0.44
19:X:244:SER:O	19:X:247:ALA:N	2.49	0.44
14:l:65:HIS:HD2	14:l:221:PHE:HB3	1.82	0.44
14:l:90:GLN:HA	14:l:93:LEU:HD12	1.99	0.44
14:l:137:TYR:CZ	14:l:217:LYS:HE3	2.52	0.44
22:a:168:ASN:OD1	22:a:169:HIS:N	2.50	0.44
26:e:40:GLU:O	26:e:42:ASN:ND2	2.49	0.44
27:f:215:ASP:HB3	27:f:838:ARG:HH12	1.82	0.44
27:f:654:VAL:HA	27:f:657:ILE:HG12	1.99	0.44
27:f:725:SER:O	27:f:729:MET:N	2.48	0.44
13:t:70:ASP:OD1	13:t:86:ARG:NH2	2.43	0.44
28:A:274:PHE:HB2	28:A:319:MET:HA	1.98	0.44
32:D:272:THR:HA	32:D:316:THR:HG22	1.99	0.44
3:O:217:ASP:CA	3:O:230:ARG:O	2.66	0.44
16:U:157:THR:HG23	16:U:159:ARG:H	1.81	0.44
16:U:579:ARG:HB3	16:U:614:VAL:HG21	2.00	0.44
6:h:36:VAL:HG13	6:h:174:LEU:HD11	1.99	0.44
17:V:318:GLN:H	17:V:318:GLN:CD	2.24	0.44
17:V:399:ARG:HB3	25:d:141:GLN:NE2	2.32	0.44
18:W:82:LEU:HA	18:W:85:GLU:HG2	2.00	0.44
19:X:145:GLU:HA	19:X:148:HIS:ND1	2.33	0.44
19:X:401:LEU:O	19:X:404:ILE:HB	2.16	0.44
5:p:131:MET:HE2	5:p:133:THR:HG22	2.00	0.44
27:f:215:ASP:N	27:f:215:ASP:OD1	2.48	0.44
31:C:375:ARG:HG2	31:C:377:HIS:H	1.82	0.44
33:E:327:ASP:OD2	33:E:330:ALA:N	2.51	0.44
1:N:79:ARG:NH2	1:N:86:THR:OG1	2.51	0.44
4:G:54:LYS:HE3	4:G:214:GLU:HA	1.99	0.44
9:R:192:VAL:HG21	7:q:137:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:13:ILE:HA	18:W:16:MET:HG2	2.00	0.44
18:W:265:GLN:HB2	18:W:333:LEU:HD13	1.99	0.44
12:k:21:LEU:HB2	12:k:24:VAL:HG12	1.99	0.44
15:m:203:ASP:HB3	15:m:206:LYS:HG2	1.98	0.44
1:n:38:MET:SD	1:n:190:THR:HG23	2.57	0.44
22:a:211:PHE:HB3	22:a:275:LEU:HD13	2.00	0.44
3:o:84:ILE:HG12	3:o:145:GLY:HA3	2.00	0.44
3:o:141:LEU:HB2	3:o:156:ILE:HB	1.99	0.44
28:A:96:ALA:O	30:B:132:TYR:HB3	2.18	0.44
33:E:381:GLU:OE1	33:E:381:GLU:N	2.47	0.44
9:R:103:THR:HG22	9:R:159:MET:H	1.83	0.44
15:M:176:GLU:HA	15:M:179:LYS:HG2	1.99	0.44
10:j:115:LYS:HE2	10:j:149:PRO:HA	1.98	0.44
21:Z:95:TYR:HB3	21:Z:122:VAL:HB	2.00	0.44
22:a:292:THR:OG1	22:a:294:GLU:OE1	2.34	0.44
27:f:326:LEU:HD13	27:f:326:LEU:N	2.33	0.44
31:C:368:MET:HE2	32:D:179:GLU:HB3	1.99	0.44
12:K:68:VAL:HG21	12:K:89:ILE:HD13	2.00	0.44
16:U:172:ASP:HB3	16:U:174:PRO:HD3	2.00	0.44
16:U:758:PRO:HA	16:U:761:VAL:HG22	2.00	0.44
17:V:148:ARG:NH1	17:V:193:GLN:O	2.51	0.44
17:V:160:LEU:O	17:V:164:GLU:HB2	2.18	0.44
10:j:154:HIS:CG	12:k:59:MET:HE1	2.53	0.44
18:W:375:MET:HA	18:W:378:MET:HG3	2.00	0.44
23:b:27:GLN:HA	23:b:30:GLN:HB3	2.00	0.44
26:e:68:GLU:N	26:e:68:GLU:OE1	2.51	0.44
27:f:328:SER:C	27:f:331:LEU:HB3	2.43	0.44
27:f:394:ASP:N	27:f:394:ASP:OD1	2.50	0.44
28:A:390:THR:HA	30:B:216:ILE:HD11	2.00	0.44
32:D:91:GLN:OE1	32:D:248:ARG:NH1	2.51	0.44
4:G:19:GLU:HG2	4:G:21:ARG:HG2	1.99	0.44
11:S:239:ARG:NH2	11:S:241:ASP:OD2	2.50	0.44
14:L:26:MET:HE1	14:L:148:CYS:HB2	2.00	0.44
4:g:112:ASP:OD1	4:g:112:ASP:N	2.48	0.44
17:V:473:GLN:HG2	21:Z:257:MET:HG3	1.99	0.44
18:W:111:TYR:O	18:W:115:ILE:HG12	2.18	0.44
19:X:364:LYS:HA	19:X:364:LYS:HD2	1.70	0.44
14:l:36:VAL:HG13	14:l:172:LEU:HD11	2.00	0.44
21:Z:45:LYS:HB2	21:Z:47:VAL:HG12	2.00	0.44
22:a:194:GLN:HE22	22:a:228:THR:HG1	1.66	0.44
5:p:27:ARG:HB2	5:p:183:MET:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:s:221:LEU:O	11:s:235:THR:HA	2.18	0.44
4:G:21:ARG:HD2	32:D:417:TYR:CZ	2.53	0.43
12:K:52:LYS:HD3	12:K:216:GLU:HB2	1.99	0.43
12:K:169:ALA:O	12:K:174:SER:OG	2.28	0.43
16:U:596:ASN:OD1	16:U:596:ASN:N	2.50	0.43
6:h:44:VAL:HB	6:h:137:CYS:HB2	1.99	0.43
18:W:338:THR:HA	18:W:342:GLY:HA3	1.98	0.43
14:l:66:VAL:HG13	14:l:89:ARG:HG3	2.00	0.43
7:q:88:LEU:HD22	7:q:122:ALA:HB2	1.99	0.43
9:r:60:THR:HG21	9:r:105:ALA:HA	2.00	0.43
27:f:805:ASP:OD1	27:f:805:ASP:N	2.39	0.43
13:t:235:ALA:HA	13:t:243:GLU:O	2.18	0.43
31:C:38:LYS:HZ1	32:D:55:GLU:HA	1.83	0.43
32:D:105:SER:OG	32:D:109:SER:O	2.26	0.43
1:N:71:ILE:HG21	1:N:97:LEU:HD21	1.99	0.43
16:U:43:ASP:OD1	16:U:43:ASP:N	2.42	0.43
16:U:413:LYS:HA	16:U:449:ILE:HG12	2.01	0.43
17:V:300:LEU:HA	17:V:397:ARG:NH2	2.32	0.43
18:W:147:LYS:O	18:W:151:THR:HG23	2.18	0.43
18:W:433:ASN:O	18:W:437:SER:HB3	2.18	0.43
14:l:80:ASP:HB3	14:l:128:TYR:HB3	2.00	0.43
20:Y:228:MET:HE2	20:Y:263:LEU:HD21	1.99	0.43
21:Z:16:LEU:CD1	21:Z:16:LEU:N	2.80	0.43
22:a:62:ASN:OD1	22:a:63:PHE:N	2.51	0.43
23:b:3:LEU:HD13	23:b:104:ASN:HB2	2.00	0.43
23:b:47:ASN:HA	23:b:105:HIS:CE1	2.48	0.43
23:b:161:ASN:HD22	23:b:168:SER:HB3	1.83	0.43
24:c:299:CYS:O	24:c:302:ALA:HB3	2.18	0.43
26:e:52:PHE:CZ	26:e:55:GLN:HA	2.53	0.43
27:f:392:THR:O	27:f:396:ASN:N	2.51	0.43
27:f:565:ASN:HA	27:f:776:LEU:HD11	2.00	0.43
30:B:153:ASN:HB3	30:B:157:HIS:H	1.82	0.43
31:C:280:LEU:HG	31:C:280:LEU:O	2.17	0.43
2:F:297:ASP:HB2	33:E:284:THR:HG22	2.00	0.43
3:O:124:ARG:NH2	4:G:103:TYR:O	2.48	0.43
10:J:81:ARG:HA	10:J:84:ILE:HB	2.01	0.43
14:L:54:SER:H	14:L:57:ALA:HB3	1.83	0.43
4:g:212:PRO:HB2	4:g:232:GLU:HG2	1.99	0.43
16:U:325:MET:O	16:U:329:LEU:HB2	2.17	0.43
18:W:231:ILE:HD13	18:W:247:TYR:HE1	1.83	0.43
12:k:100:TRP:CD1	9:r:116:ARG:HH22	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:k:145:GLY:HA2	12:k:220:VAL:HG11	2.00	0.43
14:l:199:LEU:HB2	14:l:239:ARG:HH22	1.84	0.43
1:n:157:GLN:HE21	1:n:160:ALA:HB2	1.82	0.43
5:p:78:GLU:HB3	5:p:80:ARG:HG2	2.00	0.43
5:p:185:VAL:HG23	5:p:202:ALA:HB2	2.00	0.43
7:q:118:MET:HE1	7:q:124:LEU:HD23	2.01	0.43
27:f:603:SER:HB2	27:f:639:LYS:HZ2	1.82	0.43
27:f:818:LEU:HD12	27:f:820:GLY:H	1.83	0.43
28:A:402:LYS:HA	30:B:214:MET:HE1	1.99	0.43
31:C:240:GLU:OE1	31:C:241:HIS:NE2	2.51	0.43
32:D:200:ARG:HD2	32:D:299:PHE:HD2	1.83	0.43
33:E:285:LEU:HD12	33:E:289:LEU:HD23	1.99	0.43
1:N:63:ARG:NH2	13:t:223:TYR:HB3	2.34	0.43
3:O:165:LEU:HD12	3:O:168:VAL:HG12	2.00	0.43
9:R:91:LYS:HE3	9:R:245:ARG:HH22	1.82	0.43
14:L:183:ASN:OD1	14:L:186:GLU:N	2.41	0.43
14:L:197:GLU:HG3	14:L:239:ARG:HH12	1.83	0.43
17:V:29:PRO:HB3	17:V:85:ALA:HB2	2.01	0.43
17:V:65:ARG:O	17:V:69:THR:HG23	2.18	0.43
18:W:141:GLU:HG3	18:W:144:ARG:HE	1.82	0.43
21:Z:262:LEU:O	21:Z:266:ILE:HG12	2.18	0.43
22:a:41:VAL:O	22:a:45:VAL:HG23	2.18	0.43
22:a:169:HIS:HD2	22:a:206:LEU:HD23	1.83	0.43
3:o:45:THR:HG21	3:o:205:GLY:HA3	2.00	0.43
5:p:158:MET:HE3	5:p:162:HIS:CE1	2.53	0.43
9:r:141:LEU:O	9:r:145:MET:HG3	2.18	0.43
11:s:48:PHE:HA	11:s:226:VAL:O	2.19	0.43
13:t:233:GLN:HB3	13:t:244:ILE:HD11	1.99	0.43
30:B:89:GLU:OE2	30:B:98:LYS:NZ	2.36	0.43
31:C:161:ILE:O	31:C:165:ILE:HG22	2.18	0.43
32:D:80:LYS:HE2	32:D:80:LYS:HB2	1.92	0.43
32:D:328:ASP:OD1	32:D:328:ASP:N	2.51	0.43
2:F:79:LYS:HD3	2:F:79:LYS:HA	1.69	0.43
4:G:14:THR:O	4:G:14:THR:OG1	2.36	0.43
4:G:49:VAL:HG21	4:G:195:VAL:HG12	2.00	0.43
4:G:116:LYS:HZ2	6:H:84:ARG:HD3	1.84	0.43
4:G:144:ASP:HB2	4:G:147:GLN:HB2	2.00	0.43
6:H:58:ASP:OD1	6:H:61:SER:N	2.52	0.43
11:S:119:MET:HE1	12:K:102:THR:HB	2.00	0.43
13:T:254:TRP:CZ3	1:n:63:ARG:HD3	2.53	0.43
16:U:19:LEU:HA	16:U:22:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:388:ASP:OD1	16:U:388:ASP:N	2.49	0.43
17:V:62:HIS:HA	17:V:65:ARG:HB3	2.00	0.43
17:V:92:ARG:NH2	17:V:118:GLN:OE1	2.34	0.43
19:X:93:LEU:HD21	19:X:113:CYS:SG	2.58	0.43
19:X:111:LEU:HA	19:X:114:ILE:HD12	2.00	0.43
19:X:163:LYS:HE3	19:X:163:LYS:HB3	1.77	0.43
14:l:45:VAL:HG22	14:l:214:ILE:HG23	2.00	0.43
20:Y:268:TYR:HA	20:Y:271:PHE:HB3	1.99	0.43
22:a:134:THR:O	22:a:138:VAL:HG23	2.18	0.43
24:c:232:GLN:HE21	24:c:298:GLN:HE21	1.67	0.43
9:r:132:ARG:HH21	9:r:133:ILE:HG22	1.82	0.43
11:s:55:THR:O	11:s:68:SER:N	2.43	0.43
27:f:557:TRP:HE1	27:f:784:ASP:HB3	1.83	0.43
27:f:606:VAL:HA	27:f:609:VAL:HB	2.01	0.43
27:f:673:ARG:HH21	27:f:712:LYS:HB2	1.82	0.43
27:f:758:ASN:OD1	27:f:855:GLN:NE2	2.46	0.43
27:f:779:CYS:HA	27:f:782:HIS:NE2	2.34	0.43
1:N:194:LEU:HD23	1:N:208:ILE:HG23	2.00	0.43
2:F:153:VAL:HG22	2:F:160:ILE:HG22	2.01	0.43
2:F:203:VAL:O	2:F:207:ASN:N	2.49	0.43
4:G:36:GLY:HA2	4:G:170:VAL:HG21	2.00	0.43
7:Q:62:LYS:HE2	10:J:96:LEU:HA	2.01	0.43
8:I:87:THR:O	8:I:91:ARG:HG2	2.18	0.43
11:S:55:THR:O	11:S:68:SER:N	2.51	0.43
8:i:122:THR:HG22	8:i:129:PRO:HB3	2.01	0.43
8:i:155:ASN:OD1	8:i:156:TYR:N	2.51	0.43
15:M:36:THR:HA	15:M:167:GLY:HA3	2.00	0.43
17:V:255:LEU:HD11	17:V:269:LYS:HG3	1.99	0.43
17:V:376:ASN:O	17:V:379:LEU:HB2	2.19	0.43
18:W:366:MET:O	18:W:370:TYR:HB2	2.19	0.43
19:X:137:TYR:OH	19:X:142:ARG:O	2.35	0.43
14:l:104:PRO:HB2	14:l:107:ARG:HG2	2.01	0.43
15:m:114:ASP:O	15:m:118:MET:HG2	2.19	0.43
21:Z:16:LEU:CD2	21:Z:124:ILE:CD1	2.95	0.43
22:a:35:HIS:CE1	22:a:71:VAL:HG22	2.53	0.43
22:a:359:ASP:HB3	24:c:308:VAL:HG12	1.99	0.43
3:o:153:LEU:HD21	3:o:168:VAL:HG22	2.00	0.43
24:c:232:GLN:CD	24:c:233:ASP:H	2.26	0.43
11:s:226:VAL:HG22	11:s:231:ILE:HG12	1.99	0.43
27:f:261:ARG:HH11	27:f:269:ALA:HB3	1.84	0.43
27:f:585:GLU:HG3	27:f:588:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:169:PRO:O	30:B:172:THR:OG1	2.32	0.43
31:C:201:ARG:NH1	31:C:201:ARG:O	2.51	0.43
33:E:114:GLU:OE1	33:E:114:GLU:N	2.41	0.43
1:N:102:ILE:HD12	1:N:102:ILE:HA	1.88	0.43
2:F:379:VAL:HA	2:F:417:HIS:HB2	2.01	0.43
3:O:199:SER:CB	3:O:232:TYR:CE2	2.86	0.43
8:I:33:THR:HA	8:I:165:GLY:HA2	2.00	0.43
16:U:564:ASP:HA	16:U:567:ILE:HG12	2.01	0.43
21:Z:9:VAL:HG23	21:Z:48:LEU:HB3	2.01	0.43
3:o:258:LYS:HA	3:o:258:LYS:HD3	1.69	0.43
3:o:262:LEU:HD11	5:p:195:ILE:HG13	2.01	0.43
5:p:121:ILE:HB	5:p:137:VAL:HG22	2.00	0.43
24:c:196:LEU:HD22	24:c:198:ARG:HH22	1.83	0.43
27:f:703:ARG:HH12	27:f:742:ALA:HB2	1.83	0.43
27:f:756:PRO:HG3	27:f:759:LEU:HB2	2.01	0.43
32:D:58:GLU:OE2	32:D:62:LYS:NZ	2.38	0.43
32:D:214:MET:CE	35:D:501:ATP:C4	2.81	0.43
33:E:53:VAL:HG12	33:E:102:MET:HE1	1.99	0.43
33:E:171:LEU:HD11	33:E:298:LYS:HG3	2.00	0.43
2:F:395:GLN:O	2:F:399:VAL:HG23	2.19	0.43
2:F:424:ILE:HD12	2:F:424:ILE:HA	1.86	0.43
5:P:12:MET:HE1	5:P:136:PHE:HB2	2.01	0.43
7:Q:155:ARG:O	7:Q:155:ARG:NH1	2.47	0.43
10:J:83:VAL:HG13	10:J:111:ILE:HD11	1.99	0.43
12:K:182:GLN:NE2	14:L:56:LEU:HG	2.34	0.43
15:M:236:ALA:HA	15:M:239:TYR:CZ	2.54	0.43
4:g:11:ARG:O	4:g:24:GLN:NE2	2.52	0.43
4:g:75:ASN:OD1	4:g:76:ILE:N	2.52	0.43
17:V:408:ARG:O	17:V:411:SER:OG	2.30	0.43
17:V:424:GLN:OE1	17:V:424:GLN:N	2.49	0.43
10:j:42:VAL:HB	10:j:191:VAL:HG21	2.01	0.43
1:n:41:GLN:HB2	1:n:145:VAL:HG23	2.01	0.43
5:p:33:GLN:HE22	5:p:35:VAL:HG22	1.84	0.43
24:c:169:VAL:HG23	24:c:170:LEU:HD12	2.01	0.43
27:f:373:ALA:HA	27:f:376:PHE:HD2	1.84	0.43
28:A:303:ILE:HD13	28:A:303:ILE:HA	1.84	0.43
28:A:368:ILE:HD12	28:A:370:PHE:CG	2.53	0.43
31:C:194:THR:O	31:C:194:THR:HG22	2.17	0.43
33:E:252:GLU:HA	33:E:255:ARG:HB2	2.01	0.43
2:F:126:THR:OG1	2:F:127:SER:N	2.51	0.43
4:G:60:LEU:HD21	15:M:178:GLU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:105:ILE:HD11	8:I:109:GLN:HB2	2.01	0.43
11:S:111:MET:HB3	11:S:116:ILE:HD11	2.01	0.43
11:S:239:ARG:HH21	3:o:62:ARG:HH21	1.66	0.43
13:T:99:SER:O	13:T:153:ASN:HA	2.19	0.43
15:M:71:ASP:OD1	15:M:72:ARG:N	2.49	0.43
15:M:171:GLN:HA	15:M:174:LYS:HZ3	1.84	0.43
15:M:236:ALA:HA	15:M:239:TYR:CE1	2.53	0.43
17:V:131:LEU:HA	17:V:134:PHE:HB2	2.01	0.43
17:V:495:ARG:NH2	17:V:498:PRO:HG2	2.33	0.43
10:j:172:LEU:HB2	12:k:58:LEU:HD11	2.00	0.43
19:X:118:LYS:NZ	19:X:126:ARG:HD2	2.34	0.43
19:X:201:TYR:O	32:D:339:ARG:NE	2.52	0.43
19:X:202:CYS:O	19:X:204:PRO:HD3	2.19	0.43
19:X:215:GLY:HA2	19:X:218:HIS:CE1	2.53	0.43
19:X:309:TYR:O	19:X:313:LEU:N	2.52	0.43
21:Z:189:GLN:OE1	21:Z:189:GLN:N	2.48	0.43
22:a:79:ILE:HG13	22:a:83:VAL:HG13	2.00	0.43
3:o:169:THR:OG1	3:o:178:MET:HG2	2.19	0.43
23:b:108:ARG:HA	23:b:108:ARG:HH11	1.84	0.43
27:f:78:LEU:HA	27:f:82:ILE:HD11	2.00	0.43
27:f:324:VAL:CG2	27:f:455:VAL:HG13	2.49	0.43
28:A:345:LEU:HD11	28:A:381:THR:HA	1.99	0.43
1:N:35:THR:HG21	1:N:80:SER:HA	2.01	0.43
1:N:35:THR:O	1:N:164:SER:N	2.52	0.43
1:N:117:PHE:HE2	1:N:134:ILE:HD13	1.82	0.43
10:J:16:LEU:O	10:J:19:VAL:HG22	2.19	0.43
8:i:68:LEU:HB2	8:i:72:MET:HB2	2.01	0.43
15:M:176:GLU:HB3	15:M:197:ILE:HD12	2.01	0.43
15:M:203:ASP:O	15:M:205:VAL:N	2.52	0.43
4:g:88:ARG:HD2	4:g:89:SER:N	2.34	0.43
10:j:41:VAL:HG23	10:j:211:MET:HB3	2.01	0.43
18:W:152:ILE:HG13	18:W:165:ILE:HD11	2.00	0.43
14:l:79:ALA:HA	14:l:82:ARG:HE	1.83	0.43
20:Y:113:ARG:HH12	20:Y:147:ILE:HD11	1.84	0.43
20:Y:168:ILE:HD11	20:Y:180:LEU:HD13	2.01	0.43
15:m:77:ALA:HB3	15:m:137:MET:HB2	2.01	0.43
15:m:214:LEU:HD12	15:m:233:ARG:HG3	2.01	0.43
24:c:288:VAL:HA	24:c:291:LEU:HD12	2.01	0.43
7:q:37:LYS:HA	7:q:37:LYS:HD2	1.72	0.43
9:r:197:VAL:HG21	9:r:221:GLN:HG3	2.00	0.43
13:t:233:GLN:HG2	13:t:246:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:218:PRO:CG	30:B:343:ARG:NH2	2.81	0.43
28:A:307:ASP:HB2	28:A:336:ARG:HH21	1.83	0.43
28:A:381:THR:O	28:A:385:ILE:HG12	2.19	0.43
30:B:328:ILE:O	30:B:329:MET:HE2	2.19	0.43
32:D:203:LEU:HA	32:D:309:MET:HB2	2.00	0.43
32:D:385:LEU:HD11	32:D:401:LYS:HD2	2.00	0.43
33:E:210:GLU:OE1	33:E:210:GLU:N	2.52	0.43
33:E:247:THR:OG1	33:E:248:SER:N	2.51	0.43
2:F:368:ILE:HG23	2:F:371:ARG:HH22	1.84	0.42
6:H:150:ASP:OD2	6:H:152:SER:OG	2.24	0.42
13:T:155:MET:N	13:T:155:MET:SD	2.92	0.42
14:L:186:GLU:O	14:L:190:HIS:ND1	2.46	0.42
4:g:10:ASP:HA	4:g:15:ILE:HG13	2.01	0.42
17:V:153:LYS:O	17:V:157:THR:HG23	2.19	0.42
14:l:34:ALA:HA	14:l:162:GLY:HA3	2.01	0.42
14:l:61:LYS:HD3	14:l:61:LYS:HA	1.84	0.42
21:Z:109:ASN:ND2	21:Z:140:SER:HB2	2.34	0.42
22:a:169:HIS:CD2	22:a:207:GLY:HA2	2.54	0.42
5:p:62:THR:O	5:p:66:ARG:HG2	2.19	0.42
5:p:93:ASN:O	5:p:97:GLU:HG3	2.18	0.42
25:d:10:ASN:OD1	25:d:11:ARG:N	2.53	0.42
27:f:143:ARG:O	27:f:147:SER:OG	2.24	0.42
27:f:449:GLY:HA3	27:f:484:GLY:CA	2.49	0.42
27:f:685:THR:OG1	27:f:686:LEU:N	2.51	0.42
28:A:280:ILE:HD12	28:A:280:ILE:HA	1.90	0.42
30:B:234:LEU:HD22	35:B:501:ATP:H2'	2.00	0.42
2:F:218:GLN:NE2	33:E:344:ARG:HH11	2.17	0.42
2:F:415:LEU:HD23	2:F:419:ASP:HB3	2.01	0.42
3:O:262:LEU:HD11	5:P:195:ILE:HG13	2.02	0.42
6:H:39:LYS:N	6:H:159:LYS:O	2.50	0.42
16:U:101:ILE:O	16:U:105:ILE:HG12	2.19	0.42
6:h:222:THR:HG23	6:h:225:GLU:H	1.84	0.42
18:W:406:VAL:HA	18:W:413:ILE:HG21	2.01	0.42
21:Z:16:LEU:CD2	21:Z:124:ILE:HD13	2.49	0.42
23:b:104:ASN:OD1	23:b:104:ASN:N	2.52	0.42
24:c:172:HIS:CD2	24:c:174:PRO:HD2	2.54	0.42
25:d:138:SER:O	25:d:142:TYR:HB2	2.19	0.42
11:s:225:ILE:O	11:s:231:ILE:HA	2.19	0.42
27:f:576:ILE:HA	27:f:580:LEU:HD23	2.00	0.42
27:f:826:GLN:N	27:f:864:GLY:HA2	2.34	0.42
32:D:306:LYS:HA	32:D:306:LYS:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:355:SER:HB3	32:D:393:ILE:HG21	2.00	0.42
2:F:197:GLU:HA	2:F:200:GLU:HG3	2.00	0.42
3:O:63:ALA:O	3:O:70:ALA:N	2.49	0.42
6:H:74:LEU:HA	6:H:135:LEU:O	2.19	0.42
8:i:149:GLN:OE1	8:i:162:THR:OG1	2.29	0.42
4:g:54:LYS:HB2	4:g:216:GLU:HG3	2.01	0.42
4:g:65:THR:HG21	15:m:160:GLY:HA3	2.00	0.42
4:g:72:ILE:HG22	4:g:73:THR:HG23	2.01	0.42
16:U:524:LYS:HB2	16:U:559:ARG:NH2	2.34	0.42
6:h:74:LEU:HG	6:h:83:TYR:HE1	1.84	0.42
17:V:80:LYS:O	17:V:87:SER:N	2.52	0.42
19:X:414:LEU:HD22	24:c:259:VAL:HG11	2.01	0.42
15:m:53:LEU:HD11	15:m:168:LYS:HZ3	1.84	0.42
22:a:281:THR:HG22	22:a:333:MET:HG3	2.00	0.42
24:c:296:ILE:O	24:c:300:LEU:N	2.46	0.42
9:r:71:VAL:HG11	9:r:161:CYS:HB3	2.02	0.42
11:s:43:ILE:HG22	11:s:163:PHE:HB3	2.01	0.42
27:f:434:TYR:O	27:f:434:TYR:CD2	2.73	0.42
27:f:684:PRO:HA	27:f:687:ARG:HB3	2.02	0.42
30:B:254:GLU:HA	31:C:271:ARG:NH2	2.33	0.42
33:E:180:LYS:HG3	35:E:401:ATP:PB	2.58	0.42
1:N:167:SER:HA	1:N:170:TYR:CZ	2.55	0.42
5:P:29:GLY:HA2	5:P:35:VAL:HG23	2.01	0.42
9:R:121:GLN:HA	9:R:124:ILE:HD12	2.01	0.42
9:R:161:CYS:HA	9:R:169:GLY:O	2.19	0.42
16:U:507:VAL:HA	16:U:543:LYS:NZ	2.35	0.42
6:h:39:LYS:HG3	6:h:44:VAL:HG22	2.00	0.42
6:h:148:GLN:HE21	6:h:156:PHE:HB2	1.85	0.42
22:a:57:ILE:HD12	22:a:57:ILE:HA	1.94	0.42
22:a:163:TYR:CG	22:a:172:TYR:HB2	2.54	0.42
3:o:252:THR:HG21	5:p:168:SER:HB3	2.01	0.42
11:s:86:HIS:CD2	13:t:175:VAL:HG13	2.50	0.42
27:f:442:SER:CB	27:f:476:THR:O	2.67	0.42
27:f:463:LEU:CB	27:f:489:TYR:HE2	2.18	0.42
27:f:758:ASN:OD1	27:f:809:ILE:CB	2.67	0.42
28:A:86:THR:O	28:A:89:SER:OG	2.32	0.42
30:B:181:GLN:O	30:B:241:ASN:ND2	2.53	0.42
30:B:392:GLY:HA3	35:B:501:ATP:C5	2.54	0.42
32:D:40:LEU:HD23	32:D:41:TYR:HB2	2.01	0.42
33:E:53:VAL:O	33:E:102:MET:HE1	2.19	0.42
2:F:233:LYS:HA	2:F:236:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:41:VAL:HG23	10:J:211:MET:HB3	2.01	0.42
10:J:61:LYS:HE2	10:J:61:LYS:HB2	1.74	0.42
10:J:73:PHE:HB2	10:J:129:ILE:HD11	2.02	0.42
10:J:173:GLU:OE2	12:K:58:LEU:HG	2.20	0.42
12:K:114:GLN:HE21	14:L:82:ARG:HD2	1.84	0.42
14:L:196:ARG:HG2	14:L:239:ARG:HH11	1.85	0.42
16:U:108:TYR:OH	16:U:159:ARG:NH2	2.52	0.42
16:U:543:LYS:HG2	16:U:546:ARG:NH2	2.35	0.42
6:h:49:GLU:O	6:h:64:LYS:NZ	2.42	0.42
17:V:43:THR:HG23	17:V:65:ARG:HG2	2.01	0.42
17:V:273:LYS:HA	17:V:275:VAL:HG23	2.01	0.42
18:W:359:VAL:HG23	18:W:382:LEU:HD22	2.02	0.42
12:k:116:VAL:HG11	12:k:143:PHE:CZ	2.55	0.42
15:m:199:TYR:HB3	15:m:244:LEU:HD11	2.02	0.42
25:d:217:LEU:HD13	25:d:222:TYR:CE1	2.54	0.42
9:r:125:TYR:HA	9:r:128:ARG:HG2	2.01	0.42
27:f:106:LEU:HB3	27:f:141:LYS:HD2	2.01	0.42
27:f:236:CYS:O	27:f:240:VAL:HG23	2.19	0.42
27:f:416:MET:SD	27:f:804:LEU:CG	3.07	0.42
27:f:418:LEU:HD23	27:f:418:LEU:N	2.31	0.42
13:t:72:LEU:HD11	13:t:79:ALA:HB1	2.02	0.42
2:F:350:ARG:NH2	33:E:352:MET:HG2	2.32	0.42
4:G:132:ARG:HA	4:G:133:PRO:HD3	1.89	0.42
4:g:88:ARG:HH21	15:m:121:HIS:HB3	1.84	0.42
16:U:343:ILE:HD12	16:U:343:ILE:HA	1.93	0.42
17:V:290:TYR:OH	17:V:294:ARG:NH1	2.53	0.42
10:j:235:GLU:O	10:j:239:ASN:ND2	2.52	0.42
14:l:9:ASP:HB3	14:l:12:VAL:HG23	2.02	0.42
21:Z:192:THR:HG23	22:a:375:LEU:HD11	2.01	0.42
22:a:35:HIS:CE1	23:b:14:GLU:HG2	2.55	0.42
23:b:15:TYR:CD2	23:b:116:PRO:HD2	2.55	0.42
23:b:108:ARG:NH1	23:b:137:ASN:H	2.15	0.42
5:p:15:LYS:HB2	5:p:121:ILE:HD13	2.02	0.42
27:f:221:ILE:HA	27:f:224:ASN:HB2	2.01	0.42
32:D:146:GLU:O	32:D:252:ARG:NH2	2.49	0.42
2:F:225:MET:HE3	2:F:225:MET:HB3	1.96	0.42
2:F:287:GLU:OE1	28:A:300:LEU:HD13	2.20	0.42
4:G:123:GLN:HG3	6:H:81:PRO:HB2	2.01	0.42
6:H:45:VAL:HG21	6:H:188:ILE:HG22	2.02	0.42
7:Q:18:ASP:OD1	7:Q:18:ASP:N	2.52	0.42
9:R:114:TRP:HB3	9:R:145:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:24:VAL:O	12:K:28:ILE:HG12	2.19	0.42
14:L:167:SER:O	14:L:170:THR:OG1	2.26	0.42
8:i:38:LEU:HA	8:i:43:VAL:HG23	2.00	0.42
16:U:141:CYS:SG	31:C:19:GLY:N	2.91	0.42
17:V:433:ASP:HB3	25:d:147:SER:HA	2.01	0.42
17:V:477:HIS:HA	25:d:245:GLN:HE22	1.85	0.42
15:m:68:PHE:HB2	15:m:76:MET:HB3	2.01	0.42
15:m:75:GLY:HA3	15:m:225:HIS:CD2	2.55	0.42
1:n:161:ILE:HG22	1:n:166:SER:HB2	2.01	0.42
22:a:169:HIS:ND1	22:a:208:GLU:OE1	2.52	0.42
3:o:259:ILE:HG23	5:p:194:LYS:HB2	2.02	0.42
24:c:196:LEU:HB3	24:c:198:ARG:NH2	2.33	0.42
27:f:597:VAL:HB	27:f:635:LYS:HE3	2.01	0.42
30:B:142:ASP:OD1	30:B:143:LEU:N	2.53	0.42
30:B:429:LYS:HD3	30:B:429:LYS:HA	1.90	0.42
31:C:51:GLU:O	31:C:54:ALA:HB3	2.19	0.42
2:F:295:ARG:HG2	2:F:307:GLN:HG3	2.02	0.42
2:F:421:MET:O	2:F:424:ILE:HG22	2.19	0.42
4:G:244:GLU:HG2	4:G:245:ARG:HG2	2.02	0.42
16:U:774:PRO:O	16:U:777:HIS:HB2	2.20	0.42
16:U:780:SER:HA	16:U:783:TYR:HD2	1.85	0.42
17:V:385:LYS:HA	17:V:385:LYS:HD2	1.88	0.42
20:Y:113:ARG:HA	20:Y:113:ARG:HD3	1.77	0.42
21:Z:25:ARG:NH1	24:c:71:ASP:OD2	2.52	0.42
22:a:257:GLN:NE2	22:a:259:PRO:O	2.39	0.42
22:a:301:LYS:HE3	22:a:301:LYS:HB2	1.88	0.42
27:f:326:LEU:CG	27:f:329:ASN:HB3	2.50	0.42
27:f:579:ALA:O	27:f:583:VAL:HG13	2.20	0.42
28:A:347:ASP:O	28:A:351:ARG:NH1	2.53	0.42
30:B:228:PRO:HB3	30:B:332:ASN:HD22	1.84	0.42
31:C:155:ASP:HA	31:C:158:ILE:HG12	2.02	0.42
32:D:40:LEU:O	32:D:42:SER:N	2.52	0.42
8:I:43:VAL:HG21	8:I:147:LEU:HD11	2.02	0.42
9:R:255:HIS:HD2	5:p:204:MET:HE3	1.85	0.42
14:L:18:ARG:NH2	14:L:23:GLU:OE2	2.52	0.42
8:i:17:ARG:HH22	10:j:28:LYS:HE2	1.85	0.42
8:i:23:TYR:HA	8:i:26:GLU:HG2	2.01	0.42
16:U:17:PRO:O	16:U:21:GLU:HG2	2.20	0.42
17:V:61:GLU:O	17:V:64:GLN:HG3	2.20	0.42
17:V:498:PRO:HB3	21:Z:282:ASN:HD21	1.85	0.42
10:j:64:ALA:HA	10:j:70:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:260:SER:H	18:W:263:TRP:HB3	1.84	0.42
19:X:377:ILE:HG12	20:Y:312:ARG:HB3	2.01	0.42
20:Y:15:PRO:HB2	20:Y:113:ARG:HE	1.85	0.42
21:Z:12:HIS:ND1	21:Z:50:VAL:O	2.39	0.42
3:o:124:ARG:HG2	3:o:127:LYS:NZ	2.34	0.42
25:d:49:ILE:HG12	25:d:52:ARG:HE	1.84	0.42
25:d:50:LEU:O	25:d:54:ILE:HG12	2.19	0.42
27:f:57:GLU:HA	27:f:93:PRO:HB3	2.00	0.42
13:t:54:THR:O	13:t:99:SER:OG	2.30	0.42
13:t:192:GLN:HA	13:t:195:LEU:HB2	2.02	0.42
30:B:342:ILE:HG22	30:B:350:LYS:HE3	2.00	0.42
33:E:142:ILE:HG12	33:E:183:LEU:CD2	2.49	0.42
2:F:93:VAL:HG21	2:F:145:LEU:HD21	2.01	0.42
16:U:187:LEU:HD22	32:D:45:LYS:HG3	2.02	0.42
16:U:742:HIS:O	16:U:883:ARG:NH2	2.31	0.42
17:V:346:LEU:HD12	17:V:346:LEU:HA	1.93	0.42
10:j:183:THR:HG23	10:j:186:LEU:H	1.84	0.42
19:X:400:ALA:O	19:X:403:THR:OG1	2.27	0.42
15:m:41:ARG:HB2	15:m:46:VAL:HG22	2.02	0.42
21:Z:205:LEU:HA	21:Z:208:ILE:HG12	2.01	0.42
22:a:152:HIS:HE2	22:a:178:ARG:HB3	1.84	0.42
3:o:63:ALA:HB3	3:o:71:ASP:HB3	2.02	0.42
25:d:122:LEU:HD13	25:d:126:ASP:H	1.84	0.42
9:r:90:VAL:HB	9:r:92:LYS:HZ2	1.84	0.42
27:f:43:GLN:HG3	27:f:121:PHE:HB2	2.02	0.42
28:A:358:HIS:NE2	28:A:385:ILE:HG22	2.35	0.42
31:C:184:LYS:HB3	31:C:280:LEU:HD23	2.00	0.42
33:E:182:LEU:N	35:E:401:ATP:O2A	2.53	0.42
7:Q:173:LEU:HA	7:q:173:LEU:HA	2.02	0.41
8:I:18:LEU:HB2	8:I:21:VAL:HG22	2.01	0.41
10:J:82:ILE:HD11	10:J:127:PHE:HE1	1.84	0.41
13:T:112:LEU:HA	13:T:115:MET:HE2	2.02	0.41
8:i:218:ARG:NH1	8:i:223:THR:OG1	2.41	0.41
16:U:607:VAL:O	16:U:615:ARG:NH1	2.40	0.41
14:l:203:GLN:HE22	14:l:209:ASN:HD21	1.68	0.41
21:Z:8:LYS:HG3	21:Z:47:VAL:HG23	2.02	0.41
21:Z:133:LEU:HD12	24:c:222:LYS:HG3	2.01	0.41
28:A:240:VAL:HB	28:A:274:PHE:HD1	1.85	0.41
5:P:22:ILE:HG12	5:P:42:ILE:HD13	2.02	0.41
6:H:108:ALA:O	6:H:111:VAL:HB	2.20	0.41
4:g:228:ARG:NH1	4:g:230:LEU:HD23	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:12:LEU:HB2	16:U:44:LYS:HD3	2.02	0.41
16:U:366:HIS:CE1	16:U:395:ARG:HD2	2.55	0.41
6:h:86:LEU:HD23	6:h:86:LEU:HA	1.92	0.41
6:h:122:THR:HG22	6:h:129:PRO:HB3	2.02	0.41
17:V:440:LYS:HG2	17:V:443:ARG:HH21	1.85	0.41
18:W:34:LEU:HD22	18:W:47:LEU:HD13	2.02	0.41
18:W:52:LYS:HA	18:W:55:ARG:HG2	2.00	0.41
18:W:372:ARG:HB2	22:a:325:ASP:OD1	2.20	0.41
18:W:417:ARG:HD3	18:W:418:PRO:HD2	2.02	0.41
12:k:44:GLU:HB2	12:k:191:LEU:HB2	2.01	0.41
12:k:174:SER:O	12:k:178:GLN:HB2	2.20	0.41
14:l:66:VAL:HG21	14:l:88:MET:SD	2.60	0.41
14:l:212:ILE:O	14:l:223:ILE:HA	2.20	0.41
20:Y:41:LEU:HD12	20:Y:41:LEU:HA	1.90	0.41
22:a:229:ASP:OD1	22:a:229:ASP:N	2.45	0.41
22:a:268:LEU:O	22:a:272:ILE:HG12	2.20	0.41
22:a:361:LYS:HA	22:a:364:GLU:HG3	2.02	0.41
13:t:73:GLY:HA3	13:t:84:ILE:HD11	2.03	0.41
13:t:225:ASP:HB3	13:t:228:SER:HB3	2.01	0.41
3:O:102:ILE:HD12	3:O:125:MET:HG3	2.03	0.41
8:I:13:SER:OG	8:I:17:ARG:N	2.53	0.41
12:K:13:ASN:HB3	14:L:126:ARG:HD3	2.02	0.41
13:T:194:LEU:HA	13:T:197:GLU:HG2	2.01	0.41
15:M:174:LYS:HA	15:M:177:ILE:HD12	2.03	0.41
10:j:69:VAL:HG22	10:j:104:VAL:HG22	2.02	0.41
18:W:10:ASP:HA	18:W:13:ILE:HG12	2.02	0.41
12:k:143:PHE:O	12:k:153:LEU:HA	2.19	0.41
20:Y:17:LEU:HD21	20:Y:146:ARG:HG2	2.02	0.41
20:Y:117:LYS:HA	20:Y:120:ALA:HB3	2.02	0.41
21:Z:192:THR:HA	21:Z:195:VAL:HG22	2.01	0.41
1:n:35:THR:O	1:n:164:SER:N	2.52	0.41
22:a:28:LEU:O	22:a:32:LYS:N	2.53	0.41
25:d:124:ALA:HA	25:d:127:ILE:HG12	2.01	0.41
27:f:24:THR:HG23	27:f:31:LYS:HE2	2.03	0.41
27:f:330:PHE:O	27:f:333:LEU:HG	2.19	0.41
27:f:705:ASN:OD1	27:f:706:ILE:N	2.50	0.41
28:A:335:GLY:N	28:A:338:ASP:OD1	2.34	0.41
31:C:52:LEU:HA	31:C:55:LYS:HE2	2.02	0.41
31:C:222:LYS:HZ1	32:D:290:LEU:HD11	1.84	0.41
31:C:234:LEU:HD12	31:C:234:LEU:HA	1.93	0.41
31:C:328:ILE:HA	31:C:331:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:E:175:PRO:C	33:E:178:THR:HG22	2.45	0.41
7:Q:43:LEU:HD23	7:Q:43:LEU:HA	1.90	0.41
7:Q:155:ARG:HA	7:Q:155:ARG:HD2	1.81	0.41
19:X:256:LEU:HD11	19:X:322:HIS:CE1	2.55	0.41
20:Y:319:MET:O	20:Y:323:PHE:N	2.39	0.41
15:m:135:SER:HB3	15:m:151:MET:HE1	2.03	0.41
21:Z:103:LYS:O	21:Z:106:ILE:HG22	2.20	0.41
3:o:102:ILE:HG13	3:o:126:LEU:HD23	2.01	0.41
23:b:30:GLN:HA	23:b:75:LEU:HD11	2.02	0.41
24:c:295:ASN:O	24:c:299:CYS:N	2.48	0.41
27:f:106:LEU:HD23	27:f:141:LYS:HD2	2.01	0.41
27:f:643:PRO:HB2	27:f:647:GLY:H	1.85	0.41
27:f:739:ALA:HA	27:f:743:ALA:HB2	2.02	0.41
28:A:170:PRO:HG2	28:A:227:ARG:HB3	2.01	0.41
28:A:425:ALA:HA	30:B:339:PRO:HB2	2.01	0.41
30:B:223:ILE:HD13	30:B:329:MET:HB2	2.03	0.41
31:C:69:GLN:HA	32:D:136:SER:HA	2.02	0.41
2:F:256:LEU:HD23	2:F:256:LEU:H	1.85	0.41
5:P:91:VAL:HG12	5:P:124:LEU:HD22	2.01	0.41
8:I:218:ARG:HA	8:I:223:THR:HA	2.03	0.41
8:i:192:LEU:O	8:i:196:VAL:HG23	2.21	0.41
4:g:49:VAL:HG22	4:g:219:VAL:HG12	2.01	0.41
16:U:496:LEU:O	16:U:500:ASN:ND2	2.53	0.41
17:V:285:TRP:CD1	17:V:315:LYS:HE2	2.56	0.41
10:j:173:GLU:HG3	12:k:58:LEU:HG	2.01	0.41
12:k:209:LYS:HE3	12:k:209:LYS:HB3	1.88	0.41
19:X:116:TRP:O	19:X:120:GLU:HG2	2.20	0.41
20:Y:278:VAL:O	20:Y:282:MET:HB2	2.21	0.41
20:Y:287:LEU:O	20:Y:287:LEU:HG	2.16	0.41
25:d:3:GLU:HG2	25:d:25:ARG:NH2	2.35	0.41
27:f:53:GLN:HA	27:f:58:MET:HB3	2.02	0.41
13:t:171:ASP:OD1	13:t:175:VAL:N	2.54	0.41
28:A:261:PHE:HB3	28:A:265:ARG:NH2	2.35	0.41
28:A:299:MET:O	28:A:302:LEU:HG	2.21	0.41
30:B:389:ASP:OD1	30:B:389:ASP:N	2.46	0.41
32:D:66:LYS:HD3	32:D:66:LYS:HA	1.88	0.41
6:H:205:GLU:OE2	6:H:223:PRO:HB2	2.20	0.41
8:I:119:GLN:HA	8:I:122:THR:HG22	2.02	0.41
12:K:114:GLN:OE1	12:K:118:ASN:ND2	2.47	0.41
13:T:224:ARG:HA	13:T:224:ARG:HD3	1.80	0.41
14:L:157:ARG:HD2	14:L:176:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:183:LEU:HA	16:U:186:SER:HB3	2.02	0.41
17:V:285:TRP:HD1	17:V:315:LYS:HE2	1.85	0.41
17:V:477:HIS:ND1	25:d:245:GLN:OE1	2.53	0.41
18:W:170:GLN:H	18:W:170:GLN:HG3	1.69	0.41
19:X:98:ASP:OD1	19:X:98:ASP:N	2.50	0.41
11:s:47:ASP:OD1	11:s:47:ASP:N	2.54	0.41
27:f:93:PRO:HG2	27:f:97:LYS:HE3	2.01	0.41
27:f:542:ILE:HA	27:f:546:SER:HB3	2.01	0.41
27:f:639:LYS:HA	27:f:639:LYS:HD3	1.88	0.41
13:t:137:LEU:HD11	13:t:155:MET:HE3	2.03	0.41
30:B:271:PHE:CE2	30:B:315:GLN:HB3	2.56	0.41
33:E:180:LYS:O	33:E:183:LEU:HB2	2.20	0.41
3:O:67:MET:SD	3:O:67:MET:O	2.79	0.41
3:O:105:ASN:HB3	3:O:125:MET:HE1	2.03	0.41
3:O:236:ASN:ND2	11:s:241:ASP:OD1	2.53	0.41
5:P:173:ASN:ND2	11:s:179:ASN:HD22	2.19	0.41
6:H:86:LEU:HD23	6:H:86:LEU:HA	1.81	0.41
7:Q:183:ILE:HA	7:Q:187:GLY:O	2.20	0.41
11:S:54:ASP:HB3	11:S:217:THR:HG23	2.03	0.41
14:L:117:GLN:HG3	15:M:83:ALA:HB1	2.03	0.41
16:U:9:ILE:HD11	16:U:30:VAL:HG11	2.02	0.41
16:U:35:TRP:CE3	16:U:70:HIS:HB2	2.51	0.41
16:U:471:ASP:HA	16:U:474:ARG:HG3	2.02	0.41
16:U:619:VAL:HA	16:U:622:LEU:HD13	2.03	0.41
19:X:71:LYS:NZ	19:X:109:LEU:HD21	2.35	0.41
23:b:7:MET:CE	23:b:52:ILE:HG12	2.43	0.41
5:p:109:ILE:HB	5:p:122:CYS:SG	2.61	0.41
11:s:197:ASP:OD1	11:s:197:ASP:N	2.54	0.41
27:f:137:ARG:HH21	27:f:159:VAL:HG22	1.86	0.41
29:u:406:ARG:HG2	29:u:406:ARG:H	1.42	0.41
30:B:183:THR:OG1	30:B:184:TYR:N	2.53	0.41
30:B:254:GLU:OE2	30:B:254:GLU:N	2.44	0.41
32:D:123:LEU:HD11	32:D:142:VAL:HG21	2.02	0.41
32:D:259:PRO:HB3	32:D:304:ASN:HB2	2.02	0.41
33:E:69:PHE:HB2	33:E:81:VAL:O	2.19	0.41
1:N:118:LYS:NZ	1:N:152:GLY:O	2.49	0.41
2:F:200:GLU:HA	2:F:204:LEU:HG	2.02	0.41
4:G:173:THR:O	4:G:176:THR:OG1	2.30	0.41
9:R:149:TYR:HB2	9:R:154:LEU:HD11	2.03	0.41
12:K:69:GLU:HB2	12:K:226:PHE:CE2	2.56	0.41
13:T:46:THR:HG23	13:T:152:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:171:GLN:HE21	33:E:372:ARG:HB3	1.85	0.41
4:g:132:ARG:HD2	15:m:15:PHE:CE1	2.56	0.41
16:U:616:ARG:HH22	24:c:183:HIS:CD2	2.39	0.41
6:h:145:TYR:HB3	6:h:147:PHE:HE1	1.86	0.41
18:W:158:ASP:OD1	18:W:161:GLU:HG2	2.21	0.41
19:X:281:GLY:O	19:X:284:THR:OG1	2.32	0.41
20:Y:110:TYR:CZ	20:Y:114:ILE:HG13	2.55	0.41
22:a:319:LEU:HG	22:a:337:GLN:HG2	2.02	0.41
22:a:324:ILE:HG23	22:a:331:VAL:HG22	2.02	0.41
7:q:77:PRO:HD2	7:q:108:ASP:HB2	2.02	0.41
7:q:106:GLY:HA2	7:q:183:ILE:HG21	2.03	0.41
27:f:398:TRP:HD1	27:f:401:LYS:HE3	1.85	0.41
30:B:66:GLU:HA	30:B:69:LYS:HG2	2.03	0.41
30:B:133:VAL:HG11	30:B:157:HIS:HB2	2.03	0.41
31:C:32:GLN:NE2	32:D:47:LEU:HD11	2.36	0.41
31:C:230:MET:SD	31:C:233:GLU:HG3	2.60	0.41
32:D:155:THR:HA	32:D:158:GLN:HB2	2.02	0.41
32:D:388:ARG:NH2	33:E:147:GLU:OE1	2.47	0.41
35:D:501:ATP:H2'	35:D:501:ATP:O5'	2.20	0.41
2:F:94:ILE:HG23	33:E:117:PRO:HD3	2.01	0.41
5:P:27:ARG:HB2	5:P:183:MET:HB2	2.01	0.41
5:P:33:GLN:OE1	5:P:33:GLN:N	2.51	0.41
8:I:248:GLU:OE1	8:I:248:GLU:N	2.53	0.41
9:R:192:VAL:HB	7:q:138:LEU:HD23	2.03	0.41
9:R:255:HIS:CD2	5:p:204:MET:HE3	2.55	0.41
11:S:66:ARG:NH1	11:S:219:ASP:OD1	2.48	0.41
13:T:136:TRP:CH2	14:L:99:PHE:HA	2.55	0.41
14:L:156:CYS:SG	14:L:159:MET:HB2	2.61	0.41
4:g:138:MET:HB2	4:g:154:CYS:SG	2.61	0.41
16:U:16:GLU:O	16:U:20:LYS:HG2	2.21	0.41
16:U:573:ASP:HB3	16:U:578:LEU:HD22	2.02	0.41
16:U:807:LYS:HG3	16:U:809:SER:H	1.85	0.41
6:h:46:LEU:HD13	6:h:75:VAL:HG12	2.02	0.41
6:h:86:LEU:HD22	6:h:114:VAL:HG13	2.03	0.41
10:j:204:LYS:HB2	10:j:204:LYS:HE2	1.84	0.41
18:W:167:GLN:NE2	18:W:168:GLU:OE1	2.54	0.41
19:X:328:ASP:OD1	19:X:329:ASN:N	2.54	0.41
14:l:70:ILE:HD11	14:l:105:VAL:HG22	2.03	0.41
14:l:87:PHE:O	14:l:90:GLN:HG3	2.20	0.41
15:m:29:LYS:HD3	15:m:29:LYS:HA	1.87	0.41
22:a:76:LEU:O	22:a:79:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:52:LYS:HE3	3:o:190:GLU:HA	2.03	0.41
7:q:160:LEU:O	7:q:164:LEU:HG	2.21	0.41
25:d:225:PHE:CE2	25:d:227:SER:HB3	2.55	0.41
27:f:621:ASP:N	27:f:626:GLU:OE2	2.54	0.41
13:t:181:SER:HB2	13:t:195:LEU:HD13	2.03	0.41
30:B:249:ARG:NH2	31:C:279:GLN:OE1	2.51	0.41
30:B:360:THR:O	30:B:364:ILE:HG12	2.21	0.41
31:C:31:LEU:HD22	32:D:47:LEU:HD12	2.02	0.41
32:D:47:LEU:HD22	32:D:47:LEU:HA	1.87	0.41
32:D:337:ASP:OD1	32:D:338:ARG:N	2.47	0.41
35:D:501:ATP:H5'1	35:D:501:ATP:N3	2.36	0.41
2:F:399:VAL:HG22	2:F:424:ILE:HD13	2.03	0.41
5:P:56:LEU:HB3	5:P:59:ASP:HB2	2.03	0.41
9:R:68:ARG:HE	9:R:69:HIS:CE1	2.39	0.41
9:R:118:LEU:HB2	9:R:142:LEU:HD21	2.02	0.41
11:S:215:VAL:HG22	3:o:210:LEU:HD22	2.03	0.41
14:L:133:LEU:HD23	14:L:133:LEU:HA	1.89	0.41
15:M:202:HIS:CE1	15:M:204:GLU:HA	2.56	0.41
16:U:759:SER:HA	16:U:782:ALA:HA	2.03	0.41
16:U:789:ILE:O	16:U:911:ILE:HA	2.21	0.41
18:W:382:LEU:HA	18:W:382:LEU:HD23	1.79	0.41
12:k:146:VAL:HG11	12:k:222:PRO:HA	2.03	0.41
14:l:123:TYR:HB2	15:m:128:ALA:HA	2.02	0.41
23:b:132:LYS:HD2	23:b:132:LYS:HA	1.87	0.41
24:c:207:TYR:CZ	24:c:209:LYS:HA	2.56	0.41
27:f:478:ARG:O	27:f:481:SER:HB3	2.20	0.41
27:f:643:PRO:O	27:f:646:MET:HB3	2.21	0.41
13:t:75:TYR:N	13:t:78:LEU:O	2.52	0.41
13:t:89:ARG:HD2	13:t:242:VAL:HB	2.02	0.41
28:A:57:LYS:HD2	28:A:57:LYS:HA	1.86	0.41
29:u:407:LYS:HE2	29:u:411:ASP:OD2	2.20	0.41
30:B:287:ILE:HG22	30:B:337:LEU:HD11	2.02	0.41
33:E:180:LYS:NZ	33:E:279:THR:O	2.54	0.41
1:N:175:ALA:HB2	1:n:196:LEU:HD11	2.03	0.40
2:F:323:ASN:OD1	2:F:323:ASN:N	2.55	0.40
2:F:363:ALA:HB1	2:F:381:TYR:HB3	2.03	0.40
7:Q:31:ASP:OD1	7:Q:31:ASP:N	2.54	0.40
10:J:61:LYS:HD3	10:J:73:PHE:CZ	2.56	0.40
11:S:42:ALA:HB2	11:S:51:VAL:HG12	2.03	0.40
11:S:94:LYS:HG2	14:L:97:PHE:CE1	2.56	0.40
16:U:232:ILE:HA	16:U:235:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:180:ARG:HD3	17:V:180:ARG:HA	1.90	0.40
10:j:119:THR:HA	10:j:126:PRO:HG3	2.02	0.40
19:X:90:ARG:NH2	19:X:125:LEU:HD12	2.35	0.40
14:l:107:ARG:HH21	13:t:126:HIS:HB2	1.86	0.40
20:Y:271:PHE:O	20:Y:274:SER:OG	2.27	0.40
20:Y:367:GLN:HA	20:Y:370:ILE:HG22	2.02	0.40
7:q:5:ILE:HG23	7:q:16:ALA:HB3	2.03	0.40
27:f:438:ASP:HB3	27:f:476:THR:CB	2.51	0.40
27:f:537:THR:O	27:f:541:THR:OG1	2.31	0.40
27:f:786:GLN:HG2	27:f:787:LEU:H	1.85	0.40
32:D:249:ASP:OD1	32:D:250:VAL:N	2.54	0.40
1:N:226:ASP:OD1	1:N:226:ASP:N	2.52	0.40
2:F:132:TYR:CD1	33:E:55:GLN:HG3	2.56	0.40
7:Q:186:ASN:HB2	7:Q:189:HIS:HE2	1.85	0.40
7:Q:197:PRO:HB2	7:q:197:PRO:HG2	2.03	0.40
10:J:9:VAL:HG12	12:K:10:ARG:HH21	1.85	0.40
10:J:125:ARG:HA	10:J:126:PRO:HD3	1.88	0.40
15:M:9:ASP:HB3	15:M:22:PHE:HD2	1.86	0.40
17:V:128:ARG:HD3	17:V:171:VAL:HG21	2.03	0.40
17:V:144:ASP:OD1	17:V:144:ASP:N	2.45	0.40
17:V:387:GLN:HA	17:V:392:TYR:HE1	1.87	0.40
10:j:44:GLY:HA3	10:j:195:LEU:HD11	2.03	0.40
18:W:312:MET:CE	18:W:361:HIS:ND1	2.85	0.40
12:k:15:PHE:CE2	14:l:126:ARG:HD2	2.57	0.40
19:X:163:LYS:HE2	19:X:199:ALA:HB3	2.03	0.40
19:X:216:ILE:HD13	19:X:216:ILE:HA	1.92	0.40
20:Y:136:HIS:O	20:Y:140:ILE:HG12	2.21	0.40
25:d:192:THR:O	25:d:196:ARG:HG3	2.21	0.40
27:f:431:LYS:HE3	27:f:432:TYR:CZ	2.57	0.40
31:C:373:GLU:H	31:C:373:GLU:HG2	1.74	0.40
2:F:88:TYR:O	28:A:121:PHE:HB2	2.22	0.40
2:F:300:LYS:HG2	2:F:300:LYS:O	2.22	0.40
4:G:190:THR:O	4:G:194:THR:N	2.48	0.40
5:P:4:MET:HE3	5:P:4:MET:O	2.22	0.40
5:P:126:LEU:HD22	5:P:126:LEU:HA	1.89	0.40
9:R:199:ASP:OD1	7:q:170:ARG:NH1	2.54	0.40
12:K:72:ALA:O	12:K:226:PHE:N	2.48	0.40
16:U:8:ILE:HA	16:U:37:GLU:OE2	2.20	0.40
16:U:514:LEU:HD13	16:U:550:VAL:HG11	2.03	0.40
17:V:105:SER:O	17:V:109:ASN:ND2	2.55	0.40
17:V:318:GLN:HE21	17:V:319:HIS:CD2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:36:ARG:O	10:j:176:TYR:OH	2.40	0.40
18:W:243:ILE:HG13	18:W:273:TYR:HE1	1.87	0.40
18:W:341:PHE:HA	18:W:347:GLY:HA2	2.02	0.40
18:W:367:ALA:HA	18:W:415:PHE:HD2	1.86	0.40
21:Z:34:ARG:HB3	21:Z:96:HIS:HB2	2.04	0.40
26:e:57:ARG:HD3	26:e:57:ARG:H	1.85	0.40
27:f:845:ARG:NH1	27:f:848:GLN:H	2.20	0.40
13:t:134:HIS:NE2	13:t:176:ALA:HB1	2.37	0.40
28:A:345:LEU:HD12	28:A:345:LEU:HA	1.84	0.40
28:A:372:LEU:HA	28:A:375:ARG:HD2	2.03	0.40
30:B:229:GLY:HA3	31:C:307:ARG:HH21	1.86	0.40
30:B:250:VAL:HG23	31:C:232:ARG:HH12	1.85	0.40
33:E:367:PHE:O	33:E:370:ALA:HB3	2.21	0.40
9:R:239:ARG:NH2	9:R:241:ASP:OD2	2.55	0.40
12:K:94:VAL:O	12:K:98:ASN:ND2	2.54	0.40
13:T:134:HIS:O	13:T:138:THR:HG23	2.22	0.40
4:g:105:TYR:HA	3:o:121:THR:HG23	2.03	0.40
16:U:103:LYS:HE3	16:U:103:LYS:HB2	1.74	0.40
17:V:365:GLN:HE21	17:V:365:GLN:HB2	1.76	0.40
15:m:192:LYS:HB3	15:m:239:TYR:CD2	2.56	0.40
23:b:9:CYS:HB2	23:b:111:ALA:HA	2.03	0.40
9:r:111:CYS:SG	9:r:156:MET:HG2	2.61	0.40
27:f:307:LEU:O	27:f:310:ASP:HB3	2.21	0.40
27:f:325:GLN:O	27:f:327:ASN:N	2.54	0.40
27:f:470:VAL:N	27:f:481:SER:OG	2.54	0.40
28:A:52:ILE:HG23	30:B:69:LYS:HD3	2.03	0.40
28:A:414:ASN:OD1	28:A:415:LYS:N	2.55	0.40
31:C:305:LEU:HA	31:C:310:ARG:HG2	2.03	0.40
32:D:67:ASN:C	32:D:67:ASN:HD22	2.29	0.40
1:N:194:LEU:HD12	1:N:194:LEU:HA	1.96	0.40
3:O:153:LEU:HD21	3:O:168:VAL:HG22	2.02	0.40
3:O:154:TYR:CE1	3:O:164:LYS:HE2	2.57	0.40
5:P:187:VAL:O	5:P:197:THR:HA	2.21	0.40
9:R:97:ASN:ND2	9:R:100:LEU:HB2	2.36	0.40
12:K:88:LEU:HD23	12:K:119:LEU:HD23	2.03	0.40
16:U:326:ILE:O	16:U:330:SER:OG	2.29	0.40
16:U:332:GLU:O	16:U:335:ILE:N	2.53	0.40
16:U:368:ALA:HB2	16:U:728:PHE:HD1	1.86	0.40
17:V:37:MET:HB2	17:V:89:LYS:HE3	2.04	0.40
10:j:90:GLU:OE2	10:j:106:TYR:OH	2.29	0.40
18:W:377:ARG:O	18:W:380:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:268:TYR:CE2	20:Y:307:LEU:HD12	2.56	0.40
21:Z:234:PHE:HA	21:Z:237:LEU:HD23	2.03	0.40
24:c:257:LYS:HA	24:c:257:LYS:HD3	1.92	0.40
9:r:80:THR:HG22	9:r:85:ILE:HA	2.04	0.40
13:t:64:GLY:HA3	13:t:238:THR:HG22	2.03	0.40
28:A:182:GLU:OE2	28:A:183:GLN:NE2	2.55	0.40
30:B:85:MET:HE3	30:B:85:MET:HB3	1.96	0.40
30:B:234:LEU:HB2	30:B:237:LYS:NZ	2.36	0.40
30:B:234:LEU:HB2	35:B:501:ATP:PA	2.61	0.40
32:D:82:ILE:HG21	32:D:116:LEU:HD21	2.03	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	N	199/239 (83%)	194 (98%)	5 (2%)	0	100	100
1	n	199/239 (83%)	194 (98%)	5 (2%)	0	100	100
2	F	371/439 (84%)	334 (90%)	37 (10%)	0	100	100
3	O	218/277 (79%)	209 (96%)	8 (4%)	1 (0%)	25	63
3	o	218/277 (79%)	211 (97%)	6 (3%)	1 (0%)	25	63
4	G	236/246 (96%)	224 (95%)	12 (5%)	0	100	100
4	g	237/246 (96%)	230 (97%)	7 (3%)	0	100	100
5	P	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
5	p	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
6	H	224/234 (96%)	212 (95%)	11 (5%)	1 (0%)	30	67
6	h	228/234 (97%)	224 (98%)	4 (2%)	0	100	100
7	Q	195/201 (97%)	192 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	q	195/201 (97%)	188 (96%)	7 (4%)	0	100	100
8	I	247/261 (95%)	226 (92%)	19 (8%)	2 (1%)	16	53
8	i	245/261 (94%)	244 (100%)	1 (0%)	0	100	100
9	R	198/263 (75%)	193 (98%)	5 (2%)	0	100	100
9	r	198/263 (75%)	194 (98%)	4 (2%)	0	100	100
10	J	239/248 (96%)	219 (92%)	18 (8%)	2 (1%)	16	53
10	j	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
11	S	210/241 (87%)	201 (96%)	8 (4%)	1 (0%)	25	63
11	s	210/241 (87%)	201 (96%)	9 (4%)	0	100	100
12	K	224/241 (93%)	209 (93%)	15 (7%)	0	100	100
12	k	235/241 (98%)	229 (97%)	6 (3%)	0	100	100
13	T	213/264 (81%)	205 (96%)	6 (3%)	2 (1%)	14	50
13	t	213/264 (81%)	203 (95%)	9 (4%)	1 (0%)	25	63
14	L	238/263 (90%)	229 (96%)	9 (4%)	0	100	100
14	l	236/263 (90%)	231 (98%)	5 (2%)	0	100	100
15	M	240/255 (94%)	228 (95%)	10 (4%)	2 (1%)	16	53
15	m	239/255 (94%)	233 (98%)	6 (2%)	0	100	100
16	U	806/953 (85%)	742 (92%)	63 (8%)	1 (0%)	48	82
17	V	506/534 (95%)	438 (87%)	65 (13%)	3 (1%)	22	59
18	W	454/456 (100%)	414 (91%)	37 (8%)	3 (1%)	19	55
19	X	378/422 (90%)	338 (89%)	38 (10%)	2 (0%)	25	63
20	Y	376/389 (97%)	348 (93%)	28 (7%)	0	100	100
21	Z	284/324 (88%)	253 (89%)	31 (11%)	0	100	100
22	a	371/376 (99%)	328 (88%)	41 (11%)	2 (0%)	25	63
23	b	189/377 (50%)	156 (82%)	30 (16%)	3 (2%)	8	37
24	c	275/310 (89%)	242 (88%)	30 (11%)	3 (1%)	12	46
25	d	250/350 (71%)	200 (80%)	48 (19%)	2 (1%)	16	53
26	e	35/70 (50%)	25 (71%)	9 (26%)	1 (3%)	3	24
27	f	887/908 (98%)	741 (84%)	137 (15%)	9 (1%)	13	48
28	A	391/433 (90%)	328 (84%)	59 (15%)	4 (1%)	13	48
29	u	35/491 (7%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	B	382/440 (87%)	349 (91%)	33 (9%)	0	100	100
31	C	359/406 (88%)	323 (90%)	36 (10%)	0	100	100
32	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	10	41
33	E	373/389 (96%)	341 (91%)	31 (8%)	1 (0%)	37	72
All	All	13275/15361 (86%)	12206 (92%)	1017 (8%)	52 (0%)	32	67

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	X	200	ILE
23	b	117	VAL
24	c	284	LEU
25	d	201	ASN
26	e	8	VAL
27	f	326	LEU
27	f	757	ASN
28	A	95	VAL
32	D	151	ILE
32	D	153	MET
8	I	106	PRO
8	I	251	LYS
13	T	246	GLY
18	W	41	GLN
18	W	313	GLU
22	a	192	GLU
27	f	307	LEU
27	f	322	SER
28	A	86	THR
28	A	312	ARG
33	E	179	GLY
10	J	127	PHE
17	V	354	LYS
23	b	86	PHE
27	f	786	GLN
32	D	127	ASN
15	M	204	GLU
17	V	360	TYR
18	W	312	MET
19	X	143	TYR
25	d	203	PRO
27	f	474	SER

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Mol	Chain	Res	Type
27	f	755	ASP
16	U	174	PRO
3	o	232	TYR
23	b	23	PRO
27	f	323	ASN
27	f	756	PRO
28	A	366	ARG
32	D	152	MET
3	O	231	PRO
6	H	232	ALA
10	J	98	VAL
11	S	219	ASP
13	T	247	PRO
15	M	61	GLU
24	c	31	VAL
13	t	247	PRO
32	D	126	PRO
17	V	359	PRO
22	a	209	GLY
24	c	266	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	N	156/181 (86%)	156 (100%)	0	100	100
1	n	156/181 (86%)	156 (100%)	0	100	100
2	F	288/379 (76%)	287 (100%)	1 (0%)	91	92
3	O	181/228 (79%)	178 (98%)	3 (2%)	56	72
3	o	181/228 (79%)	180 (99%)	1 (1%)	84	88
4	G	183/210 (87%)	183 (100%)	0	100	100
4	g	204/210 (97%)	204 (100%)	0	100	100
5	P	173/174 (99%)	172 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	p	173/174 (99%)	173 (100%)	0	100	100
6	H	159/191 (83%)	158 (99%)	1 (1%)	84	88
6	h	188/191 (98%)	188 (100%)	0	100	100
7	Q	168/171 (98%)	168 (100%)	0	100	100
7	q	168/171 (98%)	168 (100%)	0	100	100
8	I	185/221 (84%)	185 (100%)	0	100	100
8	i	207/221 (94%)	207 (100%)	0	100	100
9	R	156/202 (77%)	156 (100%)	0	100	100
9	r	156/202 (77%)	156 (100%)	0	100	100
10	J	150/211 (71%)	150 (100%)	0	100	100
10	j	203/211 (96%)	203 (100%)	0	100	100
11	S	177/199 (89%)	177 (100%)	0	100	100
11	s	177/199 (89%)	177 (100%)	0	100	100
12	K	174/203 (86%)	174 (100%)	0	100	100
12	k	199/203 (98%)	199 (100%)	0	100	100
13	T	178/215 (83%)	178 (100%)	0	100	100
13	t	178/215 (83%)	177 (99%)	1 (1%)	84	88
14	L	195/224 (87%)	195 (100%)	0	100	100
14	l	204/224 (91%)	204 (100%)	0	100	100
15	M	188/212 (89%)	188 (100%)	0	100	100
15	m	198/212 (93%)	198 (100%)	0	100	100
16	U	667/816 (82%)	667 (100%)	0	100	100
17	V	391/460 (85%)	388 (99%)	3 (1%)	79	85
18	W	388/416 (93%)	386 (100%)	2 (0%)	86	90
19	X	309/362 (85%)	308 (100%)	1 (0%)	91	92
20	Y	319/344 (93%)	318 (100%)	1 (0%)	91	92
21	Z	248/295 (84%)	248 (100%)	0	100	100
22	a	328/336 (98%)	327 (100%)	1 (0%)	91	92
23	b	159/312 (51%)	158 (99%)	1 (1%)	84	88
24	c	228/268 (85%)	228 (100%)	0	100	100
25	d	206/294 (70%)	205 (100%)	1 (0%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	e	33/63 (52%)	33 (100%)	0	100	100
27	f	694/763 (91%)	683 (98%)	11 (2%)	58	74
28	A	319/372 (86%)	318 (100%)	1 (0%)	91	92
29	u	33/398 (8%)	30 (91%)	3 (9%)	7	25
30	B	328/385 (85%)	325 (99%)	3 (1%)	75	83
31	C	305/352 (87%)	304 (100%)	1 (0%)	91	92
32	D	320/366 (87%)	317 (99%)	3 (1%)	75	83
33	E	290/341 (85%)	287 (99%)	3 (1%)	73	81
All	All	10868/13006 (84%)	10825 (100%)	43 (0%)	88	91

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	416	THR
3	O	106	LEU
3	O	229	LEU
3	O	230	ARG
5	P	126	LEU
6	H	74	LEU
17	V	170	LEU
17	V	358	MET
17	V	365	GLN
18	W	106	GLN
18	W	308	LEU
19	X	401	LEU
20	Y	287	LEU
22	a	129	GLN
3	o	230	ARG
23	b	44	ASN
25	d	190	LEU
27	f	305	LEU
27	f	307	LEU
27	f	308	SER
27	f	309	GLU
27	f	310	ASP
27	f	326	LEU
27	f	327	ASN
27	f	328	SER
27	f	473	ASN

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Mol	Chain	Res	Type
27	f	475	ASN
27	f	476	THR
13	t	248	LEU
28	A	403	ILE
29	u	378	ASP
29	u	389	ARG
29	u	406	ARG
30	B	125	THR
30	B	233	THR
30	B	235	LEU
31	C	109	THR
32	D	47	LEU
32	D	151	ILE
32	D	292	LEU
33	E	178	THR
33	E	180	LYS
33	E	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	87	GLN
1	N	157	GLN
1	N	188	GLN
2	F	218	GLN
2	F	255	GLN
2	F	258	GLN
2	F	316	GLN
2	F	395	GLN
3	O	236	ASN
4	G	68	HIS
5	P	31	GLN
5	P	93	ASN
5	P	173	ASN
6	H	52	GLN
6	H	95	GLN
6	H	169	ASN
7	Q	71	ASN
8	I	20	GLN
8	I	40	ASN
8	I	95	GLN
8	I	102	GLN

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Mol	Chain	Res	Type
9	R	234	ASN
12	K	97	GLN
12	K	98	ASN
14	L	60	GLN
8	i	84	ASN
8	i	102	GLN
15	M	69	ASN
15	M	102	ASN
15	M	148	GLN
15	M	171	GLN
16	U	58	GLN
16	U	79	ASN
16	U	115	ASN
16	U	135	ASN
16	U	247	GLN
16	U	463	ASN
16	U	491	GLN
16	U	665	ASN
6	h	148	GLN
6	h	189	HIS
17	V	33	GLN
17	V	109	ASN
17	V	257	ASN
17	V	281	ASN
17	V	319	HIS
17	V	459	GLN
10	j	18	GLN
10	j	85	ASN
10	j	239	ASN
18	W	106	GLN
18	W	236	HIS
18	W	246	HIS
18	W	416	GLN
19	X	44	GLN
19	X	144	GLN
19	X	198	ASN
19	X	268	GLN
19	X	406	ASN
14	l	20	HIS
14	l	166	GLN
14	l	203	GLN
20	Y	49	ASN

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Mol	Chain	Res	Type
20	Y	64	GLN
20	Y	154	ASN
15	m	111	HIS
15	m	148	GLN
21	Z	77	ASN
21	Z	109	ASN
21	Z	174	HIS
21	Z	202	ASN
21	Z	229	GLN
21	Z	282	ASN
22	a	40	GLN
22	a	86	GLN
22	a	91	ASN
22	a	152	HIS
22	a	194	GLN
22	a	287	ASN
22	a	370	GLN
3	o	123	ASN
3	o	236	ASN
23	b	30	GLN
23	b	34	ASN
23	b	44	ASN
5	p	33	GLN
5	p	65	GLN
5	p	81	GLN
24	c	128	ASN
24	c	221	HIS
24	c	232	GLN
7	q	8	GLN
7	q	63	ASN
7	q	101	ASN
7	q	168	GLN
11	s	86	HIS
11	s	185	ASN
27	f	53	GLN
27	f	199	ASN
27	f	245	ASN
27	f	291	GLN
27	f	327	ASN
27	f	329	ASN
27	f	770	HIS
27	f	855	GLN

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Mol	Chain	Res	Type
13	t	48	ASN
13	t	106	GLN
13	t	202	GLN
13	t	233	GLN
28	A	54	GLN
28	A	150	HIS
28	A	247	GLN
28	A	353	HIS
30	B	57	GLN
30	B	92	GLN
31	C	32	GLN
31	C	36	ASN
31	C	40	GLN
31	C	53	ASN
31	C	64	GLN
31	C	67	GLN
31	C	111	ASN
31	C	278	ASN
31	C	377	HIS
32	D	67	ASN
32	D	173	GLN
32	D	193	GLN
32	D	222	HIS
32	D	237	GLN
32	D	257	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

6 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
34	ADP	F	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.34	4 (13%)
34	ADP	C	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)
35	ATP	E	401	-	26,33,33	0.57	0	31,52,52	0.82	2 (6%)
35	ATP	D	501	-	26,33,33	0.72	0	31,52,52	0.89	1 (3%)
35	ATP	A	501	-	26,33,33	0.63	0	31,52,52	0.85	2 (6%)
35	ATP	B	501	-	26,33,33	0.65	0	31,52,52	0.84	1 (3%)

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
34	ADP	F	501	-	-	4/12/32/32	0/3/3/3
34	ADP	C	501	-	-	3/12/32/32	0/3/3/3
35	ATP	E	401	-	-	1/18/38/38	0/3/3/3
35	ATP	D	501	-	-	10/18/38/38	0/3/3/3
35	ATP	A	501	-	-	6/18/38/38	0/3/3/3
35	ATP	B	501	-	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	501	ADP	C5-C4	2.39	1.47	1.40
34	F	501	ADP	C5-C4	2.34	1.47	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	501	ADP	C3'-C2'-C1'	3.75	106.62	100.98
34	F	501	ADP	C3'-C2'-C1'	3.42	106.13	100.98
34	C	501	ADP	PA-O3A-PB	-3.03	122.44	132.83
34	F	501	ADP	N3-C2-N1	-2.97	124.03	128.68
34	C	501	ADP	N3-C2-N1	-2.94	124.08	128.68
34	C	501	ADP	C4-C5-N7	-2.58	106.71	109.40
34	F	501	ADP	PA-O3A-PB	-2.55	124.07	132.83
34	F	501	ADP	C4-C5-N7	-2.49	106.80	109.40
35	A	501	ATP	C5-C6-N6	2.35	123.92	120.35
35	B	501	ATP	C5-C6-N6	2.32	123.89	120.35
35	E	401	ATP	C5-C6-N6	2.31	123.86	120.35
35	A	501	ATP	PB-O3B-PG	2.23	140.49	132.83
35	D	501	ATP	C5-C6-N6	2.19	123.68	120.35
35	E	401	ATP	PB-O3B-PG	2.17	140.26	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	F	501	ADP	C5'-O5'-PA-O1A
34	C	501	ADP	PB-O3A-PA-O5'
34	C	501	ADP	O4'-C4'-C5'-O5'
34	C	501	ADP	C3'-C4'-C5'-O5'
35	A	501	ATP	PB-O3B-PG-O2G
35	A	501	ATP	PB-O3B-PG-O3G
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	O4'-C4'-C5'-O5'
35	A	501	ATP	C3'-C4'-C5'-O5'
35	D	501	ATP	C5'-O5'-PA-O1A
34	F	501	ADP	O4'-C4'-C5'-O5'
34	F	501	ADP	C3'-C4'-C5'-O5'
35	D	501	ATP	C4'-C5'-O5'-PA
35	D	501	ATP	O4'-C4'-C5'-O5'
35	D	501	ATP	C3'-C4'-C5'-O5'
35	D	501	ATP	PG-O3B-PB-O1B
35	B	501	ATP	PB-O3A-PA-O5'
35	D	501	ATP	C5'-O5'-PA-O3A
34	F	501	ADP	C4'-C5'-O5'-PA
35	D	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	PG-O3B-PB-O2B
35	E	401	ATP	PB-O3A-PA-O2A
35	D	501	ATP	PA-O3A-PB-O1B
35	A	501	ATP	C5'-O5'-PA-O3A

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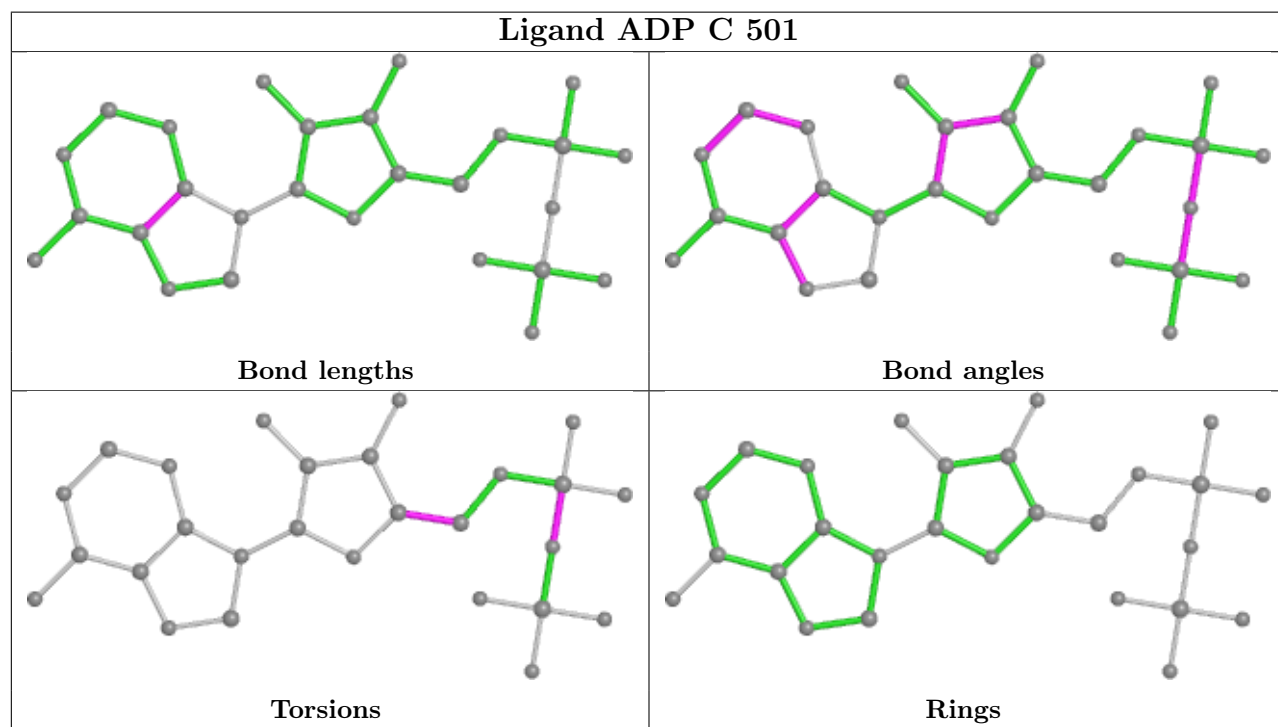
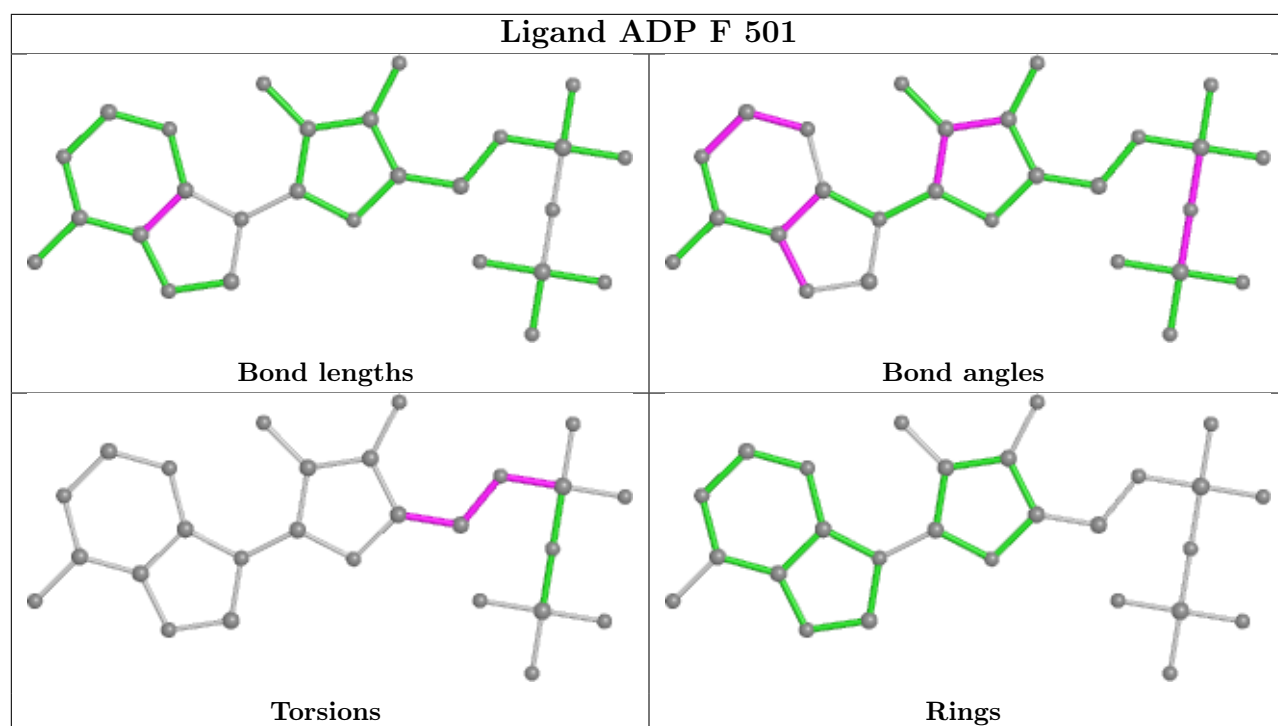
Mol	Chain	Res	Type	Atoms
35	B	501	ATP	PA-O3A-PB-O1B
35	B	501	ATP	PA-O3A-PB-O2B
35	D	501	ATP	PA-O3A-PB-O2B

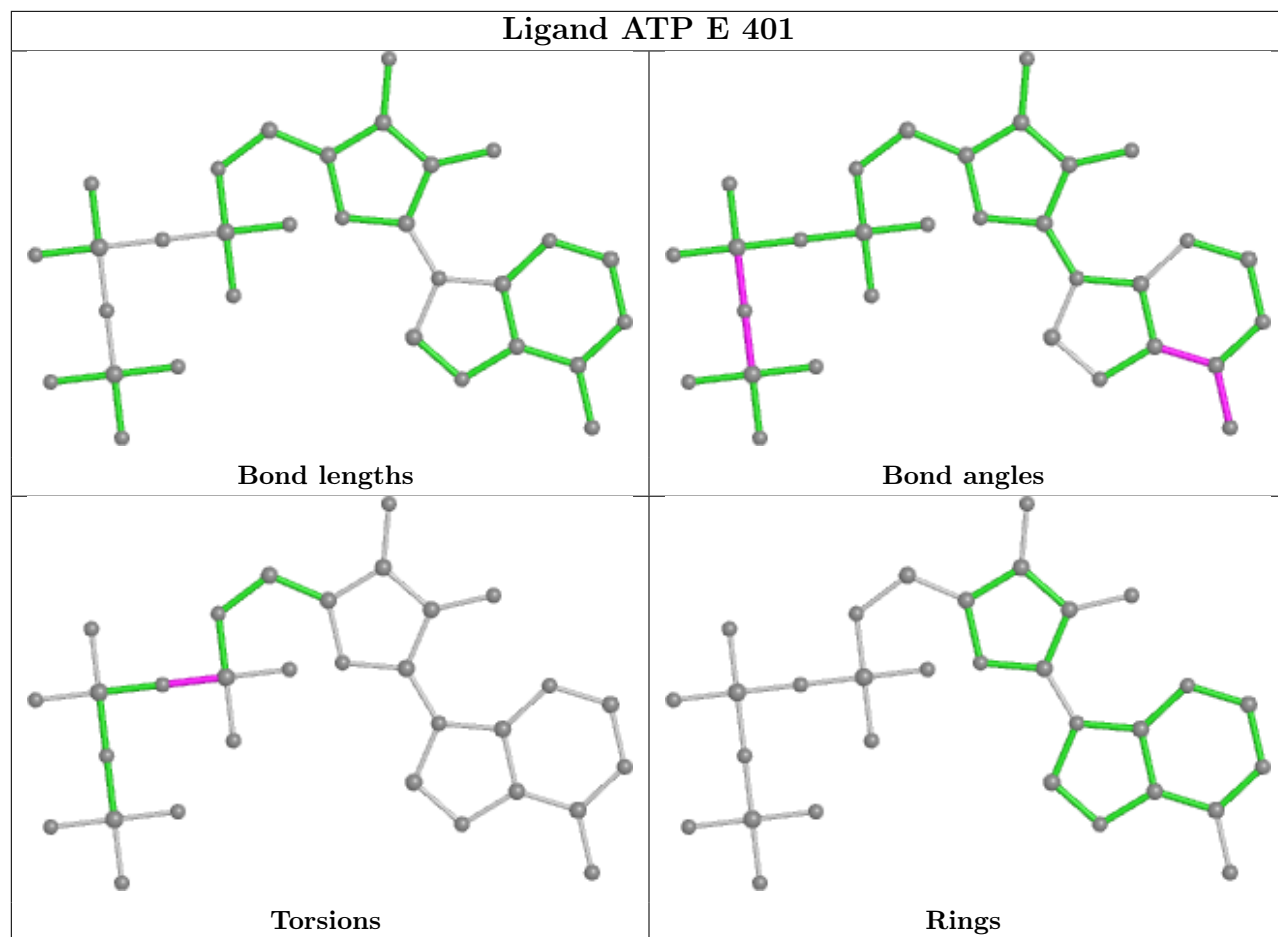
There are no ring outliers.

5 monomers are involved in 63 short contacts:

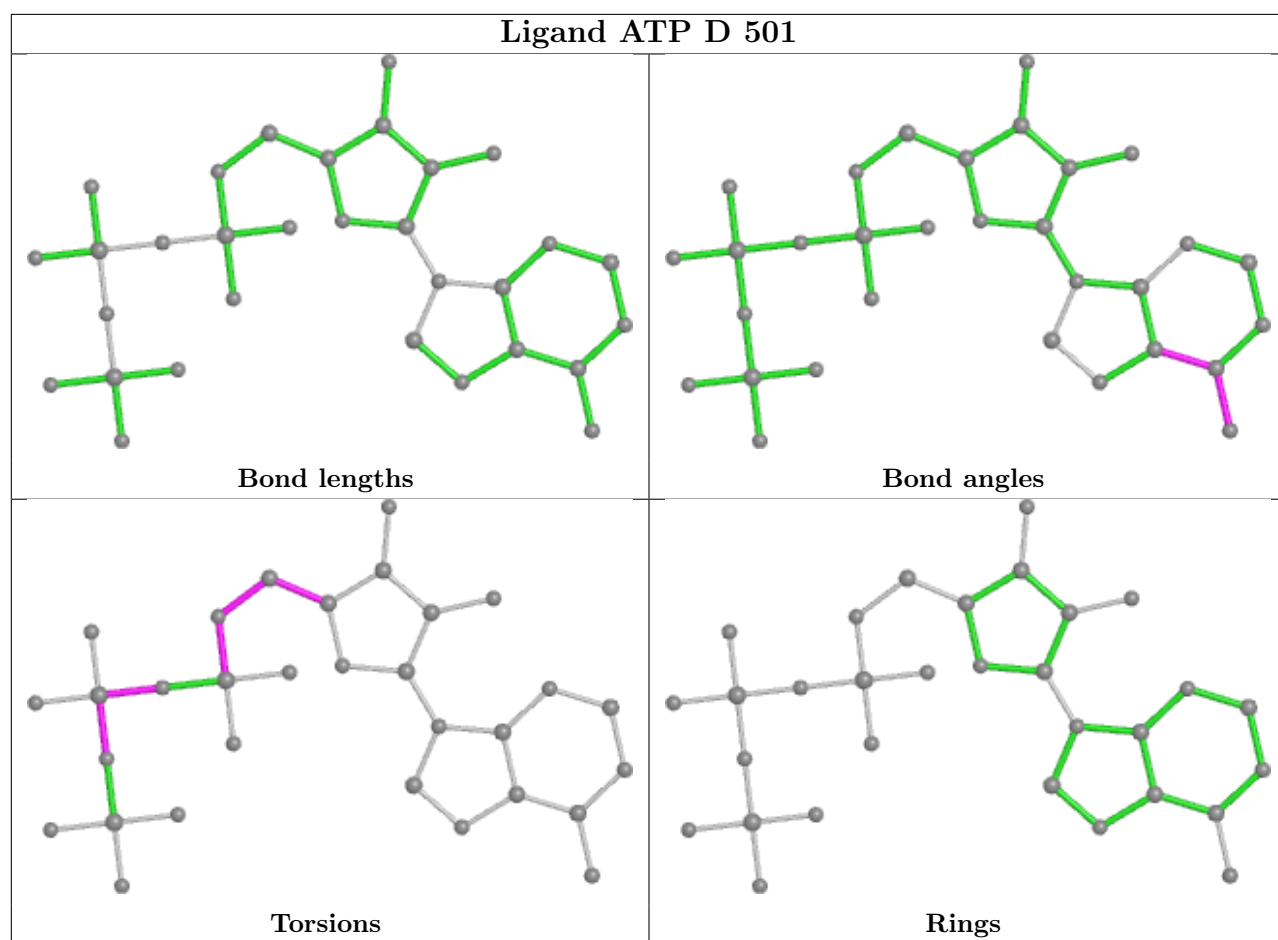
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	F	501	ADP	9	0
35	E	401	ATP	8	0
35	D	501	ATP	34	0
35	A	501	ATP	5	0
35	B	501	ATP	7	0

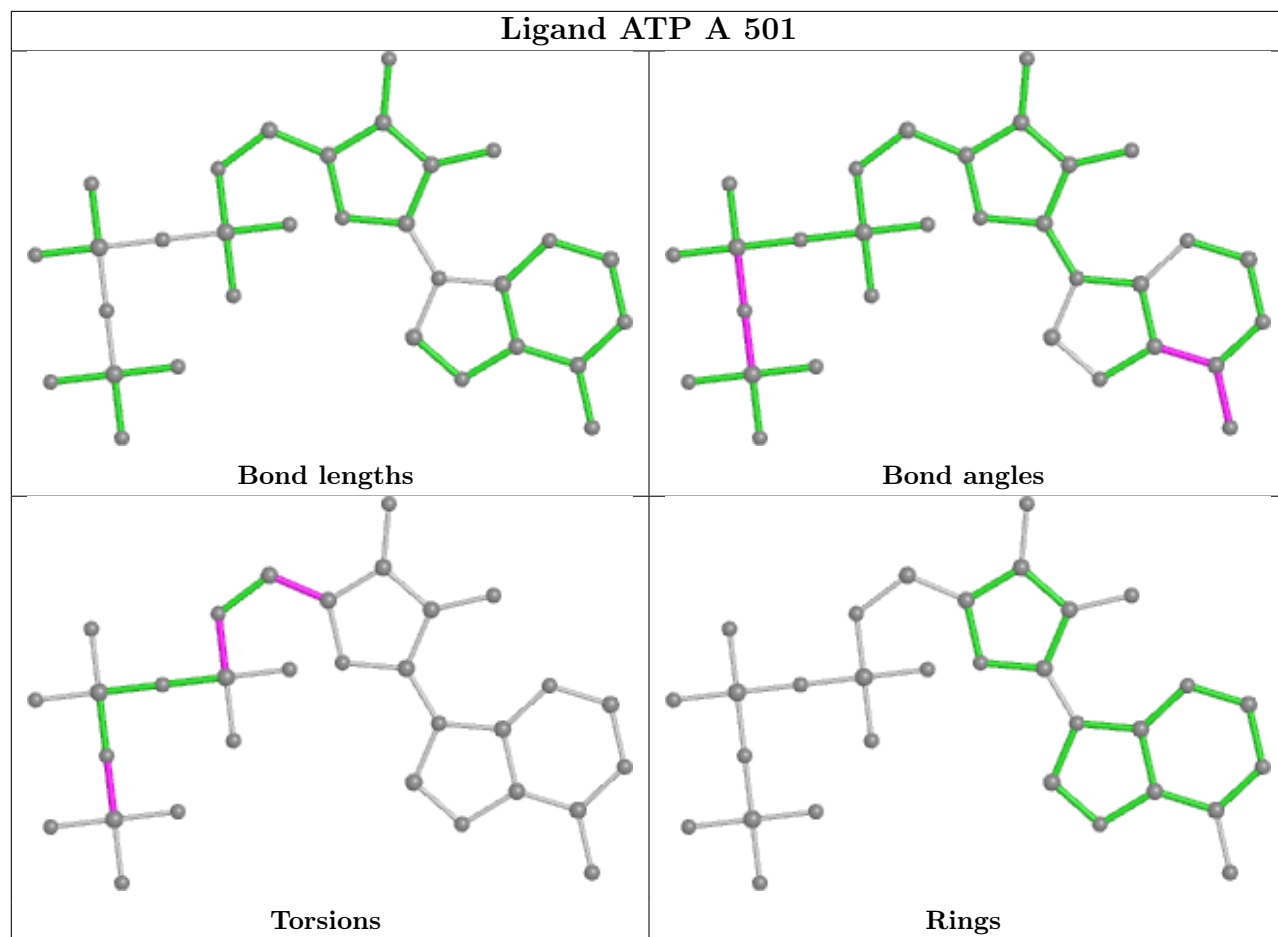
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

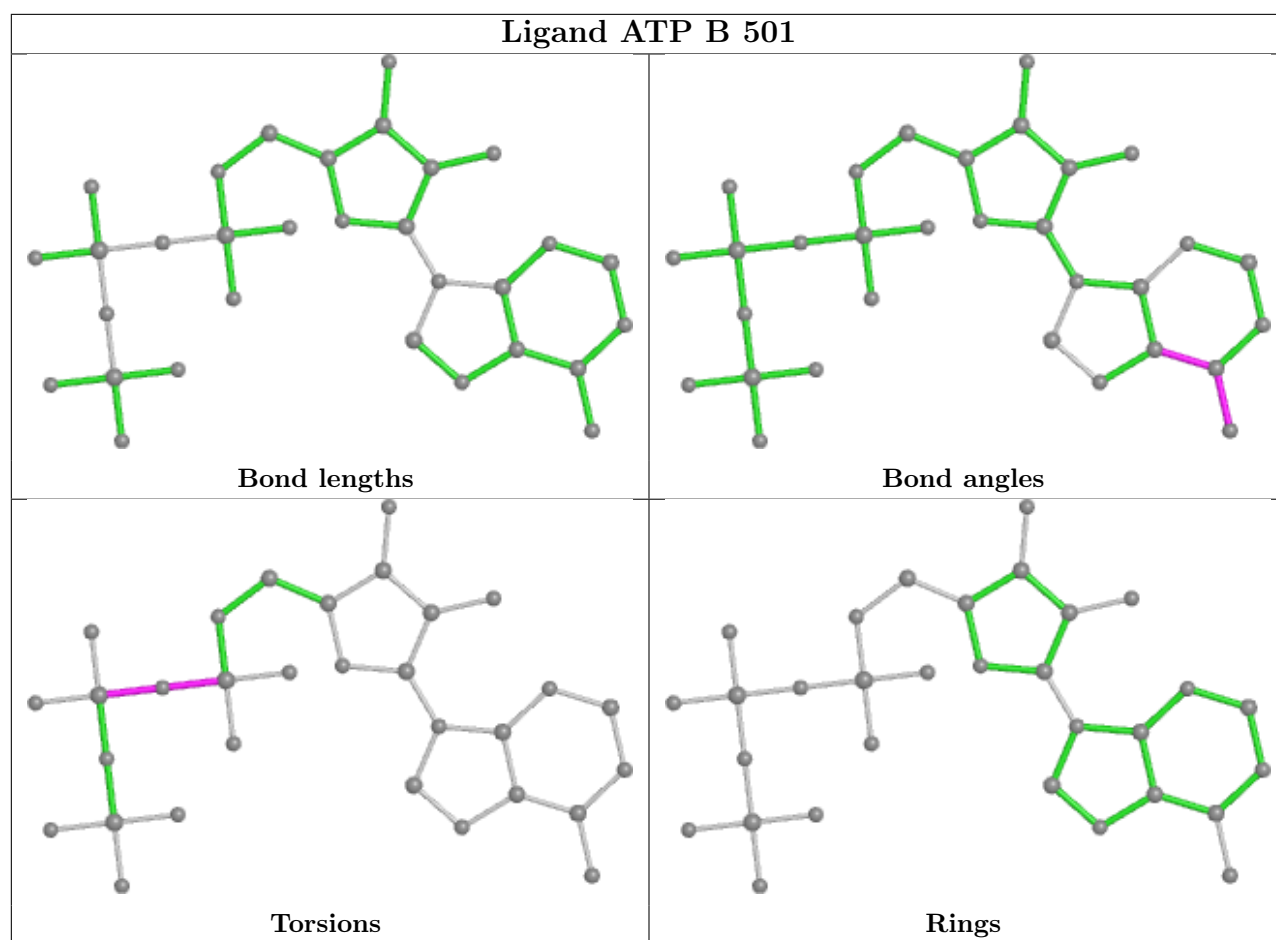












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

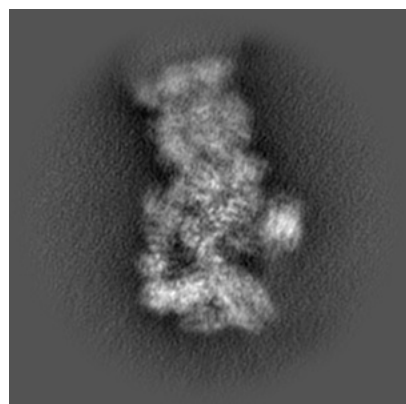
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64103. These allow visual inspection of the internal detail of the map and identification of artifacts.

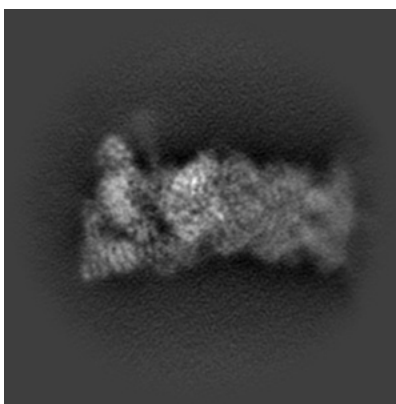
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

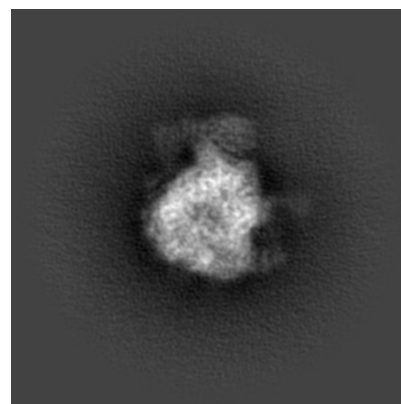
#### 6.1.1 Primary map



X

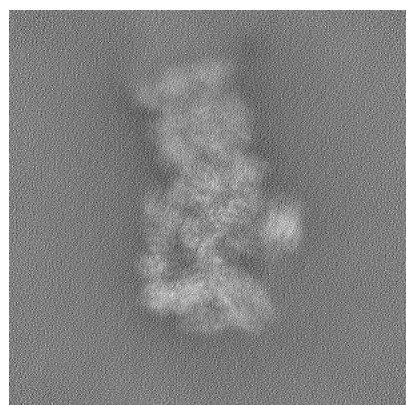


Y

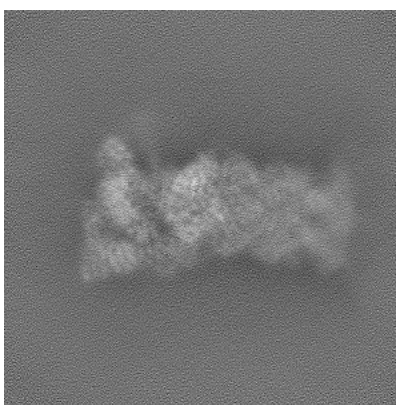


Z

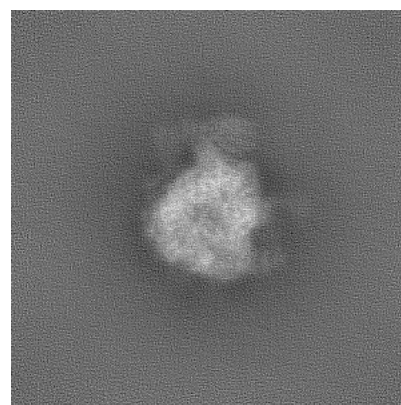
#### 6.1.2 Raw map



X



Y

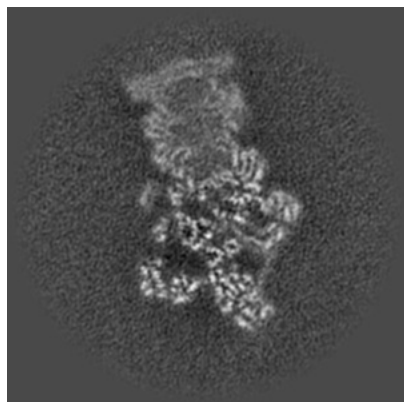


Z

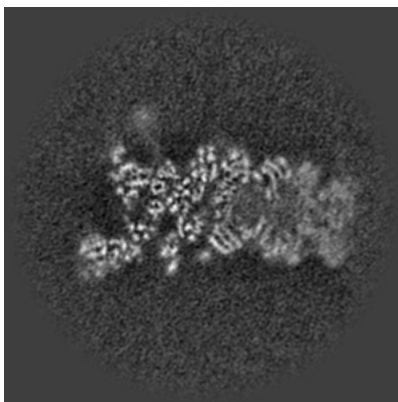
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

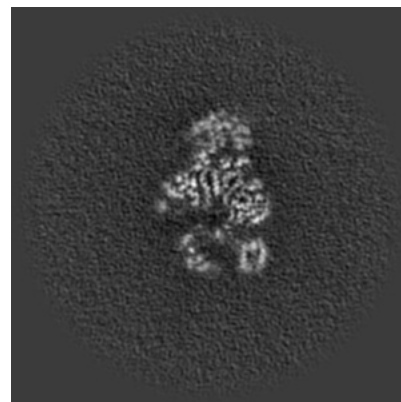
### 6.2.1 Primary map



X Index: 210

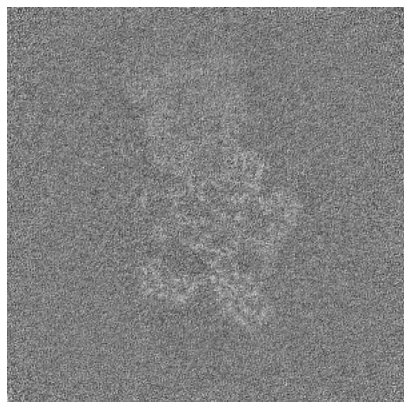


Y Index: 210

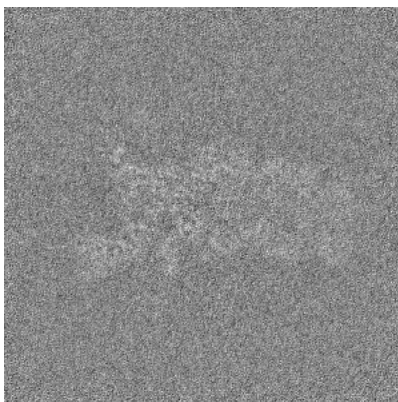


Z Index: 210

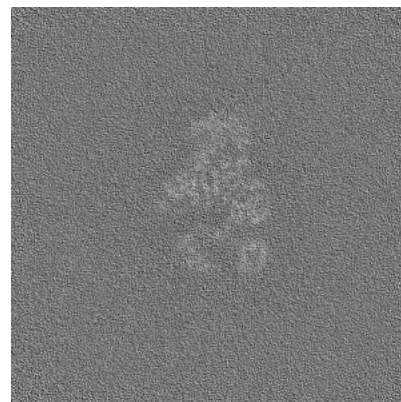
### 6.2.2 Raw map



X Index: 210



Y Index: 210



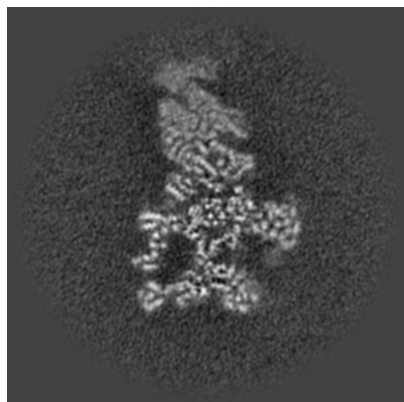
Z Index: 210

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

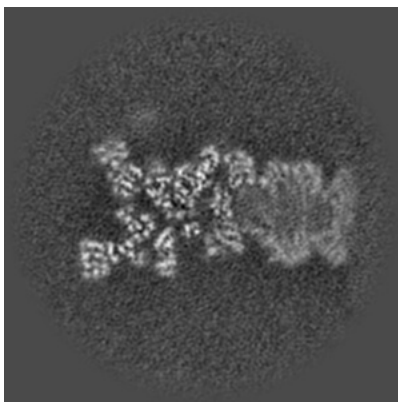


## 6.3 Largest variance slices [i](#)

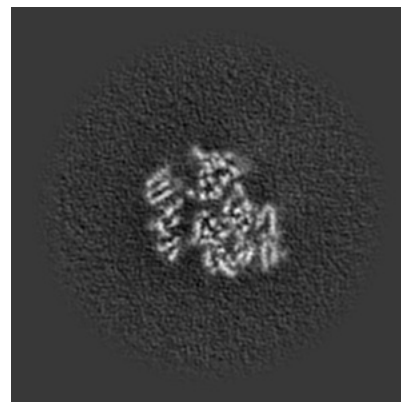
### 6.3.1 Primary map



X Index: 238

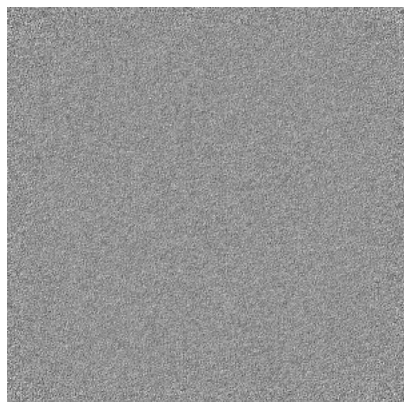


Y Index: 203

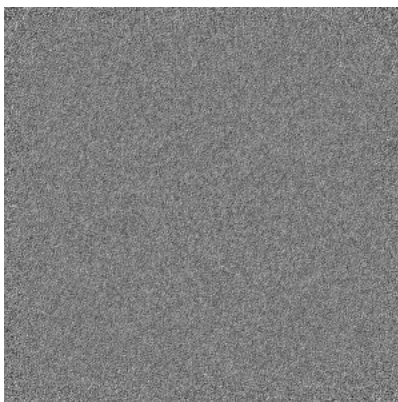


Z Index: 123

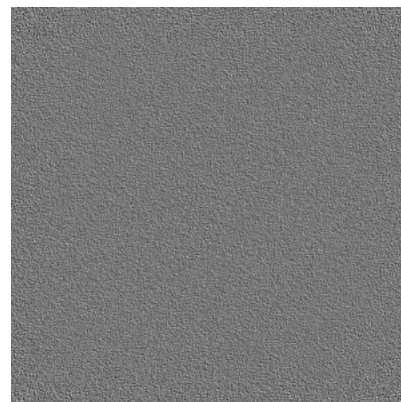
### 6.3.2 Raw map



X Index: 0



Y Index: 0

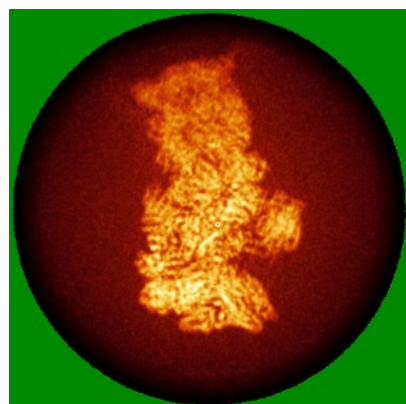


Z Index: 419

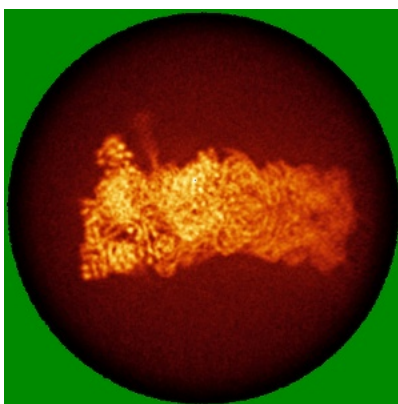
The images above show the largest variance slices of the map in three orthogonal directions.

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

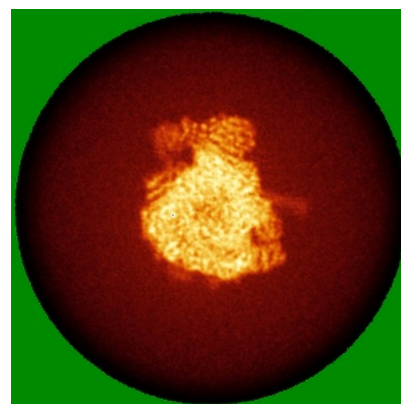
### 6.4.1 Primary map



X

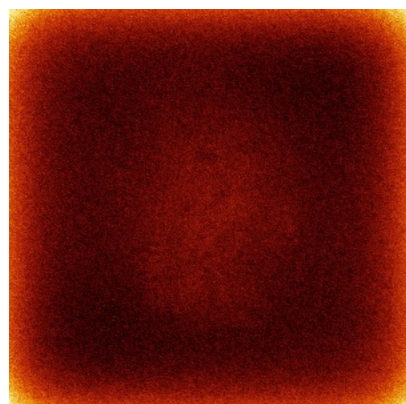


Y

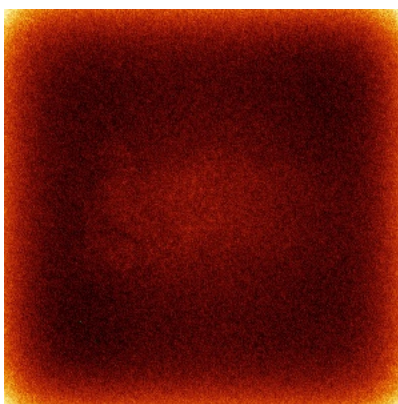


Z

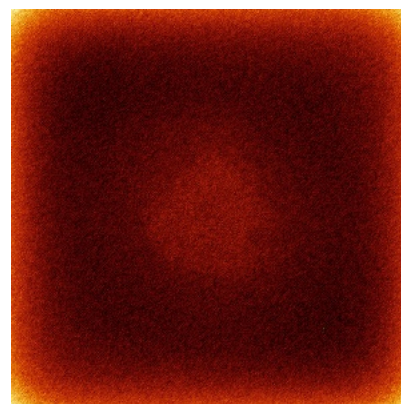
### 6.4.2 Raw map



X



Y

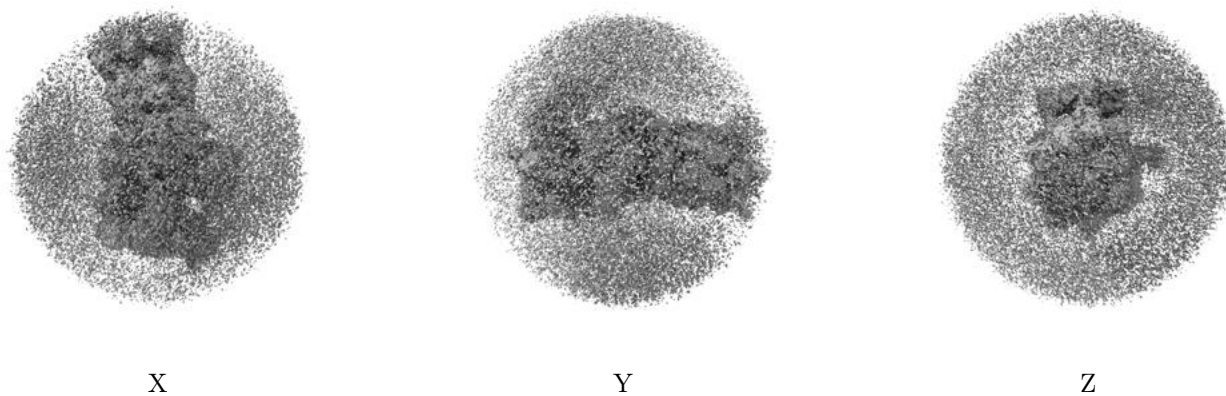


Z

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.

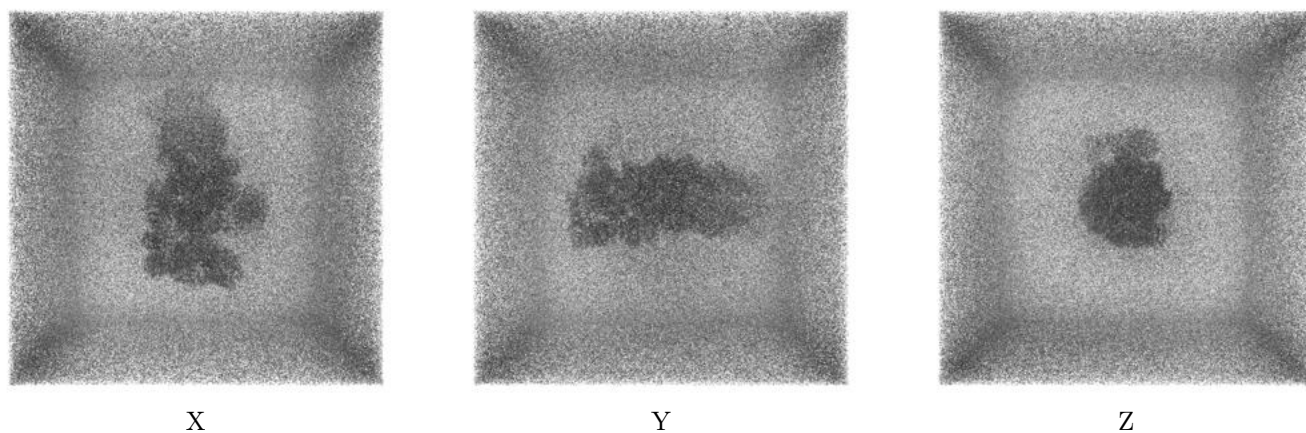
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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](#)

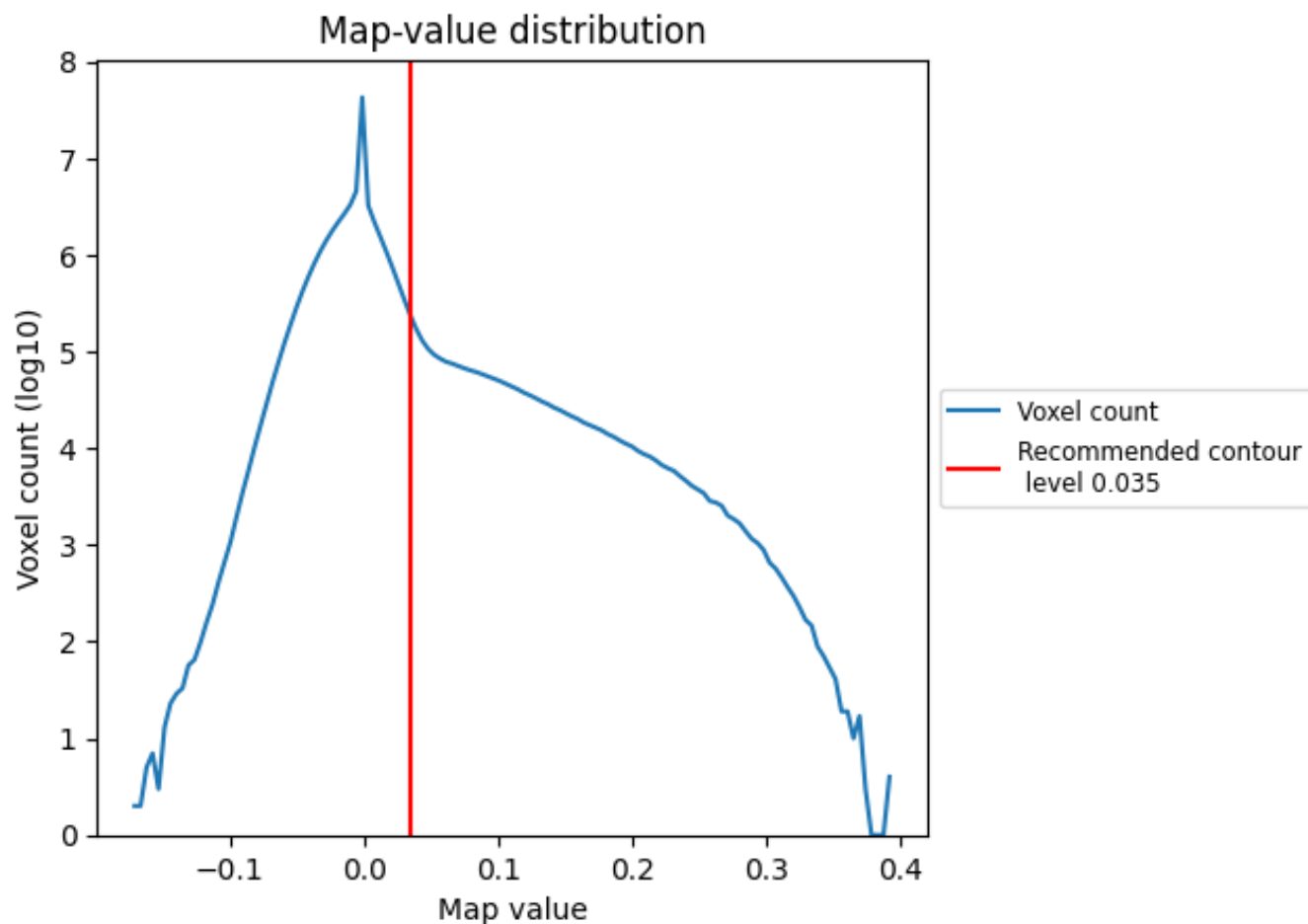
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

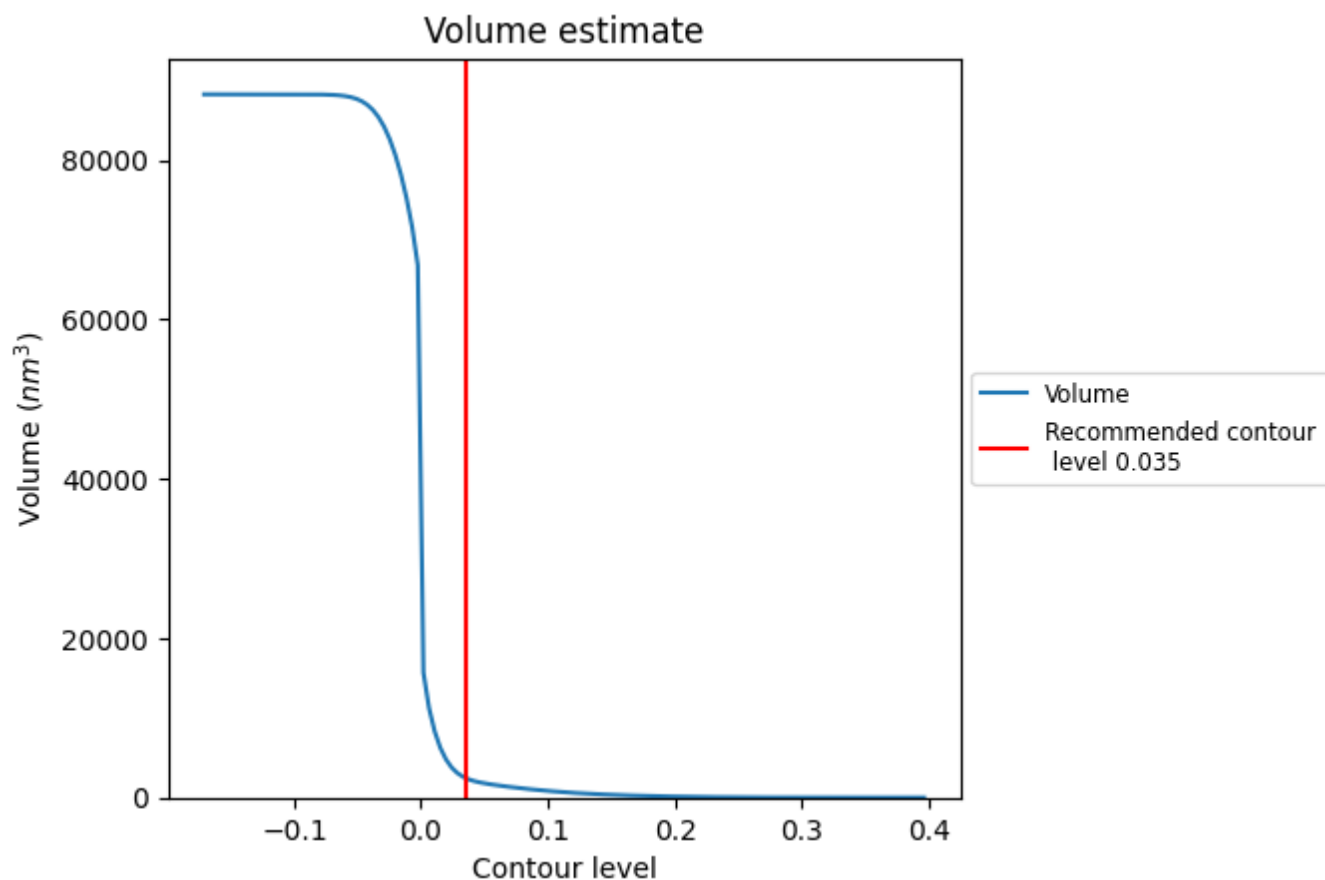
This section contains the results of statistical analysis of the map.

### 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.

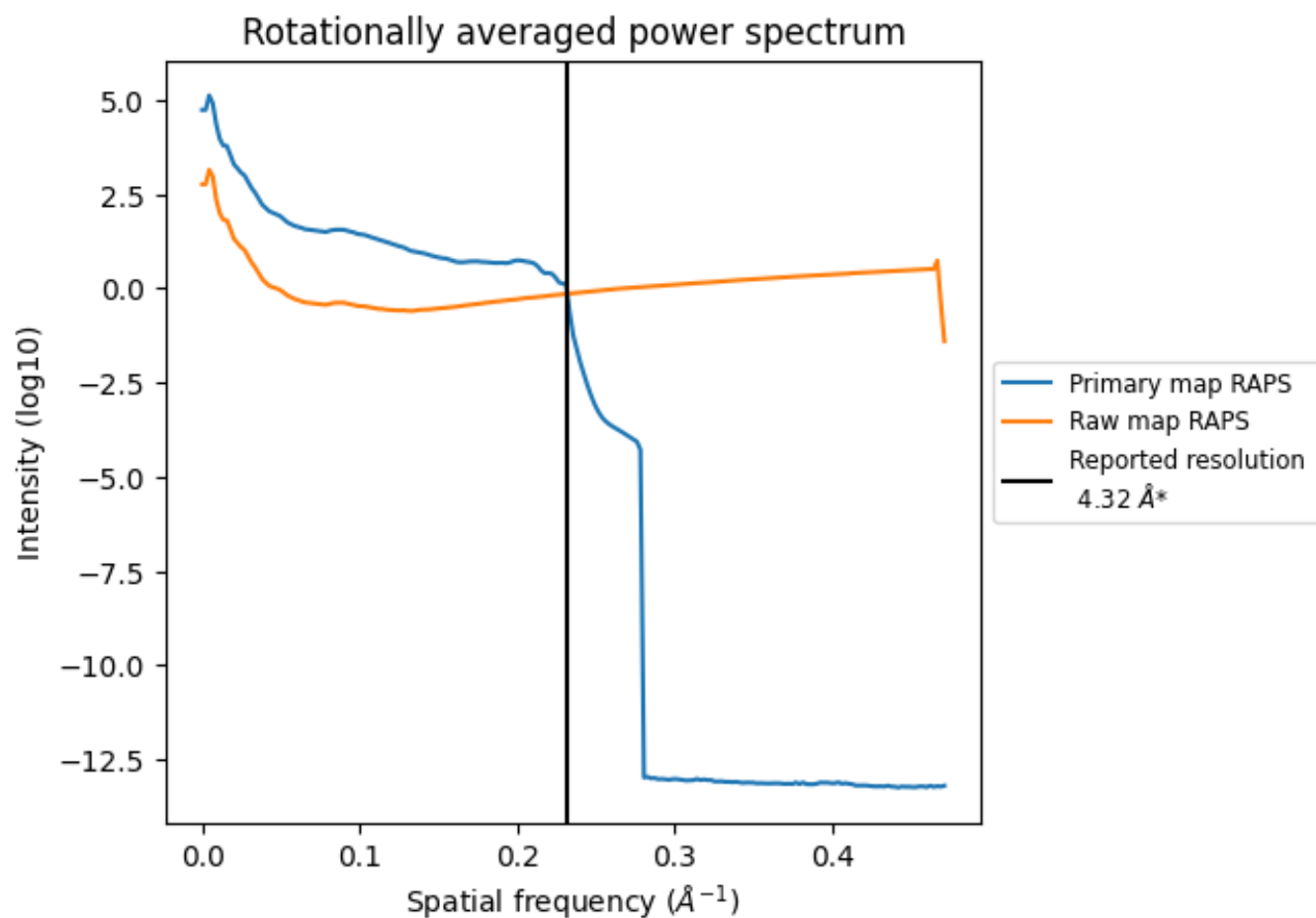
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2478 nm<sup>3</sup>; this corresponds to an approximate mass of 2238 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 ⓘ

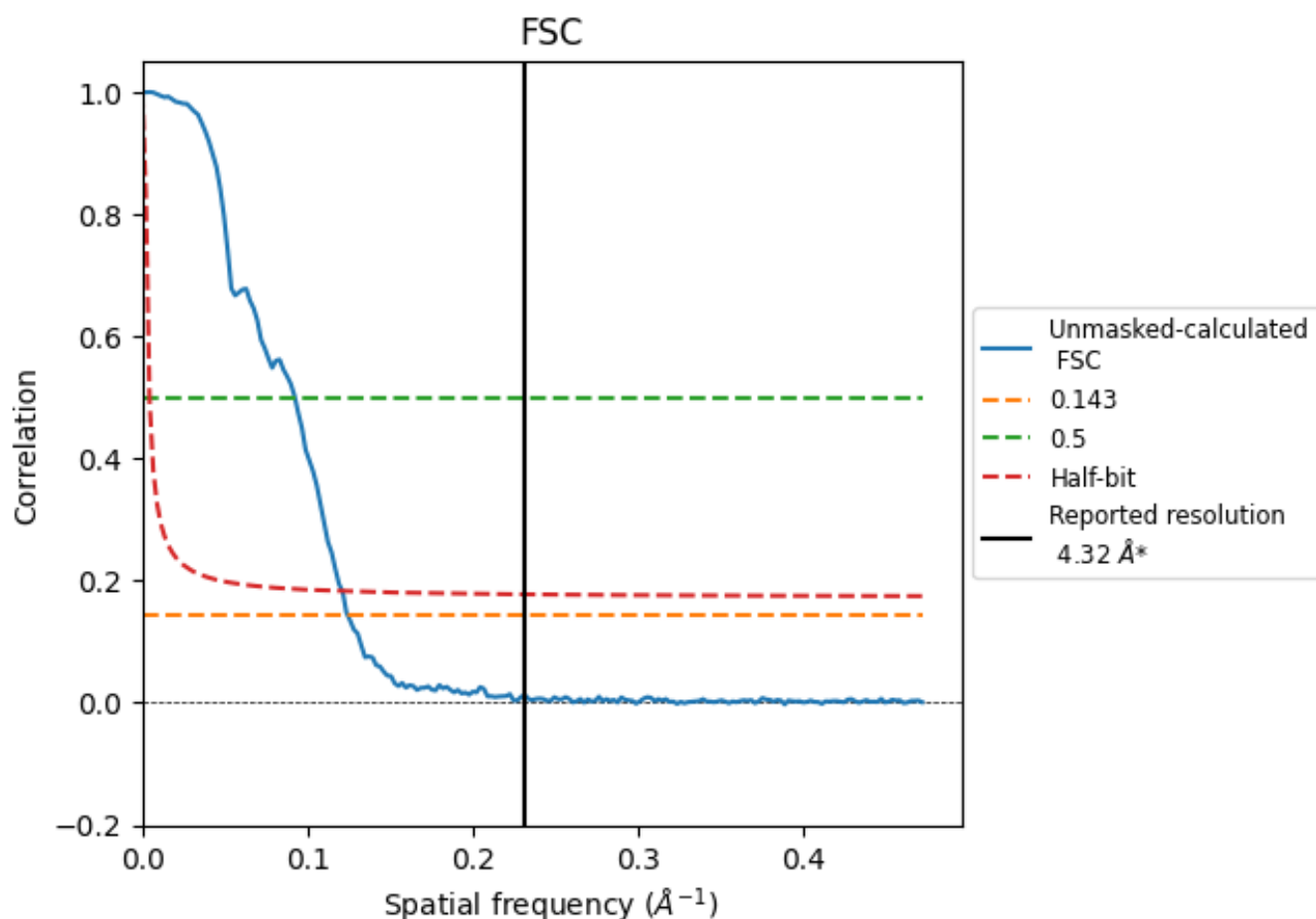


\*Reported resolution corresponds to spatial frequency of 0.231 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

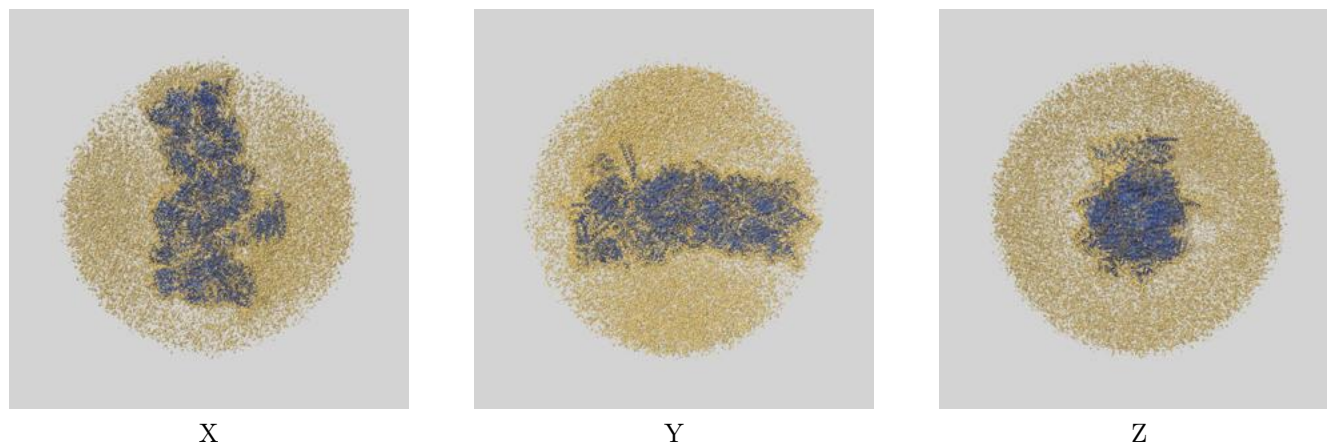
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.05	10.83	8.26

\*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 8.05 differs from the reported value 4.32 by more than 10 %

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

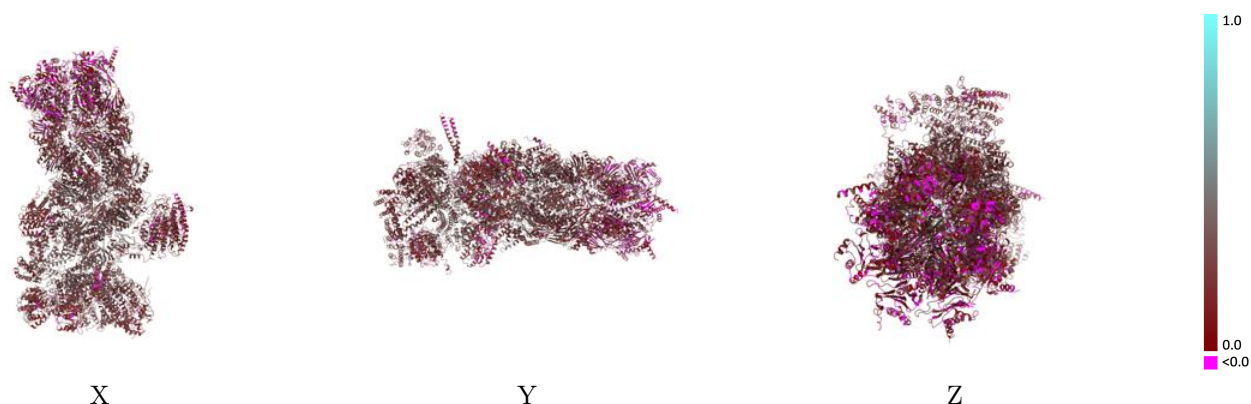
This section contains information regarding the fit between EMDB map EMD-64103 and PDB model 9UF8. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



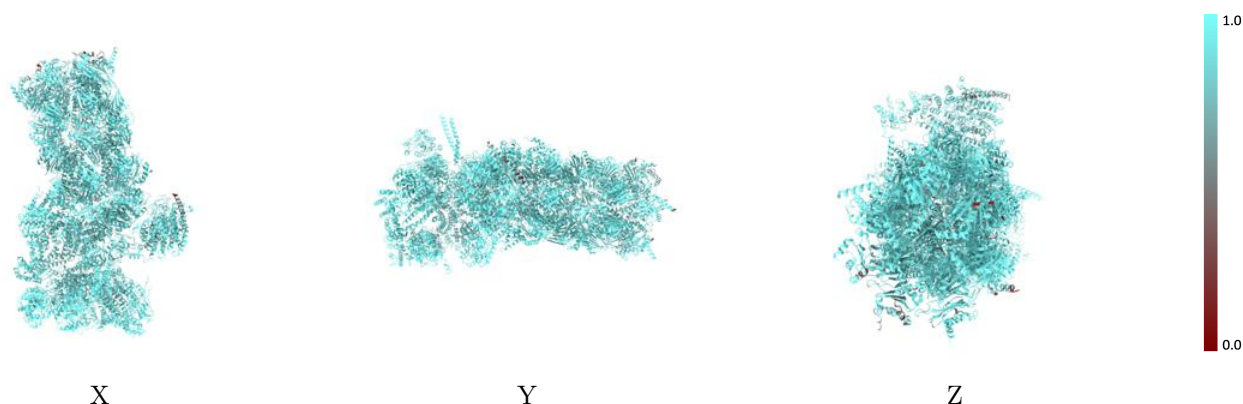
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



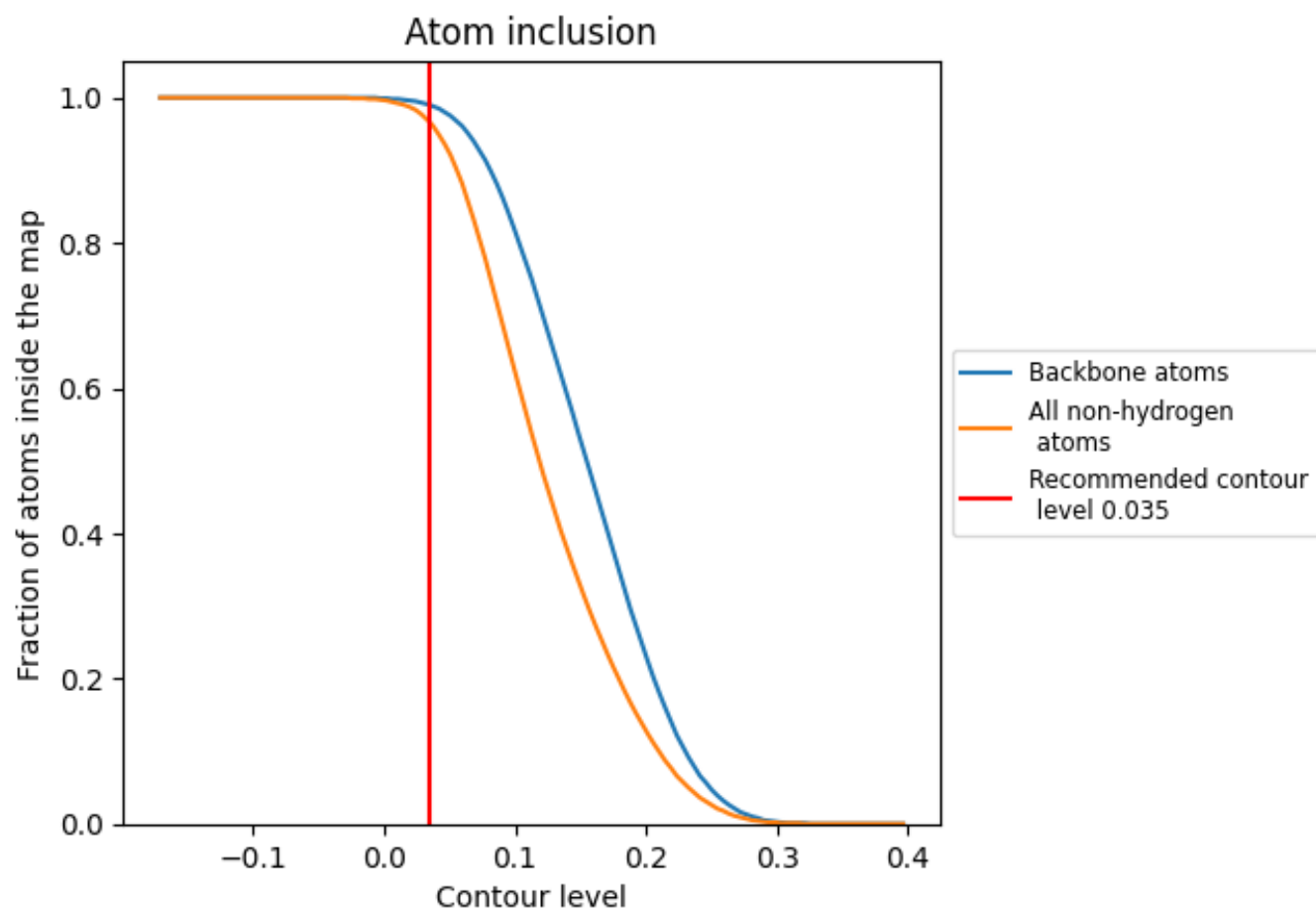
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.2340
A	 0.9640	 0.2960
B	 0.9700	 0.2910
C	 0.9570	 0.3180
D	 0.9580	 0.3130
E	 0.9730	 0.3070
F	 0.9670	 0.3010
G	 0.9810	 0.3110
H	 0.9720	 0.3100
I	 0.9830	 0.3010
J	 0.9890	 0.2860
K	 0.9770	 0.2990
L	 0.9810	 0.2950
M	 0.9850	 0.2870
N	 0.9870	 0.2390
O	 0.9820	 0.2330
P	 0.9850	 0.2130
Q	 0.9750	 0.2300
R	 0.9850	 0.2260
S	 0.9840	 0.2400
T	 0.9800	 0.2330
U	 0.9840	 0.2520
V	 0.9590	 0.2200
W	 0.9680	 0.2360
X	 0.9820	 0.2720
Y	 0.9750	 0.2810
Z	 0.9730	 0.2900
a	 0.9900	 0.2480
b	 0.9870	 0.2080
c	 0.9620	 0.2840
d	 0.9890	 0.2340
e	 0.9740	 0.2450
f	 0.9460	 0.1830
g	 0.9200	 0.1220
h	 0.8820	 0.1160



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Chain	Atom inclusion	Q-score
i	 0.9420	 0.1310
j	 0.9330	 0.1150
k	 0.9060	 0.1290
l	 0.9030	 0.0970
m	 0.9430	 0.1330
n	 0.9910	 0.1700
o	 0.9850	 0.1680
p	 0.9840	 0.1610
q	 0.9810	 0.1730
r	 0.9790	 0.1510
s	 0.9860	 0.1820
t	 0.9880	 0.1790
u	 0.5340	 0.0840