Full wwPDB EM Validation Report

Jun 10, 2025 – 10:44 PM JST

PDB ID	:	6J30 / pdb_00006j30
EMDB ID	:	EMD-9773
Title	:	yeast proteasome in Ub-engaged state (C2)
Authors	:	Cong, Y.
Deposited on	:	2019-01-03
Resolution	:	4.50 Å(reported)

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

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

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

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

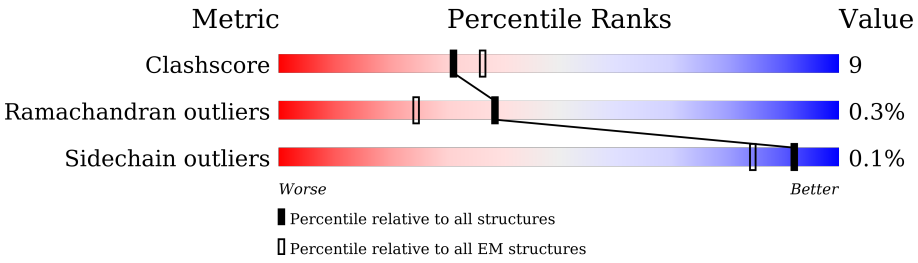
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	215	11% 73% 18% 9%
1	b	215	10% 71% 20% 9%
2	2	261	13% 70% 16% 13%
2	i	261	9% 69% 18% 13%
3	3	205	14% 67% 32%
3	h	205	14% 76% 23%
4	4	198	14% 81% 17%
4	g	198	10% 75% 23%

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Mol	Chain	Length	Quality of chain
5	5	287	10% 58% 16% 26%
5	f	287	11% 60% 14% 26%
6	6	241	11% 75% 17% 8%
6	e	241	12% 66% 27% 8%
7	7	266	9% 65% 21% 14%
7	a	266	8% 66% 21% 13%
8	A	252	19% 74% 22%
8	c	252	15% 76% 19%
9	B	250	31% 75% 25%
9	j	250	24% 80% 20%
10	C	258	28% 66% 28% 5%
10	d	258	19% 77% 17% 5%
11	D	254	20% 69% 25% 6%
11	n	254	15% 70% 24% 6%
12	E	260	22% 73% 20% 7%
12	m	260	20% 71% 22% 7%
13	F	234	20% 81% 18%
13	l	234	12% 81% 18%
14	G	288	15% 66% 19% 16%
14	k	288	11% 71% 14% 16%
15	H	467	45% 59% 17% 24%
16	I	437	52% 70% 13% 17%
17	J	405	60% 73% 19% 8%
18	K	428	55% 65% 24% 11%
19	L	437	46% 67% 18% 15%

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Mol	Chain	Length	Quality of chain
20	M	434	42% 62% 22% 15%
21	N	945	38% 71% 19% 10%
22	O	393	50% 79% 19%
23	P	445	38% 80% 17%
24	Q	434	53% 80% 20%
25	R	429	50% 75% 18% 7%
26	S	523	55% 76% 15% 9%
27	T	274	78% 78% 22%
28	U	338	29% 55% 23% 22%
29	V	306	51% 64% 27% 7%
30	W	268	38% 55% 17% 26%
31	X	156	70% 60% 12% 29%
32	Y	89	10% 26% 70%
33	Z	993	64% 65% 17% 18%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106227 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
1	b	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
2	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
3	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
4	g	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
5	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 6 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
6	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
7	a	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
8	c	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
9	j	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
11	n	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
12	m	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		
13	l	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
14	k	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	355	Total	C	N	O	S	0	0
			2787	1755	500	515	17		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	362	Total	C	N	O	S	0	0
			2822	1773	471	563	15		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 19 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	371	Total	C	N	O	S	0	0
			2937	1852	519	554	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	262	Total	C	N	O	S	0	0
			2118	1348	362	402	6		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	284	Total	C	N	O	S	0	0
			2236	1405	381	436	14		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	111	Total	C	N	O	S	0	0
			906	586	148	169	3		

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	27	Total	C	N	O	0	0
			236	143	39	54		

- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

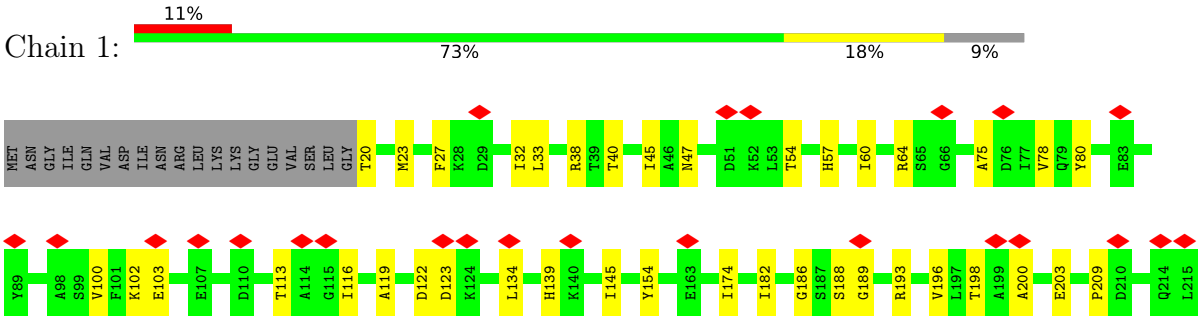
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

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.

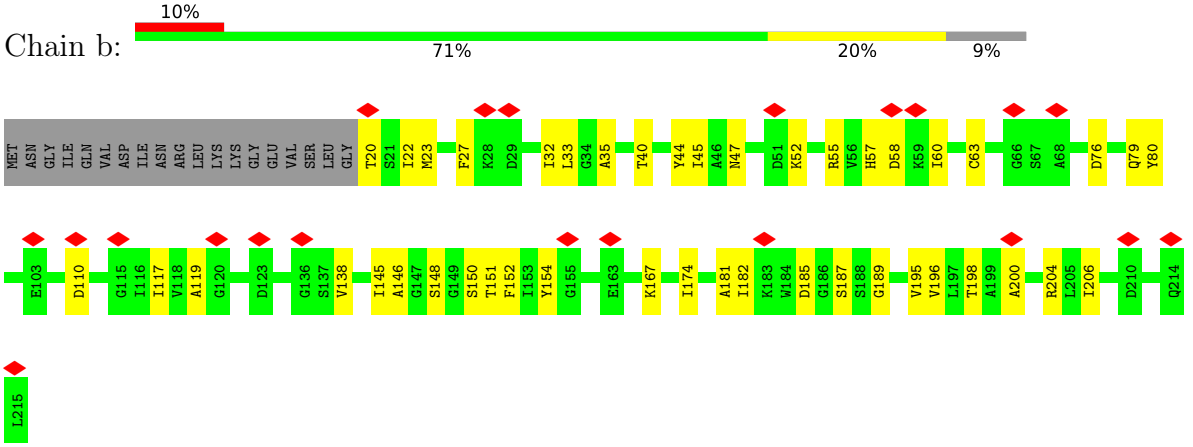
• Molecule 1: Proteasome subunit beta type-1

Chain 1:



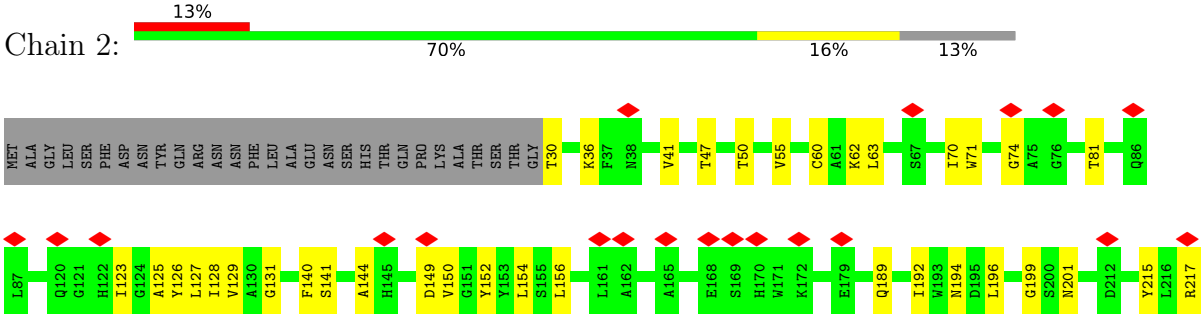
• Molecule 1: Proteasome subunit beta type-1

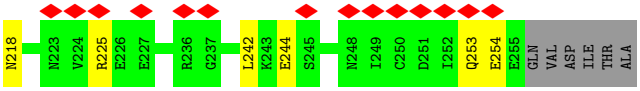
Chain b:



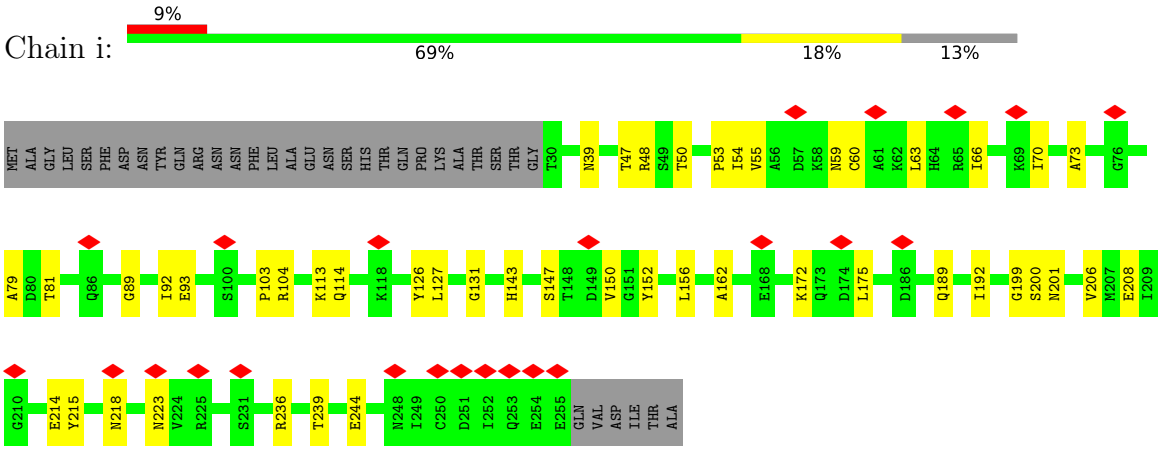
• Molecule 2: Proteasome subunit beta type-2

Chain 2:

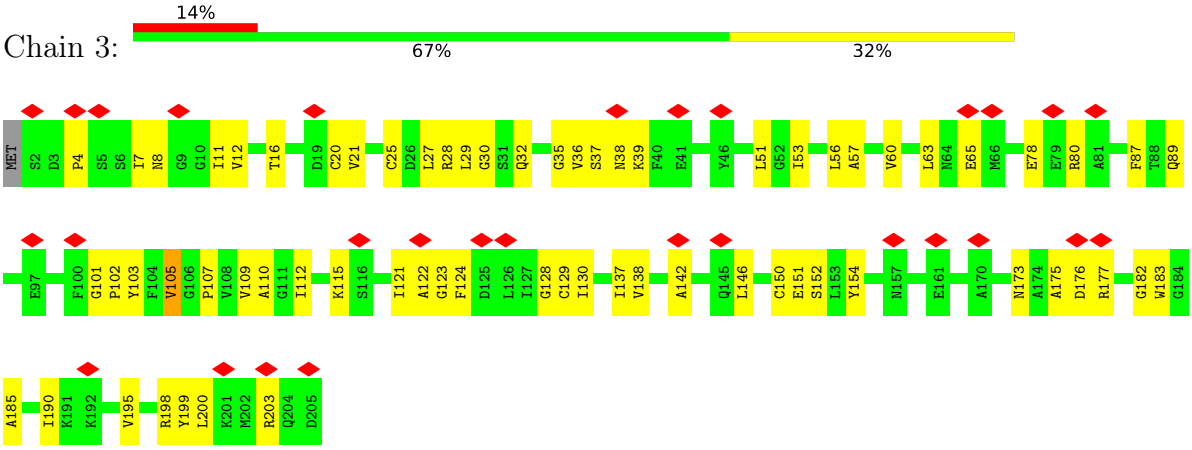




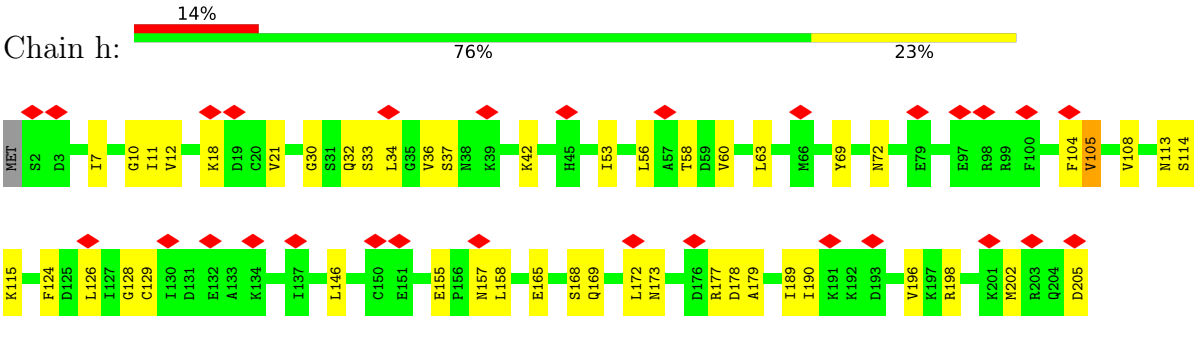
• Molecule 2: Proteasome subunit beta type-2



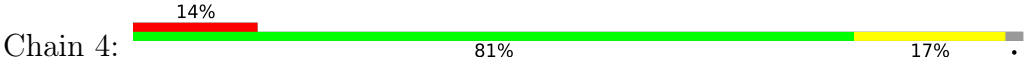
• Molecule 3: Proteasome subunit beta type-3

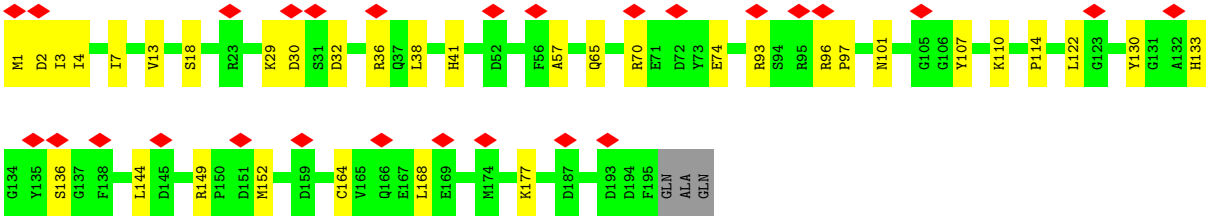


• Molecule 3: Proteasome subunit beta type-3

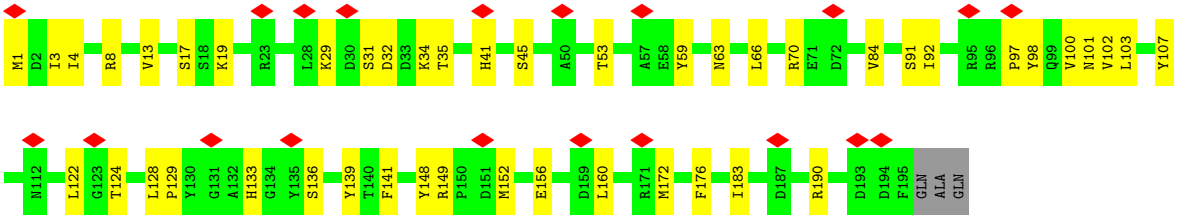


• Molecule 4: Proteasome subunit beta type-4

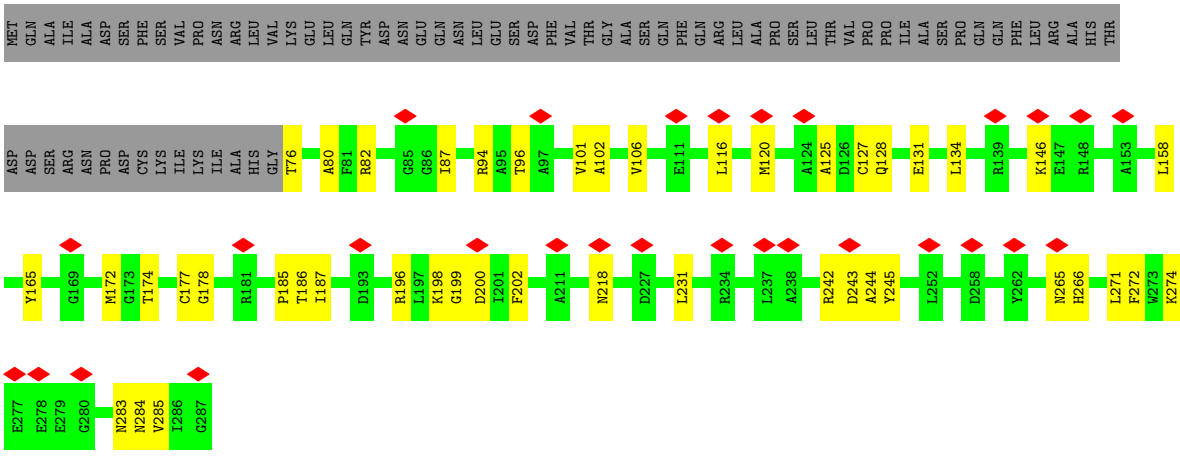




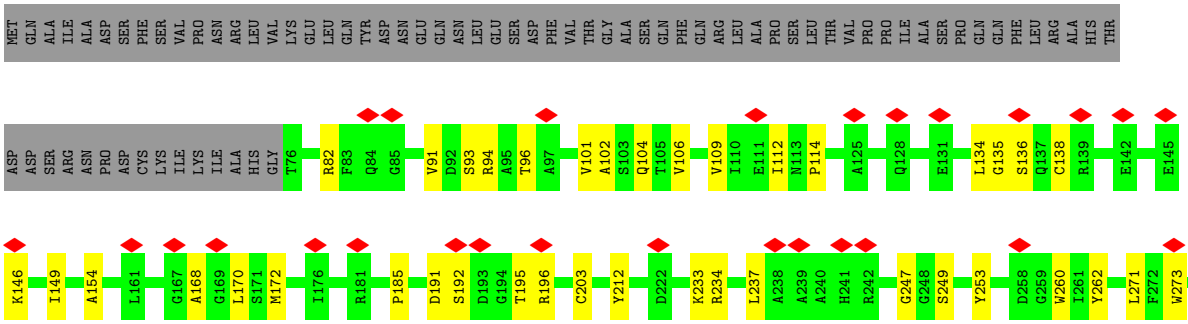
• Molecule 4: Proteasome subunit beta type-4

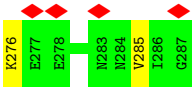


• Molecule 5: Proteasome subunit beta type-5



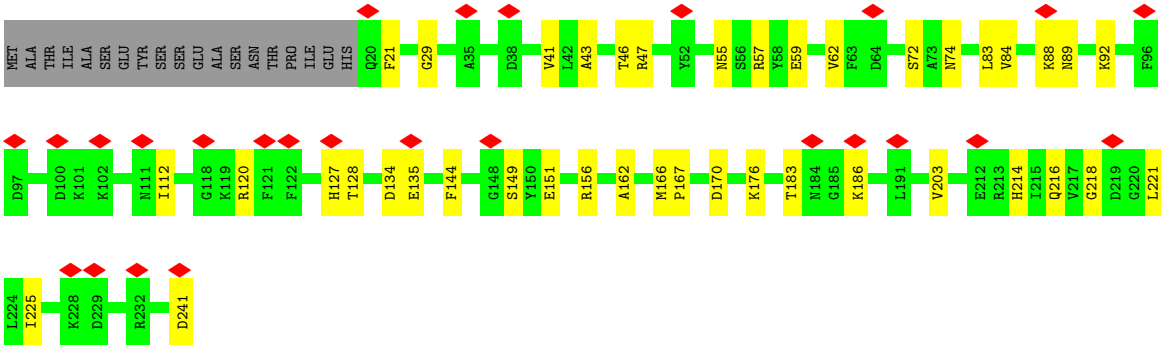
• Molecule 5: Proteasome subunit beta type-5





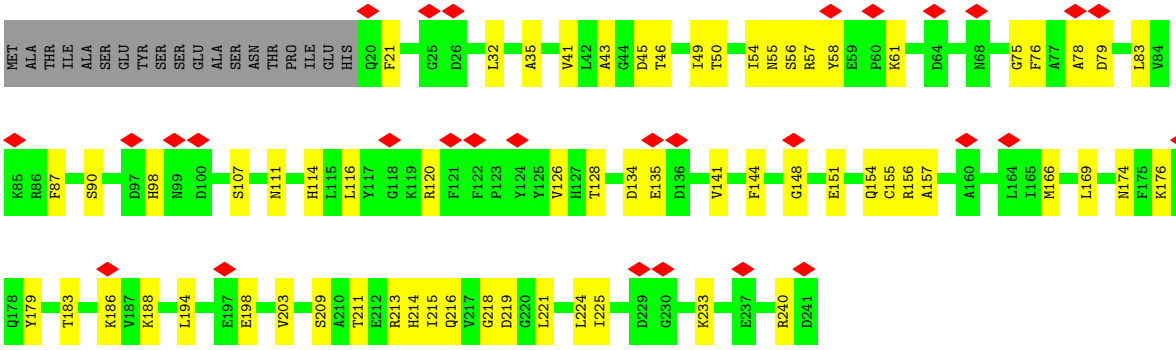
• Molecule 6: Proteasome subunit beta type-6

Chain 6:



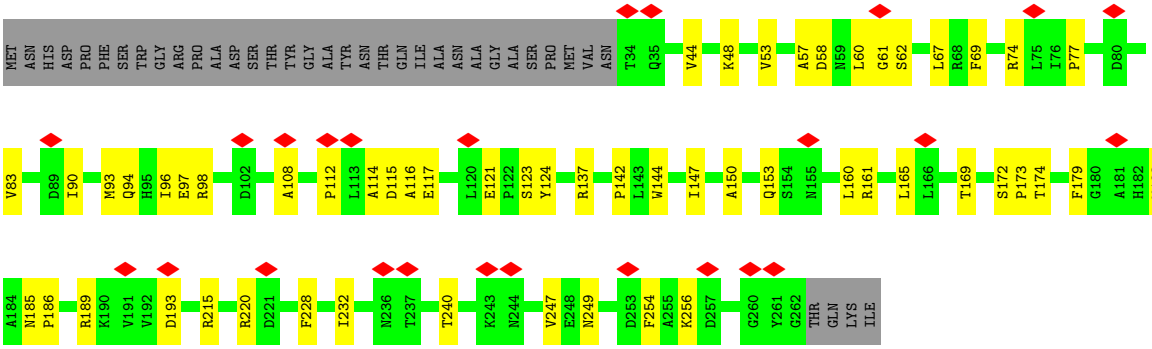
• Molecule 6: Proteasome subunit beta type-6

Chain e:



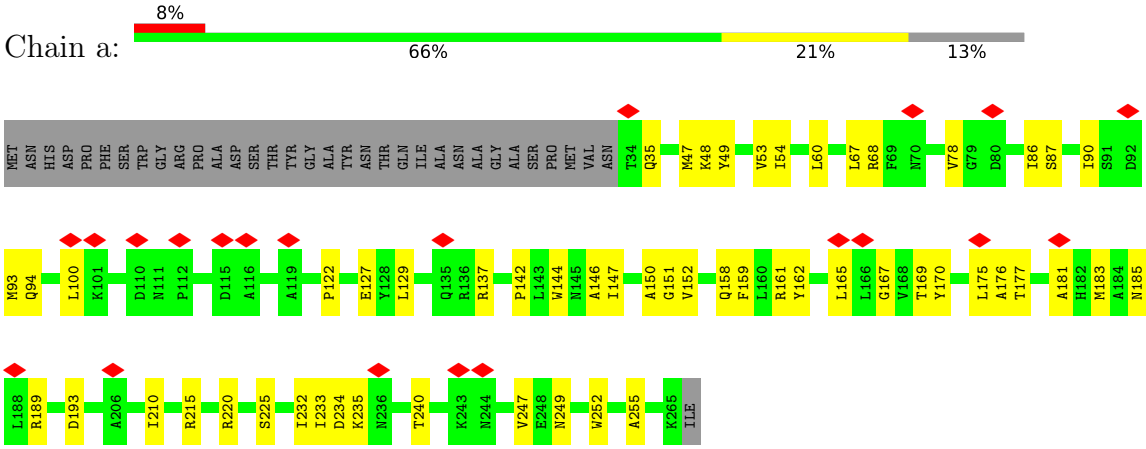
• Molecule 7: Proteasome subunit beta type-7

Chain 7:



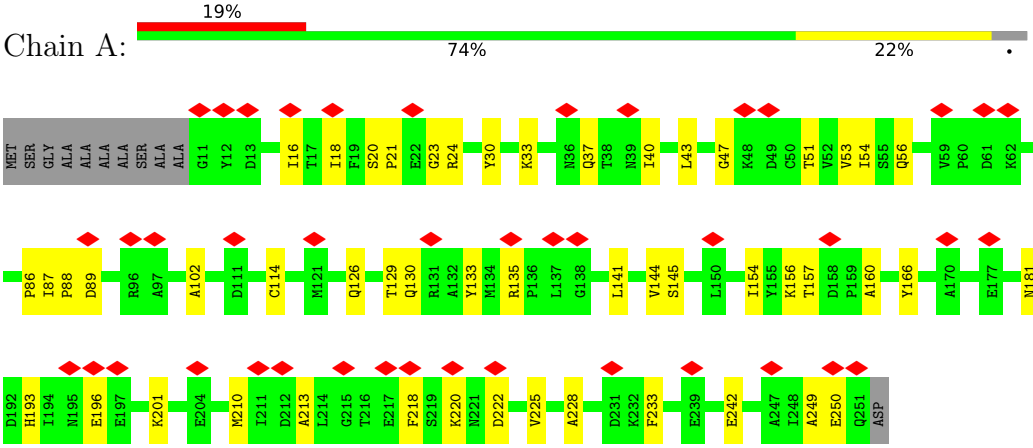
• Molecule 7: Proteasome subunit beta type-7

Chain a:



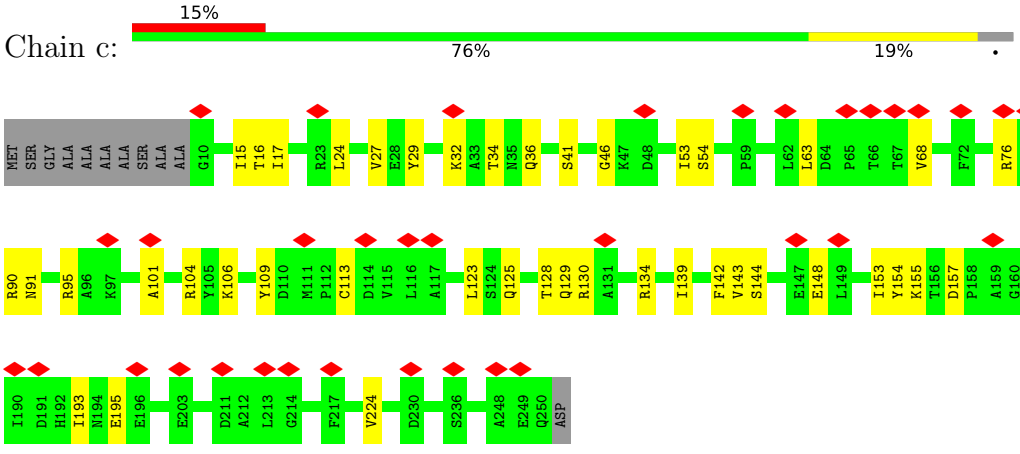
• Molecule 8: Proteasome subunit alpha type-1

Chain A:



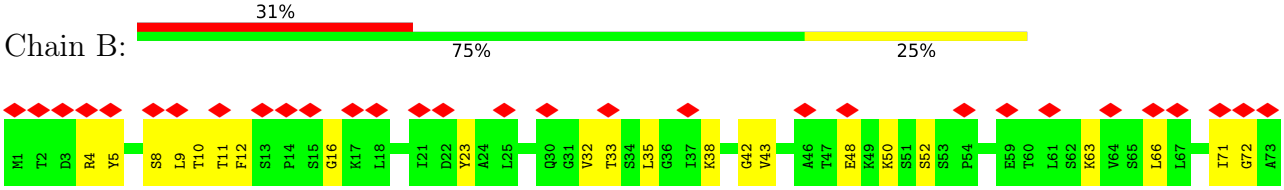
• Molecule 8: Proteasome subunit alpha type-1

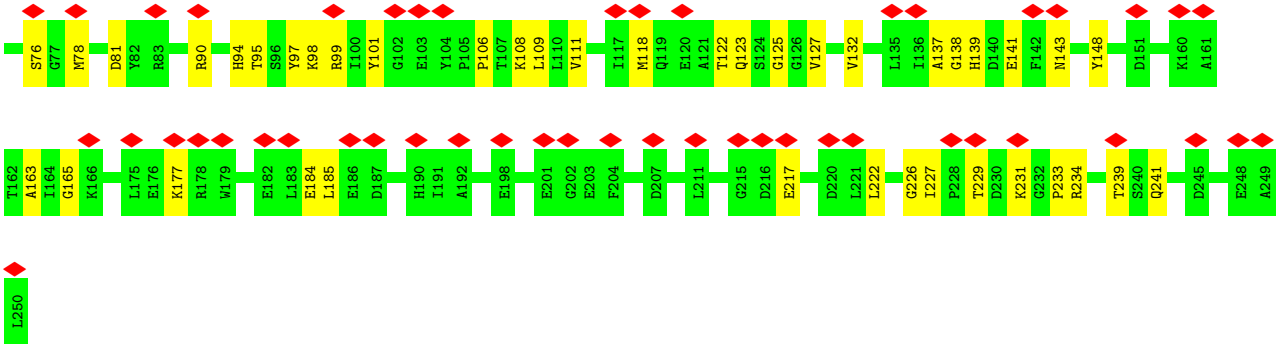
Chain c:



• Molecule 9: Proteasome subunit alpha type-2

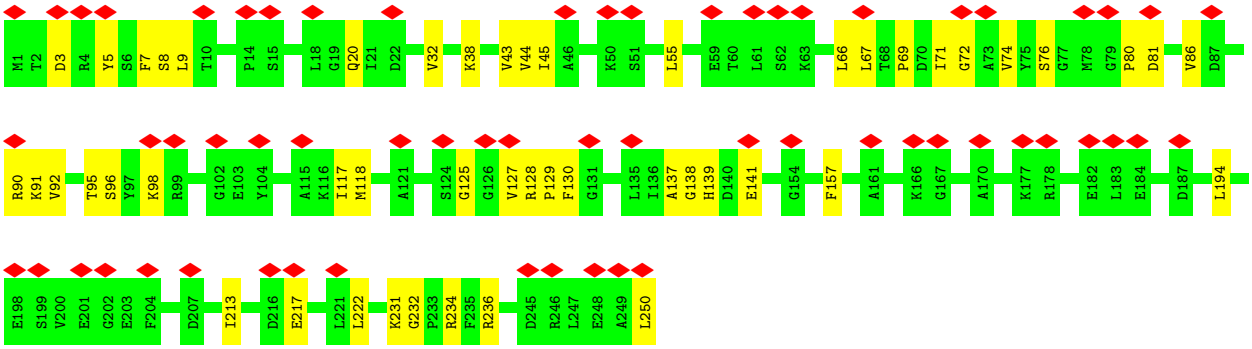
Chain B:





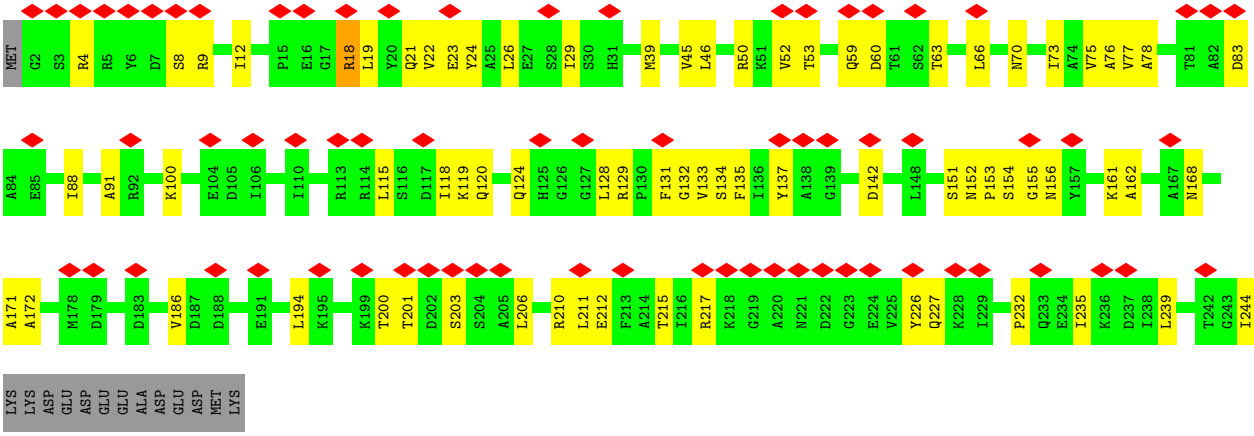
• Molecule 9: Proteasome subunit alpha type-2

Chain j:



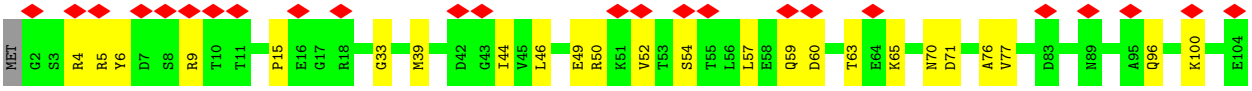
• Molecule 10: Proteasome subunit alpha type-3

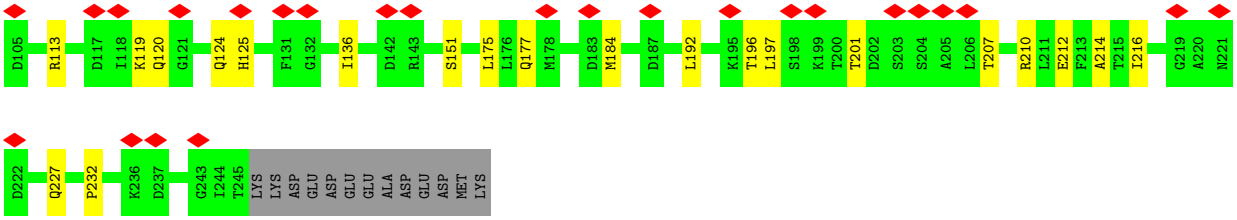
Chain C:



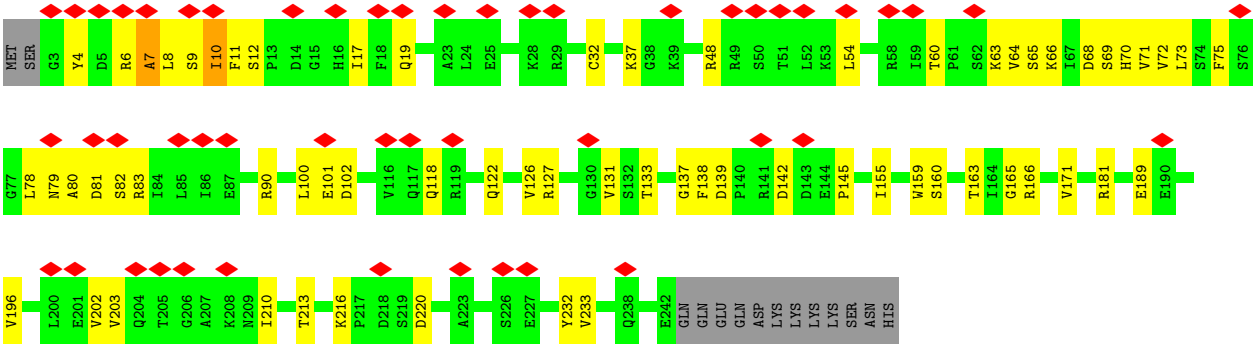
• Molecule 10: Proteasome subunit alpha type-3

Chain d:

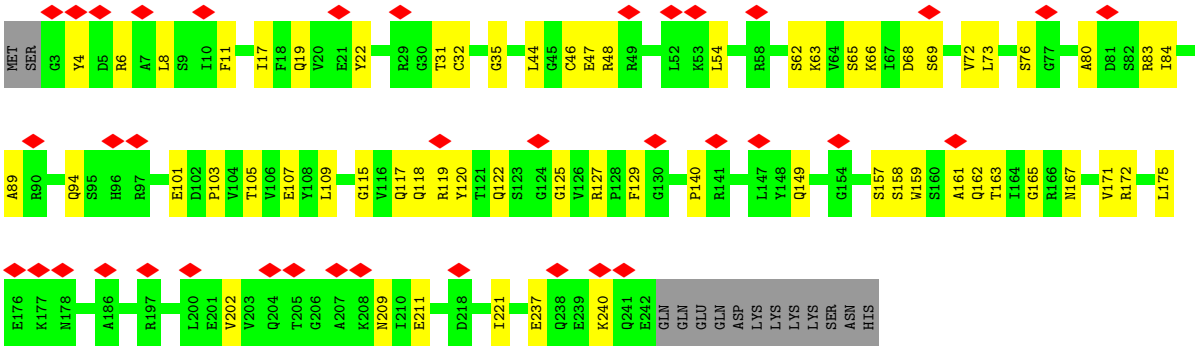




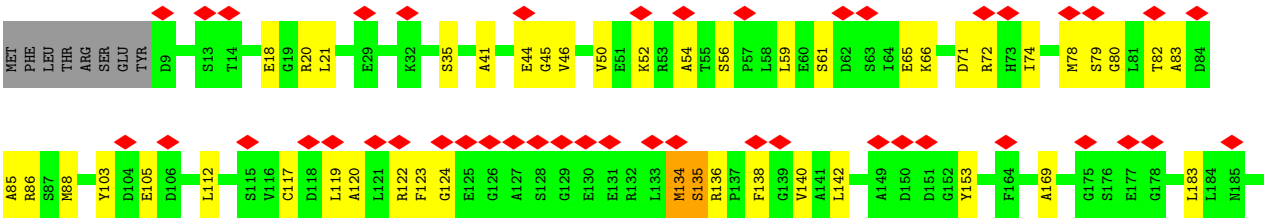
• Molecule 11: Proteasome subunit alpha type-4

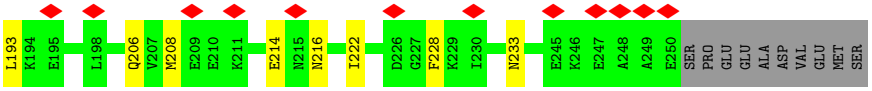


• Molecule 11: Proteasome subunit alpha type-4

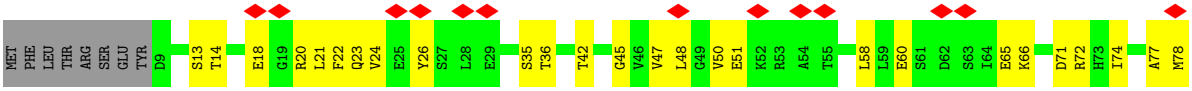


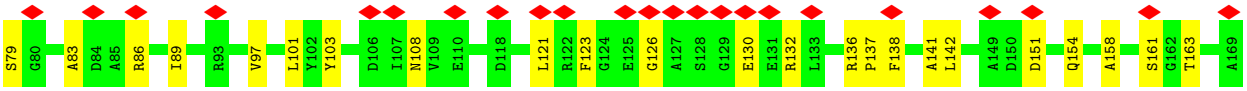
• Molecule 12: Proteasome subunit alpha type-5

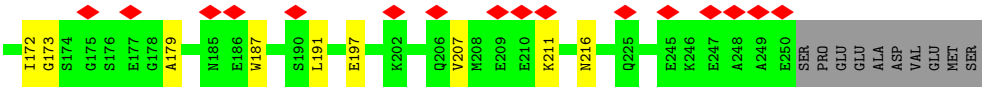




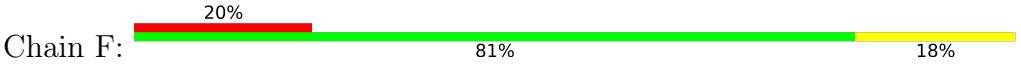
• Molecule 12: Proteasome subunit alpha type-5

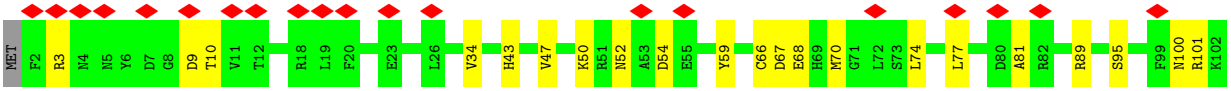


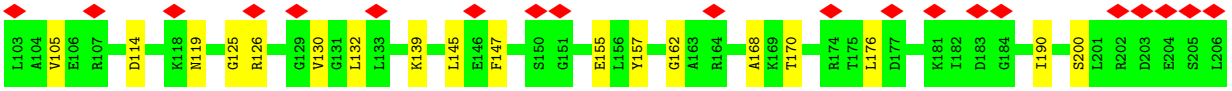




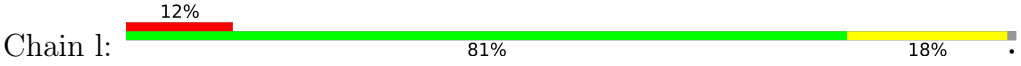
• Molecule 13: Proteasome subunit alpha type-6

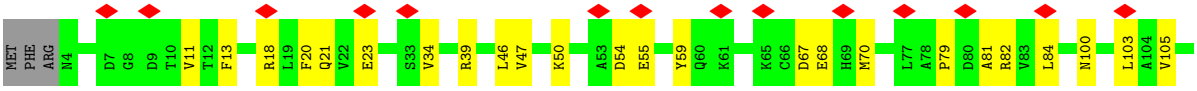


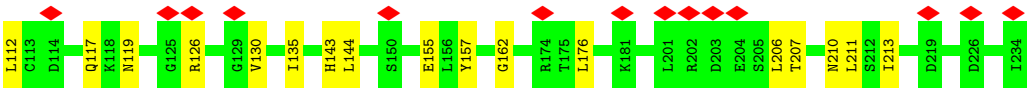




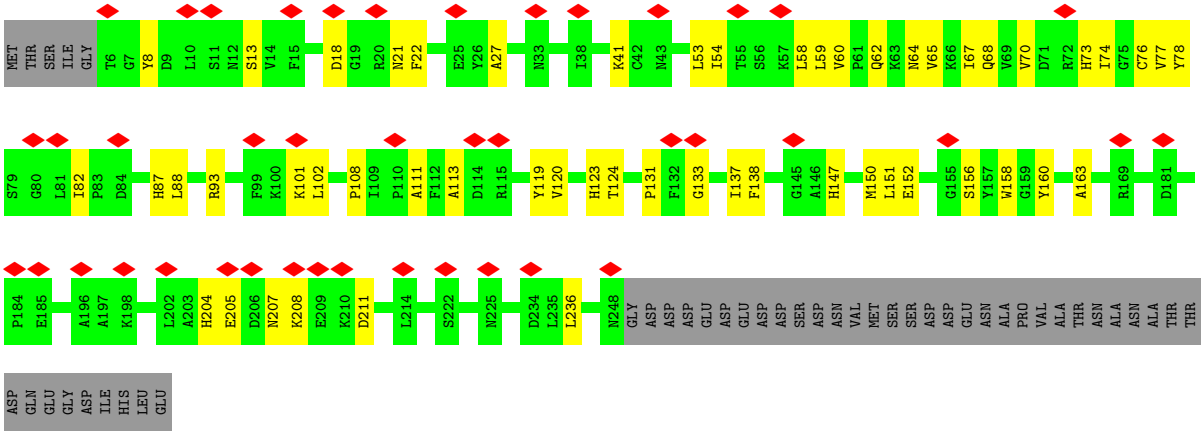
• Molecule 13: Proteasome subunit alpha type-6





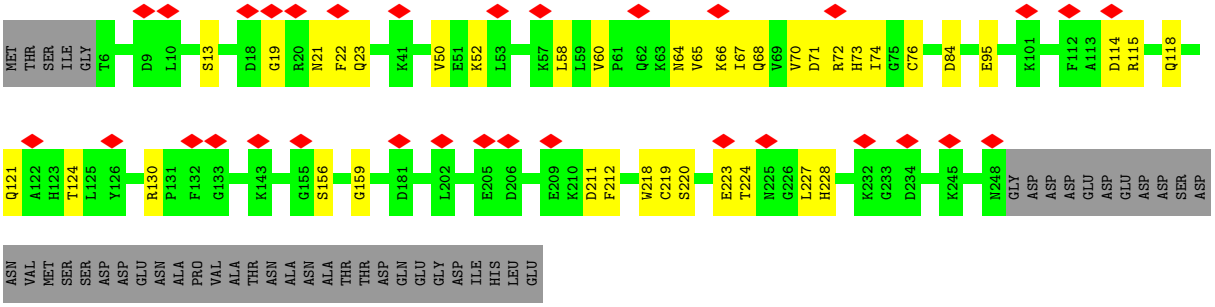


• Molecule 14: Probable proteasome subunit alpha type-7



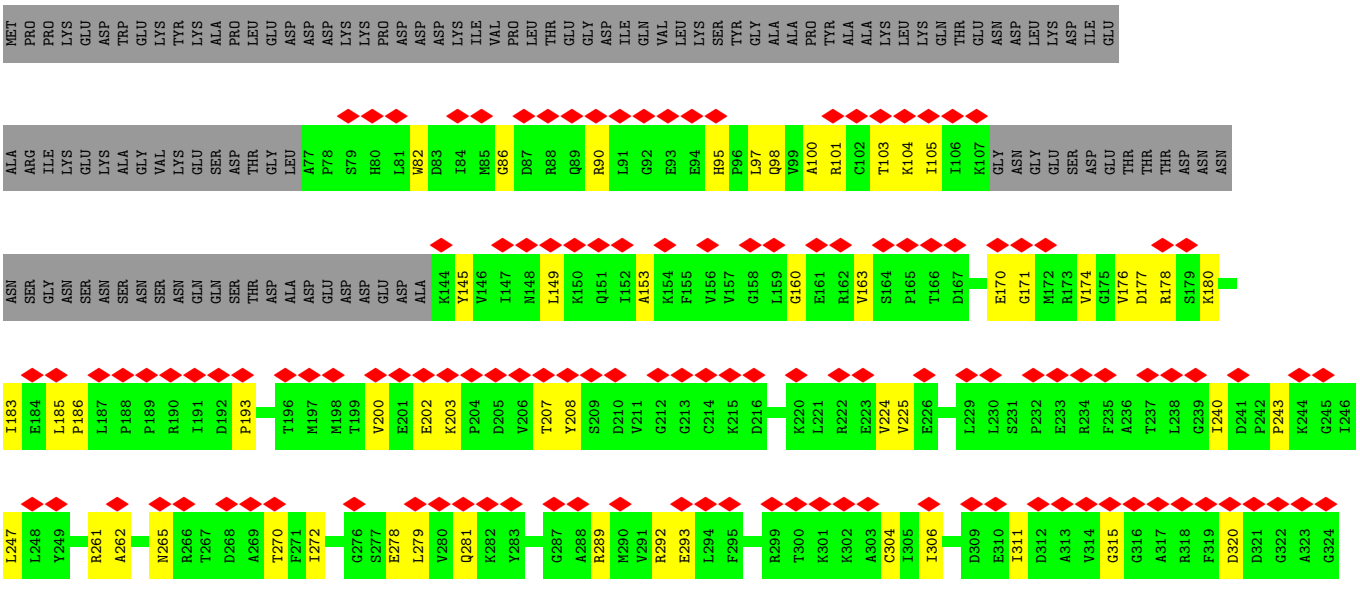
• Molecule 14: Probable proteasome subunit alpha type-7

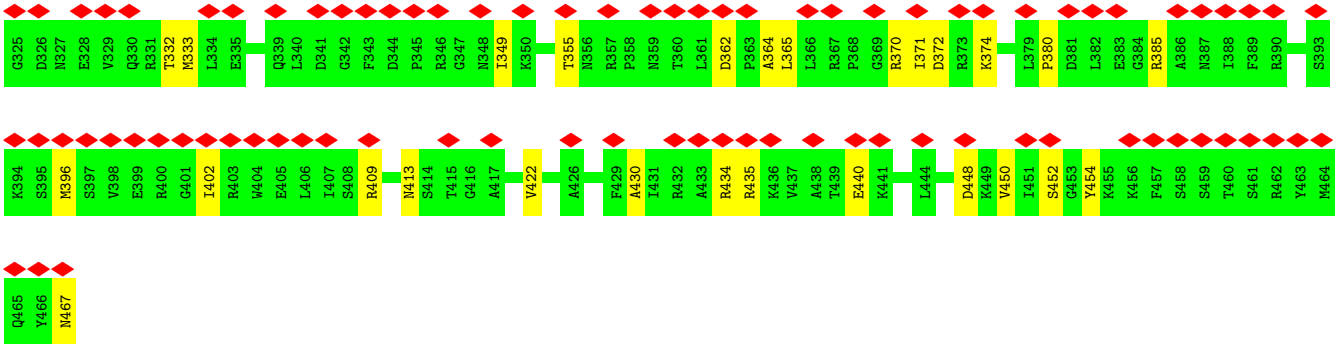
Chain k:



• Molecule 15: 26S proteasome regulatory subunit 7 homolog

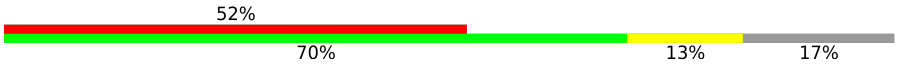
Chain H:

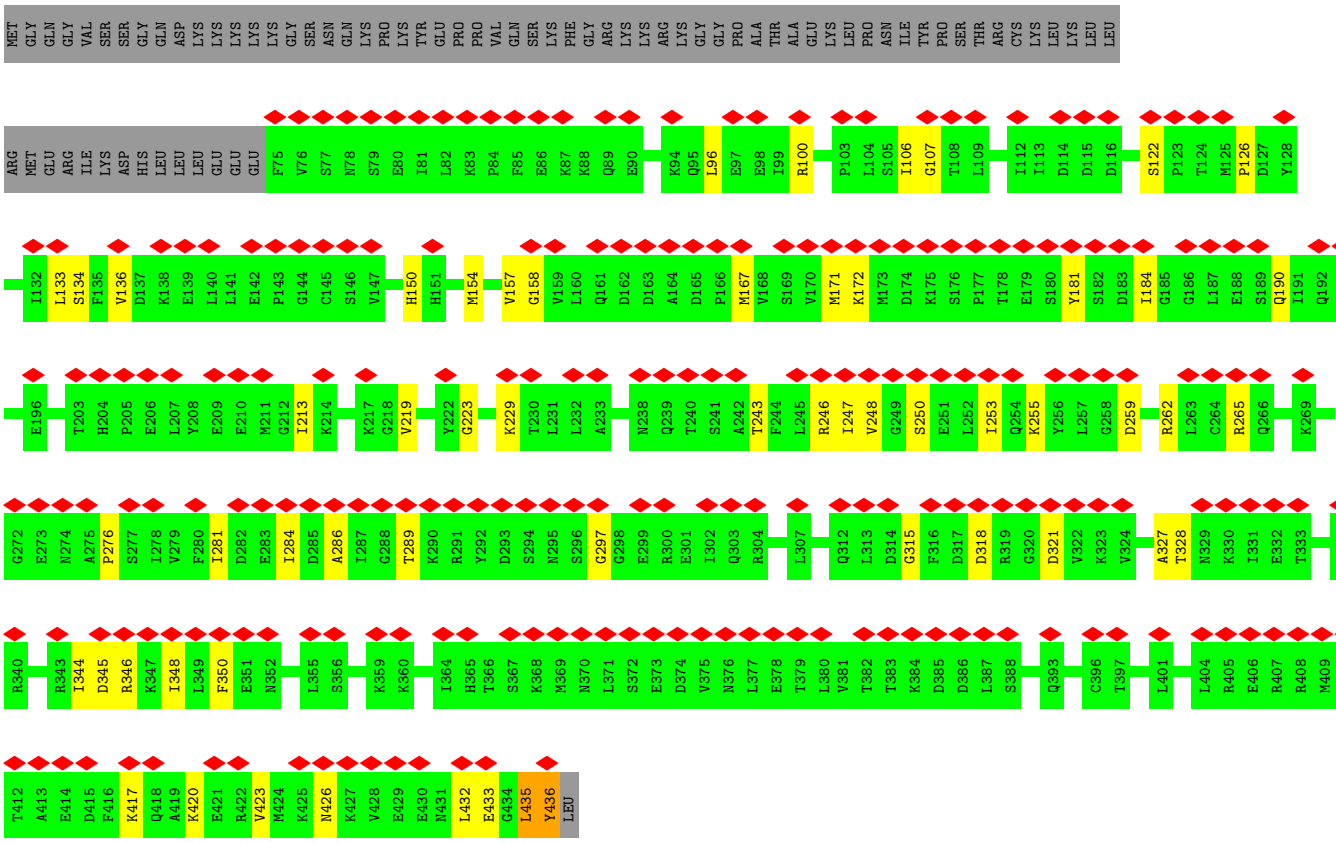




• Molecule 16: 26S proteasome regulatory subunit 4 homolog

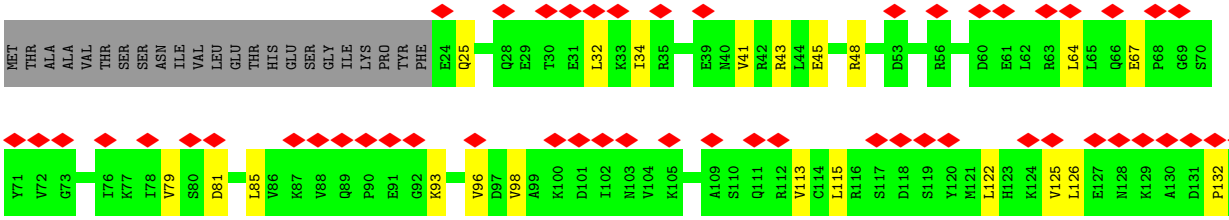
Chain I:

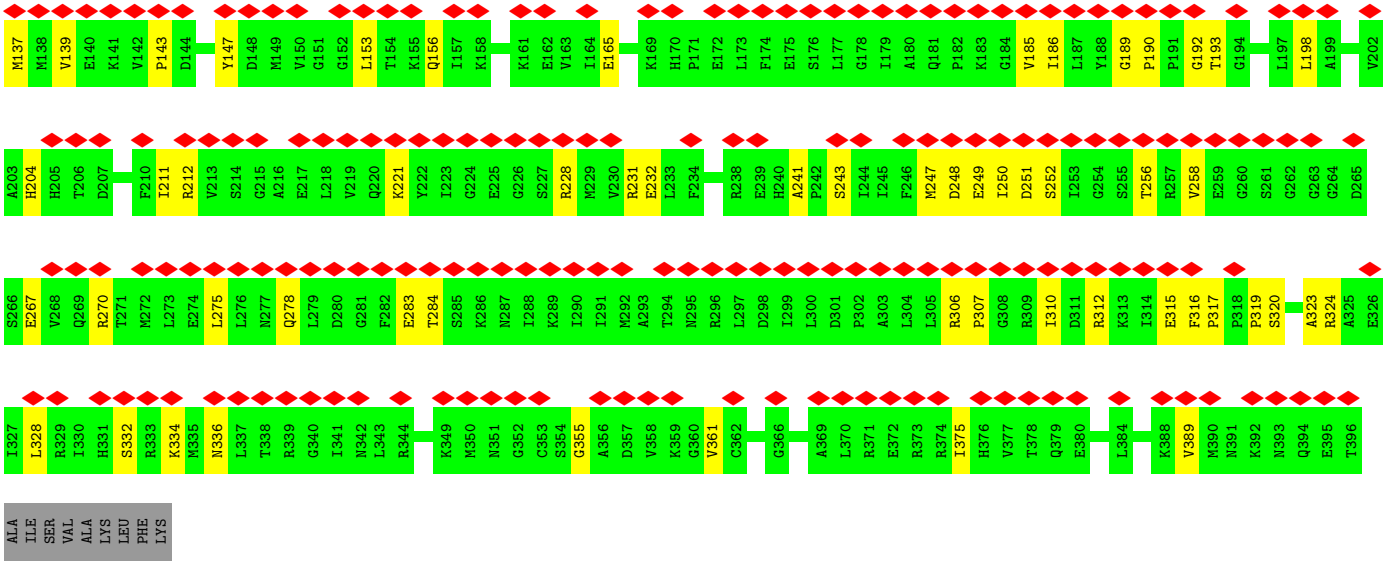




• Molecule 17: 26S proteasome regulatory subunit 8 homolog

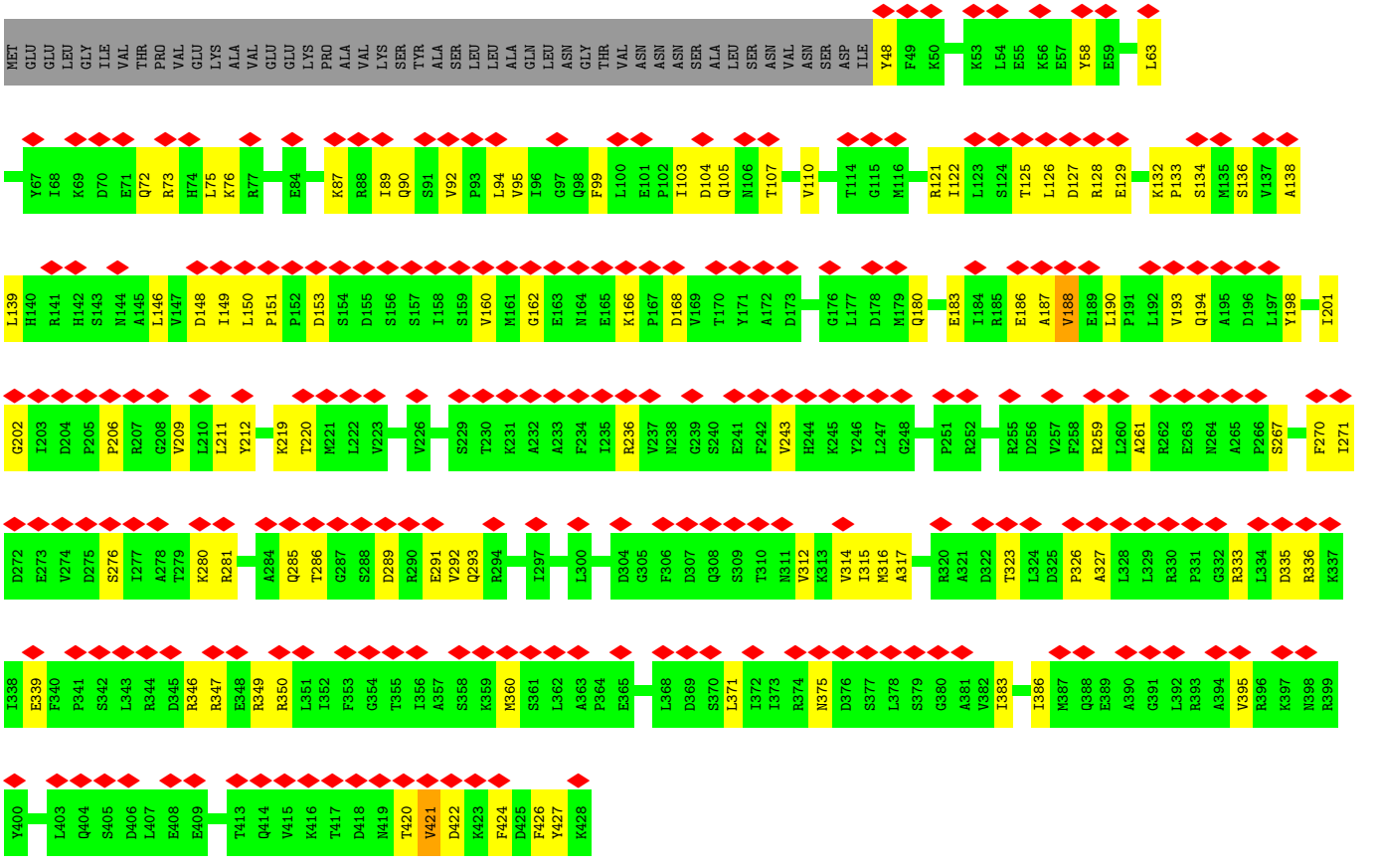
Chain J:





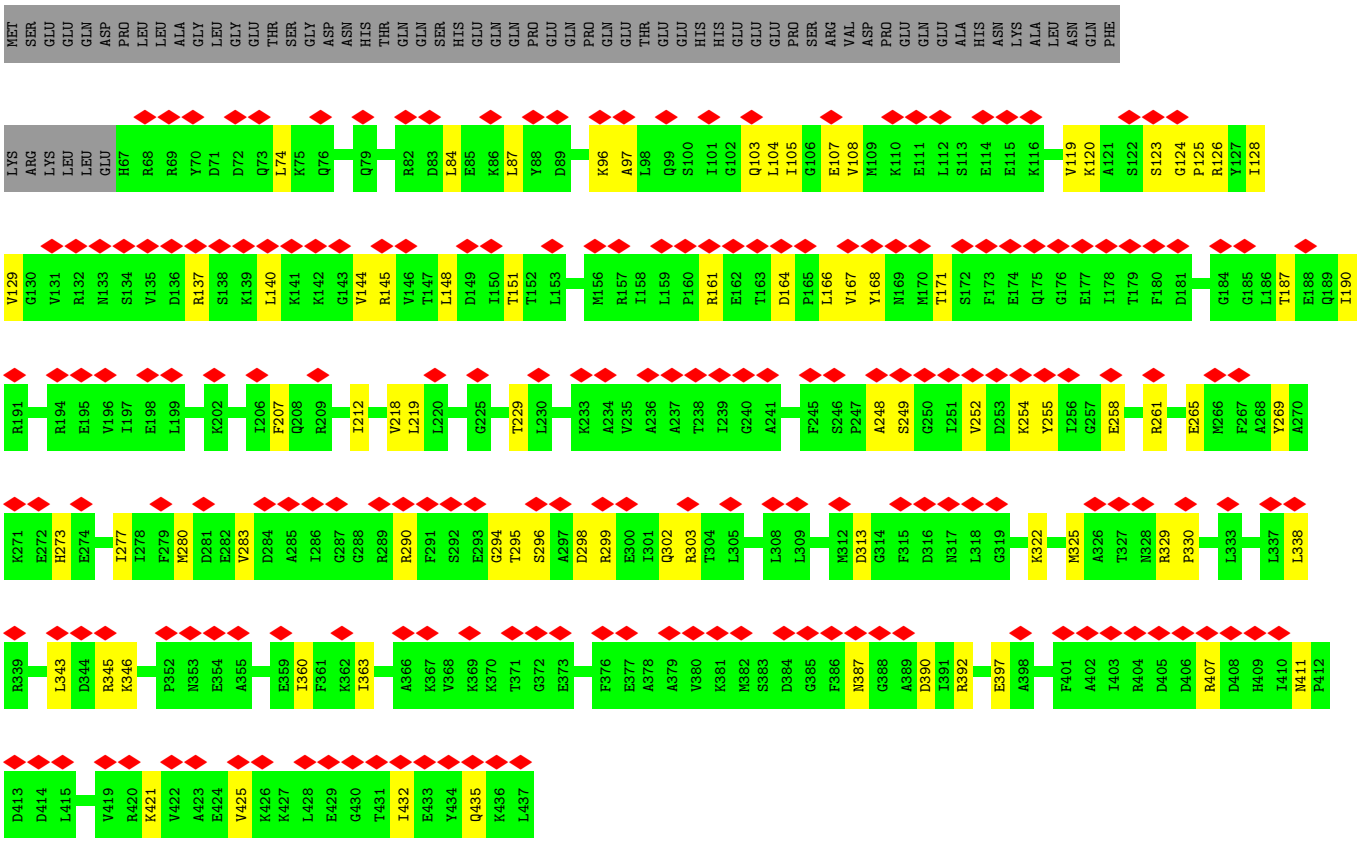
• Molecule 18: 26S proteasome regulatory subunit 6B homolog

Chain K:



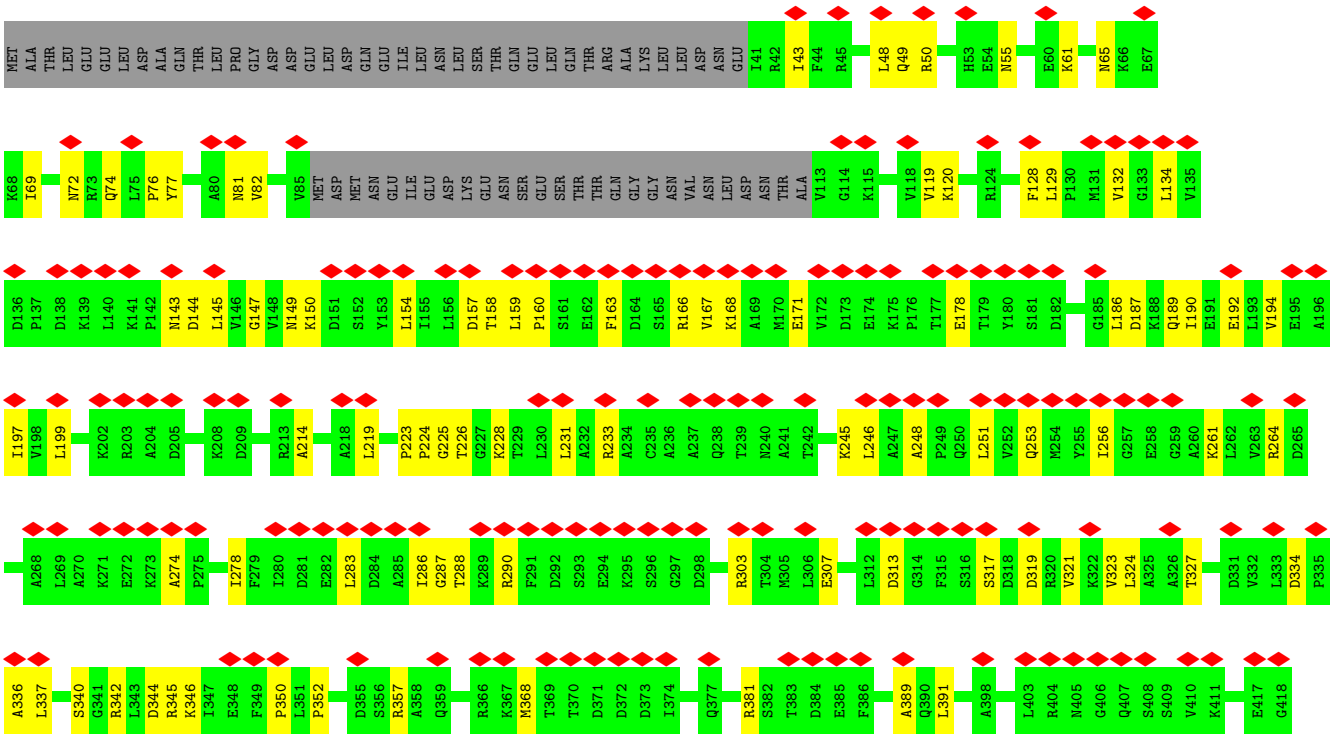
• Molecule 19: 26S proteasome subunit RPT4

Chain L:

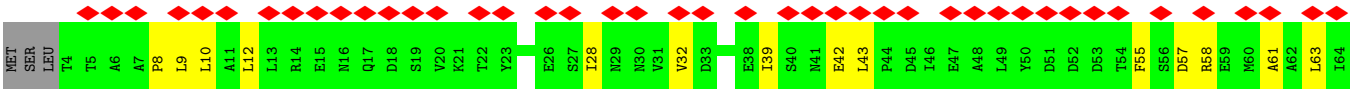


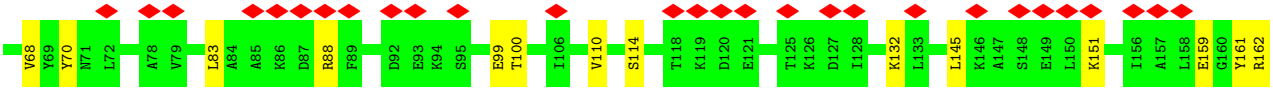
• Molecule 20: 26S proteasome regulatory subunit 6A

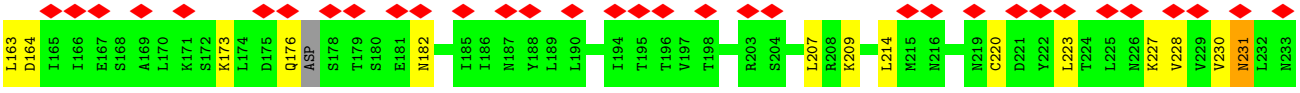
Chain M:

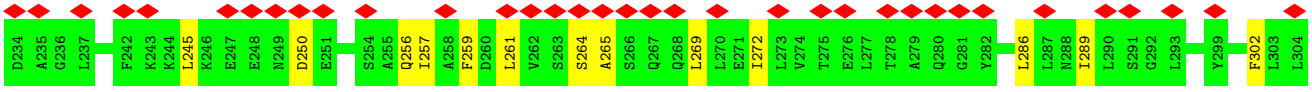


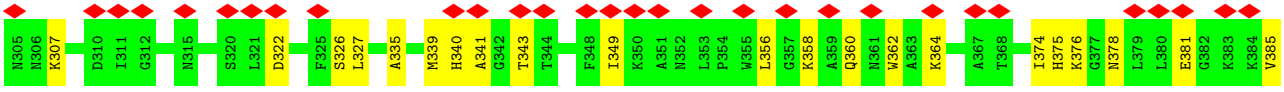
• Molecule 21: 26S proteasome regulatory subunit RPN2

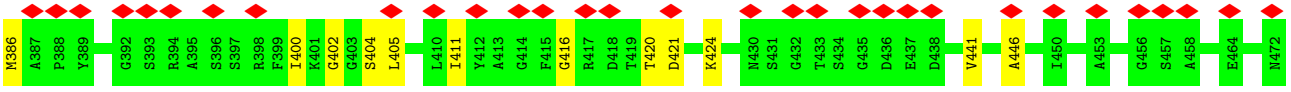


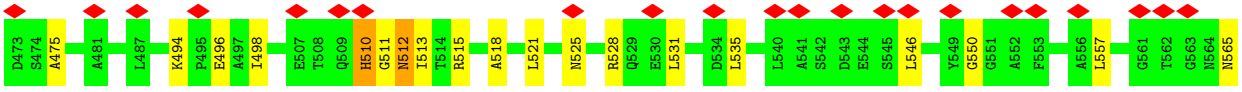


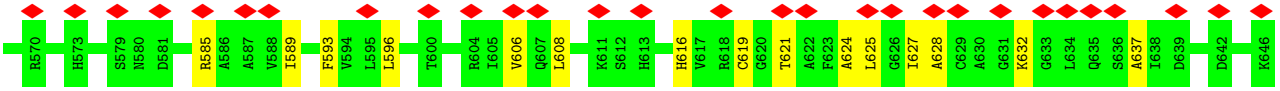


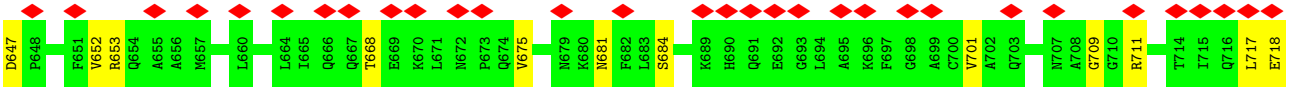


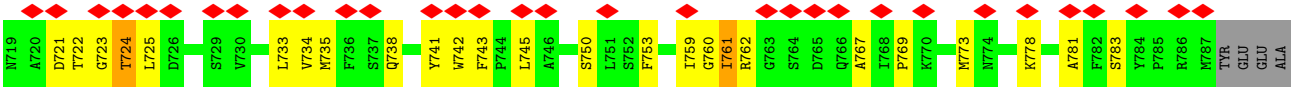


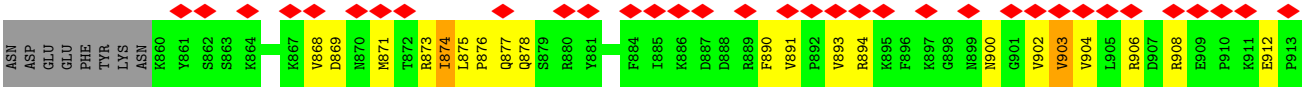


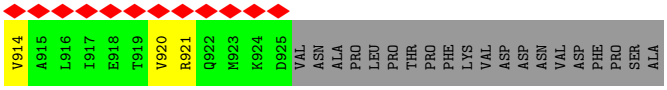






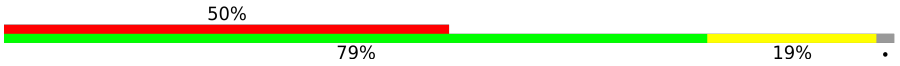


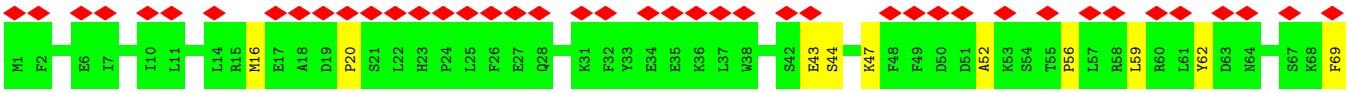


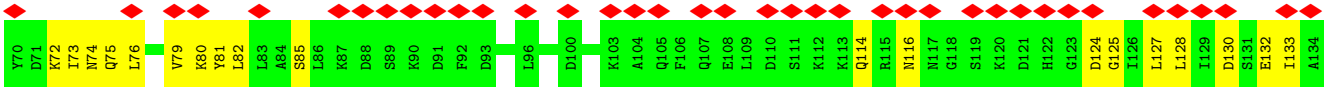


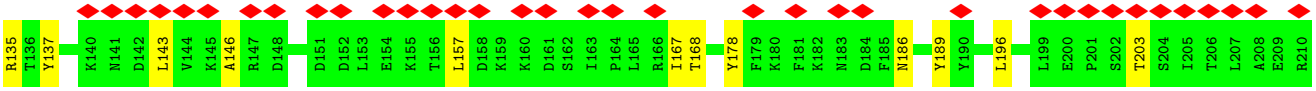
• Molecule 22: 26S proteasome regulatory subunit RPN9

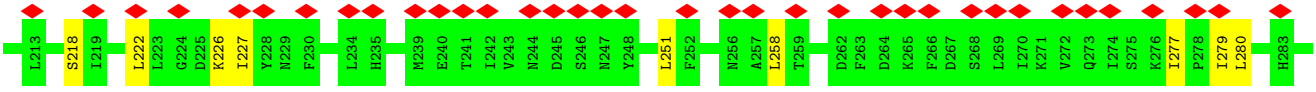
Chain O:

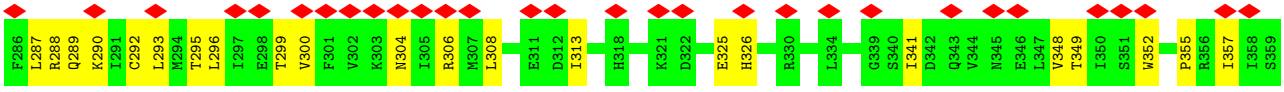


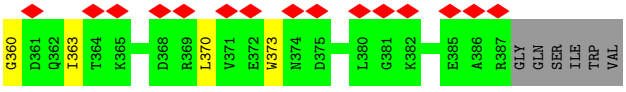






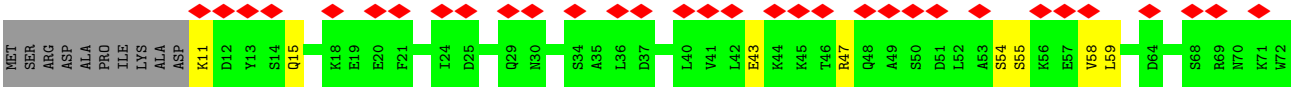


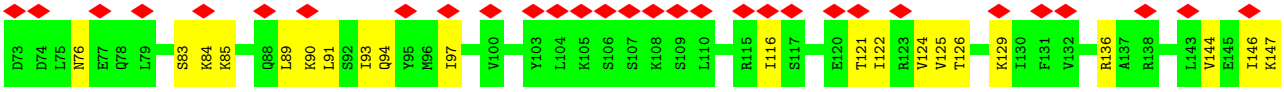


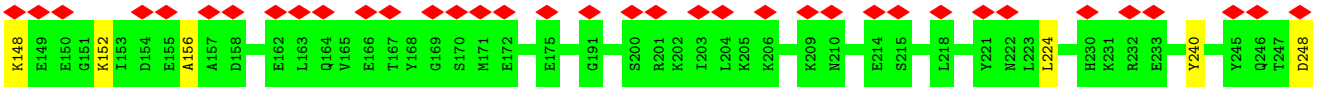


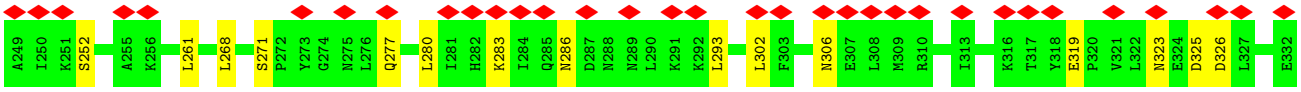
• Molecule 23: 26S proteasome regulatory subunit RPN5

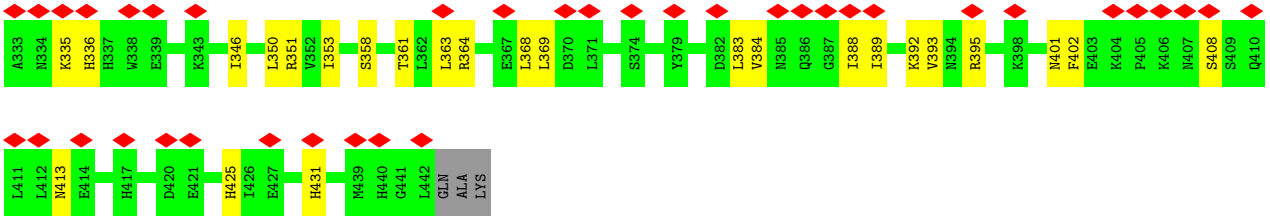
Chain P:



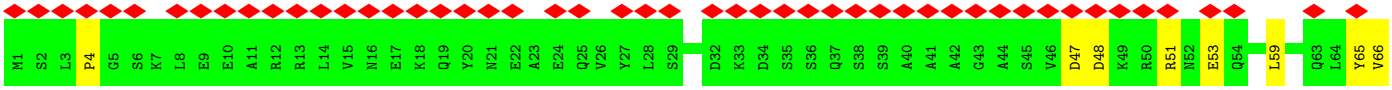


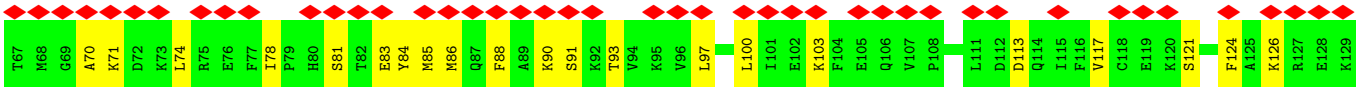


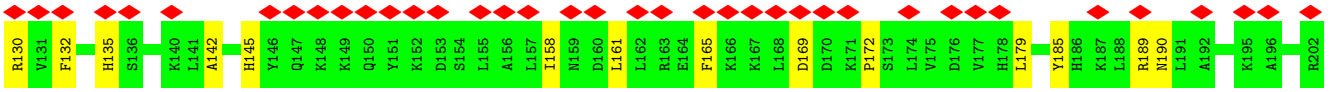


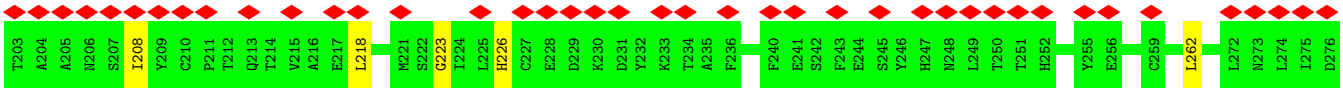


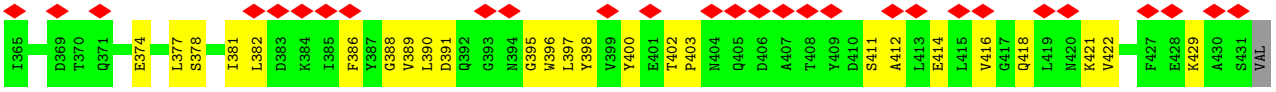
• Molecule 24: 26S proteasome regulatory subunit RPN6



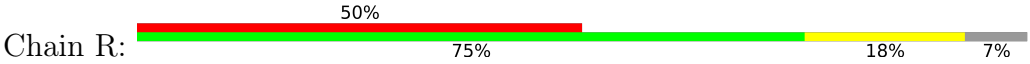


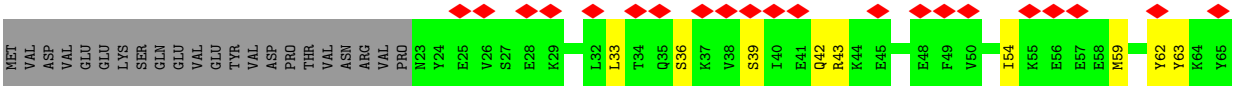


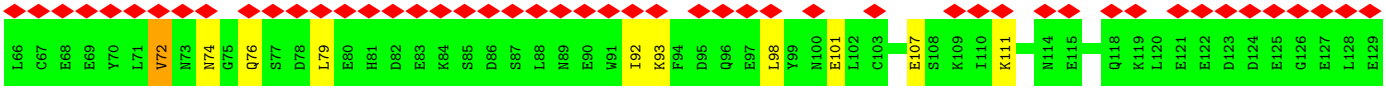


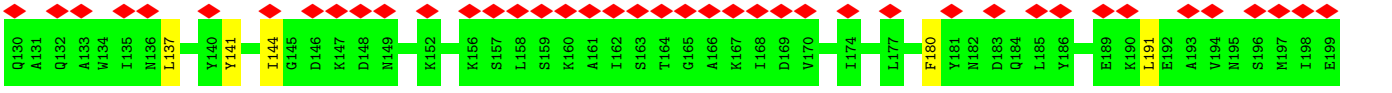


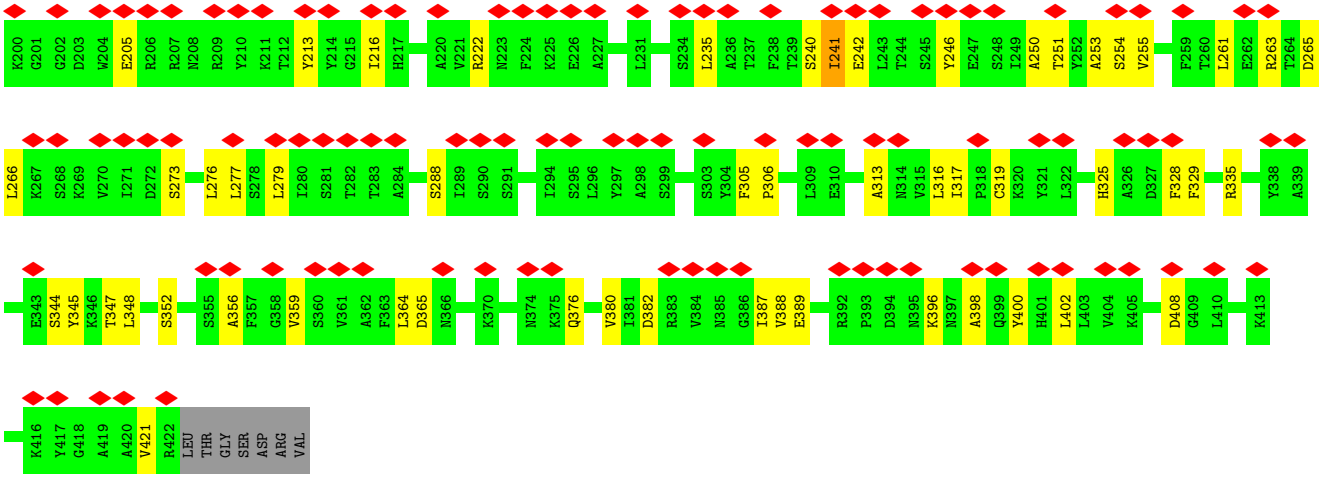
• Molecule 25: 26S proteasome regulatory subunit RPN7





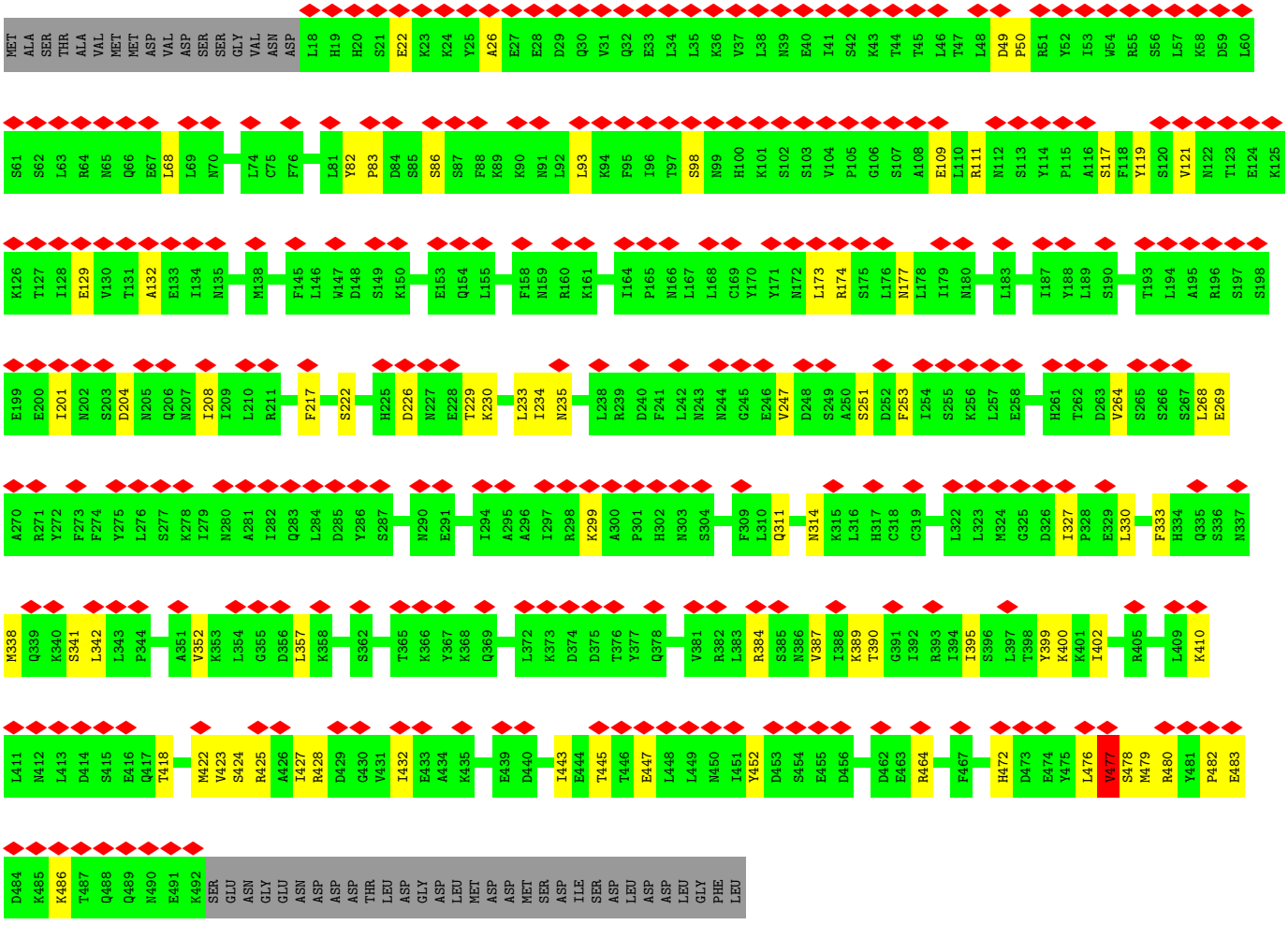






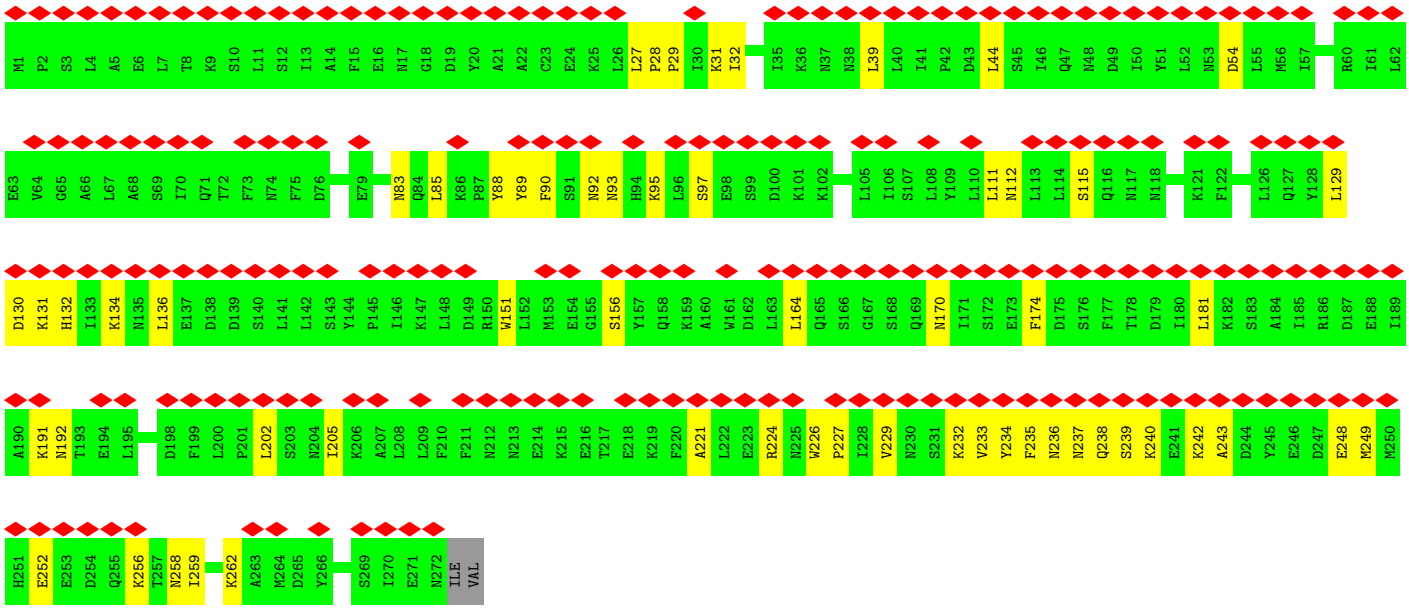
• Molecule 26: 26S proteasome regulatory subunit RPN3

Chain S:

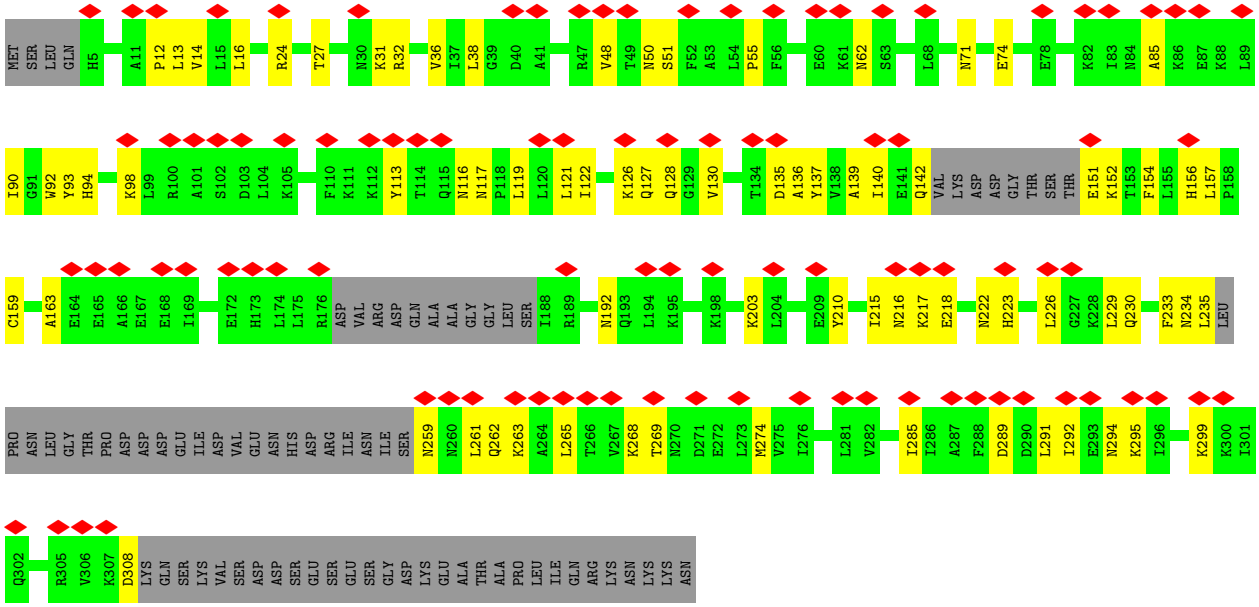


• Molecule 27: 26S proteasome regulatory subunit RPN12

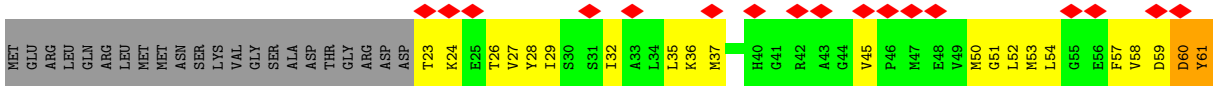
Chain T:

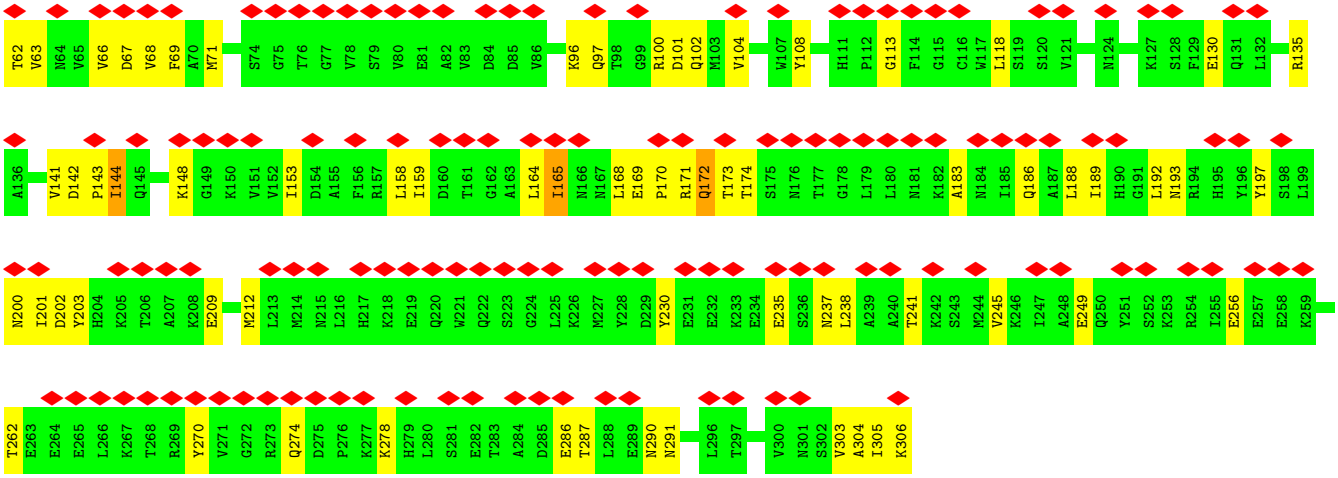


• Molecule 28: 26S proteasome regulatory subunit RPN8



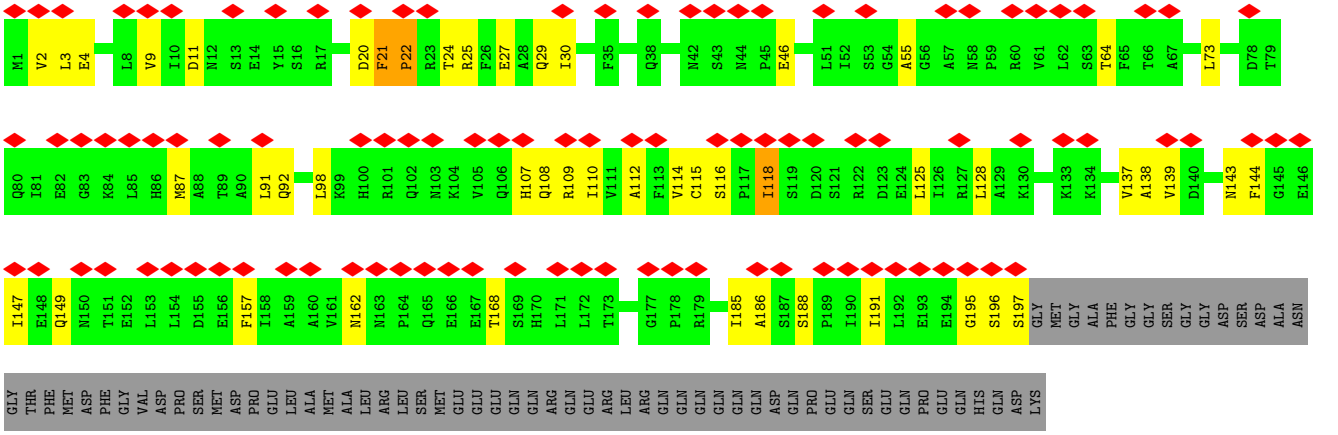
• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11





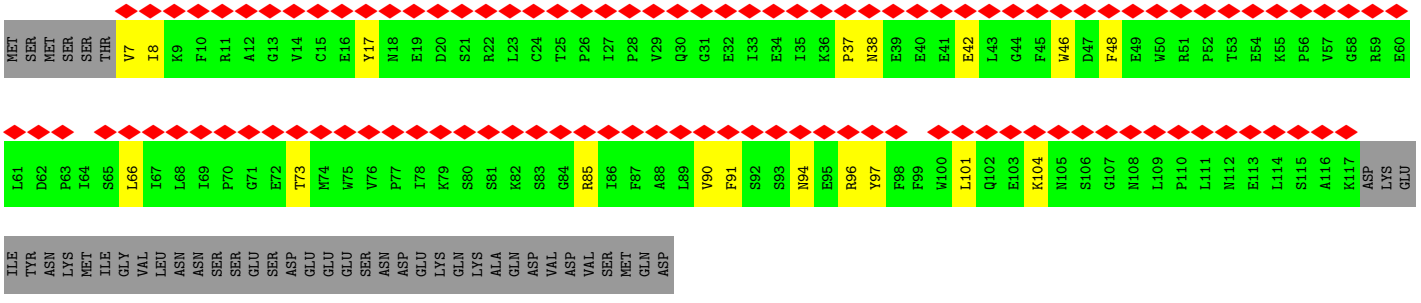
• Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W:



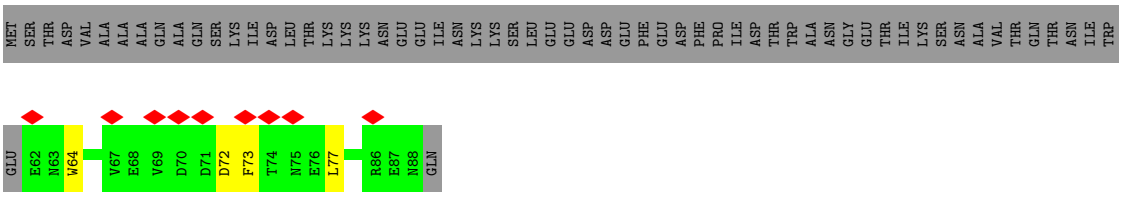
• Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X:



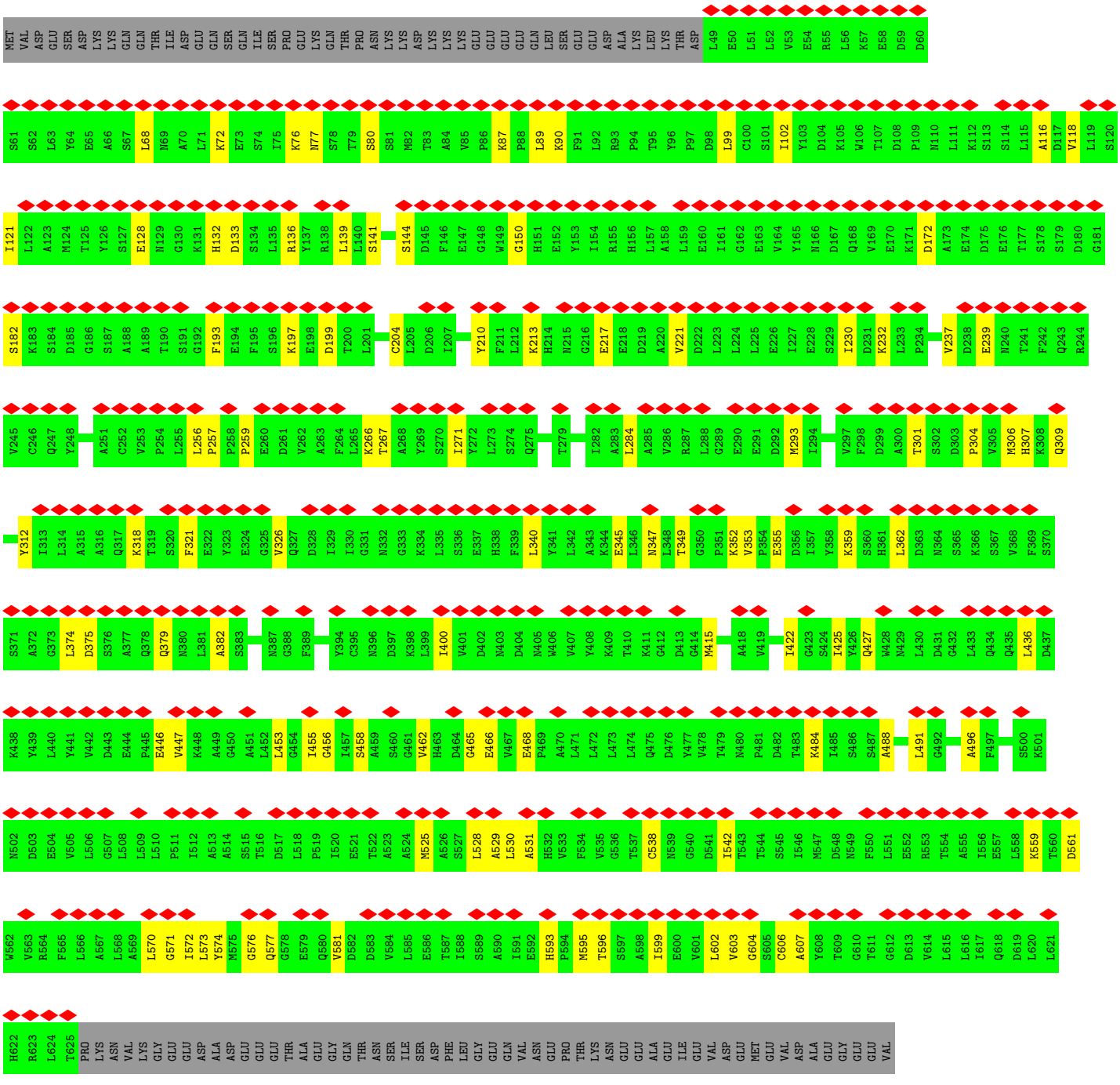
• Molecule 32: 26S proteasome complex subunit SEM1

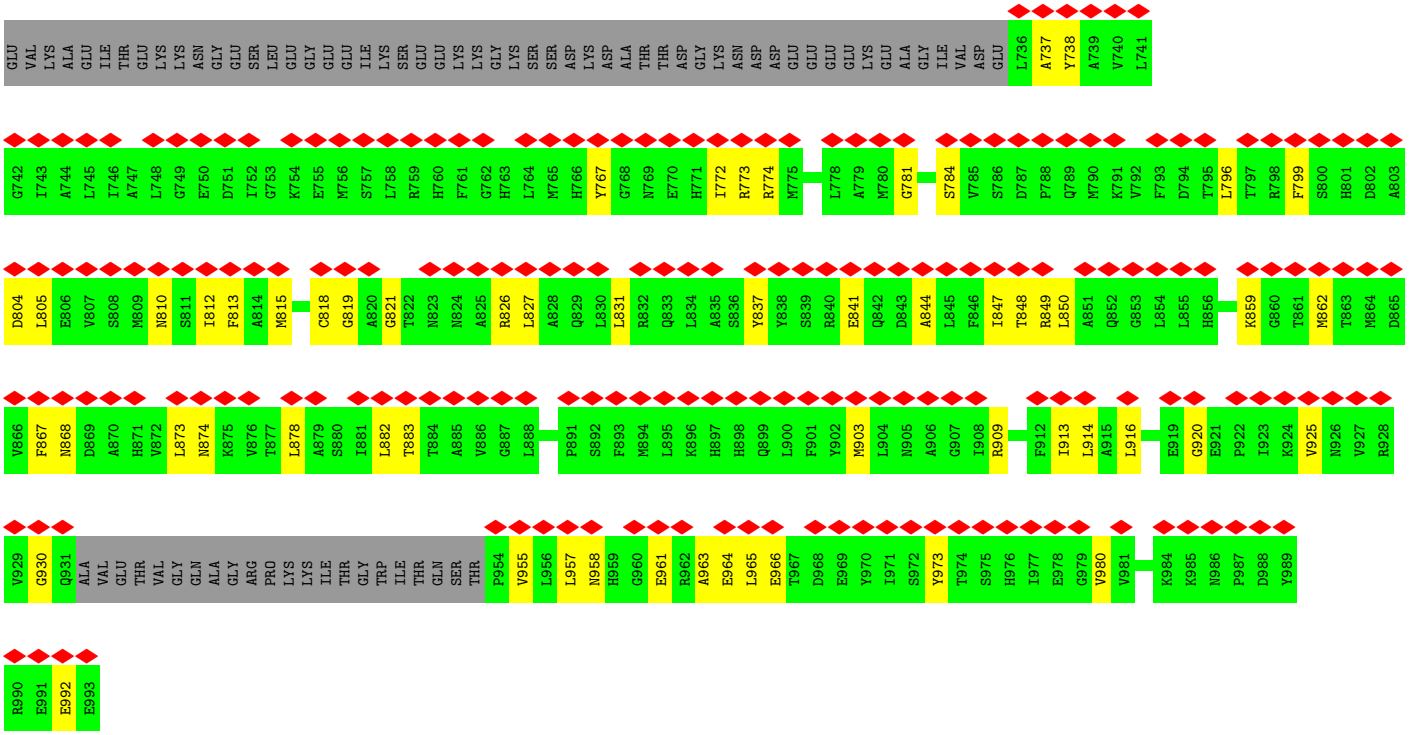
Chain Y:



• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z:




GLU VAL LYS ALA GLU ILE THR GLU LYS LYS ASN GLY GLU SER LEU GLU GLY GLU GLU ILE LYS SER GLU GLU LYS LYS GLY LYS SER SER ASP LYS ASP ALA THR THR ASP GLY LYS ASN ASP ASP GLU GLU GLU LYS GLU ALA GLY ILE VAL ASP GLU L736 A737 Y738 A739 V740 L741
G742 I743 A744 L745 I746 A747 L748 G749 E750 D751 I752 G753 K754 E755 M756 S757 L758 R759 H760 F761 G762 H763 L764 M765 H766 Y767 G768 N769 E770 H771 I772 R773 R774 M775 L778 A779 M780 G781 S784 V785 S786 D787 F788 Q789 M790 K791 V792 F793 D794 T795 L796 T797 R798 F799 S800 H801 D802 A803
D804 L805 E806 V807 S808 M809 N810 S811 I812 F813 A814 M815 C818 G819 A820 G821 T822 N823 N824 A825 R826 L827 A828 Q829 L830 L831 R832 Q833 L834 A835 S836 Y837 Y838 S839 R840 E841 Q842 D843 A844 L845 F846 I847 T848 R849 L850 A851 Q852 G853 L854 L855 H856 K859 G860 T861 M862 T863 M864 D865
V866 F867 N868 D869 A870 H871 V872 L873 N874 K875 V876 T877 L878 A879 S880 I881 L882 T883 T884 A885 V886 G887 L888 P891 S892 F893 M894 L895 K896 H897 H898 Q899 L900 F901 Y902 M903 L904 N905 A906 G907 I908 R909 F912 I913 L914 A915 L916 E919 G920 E921 P922 I923 K924 V925 N926 V927 R928
V929 G930 Q931 ALA VAL GLU THR VAL GLY GLN ALA GLY ARG PRO LYS LYS ILE THR GLY TRP ILE THR GLN SER THR P954 V955 L956 L957 N958 H959 G960 E961 R962 A963 E964 L965 E966 T967 D968 E969 Y970 I971 S972 Y973 T974 S975 H976 I977 E978 G979 V980 V981 K984 K985 N986 P987 D988 Y989
R990 E991 E992 E993

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.122	Depositor
Minimum map value	-1.006	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.686	Depositor
Map size (Å)	474.47998, 474.47998, 474.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.06	0/1541	0.21	0/2087
1	b	0.06	0/1541	0.21	0/2087
2	2	0.06	0/1750	0.21	0/2373
2	i	0.06	0/1750	0.20	0/2373
3	3	0.07	0/1611	0.24	0/2174
3	h	0.07	0/1611	0.24	0/2174
4	4	0.07	0/1589	0.24	0/2142
4	g	0.07	0/1589	0.23	0/2142
5	5	0.07	0/1681	0.22	0/2274
5	f	0.07	0/1681	0.21	0/2274
6	6	0.07	0/1795	0.23	0/2420
6	e	0.07	0/1795	0.23	0/2420
7	7	0.08	0/1821	0.24	0/2470
7	a	0.08	0/1846	0.25	0/2503
8	A	0.07	0/1945	0.22	0/2634
8	c	0.08	0/1945	0.23	0/2634
9	B	0.08	0/1952	0.28	0/2642
9	j	0.07	0/1952	0.23	0/2642
10	C	0.07	0/1934	0.24	0/2618
10	d	0.08	0/1934	0.27	0/2618
11	D	0.09	0/1910	0.28	0/2586
11	n	0.08	0/1910	0.24	0/2586
12	E	0.06	0/1886	0.21	0/2541
12	m	0.07	0/1886	0.23	0/2541
13	F	0.07	0/1823	0.24	0/2463
13	l	0.07	0/1800	0.22	0/2433
14	G	0.07	0/1932	0.22	0/2609
14	k	0.08	0/1932	0.22	0/2609
15	H	0.09	0/2834	0.28	0/3816
16	I	0.08	0/2860	0.27	0/3856
17	J	0.09	0/2964	0.28	0/3981
18	K	0.10	0/3062	0.34	0/4132
19	L	0.09	0/2981	0.29	0/4008
20	M	0.21	1/2903 (0.0%)	0.29	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
21	N	0.10	0/6670	0.29	0/9023
22	O	0.07	0/3243	0.25	0/4374
23	P	0.07	0/3599	0.23	0/4854
24	Q	0.08	0/3527	0.25	0/4748
25	R	0.08	0/3272	0.28	0/4412
26	S	0.09	0/3966	0.35	3/5355 (0.1%)
27	T	0.11	0/2279	0.36	0/3077
28	U	0.08	0/2146	0.28	0/2893
29	V	0.10	0/2271	0.33	0/3064
30	W	0.16	0/1557	0.32	0/2111
31	X	0.07	0/931	0.23	0/1262
32	Y	0.10	0/239	0.33	0/322
33	Z	0.11	1/6404 (0.0%)	0.26	0/8686
All	All	0.09	2/108050 (0.0%)	0.26	3/145952 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	274	ALA	C-N	10.45	1.58	1.33
33	Z	468	GLU	C-N	6.49	1.49	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	477	VAL	N-CA-C	12.68	123.19	111.91
26	S	477	VAL	CA-C-N	-7.12	113.00	123.11
26	S	477	VAL	C-N-CA	-7.12	113.00	123.11

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	1	1512	0	1478	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1512	0	1478	32	0
2	2	1719	0	1716	31	0
2	i	1719	0	1716	36	0
3	3	1581	0	1571	49	0
3	h	1581	0	1571	33	0
4	4	1561	0	1569	22	0
4	g	1561	0	1569	30	0
5	5	1644	0	1592	34	0
5	f	1644	0	1592	28	0
6	6	1757	0	1708	31	0
6	e	1757	0	1708	46	0
7	7	1790	0	1790	42	0
7	a	1815	0	1818	40	0
8	A	1907	0	1901	38	0
8	c	1907	0	1901	41	0
9	B	1915	0	1929	45	0
9	j	1915	0	1929	34	0
10	C	1904	0	1901	66	0
10	d	1904	0	1901	36	0
11	D	1881	0	1892	56	0
11	n	1881	0	1892	50	0
12	E	1861	0	1836	38	0
12	m	1861	0	1836	45	0
13	F	1795	0	1797	28	0
13	l	1773	0	1775	28	0
14	G	1892	0	1883	36	0
14	k	1892	0	1883	32	0
15	H	2787	0	2851	57	0
16	I	2822	0	2870	46	0
17	J	2928	0	3057	59	0
18	K	3019	0	3084	74	0
19	L	2937	0	3011	58	0
20	M	2866	0	2938	71	0
21	N	6562	0	6625	124	0
22	O	3182	0	3207	50	0
23	P	3545	0	3629	52	0
24	Q	3471	0	3495	57	0
25	R	3218	0	3216	50	0
26	S	3894	0	3938	58	0
27	T	2235	0	2207	56	0
28	U	2118	0	2177	66	0
29	V	2236	0	2242	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	W	1534	0	1542	30	0
31	X	906	0	888	14	0
32	Y	236	0	203	4	0
33	Z	6290	0	6236	102	0
All	All	106227	0	106548	1836	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 9.

All (1836) 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)
10:C:18:ARG:NE	10:C:23:GLU:HG2	1.67	1.09
29:V:59:ASP:O	29:V:60:ASP:HB2	1.56	1.05
10:C:18:ARG:CZ	10:C:23:GLU:HG2	1.91	0.98
28:U:152:LYS:HE3	28:U:154:PHE:CE1	1.99	0.96
10:C:18:ARG:NE	10:C:23:GLU:CG	2.31	0.93
3:3:107:PRO:HD2	3:3:124:PHE:HB2	1.53	0.91
28:U:152:LYS:HE3	28:U:154:PHE:HE1	1.38	0.89
21:N:475:ALA:HB1	29:V:61:TYR:CE2	2.09	0.87
21:N:230:VAL:HB	21:N:723:GLY:HA3	1.56	0.85
11:D:8:LEU:HD23	11:D:17:ILE:HG21	1.56	0.85
28:U:222:ASN:O	28:U:223:HIS:ND1	2.09	0.84
5:5:165:TYR:HB3	6:6:120:ARG:HH12	1.41	0.83
1:1:20:THR:N	1:1:188:SER:HG	1.78	0.81
29:V:61:TYR:HD1	29:V:62:THR:H	1.29	0.80
9:B:10:THR:O	9:B:12:PHE:CD2	2.36	0.79
12:E:120:ALA:HA	12:E:134:MET:HE1	1.65	0.78
10:C:18:ARG:HH11	10:C:18:ARG:HG3	1.49	0.78
29:V:118:LEU:HD22	29:V:193:ASN:HD21	1.49	0.78
10:C:53:THR:HA	10:C:210:ARG:HH12	1.49	0.77
29:V:23:THR:HG22	29:V:171:ARG:CZ	2.14	0.77
27:T:242:LYS:HG3	27:T:243:ALA:H	1.48	0.77
27:T:233:VAL:HG12	27:T:234:TYR:H	1.48	0.76
20:M:74:GLN:HG3	20:M:76:PRO:HD2	1.66	0.76
9:B:33:THR:HA	9:B:165:GLY:HA3	1.65	0.76
9:B:9:LEU:HD21	9:B:125:GLY:HA2	1.69	0.75
11:D:78:LEU:HD13	16:I:436:TYR:HE1	1.51	0.75
29:V:50:MET:HG3	29:V:71:MET:HB2	1.68	0.75
17:J:306:ARG:HD3	17:J:307:PRO:HD2	1.69	0.75
5:5:106:VAL:HA	6:6:151:GLU:HG2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:90:ARG:HB2	14:k:121:GLN:HE22	1.52	0.74
21:N:223:LEU:HD11	21:N:721:ASP:O	1.88	0.74
22:O:304:ASN:HD22	29:V:306:LYS:HE3	1.52	0.74
1:b:20:THR:N	1:b:148:SER:HG	1.84	0.73
11:n:6:ARG:HB3	11:n:125:GLY:HA3	1.70	0.73
10:d:52:VAL:HG23	10:d:59:GLN:HE21	1.54	0.73
10:C:18:ARG:NH1	16:I:432:LEU:HD23	2.04	0.72
30:W:25:ARG:NH2	30:W:115:CYS:SG	2.61	0.72
13:F:155:GLU:H	14:G:64:ASN:HD21	1.35	0.72
18:K:285:GLN:HG2	19:L:299:ARG:HH11	1.55	0.72
25:R:72:VAL:HA	25:R:76:GLN:HE22	1.54	0.72
21:N:475:ALA:CB	29:V:61:TYR:OH	2.37	0.72
25:R:33:LEU:O	25:R:74:ASN:ND2	2.23	0.72
27:T:224:ARG:HE	27:T:235:PHE:HD1	1.37	0.72
4:4:1:MET:HG2	4:4:2:ASP:H	1.54	0.72
2:i:79:ALA:HA	3:h:129:CYS:HB3	1.71	0.71
15:H:278:GLU:HB2	16:I:265:ARG:HH22	1.55	0.71
18:K:132:LYS:HD2	18:K:259:ARG:HH22	1.55	0.71
5:f:136:SER:HB3	12:m:97:VAL:HG13	1.73	0.71
26:S:428:ARG:HH12	27:T:191:LYS:HB2	1.54	0.71
10:C:18:ARG:HH12	16:I:432:LEU:HD23	1.55	0.71
21:N:307:LYS:HD3	21:N:343:THR:HG21	1.72	0.71
5:f:93:SER:HB2	5:f:249:SER:H	1.56	0.71
30:W:162:ASN:HA	30:W:168:THR:HG21	1.73	0.71
29:V:23:THR:OG1	29:V:172:GLN:HB2	1.90	0.70
18:K:160:VAL:HG12	18:K:162:GLY:H	1.56	0.70
24:Q:418:GLN:HE22	28:U:292:ILE:HD11	1.57	0.70
20:M:336:ALA:O	20:M:342:ARG:NH2	2.25	0.70
9:B:10:THR:HG23	10:C:21:GLN:HE21	1.57	0.69
11:D:37:LYS:HE2	11:D:160:SER:HA	1.73	0.69
21:N:735:MET:HB3	21:N:745:LEU:HB3	1.74	0.69
9:B:108:LYS:HE3	9:B:143:ASN:HD22	1.58	0.69
9:j:67:LEU:O	9:j:90:ARG:NH1	2.24	0.69
17:J:43:ARG:HE	26:S:480:ARG:HB3	1.56	0.69
18:K:280:LYS:HE3	18:K:281:ARG:HE	1.58	0.69
28:U:263:LYS:HG3	29:V:306:LYS:HD3	1.75	0.68
29:V:59:ASP:O	29:V:60:ASP:CB	2.38	0.68
26:S:235:ASN:HD22	26:S:268:LEU:HD22	1.58	0.68
8:c:17:ILE:HD13	9:j:9:LEU:HD21	1.75	0.68
10:d:49:GLU:O	10:d:65:LYS:NZ	2.26	0.68
12:E:123:PHE:CE1	12:E:134:MET:SD	2.87	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:63:CYS:HB2	1:b:117:ILE:HB	1.76	0.68
26:S:173:LEU:O	26:S:177:ASN:ND2	2.27	0.68
7:7:161:ARG:HD3	7:7:169:THR:HB	1.75	0.67
11:D:118:GLN:NE2	12:E:83:ALA:O	2.26	0.67
1:1:40:THR:HG22	1:1:45:ILE:HG12	1.77	0.67
15:H:185:LEU:HD12	15:H:186:PRO:HD2	1.76	0.67
33:Z:530:LEU:HB3	33:Z:542:ILE:HD11	1.76	0.67
3:h:124:PHE:HB3	3:h:128:GLY:HA2	1.75	0.67
18:K:286:THR:HB	19:L:294:GLY:HA2	1.75	0.67
21:N:475:ALA:HB1	29:V:61:TYR:HE2	1.54	0.67
11:D:32:CYS:HA	11:D:165:GLY:HA3	1.75	0.67
10:C:22:VAL:HG11	16:I:433:GLU:HG2	1.76	0.66
20:M:82:VAL:HG22	20:M:119:VAL:HG12	1.77	0.66
21:N:920:VAL:HG23	21:N:921:ARG:H	1.58	0.66
8:A:37:GLN:NE2	14:G:18:ASP:O	2.29	0.66
29:V:45:VAL:HG13	29:V:144:ILE:HG13	1.76	0.66
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.77	0.66
10:d:50:ARG:NH2	10:d:63:THR:OG1	2.28	0.66
33:Z:150:GLY:H	33:Z:210:TYR:HE1	1.42	0.66
10:C:18:ARG:CD	10:C:23:GLU:HG3	2.26	0.66
2:2:196:LEU:HB3	6:e:215:ILE:HB	1.78	0.66
10:d:50:ARG:NH1	10:d:59:GLN:O	2.29	0.66
12:E:120:ALA:HA	12:E:134:MET:CE	2.25	0.66
9:j:7:PHE:HB3	9:j:125:GLY:H	1.60	0.66
24:Q:93:THR:OG1	24:Q:130:ARG:NH2	2.29	0.65
10:C:78:ALA:HB3	10:C:134:SER:HB3	1.76	0.65
19:L:254:LYS:HB2	20:M:256:ILE:HB	1.77	0.65
11:n:66:LYS:HG2	11:n:72:VAL:HG12	1.79	0.65
17:J:32:LEU:HD21	26:S:174:ARG:HH12	1.60	0.65
21:N:762:ARG:HG3	21:N:767:ALA:HB2	1.78	0.65
30:W:143:ASN:ND2	30:W:149:GLN:O	2.30	0.65
31:X:38:ASN:HD22	31:X:42:GLU:H	1.42	0.65
5:5:146:LYS:NZ	12:E:65:GLU:OE1	2.28	0.65
21:N:223:LEU:CD1	21:N:721:ASP:O	2.45	0.65
29:V:23:THR:HG22	29:V:171:ARG:NE	2.11	0.65
3:3:8:ASN:ND2	3:3:30:GLY:O	2.25	0.65
8:A:126:GLN:NE2	9:B:81:ASP:OD1	2.30	0.65
22:O:143:LEU:HD13	22:O:178:TYR:HA	1.79	0.65
24:Q:51:ARG:HD2	24:Q:88:PHE:HA	1.76	0.65
11:D:78:LEU:HD22	16:I:436:TYR:OH	1.96	0.65
29:V:188:LEU:HB3	29:V:192:LEU:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:X:91:PHE:H	31:X:96:ARG:HD3	1.62	0.65
33:Z:925:VAL:HG13	33:Z:992:GLU:HB3	1.79	0.65
7:7:58:ASP:OD1	7:7:74:ARG:NH2	2.29	0.65
1:1:80:TYR:HB2	8:A:102:ALA:HB1	1.79	0.65
1:b:138:VAL:O	7:a:94:GLN:NE2	2.30	0.65
16:I:223:GLY:HA3	16:I:350:PHE:HB2	1.78	0.65
2:2:63:LEU:HD11	2:2:71:TRP:HB3	1.79	0.65
13:F:3:ARG:NH1	15:H:467:ASN:OD1	2.30	0.65
27:T:129:LEU:HD12	27:T:136:LEU:HD12	1.79	0.65
17:J:336:ASN:ND2	25:R:205:GLU:OE1	2.31	0.64
23:P:125:VAL:HA	23:P:136:ARG:HG2	1.78	0.64
10:C:60:ASP:HA	10:C:232:PRO:HG2	1.80	0.64
8:c:63:LEU:HD23	14:k:159:GLY:H	1.60	0.64
10:C:18:ARG:HG3	10:C:18:ARG:NH1	2.08	0.64
14:G:108:PRO:HG2	14:G:111:ALA:HB3	1.80	0.64
8:A:53:VAL:HG21	8:A:144:VAL:HG21	1.78	0.64
28:U:55:PRO:HB3	29:V:97:GLN:HB3	1.79	0.64
28:U:217:LYS:HG2	28:U:218:GLU:HG3	1.80	0.64
9:j:118:MET:HE1	9:j:130:PHE:HB2	1.80	0.64
10:C:119:LYS:HD3	10:C:153:PRO:HA	1.79	0.63
28:U:265:LEU:O	28:U:269:THR:N	2.31	0.63
7:a:137:ARG:HA	7:a:142:PRO:HG3	1.80	0.63
10:d:4:ARG:HG3	10:d:5:ARG:H	1.63	0.63
12:m:24:VAL:HG13	12:m:161:SER:HB2	1.79	0.63
18:K:271:ILE:HB	18:K:316:MET:HG2	1.81	0.63
11:D:66:LYS:HG2	11:D:72:VAL:HG12	1.79	0.63
24:Q:85:MET:HB3	24:Q:91:SER:HA	1.81	0.63
3:h:11:ILE:HD12	3:h:146:LEU:HD11	1.80	0.63
29:V:52:LEU:HD11	29:V:104:VAL:HG13	1.79	0.63
1:b:47:ASN:ND2	2:i:150:VAL:O	2.32	0.63
21:N:525:ASN:HD21	21:N:535:LEU:HD23	1.64	0.63
33:Z:819:GLY:HA3	33:Z:827:LEU:HD21	1.80	0.63
4:g:183:ILE:HB	4:g:190:ARG:HB2	1.79	0.62
7:a:161:ARG:HD3	7:a:169:THR:HB	1.79	0.62
9:B:16:GLY:HA2	10:C:24:TYR:HB3	1.80	0.62
28:U:152:LYS:CE	28:U:154:PHE:CE1	2.78	0.62
33:Z:72:LYS:NZ	33:Z:144:SER:O	2.31	0.62
1:1:47:ASN:ND2	2:2:150:VAL:O	2.32	0.62
3:3:28:ARG:HB2	3:3:183:TRP:HB2	1.81	0.62
4:g:17:SER:HB2	4:g:34:LYS:HB2	1.81	0.62
21:N:619:CYS:HB2	21:N:652:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:257:PRO:HB2	33:Z:259:PRO:HD2	1.80	0.62
4:4:29:LYS:HD2	5:5:199:GLY:HA2	1.80	0.62
5:f:170:LEU:HG	5:f:192:SER:HB2	1.80	0.62
1:b:198:THR:HG23	1:b:200:ALA:H	1.64	0.62
8:A:144:VAL:HG12	8:A:154:ILE:HG12	1.81	0.62
10:d:124:GLN:NE2	11:n:127:ARG:O	2.32	0.62
18:K:220:THR:HG21	19:L:313:ASP:HB3	1.80	0.62
25:R:359:VAL:HG21	25:R:364:LEU:HD13	1.81	0.62
28:U:259:ASN:HA	29:V:306:LYS:H	1.65	0.62
29:V:286:GLU:O	29:V:290:ASN:ND2	2.33	0.62
4:4:96:ARG:NH1	4:4:97:PRO:O	2.33	0.62
5:f:138:CYS:HB3	5:f:149:ILE:HG13	1.81	0.62
18:K:134:SER:OG	18:K:259:ARG:NH1	2.33	0.62
20:M:334:ASP:HB3	20:M:337:LEU:HG	1.81	0.62
33:Z:352:LYS:HE2	33:Z:462:VAL:HG23	1.82	0.62
11:D:78:LEU:HB2	16:I:436:TYR:CE1	2.35	0.62
22:O:306:ARG:HH12	22:O:349:THR:HB	1.64	0.62
33:Z:375:ASP:H	33:Z:379:GLN:HE21	1.45	0.62
16:I:426:ASN:HB2	17:J:306:ARG:HH12	1.65	0.62
2:2:81:THR:HG23	2:2:127:LEU:HD21	1.81	0.62
10:C:120:GLN:NE2	11:D:81:ASP:OD1	2.32	0.62
28:U:116:ASN:OD1	28:U:117:ASN:N	2.31	0.62
1:1:198:THR:HG23	1:1:200:ALA:H	1.65	0.61
5:f:106:VAL:HA	6:e:151:GLU:HG2	1.81	0.61
14:G:113:ALA:HB2	14:G:138:PHE:HZ	1.64	0.61
19:L:219:LEU:HB2	19:L:343:LEU:HD21	1.81	0.61
21:N:421:ASP:HA	21:N:424:LYS:HE2	1.81	0.61
21:N:515:ARG:HB2	21:N:546:LEU:HD22	1.82	0.61
33:Z:436:LEU:HD22	33:Z:455:ILE:HG13	1.81	0.61
5:5:283:ASN:ND2	4:g:148:TYR:O	2.33	0.61
20:M:422:VAL:HG13	20:M:426:LYS:HB2	1.80	0.61
22:O:44:SER:O	22:O:47:LYS:N	2.34	0.61
26:S:264:VAL:HB	26:S:268:LEU:HB2	1.81	0.61
26:S:389:LYS:HZ3	26:S:425:ARG:HG3	1.64	0.61
33:Z:570:LEU:HD23	33:Z:573:LEU:HD12	1.82	0.61
5:f:273:TRP:HA	5:f:276:LYS:HE2	1.83	0.61
14:G:27:ALA:HB1	14:G:133:GLY:HA2	1.81	0.61
2:i:66:ILE:HG23	2:i:89:GLY:HA2	1.82	0.61
6:e:49:ILE:HG22	6:e:54:ILE:HA	1.81	0.61
14:G:68:GLN:O	14:G:76:CYS:N	2.30	0.61
12:m:151:ASP:O	12:m:154:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:364:ALA:O	15:H:370:ARG:NH1	2.33	0.61
33:Z:347:ASN:HA	33:Z:352:LYS:HD2	1.82	0.61
9:B:184:GLU:OE1	24:Q:90:LYS:NZ	2.27	0.61
21:N:528:ARG:HB3	21:N:531:LEU:HB2	1.83	0.61
10:C:4:ARG:HG3	16:I:289:THR:HG21	1.82	0.61
12:E:85:ALA:HB2	12:E:140:VAL:HG21	1.83	0.61
4:g:66:LEU:HB2	11:n:94:GLN:HG3	1.83	0.61
21:N:227:LYS:HA	21:N:723:GLY:HA2	1.83	0.61
21:N:511:GLY:O	21:N:515:ARG:NH1	2.34	0.61
3:3:7:ILE:HG23	3:3:32:GLN:HG3	1.83	0.61
7:7:48:LYS:HG2	7:7:53:VAL:HG12	1.83	0.61
2:i:47:THR:HB	2:i:60:CYS:H	1.65	0.61
10:C:63:THR:HB	10:C:66:LEU:HB3	1.82	0.61
8:c:167:ALA:HB3	9:j:55:LEU:HD13	1.83	0.61
18:K:187:ALA:HB2	18:K:336:ARG:HE	1.66	0.61
9:j:3:ASP:HB3	11:n:4:TYR:HB2	1.83	0.61
12:m:130:GLU:HB2	12:m:132:ARG:HH12	1.66	0.61
20:M:278:ILE:HB	20:M:323:VAL:HG22	1.82	0.61
21:N:512:ASN:N	21:N:512:ASN:OD1	2.34	0.61
23:P:147:LYS:HB3	23:P:152:LYS:HB2	1.82	0.61
1:b:182:ILE:HG12	1:b:189:GLY:HA2	1.83	0.60
6:e:78:ALA:HB2	7:a:167:GLY:HA3	1.82	0.60
19:L:103:GLN:HB2	20:M:128:PHE:HB3	1.82	0.60
33:Z:774:ARG:HD3	33:Z:810:ASN:HD21	1.65	0.60
3:3:190:ILE:HA	3:3:195:VAL:HG22	1.83	0.60
33:Z:784:SER:O	33:Z:826:ARG:NH1	2.34	0.60
27:T:89:TYR:H	27:T:97:SER:HB3	1.66	0.60
3:3:27:LEU:HB3	3:3:39:LYS:HA	1.83	0.60
4:g:59:TYR:O	4:g:63:ASN:ND2	2.35	0.60
20:M:171:GLU:HG3	20:M:245:LYS:HE3	1.82	0.60
26:S:477:VAL:O	26:S:477:VAL:HG12	2.02	0.60
2:2:70:ILE:HG12	2:2:131:GLY:HA3	1.83	0.60
1:b:110:ASP:OD2	7:a:35:GLN:NE2	2.34	0.60
4:g:19:LYS:HB3	4:g:31:SER:HA	1.83	0.60
1:1:145:ILE:HD11	1:1:154:TYR:HD1	1.66	0.60
3:h:172:LEU:HD22	3:h:202:MET:HB3	1.84	0.60
15:H:243:PRO:HB3	15:H:372:ASP:HB2	1.81	0.60
21:N:230:VAL:CB	21:N:723:GLY:HA3	2.29	0.60
3:h:30:GLY:HA2	3:h:36:VAL:HG23	1.84	0.60
24:Q:185:TYR:HB3	24:Q:190:ASN:HB3	1.84	0.60
27:T:39:LEU:HD13	27:T:54:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:173:ASN:ND2	6:e:176:LYS:O	2.33	0.60
1:b:40:THR:HG22	1:b:45:ILE:HG12	1.83	0.60
11:n:163:THR:O	11:n:172:ARG:NH2	2.35	0.60
18:K:89:ILE:HG23	29:V:148:LYS:HB3	1.84	0.60
22:O:341:ILE:HG22	22:O:348:VAL:HG13	1.83	0.60
4:g:4:ILE:HG22	4:g:103:LEU:HD12	1.84	0.60
7:a:232:ILE:HB	7:a:240:THR:HB	1.84	0.60
11:n:118:GLN:HE22	12:m:86:ARG:HB3	1.66	0.60
15:H:247:LEU:HB3	15:H:374:LYS:HA	1.83	0.60
19:L:74:LEU:HD23	20:M:48:LEU:HB2	1.82	0.60
29:V:96:LYS:HA	29:V:101:ASP:HB2	1.83	0.60
33:Z:796:LEU:HD13	33:Z:815:MET:HG2	1.82	0.60
1:1:113:THR:HG23	1:1:134:LEU:HD13	1.84	0.60
3:3:103:TYR:OH	4:4:93:ARG:NH1	2.35	0.60
7:7:58:ASP:HA	7:7:228:PHE:HA	1.84	0.60
2:i:192:ILE:HG23	2:i:199:GLY:HA2	1.84	0.60
2:i:201:ASN:ND2	2:i:218:ASN:OD1	2.35	0.60
6:e:75:GLY:HA3	6:e:126:VAL:HA	1.82	0.60
9:j:92:VAL:HG21	9:j:117:ILE:HD11	1.84	0.60
11:n:162:GLN:OE1	11:n:172:ARG:NH2	2.33	0.60
2:i:104:ARG:NH2	8:c:148:GLU:OE2	2.35	0.59
9:B:217:GLU:HG2	9:B:231:LYS:HB3	1.84	0.59
14:G:70:VAL:N	14:G:74:ILE:O	2.35	0.59
21:N:261:LEU:HA	21:N:264:SER:HB2	1.84	0.59
25:R:382:ASP:HB3	25:R:387:ILE:H	1.67	0.59
6:6:29:GLY:O	6:6:216:GLN:NE2	2.35	0.59
2:i:93:GLU:O	9:j:90:ARG:NH2	2.30	0.59
10:C:155:GLY:O	11:D:83:ARG:NH1	2.34	0.59
28:U:48:VAL:HG22	28:U:90:ILE:HD11	1.84	0.59
33:Z:446:GLU:HG2	33:Z:484:LYS:HG3	1.84	0.59
5:5:244:ALA:HB1	3:h:179:ALA:HB1	1.83	0.59
6:6:43:ALA:HB1	6:6:221:LEU:HD11	1.84	0.59
6:6:57:ARG:NH1	7:7:193:ASP:O	2.34	0.59
10:C:18:ARG:HD3	10:C:23:GLU:HG3	1.85	0.59
10:C:201:THR:HG22	10:C:203:SER:H	1.67	0.59
8:c:41:SER:HA	8:c:54:SER:HA	1.84	0.59
10:d:54:SER:H	10:d:210:ARG:HH21	1.49	0.59
15:H:101:ARG:HE	15:H:171:GLY:HA2	1.67	0.59
21:N:494:LYS:HE2	21:N:496:GLU:HB3	1.84	0.59
29:V:53:MET:HA	29:V:68:VAL:HG12	1.83	0.59
33:Z:914:LEU:HB2	33:Z:980:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:76:ASP:OD2	2:i:113:LYS:NZ	2.35	0.59
7:a:129:LEU:HD13	7:a:147:ILE:HD13	1.83	0.59
10:d:70:ASN:OD1	10:d:71:ASP:N	2.34	0.59
33:Z:230:ILE:HB	33:Z:267:THR:HG21	1.82	0.59
8:c:129:GLN:HB3	9:j:127:VAL:HA	1.85	0.59
13:l:207:THR:OG1	13:l:210:ASN:ND2	2.35	0.59
15:H:98:GLN:N	15:H:176:VAL:O	2.32	0.59
8:c:87:PRO:O	14:k:121:GLN:NE2	2.35	0.59
26:S:400:LYS:HG3	26:S:445:THR:HB	1.84	0.59
20:M:192:GLU:OE1	20:M:345:ARG:NH1	2.32	0.59
27:T:248:GLU:HG3	27:T:249:MET:HG2	1.85	0.59
6:6:170:ASP:HB3	6:6:176:LYS:HD2	1.84	0.59
10:C:26:LEU:HD23	10:C:29:ILE:HD12	1.85	0.59
25:R:380:VAL:HB	25:R:389:GLU:HB3	1.85	0.59
12:m:48:LEU:HD21	12:m:77:ALA:HB2	1.83	0.59
15:H:380:PRO:O	15:H:385:ARG:NH1	2.36	0.59
28:U:71:ASN:ND2	30:W:64:THR:OG1	2.35	0.59
28:U:126:LYS:HB3	28:U:128:GLN:HE21	1.67	0.59
7:a:215:ARG:HG2	7:a:247:VAL:HG13	1.83	0.59
11:D:48:ARG:NH1	11:D:60:THR:O	2.35	0.59
8:c:15:ILE:HD12	8:c:17:ILE:HD12	1.84	0.59
12:m:18:GLU:OE1	12:m:20:ARG:NH2	2.36	0.59
15:H:103:THR:O	20:M:166:ARG:NH2	2.35	0.59
7:7:215:ARG:HG2	7:7:247:VAL:HG13	1.85	0.58
8:c:157:ASP:OD1	8:c:161:TYR:N	2.36	0.58
10:d:39:MET:HA	10:d:44:ILE:HG12	1.84	0.58
13:l:47:VAL:HG22	13:l:213:ILE:HG12	1.85	0.58
21:N:10:LEU:HB3	21:N:42:GLU:HG3	1.84	0.58
6:e:35:ALA:HB2	6:e:141:VAL:HG23	1.85	0.58
12:E:117:CYS:HA	12:E:120:ALA:HB3	1.85	0.58
8:c:63:LEU:HD12	8:c:68:VAL:HG13	1.84	0.58
18:K:276:SER:O	19:L:299:ARG:NH2	2.37	0.58
19:L:269:TYR:HB3	19:L:273:HIS:HD2	1.68	0.58
22:O:16:MET:HB3	22:O:20:PRO:HB3	1.84	0.58
33:Z:837:TYR:HB3	33:Z:848:THR:HG22	1.84	0.58
10:d:46:LEU:HB2	10:d:214:ALA:HB3	1.86	0.58
17:J:212:ARG:HB3	17:J:248:ASP:HB2	1.85	0.58
18:K:94:LEU:HB2	19:L:128:ILE:HD12	1.86	0.58
21:N:475:ALA:HB1	29:V:61:TYR:CZ	2.38	0.58
1:1:38:ARG:NH1	1:1:186:GLY:O	2.36	0.58
3:3:185:ALA:HB3	3:3:200:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:232:ILE:HB	7:7:240:THR:HB	1.84	0.58
13:F:119:ASN:ND2	13:F:126:ARG:O	2.36	0.58
10:d:216:ILE:HG12	10:d:227:GLN:HG2	1.86	0.58
3:3:11:ILE:HD12	3:3:146:LEU:HD11	1.84	0.58
17:J:189:GLY:HA3	17:J:316:PHE:HB3	1.85	0.58
20:M:283:LEU:HB3	20:M:327:THR:HB	1.85	0.58
21:N:873:ARG:HG3	21:N:874:ILE:H	1.69	0.58
22:O:74:ASN:OD1	22:O:75:GLN:N	2.36	0.58
28:U:140:ILE:HG12	28:U:142:GLN:H	1.69	0.58
28:U:152:LYS:CE	28:U:154:PHE:HE1	2.12	0.58
28:U:216:ASN:OD1	28:U:217:LYS:N	2.37	0.58
6:6:162:ALA:HB1	6:6:166:MET:HE2	1.85	0.58
7:a:152:VAL:HG22	7:a:158:GLN:HG3	1.86	0.58
10:C:77:VAL:HG21	10:C:88:ILE:HD11	1.85	0.58
26:S:418:THR:HG22	26:S:422:MET:HE2	1.86	0.58
7:7:137:ARG:HA	7:7:142:PRO:HG3	1.85	0.58
5:f:260:TRP:HZ3	5:f:262:TYR:HB2	1.69	0.58
20:M:261:LYS:HG2	20:M:264:ARG:HH21	1.68	0.58
33:Z:77:ASN:HB2	33:Z:80:SER:HB2	1.86	0.58
33:Z:813:PHE:HB2	33:Z:850:LEU:HD13	1.86	0.58
7:a:86:ILE:HG12	7:a:147:ILE:HG12	1.86	0.58
14:k:65:VAL:HG12	14:k:67:ILE:H	1.68	0.58
15:H:104:LYS:NZ	20:M:160:PRO:O	2.35	0.58
15:H:247:LEU:HB2	15:H:371:ILE:HG21	1.86	0.58
28:U:122:ILE:HD12	28:U:137:TYR:HE2	1.68	0.58
33:Z:87:LYS:HD3	33:Z:90:LYS:HG3	1.86	0.58
12:m:142:LEU:HB2	12:m:158:ALA:HB3	1.85	0.57
15:H:149:LEU:HD12	15:H:153:ALA:HB3	1.85	0.57
21:N:207:LEU:HB3	21:N:228:VAL:HG13	1.86	0.57
21:N:738:GLN:HB3	21:N:745:LEU:HD12	1.85	0.57
23:P:11:LYS:HG2	23:P:15:GLN:HG3	1.86	0.57
25:R:408:ASP:OD1	26:S:464:ARG:NH2	2.36	0.57
27:T:170:ASN:HA	27:T:174:PHE:HB2	1.86	0.57
33:Z:574:TYR:HB2	33:Z:581:VAL:HG12	1.86	0.57
33:Z:964:GLU:HG3	33:Z:965:LEU:HG	1.85	0.57
1:1:23:MET:HE2	1:1:174:ILE:HG12	1.86	0.57
2:i:63:LEU:HD23	2:i:73:ALA:HB2	1.86	0.57
3:h:155:GLU:HB3	3:h:158:LEU:HD21	1.86	0.57
8:A:126:GLN:O	8:A:129:THR:OG1	2.21	0.57
14:k:72:ARG:HH21	14:k:227:LEU:HD13	1.69	0.57
17:J:247:MET:HB2	17:J:250:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:147:GLY:HA3	20:M:157:ASP:HB3	1.86	0.57
20:M:228:LYS:NZ	20:M:327:THR:O	2.37	0.57
8:A:54:ILE:HG12	8:A:225:VAL:HG22	1.85	0.57
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.87	0.57
12:E:35:SER:HG	12:E:66:LYS:HZ3	1.51	0.57
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.85	0.57
24:Q:389:VAL:HG23	24:Q:398:TYR:HB2	1.87	0.57
10:C:162:ALA:HB3	11:D:54:LEU:HD23	1.85	0.57
18:K:73:ARG:HA	18:K:76:LYS:HE2	1.85	0.57
21:N:778:LYS:HG3	21:N:875:LEU:HB3	1.86	0.57
26:S:93:LEU:O	26:S:98:SER:OG	2.20	0.57
26:S:428:ARG:HH11	27:T:192:ASN:HB2	1.68	0.57
2:2:126:TYR:HB3	2:2:156:LEU:HD21	1.86	0.57
7:a:60:LEU:HD22	7:a:225:SER:HB3	1.85	0.57
7:a:215:ARG:NH2	7:a:249:ASN:O	2.37	0.57
7:7:121:GLU:OE2	13:F:139:LYS:NZ	2.36	0.57
2:i:39:ASN:HB3	2:i:208:GLU:HG3	1.86	0.57
11:D:166:ARG:NH2	11:D:202:VAL:O	2.37	0.57
14:k:68:GLN:O	14:k:76:CYS:N	2.36	0.57
20:M:43:ILE:HG21	30:W:27:GLU:HB3	1.87	0.57
26:S:311:GLN:NE2	26:S:341:SER:OG	2.38	0.57
31:X:48:PHE:HB2	31:X:66:LEU:HB3	1.87	0.57
6:6:128:THR:HB	6:6:144:PHE:HB2	1.84	0.57
6:e:49:ILE:HD11	6:e:216:GLN:HE21	1.69	0.57
6:e:57:ARG:NH1	7:a:193:ASP:O	2.37	0.57
10:d:60:ASP:HA	10:d:232:PRO:HG2	1.86	0.57
11:n:163:THR:HG21	11:n:171:VAL:HB	1.86	0.57
12:m:121:LEU:HB3	13:l:79:PRO:HB3	1.87	0.57
22:O:352:TRP:O	28:U:234:ASN:ND2	2.37	0.57
28:U:50:ASN:OD1	28:U:51:SER:N	2.37	0.57
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.69	0.57
9:B:222:LEU:HB2	9:B:233:PRO:HD3	1.85	0.57
11:n:17:ILE:HG12	11:n:19:GLN:H	1.70	0.57
21:N:378:ASN:HD21	21:N:381:GLU:HB2	1.68	0.57
21:N:893:VAL:HG22	21:N:908:ARG:HD2	1.87	0.57
25:R:396:LYS:HG3	25:R:400:TYR:HB2	1.87	0.57
12:E:18:GLU:OE1	12:E:20:ARG:NH2	2.36	0.57
12:m:13:SER:O	13:l:21:GLN:NE2	2.37	0.57
17:J:320:SER:H	17:J:323:ALA:HB3	1.70	0.57
18:K:104:ASP:HB3	18:K:107:THR:HB	1.86	0.57
24:Q:124:PHE:HB2	24:Q:130:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:531:ALA:HB1	33:Z:572:ILE:HB	1.87	0.57
5:5:76:THR:N	5:5:245:TYR:O	2.37	0.57
8:c:143:VAL:HG12	8:c:153:ILE:HG12	1.86	0.57
33:Z:491:LEU:HD13	33:Z:525:MET:HG3	1.87	0.57
11:n:47:GLU:O	11:n:63:LYS:NZ	2.36	0.56
21:N:742:TRP:HE3	21:N:743:PHE:HD1	1.51	0.56
24:Q:78:ILE:HG12	24:Q:100:LEU:HD13	1.87	0.56
5:f:82:ARG:NH1	5:f:185:PRO:O	2.36	0.56
6:e:174:ASN:HB3	6:e:176:LYS:HE2	1.88	0.56
15:H:160:GLY:H	15:H:163:VAL:HB	1.69	0.56
22:O:357:ILE:HG13	28:U:223:HIS:CD2	2.40	0.56
33:Z:306:MET:HG2	33:Z:973:TYR:HB3	1.86	0.56
33:Z:873:LEU:HD23	33:Z:878:LEU:HD21	1.86	0.56
3:3:152:SER:HG	6:e:209:SER:HG	1.50	0.56
10:C:18:ARG:HD2	10:C:18:ARG:C	2.30	0.56
10:C:70:ASN:OD1	10:C:73:ILE:N	2.37	0.56
9:j:20:GLN:HE21	9:j:129:PRO:HG3	1.70	0.56
12:m:163:THR:OG1	13:l:82:ARG:NH1	2.39	0.56
14:k:95:GLU:OE1	14:k:115:ARG:NH2	2.39	0.56
16:I:423:VAL:O	17:J:306:ARG:NH2	2.37	0.56
21:N:162:ARG:HE	21:N:164:ASP:HB3	1.70	0.56
29:V:23:THR:HG22	29:V:171:ARG:NH2	2.19	0.56
23:P:83:SER:HB2	23:P:90:LYS:HE3	1.87	0.56
3:h:7:ILE:HG23	3:h:32:GLN:HG3	1.88	0.56
8:A:135:ARG:NE	14:G:13:SER:O	2.38	0.56
12:E:41:ALA:HA	12:E:46:VAL:HG22	1.86	0.56
19:L:187:THR:HA	19:L:190:ILE:HB	1.87	0.56
12:E:78:MET:HA	12:E:142:LEU:HG	1.88	0.56
24:Q:142:ALA:HA	24:Q:145:HIS:HD2	1.69	0.56
3:3:51:LEU:HD11	3:3:107:PRO:HB3	1.87	0.56
7:7:144:TRP:HA	7:7:165:LEU:HD23	1.87	0.56
27:T:226:TRP:CH2	27:T:233:VAL:HA	2.41	0.56
25:R:398:ALA:HA	25:R:402:LEU:HB2	1.88	0.56
33:Z:867:PHE:O	33:Z:909:ARG:NH1	2.39	0.56
3:3:16:THR:HG22	3:3:21:VAL:HG12	1.88	0.56
29:V:235:GLU:HA	29:V:238:LEU:HG	1.88	0.56
4:4:41:HIS:HE2	4:4:74:GLU:HB3	1.71	0.56
7:a:144:TRP:HA	7:a:165:LEU:HD23	1.88	0.56
12:E:35:SER:O	12:E:79:SER:OG	2.21	0.56
15:H:224:VAL:HG23	15:H:225:VAL:HG23	1.88	0.56
17:J:85:LEU:HD11	17:J:93:LYS:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:632:LYS:NZ	21:N:717:LEU:O	2.40	0.56
24:Q:66:VAL:HA	24:Q:71:LYS:HB3	1.88	0.56
12:m:50:VAL:HG21	12:m:66:LYS:HB2	1.87	0.55
15:H:320:ASP:O	20:M:290:ARG:NH2	2.27	0.55
20:M:352:PRO:O	20:M:357:ARG:NH1	2.40	0.55
21:N:405:LEU:HD13	21:N:446:ALA:HB2	1.88	0.55
28:U:32:ARG:NH1	28:U:98:LYS:O	2.38	0.55
33:Z:604:GLY:HA2	33:Z:607:ALA:HB3	1.87	0.55
2:i:200:SER:HA	2:i:223:ASN:HD21	1.71	0.55
15:H:278:GLU:O	15:H:281:GLN:NE2	2.38	0.55
30:W:30:ILE:HG23	30:W:73:LEU:HD22	1.88	0.55
18:K:110:VAL:HG21	18:K:139:LEU:HD21	1.88	0.55
9:j:157:PHE:HB3	10:d:57:LEU:HD11	1.88	0.55
20:M:132:VAL:HG12	20:M:134:LEU:H	1.70	0.55
21:N:557:LEU:HD21	21:N:734:VAL:HG21	1.89	0.55
30:W:110:ILE:N	30:W:138:ALA:O	2.37	0.55
22:O:79:VAL:HB	22:O:127:LEU:HD23	1.88	0.55
30:W:92:GLN:HE21	30:W:128:LEU:HD21	1.70	0.55
3:h:189:ILE:HB	3:h:196:VAL:HB	1.88	0.55
17:J:221:LYS:NZ	18:K:289:ASP:O	2.36	0.55
25:R:54:ILE:HG13	25:R:59:MET:H	1.72	0.55
26:S:204:ASP:H	27:T:93:ASN:HD21	1.53	0.55
17:J:185:VAL:HG22	17:J:312:ARG:HB2	1.89	0.55
22:O:62:TYR:HB2	22:O:69:PHE:HZ	1.71	0.55
27:T:258:ASN:O	27:T:262:LYS:N	2.40	0.55
33:Z:957:LEU:HD12	33:Z:961:GLU:HB3	1.88	0.55
1:1:193:ARG:NH2	7:a:255:ALA:O	2.40	0.55
2:2:225:ARG:NH1	3:3:151:GLU:OE2	2.39	0.55
5:5:82:ARG:HH21	5:5:200:ASP:HA	1.70	0.55
25:R:107:GLU:HG2	25:R:111:LYS:HD2	1.89	0.55
3:3:27:LEU:HD13	3:3:39:LYS:HG3	1.87	0.55
12:E:88:MET:HE3	12:E:138:PHE:HD2	1.71	0.55
17:J:186:ILE:HG22	17:J:310:ILE:HG21	1.89	0.55
21:N:259:PHE:CG	21:N:904:VAL:HG11	2.42	0.55
27:T:236:ASN:OD1	27:T:237:ASN:N	2.40	0.55
11:D:6:ARG:O	12:E:135:SER:OG	2.24	0.55
10:d:197:LEU:O	10:d:201:THR:OG1	2.24	0.55
16:I:133:LEU:HD12	16:I:157:VAL:HA	1.89	0.55
28:U:127:GLN:HE22	29:V:212:MET:HA	1.72	0.55
1:b:23:MET:HE2	1:b:174:ILE:HG12	1.88	0.54
8:c:129:GLN:HG2	9:j:128:ARG:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:156:GLN:HE21	17:J:317:PRO:HD3	1.72	0.54
24:Q:172:PRO:HB3	24:Q:208:ILE:HG21	1.87	0.54
32:Y:73:PHE:HA	32:Y:77:LEU:HD13	1.89	0.54
2:i:93:GLU:OE1	9:j:98:LYS:NZ	2.35	0.54
10:C:18:ARG:CD	10:C:23:GLU:CG	2.85	0.54
11:D:71:VAL:HG22	11:D:137:GLY:HA3	1.88	0.54
11:D:78:LEU:HD13	16:I:436:TYR:CE1	2.38	0.54
12:E:80:GLY:HA3	12:E:140:VAL:HG23	1.89	0.54
12:m:179:ALA:HB2	12:m:207:VAL:HG11	1.89	0.54
13:l:84:LEU:HD22	13:l:112:LEU:HD22	1.88	0.54
18:K:212:TYR:HB2	18:K:339:GLU:HA	1.89	0.54
30:W:21:PHE:N	30:W:24:THR:O	2.36	0.54
14:G:124:THR:HG22	14:G:131:PRO:HB3	1.90	0.54
7:7:60:LEU:HD11	7:7:67:LEU:HD22	1.88	0.54
9:B:66:LEU:O	9:B:90:ARG:NH2	2.40	0.54
12:m:79:SER:HB3	12:m:141:ALA:HB3	1.90	0.54
27:T:252:GLU:HB2	27:T:256:LYS:HE3	1.89	0.54
33:Z:68:LEU:HD22	33:Z:118:VAL:HG21	1.89	0.54
2:i:114:GLN:HE22	8:c:106:LYS:HA	1.72	0.54
9:B:10:THR:O	9:B:11:THR:C	2.50	0.54
16:I:284:ILE:HB	16:I:328:THR:HB	1.89	0.54
19:L:145:ARG:H	19:L:161:ARG:HG2	1.72	0.54
26:S:314:ASN:HD22	26:S:338:MET:HE1	1.72	0.54
2:i:48:ARG:HE	2:i:199:GLY:HA3	1.73	0.54
9:B:43:VAL:HG11	9:B:137:ALA:HB1	1.90	0.54
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.89	0.54
15:H:207:THR:HA	15:H:265:ASN:HD22	1.71	0.54
21:N:340:HIS:HB2	21:N:374:ILE:HG12	1.89	0.54
33:Z:87:LYS:HE2	33:Z:89:LEU:HB2	1.88	0.54
2:2:129:VAL:HB	2:2:140:PHE:HB2	1.89	0.54
8:A:220:LYS:HD3	8:A:242:GLU:HB2	1.89	0.54
10:d:120:GLN:NE2	11:n:80:ALA:O	2.40	0.54
24:Q:421:LYS:NZ	29:V:256:GLU:O	2.40	0.54
26:S:423:VAL:HG11	26:S:443:ILE:HD13	1.89	0.54
5:f:168:ALA:HB3	6:e:120:ARG:HH22	1.72	0.54
9:B:32:VAL:O	9:B:76:SER:OG	2.21	0.54
11:D:6:ARG:O	11:D:7:ALA:HB2	2.06	0.54
11:D:6:ARG:HH21	13:F:125:GLY:H	1.56	0.54
14:k:70:VAL:N	14:k:74:ILE:O	2.41	0.54
22:O:43:GLU:HA	22:O:82:LEU:HD21	1.89	0.54
5:f:172:MET:HB3	5:f:192:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:9:LEU:HD12	10:C:128:LEU:HA	1.90	0.54
12:m:36:THR:HA	12:m:173:GLY:HA3	1.89	0.54
12:m:126:GLY:HA2	12:m:132:ARG:HG3	1.90	0.54
21:N:63:LEU:HD22	21:N:88:ARG:HB3	1.90	0.54
21:N:718:GLU:HA	21:N:725:LEU:HG	1.90	0.54
6:6:41:VAL:HG12	6:6:225:ILE:HA	1.89	0.54
2:i:172:LYS:HB3	2:i:175:LEU:HD21	1.90	0.54
7:a:122:PRO:HB2	7:a:159:PHE:HB3	1.90	0.54
8:A:249:ALA:HB1	23:P:85:LYS:HA	1.90	0.54
13:F:170:THR:HG21	20:M:381:ARG:HD3	1.90	0.54
7:a:181:ALA:O	7:a:185:ASN:ND2	2.40	0.53
9:B:95:THR:HA	9:B:99:ARG:HD2	1.90	0.53
8:c:125:GLN:O	8:c:128:THR:OG1	2.22	0.53
11:n:122:GLN:HE22	12:m:136:ARG:HG2	1.73	0.53
18:K:187:ALA:O	18:K:188:VAL:HG23	2.08	0.53
21:N:256:GLN:OE1	21:N:894:ARG:NH1	2.41	0.53
33:Z:737:ALA:HA	33:Z:772:ILE:HD13	1.88	0.53
20:M:149:ASN:OD1	20:M:150:LYS:N	2.42	0.53
28:U:93:TYR:HB3	28:U:121:LEU:HD12	1.90	0.53
28:U:121:LEU:HD23	28:U:136:ALA:HA	1.91	0.53
4:g:3:ILE:HG12	4:g:136:SER:HB2	1.89	0.53
6:e:32:LEU:HD11	6:e:169:LEU:HD11	1.89	0.53
13:l:119:ASN:ND2	13:l:126:ARG:O	2.41	0.53
26:S:445:THR:HG22	26:S:447:GLU:H	1.73	0.53
1:1:196:VAL:HB	1:1:203:GLU:HB3	1.91	0.53
8:A:40:ILE:HG23	8:A:56:GLN:HB2	1.89	0.53
10:C:39:MET:HE2	10:C:161:LYS:HA	1.90	0.53
15:H:82:TRP:CD1	16:I:134:SER:HG	2.25	0.53
16:I:255:LYS:HD3	16:I:297:GLY:HA2	1.90	0.53
19:L:338:LEU:O	19:L:346:LYS:NZ	2.35	0.53
9:B:35:LEU:HA	9:B:163:ALA:HA	1.90	0.53
13:F:114:ASP:OD1	14:G:87:HIS:ND1	2.42	0.53
20:M:317:SER:H	20:M:321:VAL:HG21	1.74	0.53
21:N:525:ASN:HA	21:N:528:ARG:HD3	1.89	0.53
22:O:168:THR:HG21	28:U:142:GLN:NE2	2.22	0.53
29:V:61:TYR:HD1	29:V:62:THR:N	2.02	0.53
13:l:176:LEU:HD22	14:k:58:LEU:HD23	1.91	0.53
15:H:193:PRO:HG3	15:H:293:GLU:HG2	1.90	0.53
15:H:261:ARG:NH2	16:I:315:GLY:O	2.42	0.53
21:N:759:ILE:HG23	21:N:761:ILE:HG12	1.91	0.53
25:R:335:ARG:HD2	25:R:376:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:362:LEU:O	33:Z:859:LYS:NZ	2.42	0.53
3:h:37:SER:HB2	4:g:128:LEU:HD21	1.89	0.53
5:f:96:THR:HA	5:f:102:ALA:H	1.73	0.53
11:D:155:ILE:HG22	12:E:82:THR:HB	1.91	0.53
14:k:220:SER:O	14:k:224:THR:OG1	2.26	0.53
15:H:448:ASP:HA	15:H:452:SER:HB2	1.91	0.53
18:K:90:GLN:HB3	18:K:94:LEU:HD21	1.91	0.53
21:N:475:ALA:HB2	29:V:61:TYR:OH	2.08	0.53
29:V:61:TYR:CD1	29:V:62:THR:N	2.69	0.53
30:W:2:VAL:HG22	30:W:196:SER:HB2	1.90	0.53
33:Z:301:THR:O	33:Z:307:HIS:NE2	2.37	0.53
33:Z:304:PRO:HB3	33:Z:340:LEU:HD13	1.91	0.53
8:c:46:GLY:HA2	8:c:193:ILE:HB	1.91	0.53
9:j:139:HIS:O	9:j:234:ARG:NH2	2.42	0.53
18:K:243:VAL:HG11	19:L:303:ARG:HH22	1.73	0.53
18:K:280:LYS:HB3	18:K:323:THR:HB	1.91	0.53
33:Z:868:ASN:HA	33:Z:909:ARG:HH12	1.74	0.53
5:5:196:ARG:NH2	11:D:101:GLU:OE1	2.42	0.53
2:i:104:ARG:HB2	8:c:109:TYR:HE2	1.74	0.53
13:l:67:ASP:HB3	13:l:70:MET:HB3	1.91	0.53
21:N:518:ALA:HB1	21:N:550:GLY:HA3	1.91	0.53
29:V:36:LYS:NZ	29:V:67:ASP:OD1	2.42	0.53
3:3:203:ARG:HH22	6:e:176:LYS:HB3	1.73	0.53
9:B:5:TYR:O	9:B:8:SER:N	2.40	0.53
25:R:255:VAL:HG11	25:R:316:LEU:HD21	1.91	0.53
30:W:114:VAL:HG11	30:W:118:ILE:HD11	1.91	0.53
33:Z:914:LEU:H	33:Z:980:VAL:HG22	1.74	0.53
8:c:161:TYR:HB2	9:j:80:PRO:HD3	1.91	0.52
21:N:647:ASP:O	21:N:653:ARG:NE	2.41	0.52
23:P:431:HIS:CG	28:U:156:HIS:HB3	2.45	0.52
25:R:39:SER:HB3	25:R:42:GLN:HG3	1.90	0.52
26:S:480:ARG:HD2	26:S:483:GLU:HB2	1.90	0.52
27:T:256:LYS:HZ3	27:T:259:ILE:HD12	1.75	0.52
2:2:192:ILE:HG12	2:2:199:GLY:HA2	1.91	0.52
4:g:53:THR:HG22	4:g:100:VAL:HG22	1.91	0.52
11:n:46:CYS:HB2	11:n:211:GLU:HB3	1.91	0.52
15:H:105:ILE:HG23	15:H:145:TYR:HE1	1.74	0.52
17:J:67:GLU:HG3	29:V:186:GLN:HE22	1.74	0.52
20:M:219:LEU:HD23	20:M:346:LYS:HG3	1.90	0.52
21:N:761:ILE:HG21	21:N:904:VAL:HG13	1.90	0.52
26:S:201:ILE:O	27:T:92:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:57:PHE:O	29:V:135:ARG:NH1	2.43	0.52
2:i:126:TYR:HB3	2:i:156:LEU:HD21	1.91	0.52
11:n:237:GLU:HA	11:n:240:LYS:HD3	1.90	0.52
13:l:143:HIS:ND1	13:l:155:GLU:OE2	2.42	0.52
22:O:341:ILE:O	23:P:358:SER:OG	2.25	0.52
26:S:234:ILE:HG23	26:S:253:PHE:HE2	1.74	0.52
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.90	0.52
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.90	0.52
15:H:315:GLY:HA2	15:H:333:MET:HG3	1.92	0.52
28:U:117:ASN:ND2	28:U:139:ALA:O	2.40	0.52
33:Z:913:ILE:HD12	33:Z:963:ALA:HB3	1.90	0.52
1:1:103:GLU:HG3	14:G:102:LEU:HD12	1.92	0.52
4:4:107:TYR:HA	4:4:114:PRO:HA	1.91	0.52
5:5:272:PHE:HZ	5:5:285:VAL:HG21	1.74	0.52
1:b:27:PHE:HE2	1:b:32:ILE:HG13	1.74	0.52
10:d:52:VAL:HG21	10:d:57:LEU:HD22	1.92	0.52
17:J:48:ARG:HH22	21:N:608:LEU:HB3	1.74	0.52
18:K:211:LEU:HD12	18:K:317:ALA:HB2	1.91	0.52
19:L:252:VAL:HG21	20:M:303:ARG:HD2	1.90	0.52
20:M:171:GLU:HG3	20:M:245:LYS:HB3	1.91	0.52
21:N:265:ALA:HB1	21:N:269:LEU:HB3	1.90	0.52
11:D:181:ARG:NH1	12:E:59:LEU:O	2.43	0.52
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.92	0.52
8:c:142:PHE:N	8:c:154:TYR:O	2.41	0.52
12:m:211:LYS:O	12:m:216:ASN:ND2	2.43	0.52
20:M:194:VAL:HG12	20:M:199:LEU:HG	1.92	0.52
20:M:428:LYS:HB3	20:M:430:VAL:HG12	1.91	0.52
21:N:110:VAL:HG11	21:N:159:GLU:HG2	1.91	0.52
33:Z:99:LEU:HD23	33:Z:102:ILE:HD12	1.91	0.52
8:A:250:GLU:HA	23:P:84:LYS:HE2	1.91	0.52
10:C:75:VAL:HG12	10:C:137:TYR:HA	1.90	0.52
17:J:319:PRO:HB2	17:J:324:ARG:HH11	1.74	0.52
18:K:187:ALA:O	18:K:188:VAL:CG2	2.58	0.52
19:L:397:GLU:OE1	20:M:345:ARG:NH2	2.34	0.52
20:M:72:ASN:O	20:M:77:TYR:OH	2.25	0.52
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.40	0.52
33:Z:139:LEU:HD22	33:Z:199:ASP:HB3	1.91	0.52
5:5:102:ALA:HB1	6:6:156:ARG:HH22	1.74	0.52
4:g:92:ILE:HD12	4:g:97:PRO:HB3	1.91	0.52
11:n:62:SER:OG	11:n:211:GLU:OE2	2.28	0.52
19:L:104:LEU:O	19:L:148:LEU:N	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:890:PHE:O	21:N:891:VAL:HG12	2.09	0.52
22:O:137:TYR:HB2	22:O:146:ALA:HB2	1.91	0.52
25:R:240:SER:O	25:R:241:ILE:HG22	2.10	0.52
26:S:472:HIS:O	26:S:476:LEU:N	2.42	0.52
5:5:199:GLY:H	5:5:202:PHE:HZ	1.57	0.52
15:H:95:HIS:O	15:H:97:LEU:N	2.42	0.52
21:N:39:ILE:HG21	21:N:68:VAL:HG21	1.92	0.52
22:O:258:LEU:HA	22:O:288:ARG:HG2	1.92	0.52
6:6:167:PRO:HG3	3:h:177:ARG:HE	1.74	0.52
10:C:22:VAL:HG11	16:I:433:GLU:CG	2.39	0.52
13:F:67:ASP:OD1	13:F:68:GLU:N	2.43	0.52
14:G:68:GLN:OE1	14:G:93:ARG:NH2	2.43	0.52
13:l:206:LEU:HD22	13:l:211:LEU:HD11	1.92	0.52
20:M:225:GLY:O	20:M:389:ALA:N	2.40	0.52
5:5:96:THR:HG22	5:5:101:VAL:HG22	1.91	0.51
1:b:146:ALA:HB2	7:a:68:ARG:HH22	1.74	0.51
5:f:102:ALA:O	6:e:156:ARG:NH1	2.32	0.51
6:e:134:ASP:OD1	6:e:135:GLU:N	2.43	0.51
10:d:120:GLN:HB3	11:n:84:ILE:HD11	1.91	0.51
11:n:8:LEU:HB2	11:n:19:GLN:HE22	1.75	0.51
11:n:149:GLN:OE1	11:n:162:GLN:NE2	2.43	0.51
24:Q:429:LYS:HG3	28:U:299:LYS:HE3	1.90	0.51
27:T:95:LYS:NZ	27:T:130:ASP:OD2	2.28	0.51
28:U:36:VAL:HA	28:U:92:TRP:HA	1.92	0.51
33:Z:382:ALA:HB1	33:Z:849:ARG:HD2	1.90	0.51
33:Z:595:MET:HG2	33:Z:737:ALA:HB3	1.91	0.51
12:E:206:GLN:OE1	15:H:409:ARG:NH2	2.42	0.51
12:m:141:ALA:HB1	12:m:172:ILE:HD12	1.92	0.51
17:J:43:ARG:NH1	26:S:478:SER:HA	2.25	0.51
27:T:248:GLU:O	27:T:249:MET:HE2	2.10	0.51
28:U:16:LEU:HB2	29:V:212:MET:HG2	1.90	0.51
5:5:127:CYS:HA	5:5:172:MET:HE3	1.92	0.51
31:X:73:THR:HG23	31:X:90:VAL:H	1.75	0.51
1:b:145:ILE:HG22	1:b:150:SER:HB2	1.92	0.51
17:J:143:PRO:O	17:J:204:HIS:ND1	2.44	0.51
28:U:230:GLN:HA	28:U:233:PHE:HD2	1.76	0.51
29:V:27:VAL:HA	29:V:63:VAL:HB	1.91	0.51
5:5:94:ARG:NH2	3:h:205:ASP:OD2	2.44	0.51
3:h:56:LEU:HD11	4:g:122:LEU:HD13	1.92	0.51
3:h:58:THR:OG1	4:g:124:THR:OG1	2.24	0.51
23:P:54:SER:HA	23:P:58:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:46:THR:HB	6:6:59:GLU:H	1.75	0.51
24:Q:93:THR:O	24:Q:97:LEU:N	2.44	0.51
33:Z:415:MET:HE2	33:Z:447:VAL:HG22	1.92	0.51
5:5:82:ARG:HH11	5:5:186:THR:HA	1.76	0.51
6:e:194:LEU:HB3	6:e:198:GLU:HB2	1.92	0.51
6:e:179:TYR:HA	6:e:188:LYS:HA	1.92	0.51
7:a:90:ILE:HG23	7:a:93:MET:HE2	1.92	0.51
17:J:139:VAL:HG22	17:J:211:ILE:HG12	1.93	0.51
19:L:108:VAL:HG22	19:L:119:VAL:HG22	1.92	0.51
29:V:141:VAL:HG22	29:V:153:ILE:HG22	1.92	0.51
3:3:30:GLY:HA2	3:3:36:VAL:HG23	1.92	0.51
1:b:80:TYR:HB2	8:c:101:ALA:HB1	1.92	0.51
9:j:71:ILE:HG12	9:j:138:GLY:HA3	1.92	0.51
18:K:122:ILE:HG23	18:K:146:LEU:HD22	1.93	0.51
25:R:250:ALA:HB1	25:R:279:LEU:HD21	1.93	0.51
25:R:348:LEU:HB2	25:R:388:VAL:HB	1.92	0.51
8:A:181:ASN:HD22	8:A:213:ALA:HB2	1.76	0.51
14:k:219:CYS:HB2	14:k:228:HIS:HD2	1.75	0.51
27:T:227:PRO:HB2	27:T:232:LYS:HE2	1.92	0.51
2:2:253:GLN:HG2	10:C:226:TYR:HA	1.93	0.50
3:3:51:LEU:HD22	3:3:87:PHE:HZ	1.76	0.50
12:m:187:TRP:HA	12:m:191:LEU:HD11	1.93	0.50
14:k:211:ASP:OD1	14:k:212:PHE:N	2.44	0.50
22:O:296:LEU:HD11	22:O:308:LEU:HD22	1.93	0.50
22:O:326:HIS:HE1	23:P:368:LEU:HD11	1.74	0.50
24:Q:391:ASP:OD1	25:R:347:THR:OG1	2.28	0.50
33:Z:957:LEU:HA	33:Z:961:GLU:HG2	1.93	0.50
11:D:63:LYS:NZ	11:D:79:ASN:OD1	2.43	0.50
13:l:67:ASP:OD1	13:l:68:GLU:N	2.44	0.50
17:J:43:ARG:HD3	26:S:479:MET:H	1.77	0.50
29:V:164:LEU:HB2	29:V:165:ILE:HD12	1.93	0.50
30:W:11:ASP:HA	30:W:55:ALA:HB3	1.93	0.50
33:Z:128:GLU:HB3	33:Z:132:HIS:CD2	2.46	0.50
33:Z:400:ILE:HG12	33:Z:422:ILE:HG12	1.92	0.50
1:1:33:LEU:HD21	1:1:119:ALA:HB3	1.93	0.50
1:1:54:THR:HG21	1:1:75:ALA:HB1	1.94	0.50
10:C:206:LEU:HD11	10:C:211:LEU:HD21	1.93	0.50
13:F:105:VAL:HG12	13:F:145:LEU:HD13	1.93	0.50
13:F:176:LEU:HD13	14:G:58:LEU:HD23	1.94	0.50
28:U:16:LEU:HD21	29:V:209:GLU:HG2	1.92	0.50
30:W:108:GLN:HB2	30:W:137:VAL:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:38:ASN:HD22	5:f:285:VAL:HG22	1.76	0.50
3:3:175:ALA:HB1	3:3:182:GLY:HA2	1.94	0.50
3:h:169:GLN:O	3:h:173:ASN:ND2	2.34	0.50
4:g:8:ARG:HG3	4:g:13:VAL:HG22	1.92	0.50
10:C:18:ARG:HD3	10:C:19:LEU:O	2.12	0.50
17:J:43:ARG:NH1	26:S:477:VAL:O	2.30	0.50
17:J:267:GLU:OE1	17:J:270:ARG:NH2	2.45	0.50
24:Q:179:LEU:HD13	24:Q:218:LEU:HD23	1.93	0.50
31:X:85:ARG:HD2	31:X:101:LEU:HD12	1.93	0.50
4:g:35:THR:HA	4:g:45:SER:HA	1.93	0.50
4:g:149:ARG:NH2	4:g:156:GLU:OE1	2.44	0.50
19:L:129:VAL:HG11	19:L:148:LEU:HD22	1.93	0.50
23:P:350:LEU:HA	23:P:353:ILE:HD12	1.93	0.50
6:6:134:ASP:OD1	6:6:135:GLU:N	2.43	0.50
10:d:207:THR:OG1	10:d:210:ARG:NH1	2.41	0.50
16:I:190:GLN:HB3	16:I:348:ILE:HG23	1.93	0.50
21:N:302:PHE:HA	21:N:871:MET:HE3	1.92	0.50
21:N:326:SER:HB3	21:N:360:GLN:HE22	1.77	0.50
23:P:248:ASP:HA	23:P:252:SER:HB3	1.93	0.50
23:P:268:LEU:HD11	23:P:277:GLN:HA	1.94	0.50
33:Z:318:LYS:HD2	33:Z:874:ASN:HD21	1.77	0.50
3:3:20:CYS:HA	3:3:112:ILE:HD11	1.93	0.50
3:3:138:VAL:HG11	3:3:146:LEU:HB2	1.93	0.50
13:F:34:VAL:HA	13:F:162:GLY:HA3	1.92	0.50
13:F:66:CYS:O	13:F:89:ARG:NH1	2.43	0.50
20:M:357:ARG:HD2	20:M:391:LEU:HD21	1.94	0.50
26:S:208:ILE:HD13	27:T:44:LEU:HD22	1.93	0.50
29:V:142:ASP:HB3	29:V:143:PRO:HD3	1.93	0.50
1:1:102:LYS:NZ	7:7:94:GLN:OE1	2.31	0.50
2:2:194:ASN:OD1	7:a:189:ARG:NH1	2.45	0.50
2:2:254:GLU:HB2	10:C:227:GLN:HG2	1.93	0.50
3:3:177:ARG:HH12	6:e:166:MET:HB3	1.77	0.50
7:7:44:VAL:HG13	7:7:57:ALA:HB2	1.94	0.50
6:e:224:LEU:HG	6:e:233:LYS:HG2	1.93	0.50
9:j:72:GLY:N	9:j:137:ALA:O	2.43	0.50
10:d:33:GLY:HA3	10:d:65:LYS:HZ3	1.77	0.50
21:N:43:LEU:HD21	21:N:68:VAL:HG11	1.93	0.50
29:V:29:ILE:HD13	29:V:37:MET:HE1	1.93	0.50
6:e:56:SER:HB2	7:a:170:TYR:HB2	1.94	0.50
15:H:200:VAL:HG13	15:H:270:THR:HG23	1.93	0.50
16:I:136:VAL:HG11	16:I:158:GLY:HA2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:29:GLN:HE21	30:W:144:PHE:HE2	1.60	0.50
2:2:189:GLN:HA	2:2:192:ILE:HD12	1.94	0.49
3:3:115:LYS:NZ	9:B:141:GLU:OE1	2.33	0.49
5:5:271:LEU:HD23	5:5:274:LYS:HD2	1.94	0.49
2:i:189:GLN:HA	2:i:192:ILE:HD12	1.93	0.49
4:g:29:LYS:HD3	4:g:32:ASP:HB2	1.94	0.49
4:g:139:TYR:HE2	4:g:172:MET:HG3	1.76	0.49
12:E:44:GLU:OE1	12:E:193:LEU:N	2.45	0.49
21:N:227:LYS:HG2	21:N:722:THR:O	2.11	0.49
27:T:221:ALA:HB1	27:T:226:TRP:HB2	1.94	0.49
28:U:234:ASN:OD1	28:U:235:LEU:N	2.45	0.49
1:b:55:ARG:HH21	1:b:58:ASP:HA	1.76	0.49
8:A:130:GLN:HB3	9:B:127:VAL:HG13	1.93	0.49
13:F:52:ASN:ND2	13:F:54:ASP:O	2.45	0.49
15:H:208:TYR:HA	15:H:262:ALA:HB1	1.94	0.49
19:L:248:ALA:HB2	19:L:283:VAL:HG22	1.94	0.49
21:N:627:ILE:HG23	21:N:733:LEU:HD13	1.93	0.49
22:O:81:TYR:HA	22:O:85:SER:HB3	1.94	0.49
24:Q:135:HIS:ND1	24:Q:169:ASP:OD2	2.44	0.49
5:5:82:ARG:NH2	5:5:199:GLY:O	2.45	0.49
11:D:189:GLU:HG3	11:D:232:TYR:HE1	1.77	0.49
13:l:18:ARG:NE	13:l:23:GLU:OE2	2.42	0.49
15:H:385:ARG:NH1	15:H:413:ASN:OD1	2.40	0.49
17:J:190:PRO:HD2	17:J:316:PHE:HD2	1.77	0.49
20:M:159:LEU:HD12	20:M:160:PRO:HD2	1.94	0.49
21:N:876:PRO:HB3	21:N:900:ASN:HB3	1.93	0.49
24:Q:295:GLY:N	24:Q:324:GLU:OE1	2.40	0.49
27:T:226:TRP:HE1	27:T:235:PHE:HB3	1.77	0.49
27:T:233:VAL:HG12	27:T:234:TYR:N	2.23	0.49
28:U:285:ILE:O	28:U:289:ASP:N	2.45	0.49
33:Z:116:ALA:HB3	33:Z:141:SER:HB2	1.95	0.49
33:Z:559:LYS:HG3	33:Z:561:ASP:H	1.77	0.49
18:K:126:LEU:HD13	18:K:149:ILE:HG13	1.94	0.49
19:L:218:VAL:HA	19:L:345:ARG:HB2	1.95	0.49
21:N:114:SER:HA	21:N:161:TYR:HD2	1.76	0.49
9:B:122:THR:HB	10:C:129:ARG:HH22	1.77	0.49
11:D:6:ARG:HD2	12:E:124:GLY:HA2	1.95	0.49
11:D:75:PHE:HB3	11:D:133:THR:HG22	1.95	0.49
13:F:226:ASP:OD1	13:F:227:GLY:N	2.46	0.49
10:d:119:LYS:NZ	10:d:151:SER:OG	2.38	0.49
15:H:289:ARG:NE	20:M:253:GLN:OE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:248:ASP:OD1	17:J:249:GLU:N	2.46	0.49
18:K:420:THR:O	18:K:421:VAL:HG22	2.11	0.49
24:Q:4:PRO:HB2	24:Q:53:GLU:HB2	1.94	0.49
2:2:149:ASP:OD1	2:2:150:VAL:N	2.45	0.49
5:5:80:ALA:HB3	5:5:202:PHE:HB2	1.95	0.49
7:7:96:ILE:HD13	7:7:147:ILE:HD11	1.94	0.49
7:7:179:PHE:HZ	1:b:44:TYR:HD1	1.59	0.49
2:i:236:ARG:HA	3:h:165:GLU:HG3	1.95	0.49
12:E:71:ASP:OD1	12:E:72:ARG:N	2.43	0.49
9:j:213:ILE:HD11	9:j:236:ARG:HD2	1.93	0.49
12:m:71:ASP:OD1	12:m:72:ARG:N	2.45	0.49
12:m:121:LEU:HD23	13:l:79:PRO:HB3	1.94	0.49
22:O:168:THR:HG21	28:U:142:GLN:HE22	1.78	0.49
28:U:38:LEU:HB2	28:U:50:ASN:HB3	1.94	0.49
3:h:115:LYS:NZ	9:j:141:GLU:OE1	2.43	0.49
4:g:70:ARG:O	10:d:113:ARG:NH1	2.42	0.49
11:D:65:SER:O	11:D:73:LEU:N	2.45	0.49
11:D:159:TRP:HZ3	12:E:56:SER:HB3	1.78	0.49
14:k:218:TRP:HH2	14:k:223:GLU:HB2	1.77	0.49
14:k:219:CYS:HB2	14:k:228:HIS:CD2	2.48	0.49
18:K:187:ALA:C	18:K:188:VAL:HG23	2.36	0.49
18:K:371:LEU:O	18:K:375:ASN:ND2	2.45	0.49
22:O:130:ASP:HA	22:O:133:ILE:HD12	1.94	0.49
25:R:325:HIS:HB2	25:R:329:PHE:CE2	2.47	0.49
26:S:330:LEU:HB2	32:Y:64:TRP:CD1	2.48	0.49
11:D:82:SER:HB3	11:D:131:VAL:HG21	1.94	0.49
11:n:161:ALA:HB1	11:n:175:LEU:HD13	1.94	0.49
20:M:61:LYS:O	20:M:65:ASN:ND2	2.45	0.49
25:R:261:LEU:HD23	25:R:266:LEU:HD23	1.94	0.49
26:S:399:TYR:HD2	26:S:402:ILE:HD12	1.78	0.49
32:Y:72:ASP:CG	32:Y:73:PHE:H	2.20	0.49
5:5:125:ALA:HA	6:6:149:SER:HB2	1.94	0.49
6:e:211:THR:HG23	6:e:218:GLY:HA2	1.94	0.49
9:B:4:ARG:HG3	9:B:5:TYR:H	1.78	0.49
8:c:34:THR:HA	8:c:84:GLY:HA2	1.93	0.49
18:K:63:LEU:HD13	21:N:565:ASN:HD22	1.77	0.49
23:P:388:ILE:HG22	23:P:389:ILE:HG23	1.95	0.49
26:S:222:SER:HA	26:S:230:LYS:HD3	1.95	0.49
28:U:262:GLN:N	29:V:306:LYS:HD2	2.28	0.49
29:V:153:ILE:HD11	29:V:201:ILE:HG21	1.95	0.49
1:1:64:ARG:HA	1:1:116:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:11:ILE:HG21	3:3:142:ALA:HB3	1.95	0.49
3:3:123:GLY:HA3	3:3:137:ILE:HG21	1.94	0.49
10:C:132:GLY:HA2	10:C:153:PRO:HB3	1.95	0.49
12:m:123:PHE:CD1	12:m:137:PRO:HB3	2.48	0.49
17:J:228:ARG:O	17:J:232:GLU:N	2.46	0.49
19:L:84:LEU:HD12	20:M:55:ASN:HD21	1.78	0.49
21:N:521:LEU:HB3	21:N:535:LEU:HD21	1.95	0.49
24:Q:388:GLY:HA2	24:Q:400:TYR:HB3	1.94	0.49
25:R:273:SER:HB3	25:R:276:LEU:HB2	1.94	0.49
27:T:224:ARG:HB2	27:T:235:PHE:HB2	1.93	0.49
30:W:114:VAL:HG12	30:W:116:SER:H	1.77	0.49
31:X:48:PHE:HD2	31:X:66:LEU:HD23	1.78	0.49
5:5:266:HIS:HB3	5:5:271:LEU:HD11	1.94	0.48
24:Q:402:THR:HB	24:Q:403:PRO:HD3	1.95	0.48
27:T:224:ARG:CZ	27:T:235:PHE:HA	2.42	0.48
28:U:119:LEU:HD11	28:U:136:ALA:HB1	1.94	0.48
30:W:87:MET:HE3	30:W:91:LEU:HD11	1.95	0.48
33:Z:796:LEU:HA	33:Z:799:PHE:HB3	1.95	0.48
8:A:51:THR:HB	8:A:228:ALA:HB3	1.96	0.48
10:C:152:ASN:O	10:C:154:SER:N	2.46	0.48
13:l:105:VAL:HG21	13:l:143:HIS:HB2	1.94	0.48
17:J:256:THR:HG22	18:K:326:PRO:HB2	1.95	0.48
18:K:347:ARG:O	18:K:350:ARG:HG2	2.13	0.48
22:O:79:VAL:HG23	22:O:80:LYS:HG2	1.94	0.48
25:R:254:SER:HB3	25:R:288:SER:HB2	1.93	0.48
5:f:146:LYS:NZ	12:m:65:GLU:OE1	2.38	0.48
7:a:127:GLU:HG2	13:l:100:ASN:HB2	1.94	0.48
16:I:172:LYS:HB3	16:I:246:ARG:HB2	1.95	0.48
20:M:357:ARG:HG2	20:M:391:LEU:HD11	1.95	0.48
23:P:124:VAL:HG22	23:P:129:LYS:HG3	1.95	0.48
23:P:392:LYS:HB3	23:P:401:ASN:H	1.78	0.48
6:6:29:GLY:N	6:6:216:GLN:HE21	2.12	0.48
18:K:104:ASP:OD1	18:K:105:GLN:N	2.43	0.48
19:L:249:SER:OG	20:M:307:GLU:OE2	2.26	0.48
33:Z:266:LYS:HA	33:Z:293:MET:HE1	1.95	0.48
1:b:33:LEU:HD21	1:b:119:ALA:HB3	1.96	0.48
9:j:91:LYS:O	9:j:95:THR:N	2.46	0.48
11:n:32:CYS:HA	11:n:165:GLY:HA3	1.96	0.48
15:H:86:GLY:HA2	15:H:90:ARG:HH11	1.79	0.48
19:L:290:ARG:HE	19:L:302:GLN:HG2	1.79	0.48
22:O:114:GLN:C	22:O:116:ASN:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:269:GLU:HB3	26:S:299:LYS:HB3	1.94	0.48
29:V:173:THR:HB	29:V:200:ASN:ND2	2.28	0.48
1:b:22:ILE:HD12	1:b:63:CYS:HB3	1.95	0.48
11:n:161:ALA:HB3	12:m:58:LEU:HD13	1.94	0.48
15:H:86:GLY:HA2	15:H:90:ARG:HD2	1.96	0.48
20:M:197:ILE:HD13	20:M:324:LEU:HD11	1.96	0.48
21:N:360:GLN:HG2	21:N:362:TRP:H	1.76	0.48
29:V:173:THR:HG22	29:V:174:THR:HG23	1.94	0.48
29:V:237:ASN:O	29:V:241:THR:N	2.26	0.48
6:e:155:CYS:HB3	6:e:169:LEU:HD13	1.96	0.48
8:A:20:SER:HB2	8:A:21:PRO:HD2	1.95	0.48
8:A:43:LEU:HD13	8:A:210:MET:HB2	1.95	0.48
11:D:68:ASP:HB3	11:D:71:VAL:HB	1.96	0.48
14:G:21:ASN:OD1	14:G:22:PHE:N	2.47	0.48
15:H:434:ARG:HH11	33:Z:955:VAL:HB	1.79	0.48
17:J:375:ILE:HD11	25:R:205:GLU:HB2	1.96	0.48
18:K:92:VAL:O	18:K:94:LEU:N	2.47	0.48
25:R:365:ASP:OD1	26:S:399:TYR:OH	2.24	0.48
33:Z:133:ASP:OD1	33:Z:136:ARG:NH2	2.44	0.48
4:4:4:ILE:HD11	4:4:133:HIS:HD2	1.78	0.48
8:A:141:LEU:HB2	8:A:157:THR:HB	1.95	0.48
11:D:64:VAL:HG11	11:D:213:THR:HG21	1.95	0.48
11:D:68:ASP:OD1	11:D:69:SER:N	2.43	0.48
12:E:222:ILE:HG13	12:E:228:PHE:HD1	1.77	0.48
10:d:6:TYR:HD2	10:d:9:ARG:HD2	1.78	0.48
13:l:13:PHE:N	14:k:23:GLN:OE1	2.46	0.48
17:J:251:ASP:OD1	17:J:252:SER:N	2.46	0.48
21:N:349:ILE:HA	21:N:356:LEU:HD11	1.95	0.48
21:N:589:ILE:HA	21:N:624:ALA:HB2	1.94	0.48
26:S:425:ARG:HD2	26:S:428:ARG:HG3	1.94	0.48
28:U:259:ASN:N	29:V:304:ALA:HB1	2.28	0.48
33:Z:593:HIS:HB2	33:Z:596:THR:HG23	1.95	0.48
5:5:120:MET:HE3	5:5:128:GLN:HB2	1.94	0.48
7:7:48:LYS:HD2	7:7:173:PRO:HA	1.96	0.48
6:e:50:THR:OG1	6:e:55:ASN:ND2	2.41	0.48
15:H:163:VAL:HG21	15:H:183:ILE:HG22	1.96	0.48
23:P:43:GLU:HB3	23:P:47:ARG:NE	2.28	0.48
25:R:79:LEU:HG	25:R:93:LYS:HB2	1.96	0.48
26:S:357:LEU:HB3	26:S:384:ARG:HH22	1.79	0.48
5:5:116:LEU:HD23	5:5:178:GLY:HA3	1.96	0.48
20:M:187:ASP:HA	20:M:190:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:668:THR:OG1	21:N:711:ARG:NH2	2.47	0.48
26:S:119:TYR:CE2	26:S:121:VAL:HB	2.49	0.48
26:S:129:GLU:OE2	26:S:132:ALA:N	2.46	0.48
33:Z:599:ILE:O	33:Z:603:VAL:HG13	2.14	0.48
3:3:124:PHE:HB3	3:3:128:GLY:HA2	1.95	0.47
8:c:113:CYS:HB2	8:c:144:SER:HB3	1.96	0.47
15:H:202:GLU:HG2	15:H:203:LYS:HG3	1.96	0.47
23:P:346:ILE:HG23	23:P:369:LEU:HD22	1.96	0.47
25:R:261:LEU:HD11	25:R:265:ASP:HB2	1.96	0.47
26:S:424:SER:O	27:T:192:ASN:ND2	2.47	0.47
30:W:185:ILE:O	30:W:188:SER:OG	2.31	0.47
33:Z:427:GLN:HG3	33:Z:458:SER:HA	1.95	0.47
6:6:214:HIS:HE1	2:i:53:PRO:HB2	1.79	0.47
16:I:259:ASP:OD1	16:I:262:ARG:NH2	2.47	0.47
21:N:214:LEU:HD22	21:N:220:CYS:HB3	1.96	0.47
33:Z:213:LYS:NZ	33:Z:239:GLU:OE2	2.40	0.47
33:Z:256:LEU:HB3	33:Z:257:PRO:HD3	1.95	0.47
3:h:53:ILE:HG22	3:h:60:VAL:HG22	1.95	0.47
10:C:50:ARG:HH21	10:C:212:GLU:HG2	1.79	0.47
13:F:74:LEU:HD13	13:F:81:ALA:HB2	1.96	0.47
11:n:117:GLN:HE21	11:n:129:PHE:HB2	1.80	0.47
12:m:71:ASP:HB3	12:m:74:ILE:HB	1.95	0.47
14:k:73:HIS:CD2	14:k:74:ILE:HG13	2.49	0.47
19:L:84:LEU:HD23	19:L:87:LEU:HD12	1.95	0.47
20:M:248:ALA:HB1	20:M:286:ILE:HG12	1.96	0.47
21:N:250:ASP:OD2	21:N:906:ARG:NH2	2.47	0.47
24:Q:117:VAL:O	24:Q:121:SER:OG	2.30	0.47
33:Z:359:LYS:NZ	33:Z:425:ILE:O	2.44	0.47
33:Z:916:LEU:HB3	33:Z:920:GLY:HA2	1.97	0.47
2:2:201:ASN:ND2	2:2:218:ASN:OD1	2.42	0.47
5:5:134:LEU:HD22	5:5:158:LEU:HD22	1.95	0.47
5:f:191:ASP:HB3	5:f:195:THR:HB	1.94	0.47
10:C:18:ARG:HD2	10:C:18:ARG:O	2.14	0.47
11:D:216:LYS:HB2	11:D:220:ASP:HB3	1.95	0.47
17:J:96:VAL:HG11	17:J:115:LEU:HD11	1.95	0.47
19:L:360:ILE:HA	19:L:363:ILE:HD12	1.97	0.47
6:e:45:ASP:OD1	6:e:61:LYS:NZ	2.33	0.47
9:B:239:THR:HG22	9:B:241:GLN:H	1.79	0.47
11:D:118:GLN:OE1	12:E:86:ARG:NH2	2.38	0.47
10:d:177:GLN:HE22	11:n:54:LEU:HB2	1.80	0.47
16:I:181:TYR:HD1	16:I:184:ILE:HD11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:236:ARG:HG3	18:K:270:PHE:HD2	1.80	0.47
21:N:364:LYS:HB3	21:N:400:ILE:HD12	1.97	0.47
24:Q:158:ILE:HD13	24:Q:161:LEU:HD12	1.96	0.47
24:Q:382:LEU:HB3	25:R:263:ARG:HH22	1.80	0.47
29:V:26:THR:HB	29:V:172:GLN:HE22	1.78	0.47
30:W:125:LEU:HB3	30:W:157:PHE:HD1	1.79	0.47
31:X:17:TYR:HH	31:X:97:TYR:HH	1.61	0.47
5:5:243:ASP:OD1	3:h:33:SER:OG	2.32	0.47
7:7:256:LYS:HB3	1:b:206:ILE:HG21	1.97	0.47
7:a:183:MET:O	7:a:186:PRO:HD2	2.13	0.47
13:F:190:ILE:HG23	13:F:213:ILE:HD13	1.97	0.47
8:c:34:THR:HG21	8:c:139:ILE:HD12	1.97	0.47
8:c:36:GLN:HG3	14:k:19:GLY:HA3	1.95	0.47
10:d:4:ARG:C	10:d:6:TYR:H	2.23	0.47
10:d:65:LYS:HA	10:d:77:VAL:HB	1.96	0.47
21:N:902:VAL:O	21:N:903:VAL:HG22	2.15	0.47
4:4:29:LYS:HD3	4:4:32:ASP:HB2	1.96	0.47
1:b:195:VAL:HG22	1:b:204:ARG:HA	1.97	0.47
7:a:78:VAL:HG21	7:a:100:LEU:HB3	1.97	0.47
8:A:69:VAL:HG22	14:G:158:TRP:CD1	2.49	0.47
9:B:50:LYS:HE2	9:B:52:SER:HB2	1.96	0.47
9:B:118:MET:HE2	9:B:132:VAL:HG23	1.96	0.47
10:C:115:LEU:HD23	10:C:118:ILE:HD12	1.97	0.47
13:F:50:LYS:HB3	13:F:59:TYR:HB3	1.97	0.47
8:c:87:PRO:HB3	14:k:156:SER:HB3	1.96	0.47
11:n:158:SER:OG	12:m:60:GLU:OE1	2.32	0.47
13:l:70:MET:HE1	13:l:103:LEU:HD23	1.96	0.47
16:I:107:GLY:HA2	16:I:122:SER:HA	1.95	0.47
16:I:253:ILE:HG21	16:I:286:ALA:HA	1.97	0.47
17:J:193:THR:HA	17:J:355:GLY:H	1.78	0.47
18:K:129:GLU:OE1	29:V:278:LYS:NZ	2.45	0.47
19:L:432:ILE:HG23	19:L:435:GLN:OE1	2.15	0.47
21:N:70:TYR:HE1	21:N:100:THR:HG21	1.80	0.47
21:N:475:ALA:HB1	29:V:61:TYR:OH	2.14	0.47
23:P:283:LYS:HE2	23:P:286:ASN:HB2	1.97	0.47
23:P:351:ARG:HA	23:P:389:ILE:HD13	1.96	0.47
24:Q:47:ASP:OD1	24:Q:48:ASP:N	2.47	0.47
24:Q:113:ASP:O	24:Q:117:VAL:HG23	2.14	0.47
33:Z:602:LEU:HB2	33:Z:738:TYR:HE2	1.79	0.47
6:6:47:ARG:CZ	6:6:218:GLY:HA3	2.44	0.47
9:B:38:LYS:HG3	9:B:43:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:59:LEU:HB3	24:Q:103:LYS:HE3	1.97	0.47
28:U:265:LEU:HD22	28:U:268:LYS:HD3	1.95	0.47
30:W:3:LEU:HD22	30:W:46:GLU:HB2	1.96	0.47
13:F:67:ASP:HB3	13:F:70:MET:HB2	1.97	0.47
14:G:205:GLU:HA	14:G:208:LYS:HE3	1.96	0.47
8:c:53:ILE:HG12	8:c:224:VAL:HG22	1.96	0.47
13:l:54:ASP:OD1	13:l:55:GLU:N	2.45	0.47
16:I:243:THR:HB	16:I:276:PRO:HB3	1.96	0.47
21:N:498:ILE:HG23	21:N:535:LEU:HD22	1.97	0.47
22:O:289:GLN:HG2	22:O:293:LEU:HG	1.96	0.47
27:T:85:LEU:HA	27:T:88:TYR:HD2	1.79	0.47
27:T:111:LEU:HD22	27:T:181:LEU:HD11	1.95	0.47
14:G:120:VAL:HG21	14:G:151:LEU:HD21	1.97	0.47
15:H:454:TYR:OH	16:I:345:ASP:O	2.22	0.47
17:J:98:VAL:HA	17:J:122:LEU:HB3	1.97	0.47
21:N:912:GLU:O	21:N:914:VAL:N	2.48	0.47
24:Q:161:LEU:HB3	24:Q:165:PHE:CE2	2.50	0.47
24:Q:262:LEU:HD23	24:Q:296:ILE:HD13	1.96	0.47
33:Z:827:LEU:O	33:Z:831:LEU:N	2.43	0.47
9:B:106:PRO:HG2	9:B:109:LEU:HB3	1.95	0.46
10:C:135:PHE:HB2	10:C:151:SER:HB3	1.96	0.46
12:m:14:THR:HG22	12:m:22:PHE:HE2	1.79	0.46
14:k:21:ASN:OD1	14:k:22:PHE:N	2.48	0.46
21:N:341:ALA:HA	21:N:374:ILE:HA	1.97	0.46
23:P:395:ARG:HD2	24:Q:358:GLU:H	1.79	0.46
24:Q:65:TYR:HD2	24:Q:74:LEU:HD13	1.81	0.46
24:Q:81:SER:HA	24:Q:84:TYR:HD2	1.79	0.46
29:V:113:GLY:HA2	29:V:144:ILE:HD11	1.97	0.46
33:Z:197:LYS:HG3	33:Z:199:ASP:H	1.81	0.46
33:Z:237:VAL:HB	33:Z:271:ILE:HG12	1.97	0.46
2:2:74:GLY:HA3	2:2:81:THR:HG21	1.97	0.46
3:3:56:LEU:HD11	4:4:122:LEU:HD13	1.98	0.46
3:h:104:PHE:HD1	3:h:126:LEU:HD13	1.80	0.46
17:J:228:ARG:NE	17:J:232:GLU:OE1	2.46	0.46
19:L:144:VAL:HA	19:L:161:ARG:HD3	1.96	0.46
22:O:277:ILE:HG22	22:O:279:ILE:H	1.80	0.46
3:h:63:LEU:HD11	3:h:105:VAL:HG21	1.96	0.46
17:J:241:ALA:O	17:J:243:SER:N	2.47	0.46
19:L:392:ARG:NE	20:M:340:SER:OG	2.41	0.46
23:P:125:VAL:O	23:P:136:ARG:NE	2.47	0.46
26:S:479:MET:O	26:S:482:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:345:GLU:O	33:Z:349:THR:OG1	2.33	0.46
5:5:131:GLU:OE2	5:5:174:THR:OG1	2.30	0.46
6:6:84:VAL:HG12	6:6:88:LYS:HE3	1.96	0.46
10:C:18:ARG:HE	10:C:23:GLU:CG	2.22	0.46
11:n:103:PRO:HG2	11:n:140:PRO:HG2	1.97	0.46
16:I:219:VAL:HG12	16:I:346:ARG:HB3	1.96	0.46
17:J:113:VAL:HG12	17:J:125:VAL:HA	1.97	0.46
18:K:166:LYS:O	18:K:168:ASP:N	2.48	0.46
22:O:72:LYS:HG2	22:O:73:ILE:HG12	1.98	0.46
23:P:94:GLN:HA	23:P:97:ILE:HD12	1.96	0.46
24:Q:344:GLU:HG2	24:Q:386:PHE:HE2	1.80	0.46
25:R:79:LEU:HD11	25:R:93:LYS:HD2	1.97	0.46
27:T:226:TRP:HE1	27:T:235:PHE:CB	2.28	0.46
30:W:9:VAL:HB	30:W:112:ALA:HA	1.97	0.46
1:b:20:THR:N	1:b:148:SER:OG	2.46	0.46
5:f:234:ARG:HA	5:f:237:LEU:HB3	1.97	0.46
6:e:219:ASP:HA	6:e:240:ARG:HG2	1.98	0.46
10:C:206:LEU:HD23	10:C:244:ILE:HG21	1.97	0.46
11:D:10:ILE:C	11:D:12:SER:H	2.22	0.46
8:c:155:LYS:HE3	8:c:165:TYR:HE2	1.80	0.46
10:d:76:ALA:HB3	10:d:136:ILE:HB	1.97	0.46
19:L:280:MET:HB2	19:L:325:MET:HA	1.98	0.46
20:M:129:LEU:HD22	20:M:154:LEU:HA	1.97	0.46
20:M:189:GLN:HE21	20:M:350:PRO:HD2	1.80	0.46
22:O:189:TYR:HE2	22:O:227:ILE:HB	1.79	0.46
23:P:361:THR:HG22	23:P:363:LEU:H	1.80	0.46
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.79	0.46
28:U:192:ASN:O	29:V:230:TYR:OH	2.29	0.46
1:b:152:PHE:CE2	1:b:185:ASP:HB2	2.50	0.46
14:k:121:GLN:O	14:k:124:THR:OG1	2.32	0.46
15:H:370:ARG:HG3	15:H:371:ILE:H	1.81	0.46
17:J:79:VAL:HG23	17:J:81:ASP:H	1.80	0.46
17:J:126:LEU:HD22	18:K:103:ILE:HG21	1.98	0.46
21:N:386:MET:HB3	21:N:404:SER:HB2	1.97	0.46
21:N:742:TRP:HE3	21:N:743:PHE:CD1	2.32	0.46
21:N:783:SER:O	21:N:873:ARG:NH1	2.48	0.46
25:R:222:ARG:HG2	25:R:325:HIS:CE1	2.50	0.46
27:T:112:ASN:O	27:T:115:SER:OG	2.31	0.46
33:Z:374:LEU:HD11	33:Z:849:ARG:HH12	1.81	0.46
33:Z:812:ILE:HD13	33:Z:848:THR:HA	1.98	0.46
4:4:101:ASN:HB3	4:4:133:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:128:THR:HB	6:e:144:PHE:HB2	1.97	0.46
9:j:8:SER:H	9:j:125:GLY:N	2.13	0.46
10:d:184:MET:HE1	10:d:192:LEU:HD22	1.97	0.46
12:m:42:THR:OG1	12:m:45:GLY:O	2.31	0.46
13:l:157:TYR:CE2	14:k:60:VAL:HG22	2.51	0.46
17:J:132:PRO:HA	17:J:137:MET:HB3	1.96	0.46
20:M:288:THR:OG1	20:M:290:ARG:HG2	2.16	0.46
21:N:718:GLU:HG3	21:N:725:LEU:HD12	1.96	0.46
24:Q:374:GLU:O	25:R:345:TYR:OH	2.32	0.46
25:R:251:THR:OG1	25:R:319:CYS:SG	2.72	0.46
3:3:28:ARG:HD2	3:3:183:TRP:HD1	1.81	0.46
4:4:13:VAL:HG23	4:4:114:PRO:HB2	1.98	0.46
5:5:242:ARG:HH22	5:5:284:ASN:HD22	1.63	0.46
7:7:53:VAL:HG21	7:7:150:ALA:HB1	1.98	0.46
15:H:430:ALA:HA	15:H:435:ARG:HB2	1.97	0.46
18:K:267:SER:H	18:K:312:VAL:HG22	1.79	0.46
19:L:387:ASN:ND2	19:L:390:ASP:O	2.49	0.46
21:N:416:GLY:O	21:N:420:THR:N	2.49	0.46
26:S:201:ILE:O	27:T:93:ASN:ND2	2.49	0.46
33:Z:596:THR:HA	33:Z:599:ILE:HD12	1.98	0.46
2:2:36:LYS:HB2	2:2:152:TYR:CE1	2.51	0.46
7:7:183:MET:O	7:7:186:PRO:HD2	2.15	0.46
1:b:151:THR:HA	1:b:154:TYR:CE2	2.51	0.46
2:i:70:ILE:HG12	2:i:131:GLY:HA3	1.96	0.46
5:f:233:LYS:HB3	5:f:271:LEU:HD21	1.98	0.46
18:K:183:GLU:OE1	18:K:336:ARG:NH1	2.49	0.46
19:L:294:GLY:C	19:L:296:SER:H	2.24	0.46
20:M:82:VAL:O	20:M:143:ASN:N	2.47	0.46
21:N:742:TRP:CE3	21:N:743:PHE:HD1	2.31	0.46
23:P:89:LEU:HG	23:P:91:LEU:H	1.81	0.46
23:P:302:LEU:HG	23:P:306:ASN:HB2	1.97	0.46
23:P:392:LYS:HD2	23:P:401:ASN:HB2	1.98	0.46
26:S:333:PHE:HD1	26:S:342:LEU:HB3	1.81	0.46
29:V:183:ALA:H	29:V:186:GLN:HA	1.81	0.46
9:B:42:GLY:HA3	9:B:185:LEU:HD22	1.97	0.46
11:D:9:SER:C	11:D:11:PHE:H	2.24	0.46
14:G:8:TYR:HB2	14:G:22:PHE:HE2	1.81	0.46
16:I:122:SER:H	16:I:126:PRO:HD2	1.81	0.46
18:K:107:THR:HA	18:K:121:ARG:HA	1.98	0.46
19:L:105:ILE:HD11	20:M:128:PHE:HB2	1.98	0.46
19:L:164:ASP:N	19:L:269:TYR:OH	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:163:PHE:HE2	20:M:264:ARG:HH12	1.64	0.46
25:R:137:LEU:HG	25:R:141:TYR:HE2	1.81	0.46
25:R:213:TYR:HD1	25:R:216:ILE:HD12	1.81	0.46
2:2:215:TYR:HB3	9:B:226:GLY:HA3	1.98	0.45
6:6:83:LEU:HD11	6:6:112:ILE:HG23	1.97	0.45
8:A:86:PRO:HB2	8:A:89:ASP:HB2	1.96	0.45
11:D:202:VAL:HG23	11:D:203:VAL:H	1.81	0.45
14:G:88:LEU:HD21	14:G:151:LEU:HD23	1.98	0.45
20:M:223:PRO:HG2	20:M:226:THR:HG23	1.98	0.45
21:N:145:LEU:O	21:N:173:LYS:NZ	2.44	0.45
21:N:327:LEU:HD11	29:V:170:PRO:HB2	1.98	0.45
22:O:127:LEU:HD22	22:O:167:ILE:HG12	1.97	0.45
23:P:271:SER:HB3	23:P:277:GLN:HE21	1.80	0.45
23:P:350:LEU:HD23	23:P:383:LEU:HD12	1.98	0.45
33:Z:347:ASN:HB3	33:Z:353:VAL:HG23	1.98	0.45
10:C:172:ALA:HB2	10:C:200:THR:HG21	1.98	0.45
8:c:16:THR:OG1	8:c:130:ARG:O	2.29	0.45
9:j:222:LEU:HD13	9:j:232:GLY:HA2	1.97	0.45
19:L:295:THR:HG22	19:L:298:ASP:HB2	1.97	0.45
23:P:325:ASP:OD1	23:P:326:ASP:N	2.47	0.45
25:R:141:TYR:HA	25:R:144:ILE:HD12	1.99	0.45
33:Z:525:MET:O	33:Z:529:ALA:N	2.48	0.45
3:3:65:GLU:HB3	10:C:100:LYS:HG3	1.98	0.45
9:B:111:VAL:HG21	9:B:148:TYR:HD2	1.82	0.45
16:I:247:ILE:HB	16:I:281:ILE:HG12	1.97	0.45
21:N:376:LYS:HA	21:N:411:ILE:HA	1.98	0.45
33:Z:781:GLY:HA3	33:Z:818:CYS:HA	1.98	0.45
33:Z:958:ASN:H	33:Z:961:GLU:HB2	1.82	0.45
9:B:94:HIS:O	9:B:99:ARG:N	2.46	0.45
10:C:168:ASN:HB3	10:C:171:ALA:HB3	1.98	0.45
11:D:78:LEU:HB2	16:I:436:TYR:CZ	2.51	0.45
12:E:119:LEU:HD12	12:E:122:ARG:HE	1.82	0.45
14:G:73:HIS:CD2	14:G:74:ILE:HG13	2.51	0.45
9:j:5:TYR:HD2	11:n:4:TYR:HB3	1.82	0.45
16:I:436:TYR:N	16:I:436:TYR:CD1	2.83	0.45
18:K:127:ASP:OD1	18:K:128:ARG:N	2.50	0.45
26:S:395:ILE:HD12	26:S:410:LYS:HD3	1.98	0.45
27:T:221:ALA:HA	27:T:226:TRP:CD1	2.51	0.45
30:W:107:HIS:HD2	30:W:197:SER:HB3	1.82	0.45
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.97	0.45
33:Z:491:LEU:HD11	33:Z:903:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:82:ARG:HG2	5:5:87:ILE:HG12	1.98	0.45
7:7:61:GLY:N	7:7:69:PHE:O	2.45	0.45
9:j:5:TYR:HB2	11:n:4:TYR:HB3	1.98	0.45
11:n:157:SER:OG	11:n:159:TRP:NE1	2.49	0.45
15:H:240:ILE:HG22	20:M:368:MET:HG2	1.99	0.45
18:K:261:ALA:HB1	18:K:267:SER:HB3	1.97	0.45
19:L:168:TYR:HD2	20:M:143:ASN:HD22	1.64	0.45
21:N:163:LEU:HB3	21:N:209:LYS:HE3	1.98	0.45
1:1:27:PHE:HE2	1:1:32:ILE:HG13	1.80	0.45
7:7:172:SER:OG	7:7:174:THR:O	2.32	0.45
12:m:23:GLN:HB3	12:m:137:PRO:HG3	1.99	0.45
12:m:86:ARG:HA	12:m:89:ILE:HD12	1.97	0.45
15:H:105:ILE:HG23	15:H:145:TYR:CE1	2.51	0.45
17:J:334:LYS:HB3	18:K:202:GLY:HA3	1.99	0.45
18:K:327:ALA:O	18:K:333:ARG:NH1	2.50	0.45
20:M:246:LEU:HD21	20:M:251:LEU:HD21	1.98	0.45
21:N:9:LEU:HD23	21:N:12:LEU:HD12	1.97	0.45
27:T:28:PRO:HA	27:T:31:LYS:HE2	1.98	0.45
33:Z:204:CYS:HA	33:Z:232:LYS:HG2	1.99	0.45
5:5:94:ARG:NH1	5:5:244:ALA:O	2.49	0.45
10:C:124:GLN:HA	11:D:127:ARG:HG2	1.99	0.45
13:l:34:VAL:HG22	13:l:162:GLY:HA3	1.99	0.45
17:J:192:GLY:N	17:J:252:SER:O	2.50	0.45
17:J:361:VAL:HG22	17:J:389:VAL:HG21	1.98	0.45
19:L:164:ASP:O	19:L:166:LEU:N	2.49	0.45
23:P:268:LEU:HD13	23:P:280:LEU:HD12	1.98	0.45
24:Q:223:GLY:HA2	24:Q:226:HIS:HD2	1.82	0.45
29:V:51:GLY:HA3	29:V:108:TYR:CZ	2.52	0.45
3:h:72:ASN:ND2	10:d:96:GLN:OE1	2.47	0.45
10:d:63:THR:HG21	10:d:212:GLU:HG2	1.98	0.45
15:H:320:ASP:OD1	20:M:290:ARG:NH2	2.50	0.45
22:O:352:TRP:CZ2	22:O:355:PRO:HA	2.52	0.45
33:Z:321:PHE:HB3	33:Z:326:VAL:HG21	1.98	0.45
33:Z:538:CYS:HA	33:Z:577:GLN:HE22	1.82	0.45
6:6:183:THR:HB	6:6:186:LYS:HB3	1.98	0.45
5:f:96:THR:HG22	5:f:101:VAL:HA	1.99	0.45
6:e:76:PHE:HE2	6:e:78:ALA:HB3	1.82	0.45
9:B:48:GLU:O	9:B:63:LYS:NZ	2.37	0.45
13:F:9:ASP:OD1	13:F:10:THR:N	2.50	0.45
13:l:50:LYS:HB3	13:l:59:TYR:HB3	1.99	0.45
15:H:100:ALA:HB2	15:H:149:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:875:LEU:HD12	21:N:876:PRO:HD2	1.99	0.45
23:P:261:LEU:HD21	23:P:293:LEU:HD22	1.99	0.45
26:S:111:ARG:HA	26:S:117:SER:HB3	1.98	0.45
26:S:330:LEU:HB2	32:Y:64:TRP:HD1	1.82	0.45
31:X:7:VAL:HG12	31:X:8:ILE:HG13	1.99	0.45
33:Z:576:GLY:H	33:Z:606:CYS:HB3	1.81	0.45
8:A:126:GLN:HE22	9:B:81:ASP:HA	1.83	0.45
10:C:156:ASN:HA	11:D:83:ARG:HH12	1.82	0.45
11:D:12:SER:HB2	11:D:17:ILE:HA	1.98	0.45
13:l:117:GLN:HE22	14:k:84:ASP:HA	1.81	0.45
14:k:50:VAL:HG21	14:k:66:LYS:HB2	1.99	0.45
15:H:311:ILE:O	15:H:315:GLY:N	2.49	0.45
19:L:229:THR:HG21	20:M:313:ASP:HB3	1.98	0.45
20:M:214:ALA:N	20:M:319:ASP:OD2	2.50	0.45
23:P:335:LYS:HE3	23:P:336:HIS:CE1	2.52	0.45
25:R:325:HIS:O	25:R:328:PHE:HD2	2.00	0.45
26:S:217:PHE:HD2	26:S:233:LEU:HD11	1.82	0.45
27:T:131:LYS:HB3	27:T:134:LYS:HB2	1.98	0.45
28:U:259:ASN:HA	29:V:306:LYS:N	2.32	0.45
4:4:3:ILE:HG23	4:4:18:SER:HB3	1.98	0.44
7:7:215:ARG:HH12	7:7:249:ASN:HD22	1.65	0.44
1:b:167:LYS:HE3	1:b:196:VAL:HG11	1.99	0.44
6:e:90:SER:OG	6:e:111:ASN:ND2	2.50	0.44
8:A:156:LYS:HD3	8:A:166:TYR:HE2	1.82	0.44
11:D:138:PHE:HE1	11:D:145:PRO:HB3	1.81	0.44
11:n:72:VAL:HG13	11:n:221:ILE:HD13	1.99	0.44
13:l:81:ALA:HB2	13:l:130:VAL:HG21	1.97	0.44
17:J:147:TYR:OH	17:J:165:GLU:OE1	2.33	0.44
23:P:126:THR:O	23:P:136:ARG:NH2	2.50	0.44
2:i:81:THR:HG23	2:i:127:LEU:HD21	1.98	0.44
3:h:12:VAL:HB	3:h:108:VAL:HG21	1.98	0.44
8:c:155:LYS:HE3	8:c:165:TYR:CE2	2.52	0.44
10:d:175:LEU:HD12	10:d:196:THR:HG23	2.00	0.44
11:n:115:GLY:O	11:n:119:ARG:N	2.44	0.44
16:I:106:ILE:HD11	17:J:93:LYS:HB2	1.99	0.44
17:J:328:LEU:O	17:J:332:SER:N	2.51	0.44
19:L:123:SER:C	19:L:125:PRO:HD2	2.43	0.44
24:Q:117:VAL:O	24:Q:117:VAL:HG12	2.17	0.44
24:Q:422:VAL:O	28:U:295:LYS:NZ	2.49	0.44
29:V:26:THR:HB	29:V:172:GLN:NE2	2.32	0.44
29:V:27:VAL:HG22	29:V:63:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:63:LEU:HD11	3:3:105:VAL:HG21	2.00	0.44
5:5:82:ARG:HD2	5:5:185:PRO:HB2	1.99	0.44
1:b:40:THR:HG21	1:b:187:SER:HA	1.98	0.44
2:i:244:GLU:HG2	3:h:198:ARG:HG2	1.99	0.44
3:h:10:GLY:HA3	3:h:42:LYS:NZ	2.32	0.44
11:n:68:ASP:OD1	11:n:69:SER:N	2.45	0.44
12:m:35:SER:OG	12:m:51:GLU:O	2.26	0.44
15:H:279:LEU:HB3	15:H:332:THR:HG21	2.00	0.44
18:K:395:VAL:HG21	19:L:207:PHE:HE1	1.81	0.44
21:N:750:SER:HA	21:N:753:PHE:HD2	1.82	0.44
26:S:247:VAL:O	26:S:251:SER:N	2.47	0.44
28:U:27:THR:HG23	28:U:31:LYS:HB2	2.00	0.44
1:1:182:ILE:HG12	1:1:189:GLY:HA2	1.99	0.44
2:2:123:ILE:HG22	2:2:125:ALA:H	1.83	0.44
6:e:35:ALA:HB3	6:e:154:GLN:HA	1.99	0.44
13:F:95:SER:O	13:F:100:ASN:N	2.50	0.44
14:G:78:TYR:HE2	14:G:82:ILE:HA	1.83	0.44
10:d:15:PRO:HA	11:n:22:TYR:CZ	2.52	0.44
11:n:122:GLN:HG3	12:m:138:PHE:HE1	1.82	0.44
18:K:360:MET:HE1	19:L:212:ILE:HA	1.99	0.44
19:L:137:ARG:HA	19:L:140:LEU:HD12	2.00	0.44
21:N:176:GLN:HG3	21:N:182:ASN:HD22	1.83	0.44
31:X:37:PRO:HB3	31:X:46:TRP:HD1	1.83	0.44
1:b:181:ALA:O	1:b:185:ASP:HB3	2.17	0.44
6:e:157:ALA:N	6:e:166:MET:SD	2.91	0.44
10:C:232:PRO:HA	10:C:235:ILE:HD12	1.99	0.44
11:D:196:VAL:HG13	11:D:210:ILE:HD13	1.99	0.44
15:H:311:ILE:HG22	15:H:355:THR:HB	1.99	0.44
21:N:245:LEU:HD11	21:N:257:ILE:HD12	1.98	0.44
28:U:210:TYR:HE2	28:U:229:LEU:HD11	1.83	0.44
29:V:168:LEU:HD12	29:V:170:PRO:HD2	1.98	0.44
30:W:110:ILE:HB	30:W:139:VAL:HA	2.00	0.44
33:Z:930:GLY:HA2	33:Z:966:GLU:HG3	1.99	0.44
5:f:91:VAL:HG11	5:f:109:VAL:HG23	2.00	0.44
8:A:88:PRO:HB3	14:G:156:SER:HB3	1.99	0.44
12:E:169:ALA:HB1	12:E:183:LEU:HD22	1.98	0.44
10:d:120:GLN:HE22	11:n:83:ARG:HB2	1.82	0.44
12:m:21:LEU:HB3	12:m:24:VAL:HG23	1.99	0.44
18:K:291:GLU:C	18:K:293:GLN:H	2.24	0.44
24:Q:377:LEU:HD23	24:Q:390:LEU:HD21	2.00	0.44
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:352:LYS:HB3	33:Z:466:GLU:HG3	2.00	0.44
10:C:91:ALA:HB2	10:C:115:LEU:HD21	1.99	0.44
12:m:21:LEU:HG	12:m:23:GLN:H	1.83	0.44
20:M:340:SER:HA	20:M:344:ASP:OD1	2.17	0.44
21:N:375:HIS:CD2	21:N:385:VAL:HG21	2.52	0.44
21:N:773:MET:HG3	21:N:869:ASP:OD2	2.18	0.44
23:P:358:SER:O	23:P:402:PHE:N	2.51	0.44
26:S:82:TYR:CD2	26:S:86:SER:HB3	2.52	0.44
28:U:74:GLU:OE2	28:U:113:TYR:OH	2.28	0.44
33:Z:812:ILE:HD12	33:Z:847:ILE:HG22	2.00	0.44
33:Z:821:GLY:HA3	33:Z:862:MET:HB2	1.98	0.44
2:2:244:GLU:HG3	3:3:198:ARG:HG2	2.00	0.44
4:4:7:ILE:HD12	4:4:144:LEU:HD22	2.00	0.44
5:5:186:THR:HG23	5:5:198:LYS:HE3	2.00	0.44
13:F:132:LEU:HB2	13:F:147:PHE:HB3	2.00	0.44
9:j:66:LEU:HD13	9:j:69:PRO:HB3	2.00	0.44
14:k:95:GLU:HB3	14:k:115:ARG:HE	1.82	0.44
17:J:48:ARG:HD3	18:K:72:GLN:HB2	2.00	0.44
21:N:778:LYS:HD3	21:N:878:GLN:HB2	2.00	0.44
30:W:109:ARG:HH22	30:W:195:GLY:HA3	1.83	0.44
2:2:30:THR:OG1	2:2:62:LYS:NZ	2.50	0.44
7:7:108:ALA:HA	7:7:112:PRO:HB3	2.00	0.44
6:e:107:SER:HB3	12:m:103:TYR:HD1	1.83	0.44
7:a:162:TYR:HE1	7:a:177:THR:HG22	1.83	0.44
10:C:52:VAL:HG23	10:C:59:GLN:HE21	1.83	0.44
14:G:150:MET:HB3	14:G:160:TYR:CE2	2.53	0.44
8:c:95:ARG:HE	8:c:123:LEU:HD13	1.83	0.44
14:k:70:VAL:HB	14:k:74:ILE:HB	2.00	0.44
21:N:596:LEU:HD23	21:N:628:ALA:HB2	1.98	0.44
21:N:724:THR:HG23	21:N:725:LEU:H	1.83	0.44
28:U:263:LYS:HE2	29:V:306:LYS:NZ	2.32	0.44
29:V:202:ASP:OD1	29:V:203:TYR:N	2.51	0.44
33:Z:309:GLN:HA	33:Z:312:TYR:HD2	1.83	0.44
33:Z:374:LEU:HB3	33:Z:379:GLN:NE2	2.33	0.44
5:f:112:ILE:HG23	5:f:135:GLY:HA2	2.00	0.43
14:G:204:HIS:CE1	14:G:208:LYS:HA	2.53	0.43
11:n:65:SER:O	11:n:73:LEU:N	2.51	0.43
24:Q:124:PHE:O	24:Q:126:LYS:N	2.50	0.43
3:3:4:PRO:HA	3:3:7:ILE:HD12	1.98	0.43
3:3:53:ILE:HG22	3:3:60:VAL:HG22	2.00	0.43
6:6:74:ASN:HB3	6:6:127:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:253:TYR:HE1	5:f:262:TYR:HD1	1.66	0.43
8:A:114:CYS:HB2	8:A:145:SER:OG	2.18	0.43
8:c:125:GLN:NE2	9:j:81:ASP:OD1	2.51	0.43
9:j:38:LYS:HG3	9:j:43:VAL:HG22	1.99	0.43
12:m:78:MET:HA	12:m:142:LEU:HD23	2.00	0.43
20:M:178:GLU:HB3	20:M:233:ARG:HG2	2.00	0.43
21:N:58:ARG:HA	21:N:61:ALA:HB3	2.00	0.43
21:N:625:LEU:HD21	21:N:637:ALA:HB1	1.99	0.43
25:R:191:LEU:HD13	25:R:213:TYR:HB3	2.00	0.43
28:U:94:HIS:CE1	28:U:122:ILE:HG12	2.53	0.43
33:Z:307:HIS:CE1	33:Z:340:LEU:HD12	2.53	0.43
33:Z:572:ILE:HD11	33:Z:882:LEU:HB2	2.00	0.43
1:1:145:ILE:HD11	1:1:154:TYR:CD1	2.50	0.43
3:3:8:ASN:OD1	3:3:57:ALA:N	2.37	0.43
3:3:29:LEU:HB3	3:3:37:SER:HB3	2.00	0.43
4:g:41:HIS:HB2	4:g:107:TYR:HB3	2.00	0.43
5:f:203:CYS:HB2	5:f:212:TYR:CE1	2.53	0.43
6:e:41:VAL:HG12	6:e:225:ILE:HG12	2.00	0.43
8:A:77:ARG:O	8:A:78:THR:OG1	2.30	0.43
12:E:45:GLY:HA2	12:E:153:TYR:CD1	2.53	0.43
11:n:167:ASN:HD22	11:n:202:VAL:HG12	1.83	0.43
13:l:39:ARG:HD3	13:l:144:LEU:HB2	2.00	0.43
15:H:177:ASP:OD1	15:H:178:ARG:N	2.51	0.43
22:O:76:LEU:HA	22:O:79:VAL:HG22	2.00	0.43
23:P:76:ASN:HB3	23:P:121:THR:HG21	2.01	0.43
25:R:63:TYR:HE1	25:R:92:ILE:HD12	1.83	0.43
25:R:240:SER:C	25:R:242:GLU:H	2.25	0.43
29:V:159:ILE:HD11	29:V:197:TYR:HA	2.00	0.43
30:W:4:GLU:CD	30:W:109:ARG:HE	2.26	0.43
7:7:114:ALA:HB1	7:7:117:GLU:HB2	2.00	0.43
3:h:113:ASN:OD1	3:h:114:SER:N	2.52	0.43
6:e:98:HIS:HD2	12:m:108:ASN:HD22	1.64	0.43
10:C:45:VAL:HG22	10:C:215:THR:HG23	2.00	0.43
10:C:83:ASP:HB3	10:C:131:PHE:CG	2.53	0.43
13:F:77:LEU:N	13:F:130:VAL:HG12	2.33	0.43
8:c:24:LEU:HD23	8:c:27:VAL:HG23	2.01	0.43
8:c:90:ARG:NH2	14:k:114:ASP:OD1	2.51	0.43
11:n:11:PHE:HB2	12:m:23:GLN:HE22	1.84	0.43
11:n:105:THR:HG22	11:n:107:GLU:H	1.83	0.43
18:K:48:TYR:HB3	21:N:151:LYS:HD3	2.00	0.43
22:O:132:GLU:OE2	22:O:135:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:390:LEU:HB2	25:R:345:TYR:HD1	1.84	0.43
27:T:202:LEU:HD23	27:T:205:ILE:HD12	1.99	0.43
3:3:16:THR:O	3:3:154:TYR:OH	2.27	0.43
7:7:185:ASN:HB3	7:7:186:PRO:HD3	1.98	0.43
7:a:47:MET:HG2	7:a:210:ILE:HD11	2.00	0.43
8:A:78:THR:HA	8:A:233:PHE:HB2	2.01	0.43
14:G:54:ILE:HB	14:G:211:ASP:HB2	1.99	0.43
8:c:86:ILE:N	8:c:87:PRO:HD2	2.34	0.43
18:K:186:GLU:HA	18:K:190:LEU:HD12	1.99	0.43
20:M:50:ARG:HG2	30:W:73:LEU:HD12	2.01	0.43
22:O:157:LEU:HD21	22:O:168:THR:HG23	2.01	0.43
28:U:12:PRO:HD2	28:U:163:ALA:HB2	2.01	0.43
28:U:14:VAL:HG13	28:U:51:SER:HB3	2.00	0.43
29:V:274:GLN:O	29:V:278:LYS:HG3	2.18	0.43
30:W:98:LEU:HD13	30:W:108:GLN:HB3	2.01	0.43
31:X:85:ARG:HH22	31:X:104:LYS:HG3	1.82	0.43
33:Z:76:LYS:HE2	33:Z:150:GLY:HA2	2.01	0.43
2:i:206:VAL:HB	2:i:214:GLU:HB2	2.01	0.43
3:h:34:LEU:HD11	4:g:141:PHE:HE2	1.84	0.43
7:a:49:TYR:HE2	7:a:54:ILE:HG13	1.83	0.43
10:C:12:ILE:HA	11:D:19:GLN:NE2	2.34	0.43
11:n:35:GLY:HA3	11:n:44:LEU:HD23	2.01	0.43
20:M:186:LEU:HD13	20:M:231:LEU:HD11	2.00	0.43
21:N:230:VAL:CG1	21:N:723:GLY:HA3	2.49	0.43
21:N:681:ASN:HA	21:N:684:SER:HB3	2.00	0.43
25:R:235:LEU:HD12	25:R:253:ALA:HB2	2.01	0.43
26:S:427:ILE:HG22	26:S:432:ILE:HB	2.01	0.43
4:4:38:LEU:O	4:4:65:GLN:NE2	2.51	0.43
2:i:92:ILE:HG23	2:i:103:PRO:HG2	2.00	0.43
2:i:206:VAL:O	2:i:214:GLU:N	2.48	0.43
7:a:87:SER:OG	7:a:146:ALA:HB3	2.19	0.43
7:a:176:ALA:HB3	7:a:181:ALA:HA	1.99	0.43
8:A:218:PHE:HB3	8:A:222:ASP:HB2	2.01	0.43
9:B:94:HIS:HA	9:B:98:LYS:HB3	1.99	0.43
9:B:139:HIS:O	9:B:234:ARG:NH1	2.52	0.43
13:F:43:HIS:CD2	13:F:217:GLY:HA3	2.54	0.43
13:F:157:TYR:CE2	14:G:60:VAL:HG22	2.54	0.43
9:j:45:ILE:HD12	9:j:74:VAL:HB	1.99	0.43
16:I:171:MET:O	17:J:278:GLN:NE2	2.48	0.43
22:O:308:LEU:HB3	22:O:348:VAL:HB	2.00	0.43
23:P:144:VAL:HG13	23:P:156:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:189:ARG:HB3	25:R:277:LEU:HD13	2.00	0.43
28:U:263:LYS:HE2	29:V:306:LYS:HZ2	1.83	0.43
29:V:287:THR:O	29:V:291:ASN:ND2	2.49	0.43
2:2:242:LEU:N	3:3:199:TYR:O	2.49	0.43
6:6:89:ASN:HA	6:6:92:LYS:HB2	2.00	0.43
6:e:114:HIS:NE2	12:m:101:LEU:O	2.52	0.43
9:B:78:MET:HB2	9:B:81:ASP:HB2	2.00	0.43
10:C:19:LEU:HG	10:C:21:GLN:H	1.83	0.43
10:C:194:LEU:HD13	10:C:239:LEU:HD23	2.00	0.43
14:k:218:TRP:CH2	14:k:224:THR:HG23	2.54	0.43
16:I:96:LEU:O	16:I:100:ARG:N	2.51	0.43
17:J:25:GLN:HE22	21:N:99:GLU:HB3	1.84	0.43
20:M:69:ILE:HA	20:M:72:ASN:HB2	2.01	0.43
21:N:83:LEU:HD13	21:N:132:LYS:HB3	2.00	0.43
21:N:585:ARG:HB2	21:N:616:HIS:HB3	2.01	0.43
22:O:196:LEU:HD13	22:O:203:THR:HB	2.00	0.43
22:O:222:LEU:HB3	22:O:280:LEU:HD13	2.00	0.43
23:P:55:SER:HA	23:P:59:LEU:HB3	2.00	0.43
23:P:392:LYS:NZ	23:P:401:ASN:HD22	2.16	0.43
23:P:408:SER:HB2	23:P:413:ASN:HB3	2.01	0.43
24:Q:378:SER:HA	24:Q:381:ILE:HD12	2.01	0.43
26:S:486:LYS:HE2	28:U:308:ASP:HB3	2.00	0.43
2:2:126:TYR:HE1	2:2:144:ALA:H	1.67	0.43
8:A:87:ILE:N	8:A:88:PRO:HD2	2.34	0.43
9:j:32:VAL:O	9:j:76:SER:OG	2.27	0.43
9:j:92:VAL:O	9:j:96:SER:OG	2.32	0.43
15:H:362:ASP:HB3	15:H:365:LEU:HB2	1.99	0.43
17:J:64:LEU:HB3	18:K:121:ARG:HD2	2.01	0.43
18:K:426:PHE:HD1	18:K:427:TYR:H	1.67	0.43
19:L:107:GLU:OE2	19:L:145:ARG:NH2	2.52	0.43
25:R:72:VAL:O	25:R:72:VAL:HG12	2.19	0.43
27:T:88:TYR:C	27:T:90:PHE:H	2.25	0.43
28:U:24:ARG:HH11	29:V:100:ARG:HG2	1.84	0.43
29:V:23:THR:OG1	29:V:24:LYS:N	2.47	0.43
33:Z:312:TYR:CD1	33:Z:349:THR:HA	2.54	0.43
3:h:18:LYS:HB2	3:h:157:ASN:HA	2.01	0.43
6:e:21:PHE:CZ	7:a:142:PRO:HG2	2.53	0.43
6:e:203:VAL:HG12	6:e:221:LEU:HD21	2.00	0.43
14:G:54:ILE:HG12	14:G:59:LEU:HD23	2.00	0.43
14:G:119:TYR:O	14:G:123:HIS:ND1	2.47	0.43
15:H:170:GLU:HB3	20:M:166:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:229:LYS:HD2	16:I:327:ALA:HB1	2.01	0.43
17:J:48:ARG:HD2	18:K:75:LEU:HD23	2.01	0.43
19:L:255:TYR:HB2	19:L:258:GLU:HB3	1.99	0.43
25:R:352:SER:O	25:R:356:ALA:HB3	2.19	0.43
27:T:238:GLN:HG3	27:T:239:SER:N	2.34	0.43
8:A:183:GLU:HG2	8:A:187:LYS:HE3	2.00	0.42
8:c:193:ILE:HG22	8:c:195:GLU:H	1.84	0.42
19:L:421:LYS:O	19:L:425:VAL:HG23	2.19	0.42
21:N:286:LEU:HD23	21:N:289:ILE:HD12	2.00	0.42
21:N:724:THR:HG23	21:N:725:LEU:N	2.34	0.42
28:U:226:LEU:HD23	28:U:229:LEU:HD12	2.00	0.42
1:1:122:ASP:OD1	1:1:123:ASP:N	2.51	0.42
4:4:30:ASP:HB2	4:4:177:LYS:HB3	2.01	0.42
18:K:198:TYR:HA	18:K:201:ILE:HG12	2.01	0.42
21:N:227:LYS:O	21:N:231:ASN:HB2	2.20	0.42
22:O:306:ARG:NH1	22:O:349:THR:HB	2.31	0.42
24:Q:358:GLU:HG2	24:Q:360:SER:H	1.83	0.42
29:V:53:MET:HG3	29:V:108:TYR:HD1	1.84	0.42
2:2:36:LYS:HA	2:2:41:VAL:HA	2.01	0.42
3:h:69:TYR:HB2	10:d:100:LYS:HD2	2.01	0.42
15:H:304:CYS:SG	15:H:349:ILE:HG21	2.59	0.42
16:I:435:LEU:O	16:I:436:TYR:HB3	2.19	0.42
18:K:148:ASP:OD1	18:K:149:ILE:N	2.52	0.42
18:K:420:THR:C	18:K:422:ASP:H	2.27	0.42
22:O:308:LEU:O	22:O:348:VAL:N	2.47	0.42
25:R:313:ALA:HA	25:R:317:ILE:HD12	2.00	0.42
27:T:151:TRP:HE3	27:T:156:SER:HB3	1.83	0.42
27:T:227:PRO:O	27:T:229:VAL:N	2.52	0.42
2:i:239:THR:HG21	3:h:168:SER:HB3	2.01	0.42
6:e:43:ALA:HB1	6:e:221:LEU:HD11	2.00	0.42
8:A:24:ARG:HB3	18:K:427:TYR:HE1	1.84	0.42
12:E:21:LEU:HD12	20:M:432:PHE:CE2	2.54	0.42
11:n:11:PHE:CE2	12:m:26:TYR:HB2	2.54	0.42
17:J:156:GLN:NE2	17:J:315:GLU:O	2.51	0.42
22:O:289:GLN:HG3	22:O:313:ILE:HD11	2.00	0.42
23:P:54:SER:O	23:P:58:VAL:N	2.52	0.42
23:P:90:LYS:HD3	23:P:93:ILE:HD12	2.01	0.42
23:P:224:LEU:HD13	23:P:240:TYR:CG	2.55	0.42
26:S:327:ILE:HD11	26:S:390:THR:HG21	2.02	0.42
27:T:226:TRP:HA	27:T:232:LYS:HB3	2.01	0.42
33:Z:571:GLY:HA2	33:Z:574:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:149:ARG:HG2	4:4:152:MET:HG3	2.01	0.42
12:E:103:TYR:HB3	12:E:105:GLU:HG2	2.02	0.42
11:n:89:ALA:HB1	11:n:109:LEU:HD11	2.00	0.42
13:l:20:PHE:HA	13:l:23:GLU:HG2	2.01	0.42
16:I:435:LEU:C	16:I:436:TYR:HD1	2.28	0.42
17:J:41:VAL:O	17:J:45:GLU:HG2	2.19	0.42
18:K:180:GLN:HE22	18:K:219:LYS:NZ	2.17	0.42
21:N:207:LEU:HD22	21:N:228:VAL:HG22	2.01	0.42
26:S:26:ALA:HB2	26:S:68:LEU:HD12	2.02	0.42
29:V:60:ASP:HB3	29:V:61:TYR:CD2	2.55	0.42
7:7:94:GLN:HA	7:7:97:GLU:HB3	2.02	0.42
11:D:100:LEU:C	11:D:102:ASP:H	2.27	0.42
14:G:152:GLU:OE1	14:G:156:SER:OG	2.37	0.42
15:H:177:ASP:HB3	15:H:180:LYS:O	2.19	0.42
16:I:219:VAL:HA	16:I:344:ILE:HG23	2.02	0.42
21:N:668:THR:HG22	21:N:675:VAL:HB	2.02	0.42
24:Q:356:CYS:HA	24:Q:397:LEU:HB3	2.02	0.42
26:S:452:TYR:HE2	28:U:274:MET:HG3	1.84	0.42
6:6:214:HIS:ND1	2:i:54:ILE:HD13	2.35	0.42
6:e:46:THR:HB	6:e:58:TYR:HA	2.02	0.42
7:a:48:LYS:HG2	7:a:53:VAL:HG12	2.01	0.42
7:a:60:LEU:HD21	7:a:67:LEU:HD13	2.00	0.42
7:a:151:GLY:HA2	7:a:233:ILE:HG21	2.00	0.42
7:a:234:ASP:OD1	7:a:235:LYS:N	2.53	0.42
12:E:52:LYS:NZ	12:E:61:SER:HB3	2.35	0.42
14:G:62:GLN:HE22	14:G:236:LEU:HD21	1.85	0.42
14:G:67:ILE:HA	14:G:77:VAL:HG12	2.01	0.42
8:c:76:ARG:C	8:c:78:ILE:H	2.28	0.42
15:H:402:ILE:HD12	15:H:440:GLU:HB2	2.00	0.42
18:K:209:VAL:N	18:K:314:VAL:O	2.52	0.42
19:L:74:LEU:HD21	20:M:49:GLN:HB2	2.01	0.42
19:L:124:GLY:N	19:L:125:PRO:HD2	2.35	0.42
20:M:144:ASP:OD1	20:M:145:LEU:N	2.53	0.42
22:O:325:GLU:OE1	23:P:364:ARG:NH1	2.53	0.42
24:Q:359:ILE:HD12	24:Q:395:GLY:HA2	2.01	0.42
31:X:17:TYR:OH	31:X:97:TYR:OH	2.32	0.42
33:Z:284:LEU:HB3	33:Z:293:MET:HB3	2.01	0.42
33:Z:767:TYR:O	33:Z:773:ARG:NH2	2.52	0.42
2:2:50:THR:HG22	2:2:55:VAL:HG13	2.02	0.42
3:3:78:GLU:HB3	3:3:80:ARG:NH1	2.35	0.42
1:b:152:PHE:HE2	1:b:185:ASP:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:72:GLY:N	9:B:137:ALA:O	2.42	0.42
10:C:77:VAL:HG13	10:C:133:VAL:HG13	2.01	0.42
11:D:139:ASP:HB2	11:D:142:ASP:HB3	2.02	0.42
20:M:81:ASN:O	20:M:120:LYS:N	2.32	0.42
21:N:606:VAL:HB	21:N:621:THR:HB	2.01	0.42
21:N:781:ALA:HB1	21:N:868:VAL:HG11	2.01	0.42
23:P:393:VAL:H	24:Q:354:PHE:HB3	1.85	0.42
27:T:233:VAL:CG1	27:T:234:TYR:H	2.25	0.42
27:T:238:GLN:HG3	27:T:239:SER:H	1.85	0.42
6:6:62:VAL:HG22	6:6:72:SER:HB2	2.02	0.42
7:7:124:TYR:HD1	13:F:100:ASN:HB3	1.85	0.42
3:h:178:ASP:OD1	3:h:179:ALA:N	2.53	0.42
7:a:60:LEU:HB2	7:a:225:SER:HB3	2.02	0.42
23:P:425:HIS:NE2	28:U:203:LYS:HG3	2.35	0.42
33:Z:182:SER:H	33:Z:267:THR:HG22	1.84	0.42
3:3:30:GLY:HA3	3:3:35:GLY:HA2	2.02	0.42
5:5:265:ASN:OD1	5:5:266:HIS:N	2.53	0.42
7:7:60:LEU:HD11	7:7:62:SER:HB2	2.02	0.42
7:7:115:ASP:OD1	7:7:116:ALA:N	2.52	0.42
6:e:116:LEU:HD13	6:e:148:GLY:HA2	2.02	0.42
9:B:9:LEU:HD11	9:B:123:GLN:O	2.20	0.42
8:c:155:LYS:HB3	8:c:165:TYR:HE2	1.84	0.42
10:d:52:VAL:HG11	10:d:57:LEU:HD13	2.02	0.42
18:K:94:LEU:HB3	18:K:138:ALA:HB1	2.01	0.42
19:L:435:GLN:OE1	19:L:435:GLN:N	2.53	0.42
21:N:322:ASP:HB2	21:N:358:LYS:HE3	2.01	0.42
21:N:335:ALA:HB2	21:N:701:VAL:HA	2.01	0.42
22:O:56:PRO:HG2	22:O:59:LEU:HB2	2.02	0.42
26:S:352:VAL:HG22	26:S:387:VAL:HG22	2.02	0.42
28:U:13:LEU:HD13	29:V:35:LEU:HB2	2.01	0.42
29:V:67:ASP:OD1	29:V:68:VAL:N	2.52	0.42
1:1:139:HIS:HB2	7:7:69:PHE:CE1	2.55	0.41
2:2:217:ARG:HG2	2:2:218:ASN:HD22	1.84	0.41
3:3:109:VAL:HB	3:3:122:ALA:HB3	2.01	0.41
6:6:21:PHE:CZ	7:7:142:PRO:HG2	2.55	0.41
7:7:150:ALA:HB2	7:7:160:LEU:HD13	2.02	0.41
1:b:79:GLN:NE2	8:c:104:ARG:HE	2.18	0.41
2:i:47:THR:HB	2:i:59:ASN:HA	2.00	0.41
8:A:47:GLY:O	8:A:193:HIS:ND1	2.41	0.41
8:A:196:GLU:HG2	8:A:201:LYS:HB2	2.02	0.41
13:F:168:ALA:N	13:F:200:SER:OG	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:134:ARG:NE	14:k:13:SER:O	2.53	0.41
11:n:31:THR:O	11:n:76:SER:OG	2.31	0.41
15:H:292:ARG:HH21	20:M:168:LYS:NZ	2.18	0.41
17:J:43:ARG:HD2	26:S:477:VAL:HG12	2.02	0.41
17:J:231:ARG:HG2	17:J:275:LEU:HD11	2.01	0.41
22:O:47:LYS:NZ	22:O:52:ALA:H	2.18	0.41
22:O:124:ASP:OD1	22:O:125:GLY:N	2.53	0.41
22:O:186:ASN:HB3	22:O:226:LYS:HD2	2.02	0.41
25:R:36:SER:H	25:R:43:ARG:HH21	1.67	0.41
27:T:132:HIS:O	27:T:136:LEU:HB3	2.20	0.41
29:V:26:THR:HG23	29:V:200:ASN:O	2.20	0.41
3:3:8:ASN:OD1	3:3:56:LEU:HD12	2.21	0.41
5:5:218:ASN:HB2	5:5:231:LEU:HD13	2.03	0.41
4:g:29:LYS:HE2	4:g:31:SER:O	2.20	0.41
10:C:46:LEU:HD11	10:C:76:ALA:HB2	2.01	0.41
12:E:214:GLU:HG3	12:E:233:ASN:HB3	2.02	0.41
9:j:44:VAL:HG23	9:j:213:ILE:HG22	2.03	0.41
9:j:194:LEU:HG	9:j:250:LEU:HD11	2.01	0.41
15:H:100:ALA:O	15:H:174:VAL:N	2.37	0.41
15:H:422:VAL:HA	15:H:450:VAL:HG21	2.02	0.41
19:L:167:VAL:O	19:L:171:THR:HG22	2.19	0.41
21:N:760:GLY:H	21:N:769:PRO:HD2	1.85	0.41
25:R:62:TYR:HB2	25:R:180:PHE:CZ	2.55	0.41
26:S:424:SER:HB3	27:T:192:ASN:HD22	1.85	0.41
33:Z:462:VAL:HG22	33:Z:465:GLY:H	1.86	0.41
33:Z:804:ASP:OD1	33:Z:805:LEU:N	2.53	0.41
2:2:55:VAL:HB	6:e:213:ARG:HA	2.02	0.41
2:2:128:ILE:HD11	2:2:156:LEU:HB2	2.02	0.41
2:2:192:ILE:HG23	2:2:199:GLY:HA2	2.03	0.41
3:3:110:ALA:HA	3:3:121:ILE:HG22	2.01	0.41
4:4:130:TYR:HB2	4:4:144:LEU:HD13	2.03	0.41
1:b:20:THR:O	1:b:148:SER:N	2.48	0.41
4:g:1:MET:HA	4:g:176:PHE:HZ	1.85	0.41
8:A:24:ARG:HH11	18:K:424:PHE:HE2	1.67	0.41
8:A:30:TYR:HA	8:A:33:LYS:HG2	2.03	0.41
9:B:10:THR:O	9:B:12:PHE:HD2	1.96	0.41
15:H:247:LEU:HD13	15:H:374:LYS:HG2	2.02	0.41
15:H:396:MET:HB2	16:I:213:ILE:HG22	2.01	0.41
17:J:48:ARG:NH2	21:N:608:LEU:HB3	2.34	0.41
19:L:96:LYS:HG2	28:U:85:ALA:HB1	2.01	0.41
21:N:402:GLY:HA3	21:N:441:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:233:VAL:O	27:T:234:TYR:HB2	2.21	0.41
4:4:70:ARG:HA	11:D:90:ARG:NH1	2.35	0.41
5:5:177:CYS:HA	5:5:187:ILE:HG12	2.02	0.41
4:g:100:VAL:HG12	4:g:102:VAL:HG13	2.02	0.41
8:A:133:TYR:O	8:A:135:ARG:NH1	2.53	0.41
9:B:9:LEU:CD2	9:B:125:GLY:HA2	2.44	0.41
11:D:196:VAL:HG11	11:D:233:VAL:HG22	2.03	0.41
10:d:120:GLN:HE21	11:n:80:ALA:HA	1.86	0.41
11:n:118:GLN:NE2	12:m:83:ALA:O	2.54	0.41
21:N:875:LEU:HG	21:N:877:GLN:H	1.85	0.41
22:O:292:CYS:O	22:O:295:THR:OG1	2.31	0.41
27:T:227:PRO:N	27:T:232:LYS:HG3	2.36	0.41
27:T:234:TYR:O	27:T:239:SER:HA	2.19	0.41
28:U:16:LEU:HB3	29:V:32:ILE:HD11	2.02	0.41
28:U:135:ASP:HB3	28:U:156:HIS:CD2	2.55	0.41
28:U:291:LEU:HA	28:U:294:ASN:HB3	2.01	0.41
33:Z:841:GLU:H	33:Z:844:ALA:HB3	1.84	0.41
3:3:12:VAL:HG22	3:3:25:CYS:HB3	2.02	0.41
6:6:47:ARG:NH2	6:6:218:GLY:HA3	2.35	0.41
7:7:144:TRP:HE3	7:7:165:LEU:HD21	1.84	0.41
4:g:84:VAL:HG11	4:g:102:VAL:HG21	2.03	0.41
6:e:214:HIS:CE1	6:e:216:GLN:HB2	2.55	0.41
12:E:208:MET:SD	12:E:216:ASN:ND2	2.93	0.41
9:j:86:VAL:O	9:j:90:ARG:N	2.53	0.41
10:d:125:HIS:HE1	11:n:120:TYR:CZ	2.38	0.41
16:I:248:VAL:HG12	16:I:250:SER:H	1.86	0.41
18:K:151:PRO:O	18:K:153:ASP:N	2.52	0.41
25:R:305:PHE:N	25:R:306:PRO:HD2	2.36	0.41
28:U:222:ASN:CG	28:U:223:HIS:H	2.29	0.41
33:Z:172:ASP:HB3	33:Z:193:PHE:HB3	2.02	0.41
2:2:141:SER:HB3	2:2:154:LEU:HD13	2.03	0.41
3:3:89:GLN:HE22	3:3:130:ILE:HD13	1.85	0.41
1:b:57:HIS:HB3	1:b:60:ILE:HB	2.01	0.41
4:g:91:SER:HB3	4:g:98:TYR:HB2	2.03	0.41
5:f:134:LEU:HD21	5:f:154:ALA:HB1	2.02	0.41
10:C:9:ARG:HD2	11:D:4:TYR:HE2	1.86	0.41
12:m:47:VAL:HG11	12:m:197:GLU:HA	2.03	0.41
14:k:52:LYS:NZ	14:k:64:ASN:O	2.39	0.41
14:k:71:ASP:CG	14:k:72:ARG:H	2.27	0.41
18:K:136:SER:HB3	18:K:150:LEU:HD12	2.03	0.41
19:L:120:LYS:HA	19:L:126:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:223:PRO:HA	20:M:224:PRO:HD3	1.95	0.41
20:M:287:GLY:O	20:M:288:THR:HB	2.21	0.41
21:N:269:LEU:HD12	21:N:272:ILE:HD12	2.03	0.41
21:N:773:MET:HE2	21:N:869:ASP:OD1	2.21	0.41
22:O:287:LEU:HD23	22:O:290:LYS:HD3	2.03	0.41
23:P:116:ILE:HD11	23:P:146:ILE:HG21	2.01	0.41
23:P:319:GLU:OE1	23:P:323:ASN:HB3	2.21	0.41
28:U:157:LEU:O	28:U:159:CYS:N	2.53	0.41
29:V:169:GLU:O	29:V:171:ARG:N	2.50	0.41
1:1:209:PRO:HG2	7:a:252:TRP:CE2	2.55	0.41
6:6:55:ASN:O	7:7:189:ARG:NH2	2.54	0.41
6:6:203:VAL:HG12	6:6:221:LEU:HD21	2.02	0.41
7:7:77:PRO:HA	7:7:83:VAL:HA	2.03	0.41
7:7:123:SER:HB3	7:7:153:GLN:HE21	1.85	0.41
7:7:186:PRO:HG2	2:i:162:ALA:HB1	2.02	0.41
3:h:21:VAL:HG13	3:h:190:ILE:HD13	2.02	0.41
5:f:114:PRO:HA	5:f:260:TRP:CD1	2.56	0.41
6:e:35:ALA:N	6:e:154:GLN:O	2.53	0.41
9:B:97:TYR:O	9:B:101:TYR:N	2.49	0.41
10:C:124:GLN:HG2	11:D:126:VAL:HG13	2.03	0.41
14:G:41:LYS:HE3	14:G:147:HIS:HA	2.03	0.41
14:G:137:ILE:HD13	14:G:163:ALA:HB1	2.02	0.41
8:c:91:ASN:OD1	14:k:118:GLN:NE2	2.53	0.41
17:J:34:ILE:HD11	18:K:58:TYR:HB3	2.02	0.41
18:K:87:LYS:HE2	18:K:125:THR:HG21	2.03	0.41
18:K:206:PRO:HB3	18:K:335:ASP:HB3	2.03	0.41
21:N:873:ARG:CG	21:N:874:ILE:H	2.29	0.41
22:O:360:GLY:HA2	22:O:363:ILE:HD12	2.03	0.41
27:T:227:PRO:C	27:T:229:VAL:H	2.29	0.41
27:T:239:SER:OG	27:T:240:LYS:N	2.49	0.41
29:V:58:VAL:HG12	29:V:59:ASP:O	2.21	0.41
30:W:186:ALA:HA	30:W:191:ILE:HD12	2.02	0.41
3:3:150:CYS:O	3:3:154:TYR:HB3	2.21	0.41
4:4:110:LYS:NZ	10:C:142:ASP:OD2	2.49	0.41
4:4:164:CYS:O	4:4:168:LEU:HG	2.20	0.41
2:i:143:HIS:HD2	2:i:147:SER:HB3	1.85	0.41
4:g:152:MET:HE1	4:g:160:LEU:HD22	2.03	0.41
5:f:94:ARG:CZ	5:f:247:GLY:HA3	2.51	0.41
6:e:183:THR:HB	6:e:186:LYS:HB2	2.02	0.41
10:C:8:SER:HB3	10:C:12:ILE:HD12	2.02	0.41
11:D:7:ALA:HB3	12:E:136:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:50:VAL:HG21	12:E:66:LYS:HB2	2.02	0.41
12:E:54:ALA:HA	12:E:59:LEU:HD23	2.03	0.41
14:G:65:VAL:HG12	14:G:67:ILE:H	1.84	0.41
13:l:46:LEU:HG	13:l:135:ILE:HD13	2.03	0.41
23:P:122:ILE:HG22	23:P:124:VAL:H	1.86	0.41
23:P:384:VAL:HG12	24:Q:352:GLU:HG3	2.02	0.41
28:U:261:LEU:HD12	29:V:305:ILE:HB	2.02	0.41
29:V:57:PHE:CE1	29:V:135:ARG:HD3	2.56	0.41
30:W:20:ASP:HA	30:W:24:THR:C	2.46	0.41
31:X:66:LEU:HD11	31:X:91:PHE:HE2	1.86	0.41
31:X:91:PHE:HB3	31:X:94:ASN:ND2	2.35	0.41
1:1:47:ASN:HA	7:a:220:ARG:HH12	1.86	0.41
3:3:124:PHE:HA	3:3:129:CYS:O	2.21	0.41
3:3:176:ASP:O	5:f:104:GLN:NE2	2.54	0.41
6:6:43:ALA:HB2	6:6:223:ILE:HG12	2.03	0.41
6:6:84:VAL:O	6:6:88:LYS:N	2.48	0.41
3:h:34:LEU:HD11	4:g:141:PHE:CE2	2.56	0.41
5:f:109:VAL:HG21	5:f:253:TYR:HE2	1.85	0.41
5:f:196:ARG:NH1	11:n:101:GLU:OE2	2.54	0.41
6:e:83:LEU:HB3	6:e:87:PHE:CE2	2.56	0.41
11:n:11:PHE:CZ	12:m:26:TYR:HB2	2.56	0.41
11:n:48:ARG:HB2	11:n:209:ASN:HA	2.02	0.41
11:n:122:GLN:HG3	12:m:138:PHE:CE1	2.56	0.41
17:J:283:GLU:O	17:J:284:THR:OG1	2.37	0.41
18:K:99:PHE:HD2	18:K:133:PRO:HA	1.86	0.41
18:K:285:GLN:CD	19:L:302:GLN:HE22	2.29	0.41
19:L:97:ALA:HB1	20:M:132:VAL:HA	2.02	0.41
19:L:407:ARG:HH12	19:L:411:ASN:ND2	2.19	0.41
21:N:593:PHE:HA	21:N:596:LEU:HG	2.02	0.41
24:Q:378:SER:HB2	25:R:344:SER:HB2	2.03	0.41
24:Q:412:ALA:O	24:Q:416:VAL:HG22	2.20	0.41
27:T:29:PRO:HA	27:T:32:ILE:HD12	2.03	0.41
28:U:62:ASN:ND2	30:W:92:GLN:OE1	2.53	0.41
29:V:52:LEU:HD23	29:V:69:PHE:CZ	2.56	0.41
29:V:245:VAL:O	29:V:249:GLU:HB2	2.21	0.41
33:Z:72:LYS:HG3	33:Z:121:ILE:HD11	2.03	0.41
33:Z:217:GLU:O	33:Z:221:VAL:HG23	2.21	0.41
2:2:47:THR:O	2:2:60:CYS:N	2.37	0.41
8:A:16:ILE:HD12	8:A:18:ILE:HG13	2.03	0.41
8:A:160:ALA:HB3	18:K:426:PHE:CZ	2.56	0.41
9:B:177:LYS:HE2	24:Q:132:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:163:THR:HG21	11:D:171:VAL:HB	2.02	0.41
12:E:74:ILE:HG21	12:E:112:LEU:HD23	2.03	0.41
19:L:277:ILE:HG12	19:L:322:LYS:HB2	2.03	0.41
22:O:79:VAL:HG12	22:O:128:LEU:HG	2.03	0.41
26:S:22:GLU:HB3	26:S:68:LEU:HD22	2.03	0.41
26:S:49:ASP:HB2	26:S:50:PRO:HD3	2.03	0.41
27:T:191:LYS:HA	27:T:237:ASN:HB3	2.02	0.41
7:7:90:ILE:HG23	7:7:93:MET:HE2	2.02	0.40
7:a:49:TYR:CE2	7:a:54:ILE:HG13	2.55	0.40
7:a:162:TYR:HB2	7:a:175:LEU:HD13	2.03	0.40
11:D:17:ILE:HG22	11:D:19:GLN:H	1.84	0.40
11:D:118:GLN:HE21	11:D:122:GLN:NE2	2.19	0.40
12:E:119:LEU:HD13	12:E:122:ARG:HH21	1.86	0.40
14:G:53:LEU:HD21	14:G:207:ASN:HD21	1.86	0.40
17:J:153:LEU:HD13	17:J:198:LEU:HD11	2.03	0.40
20:M:157:ASP:OD1	20:M:158:THR:N	2.54	0.40
22:O:370:LEU:HA	22:O:373:TRP:HD1	1.86	0.40
24:Q:65:TYR:HA	24:Q:70:ALA:HB3	2.02	0.40
29:V:54:LEU:HB3	29:V:102:GLN:HB2	2.02	0.40
1:1:32:ILE:HG12	1:1:196:VAL:HA	2.03	0.40
4:4:3:ILE:HD12	4:4:136:SER:HB2	2.03	0.40
1:b:35:ALA:HB1	1:b:52:LYS:HB2	2.03	0.40
2:i:50:THR:HG22	2:i:55:VAL:HG22	2.03	0.40
8:A:23:GLY:HA2	9:B:23:TYR:HB3	2.02	0.40
10:C:26:LEU:HD12	16:I:432:LEU:HD12	2.03	0.40
16:I:167:MET:HE3	17:J:228:ARG:HH12	1.86	0.40
18:K:193:VAL:HG12	18:K:194:GLN:HG2	2.03	0.40
18:K:209:VAL:HB	18:K:315:ILE:HG12	2.03	0.40
19:L:329:ARG:HA	19:L:330:PRO:HD3	1.92	0.40
22:O:218:SER:HA	22:O:251:LEU:HD21	2.04	0.40
25:R:98:LEU:HA	25:R:101:GLU:HB2	2.03	0.40
26:S:357:LEU:HA	26:S:384:ARG:HH12	1.85	0.40
27:T:164:LEU:O	27:T:170:ASN:ND2	2.53	0.40
30:W:21:PHE:HB2	30:W:22:PRO:HD3	2.03	0.40
33:Z:352:LYS:O	33:Z:355:GLU:HG2	2.20	0.40
33:Z:456:GLY:HA2	33:Z:496:ALA:HB2	2.03	0.40
1:1:78:VAL:HG22	1:1:100:VAL:HG12	2.04	0.40
3:3:101:GLY:N	3:3:102:PRO:HD3	2.36	0.40
7:7:124:TYR:HE2	13:F:101:ARG:HH11	1.69	0.40
4:g:8:ARG:N	4:g:129:PRO:O	2.42	0.40
6:e:76:PHE:HD2	6:e:79:ASP:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:227:ILE:HG22	9:B:229:THR:H	1.86	0.40
9:j:217:GLU:HG2	9:j:231:LYS:HB3	2.03	0.40
15:H:272:ILE:HB	15:H:306:ILE:HA	2.03	0.40
16:I:318:ASP:OD2	16:I:321:ASP:HB2	2.22	0.40
18:K:346:ARG:HG2	18:K:349:ARG:HH22	1.86	0.40
19:L:151:THR:HG22	29:V:45:VAL:HG23	2.02	0.40
21:N:55:PHE:CZ	21:N:57:ASP:HB2	2.57	0.40
21:N:339:MET:HA	21:N:709:GLY:H	1.85	0.40
27:T:27:LEU:HB2	27:T:28:PRO:HD3	2.03	0.40
27:T:224:ARG:NH2	27:T:235:PHE:O	2.54	0.40
33:Z:528:LEU:HD13	33:Z:883:THR:HA	2.04	0.40
6:6:241:ASP:OXT	2:i:48:ARG:NH2	2.54	0.40
7:7:254:PHE:HB2	2:i:152:TYR:CE2	2.57	0.40
4:g:101:ASN:HB3	4:g:133:HIS:CG	2.56	0.40
10:C:120:GLN:HE22	11:D:81:ASP:HA	1.87	0.40
10:C:186:VAL:HG11	10:C:217:ARG:HD2	2.04	0.40
11:D:78:LEU:HG	11:D:80:ALA:H	1.87	0.40
13:l:11:VAL:HA	14:k:130:ARG:HD3	2.02	0.40
18:K:95:VAL:HB	18:K:139:LEU:HB2	2.03	0.40
21:N:510:HIS:HB2	21:N:513:ILE:HB	2.02	0.40
21:N:738:GLN:HG3	21:N:741:TYR:CD2	2.56	0.40
23:P:392:LYS:HG3	24:Q:354:PHE:CE2	2.57	0.40
24:Q:83:GLU:HA	24:Q:86:MET:HE2	2.04	0.40
24:Q:302:VAL:HG11	24:Q:338:LEU:HD13	2.03	0.40
24:Q:411:SER:HA	24:Q:414:GLU:HB3	2.03	0.40
29:V:130:GLU:HG3	29:V:158:LEU:HD23	2.03	0.40
29:V:169:GLU:HB2	29:V:170:PRO:HD3	2.04	0.40
29:V:262:THR:HA	29:V:270:TYR:HB2	2.03	0.40
7:7:220:ARG:HB3	1:b:44:TYR:CE1	2.57	0.40
2:i:63:LEU:HD12	2:i:215:TYR:HE1	1.87	0.40
7:a:53:VAL:HG21	7:a:150:ALA:HB1	2.03	0.40
11:D:70:HIS:ND1	11:D:71:VAL:HG23	2.36	0.40
8:c:29:TYR:HD1	8:c:32:LYS:HD2	1.87	0.40
16:I:150:HIS:O	16:I:154:MET:HA	2.21	0.40
18:K:383:ILE:HA	18:K:386:ILE:HD12	2.01	0.40
19:L:261:ARG:O	19:L:265:GLU:HG3	2.21	0.40
21:N:8:PRO:HB3	27:T:83:ASN:HB2	2.04	0.40
21:N:28:ILE:O	21:N:32:VAL:HG13	2.21	0.40
21:N:762:ARG:H	21:N:767:ALA:HB2	1.86	0.40
22:O:299:THR:HG22	22:O:300:VAL:HG23	2.03	0.40
23:P:144:VAL:HG12	23:P:148:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:246:TYR:CE2	25:R:279:LEU:HD13	2.56	0.40
29:V:28:TYR:HA	29:V:202:ASP:O	2.21	0.40
29:V:66:VAL:HG21	29:V:102:GLN:HG3	2.02	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	1	194/215 (90%)	188 (97%)	6 (3%)	0	100	100
1	b	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
2	2	224/261 (86%)	214 (96%)	10 (4%)	0	100	100
2	i	224/261 (86%)	220 (98%)	4 (2%)	0	100	100
3	3	202/205 (98%)	195 (96%)	6 (3%)	1 (0%)	25	64
3	h	202/205 (98%)	193 (96%)	8 (4%)	1 (0%)	25	64
4	4	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
4	g	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
5	5	210/287 (73%)	206 (98%)	4 (2%)	0	100	100
5	f	210/287 (73%)	204 (97%)	6 (3%)	0	100	100
6	6	220/241 (91%)	211 (96%)	9 (4%)	0	100	100
6	e	220/241 (91%)	211 (96%)	9 (4%)	0	100	100
7	7	227/266 (85%)	214 (94%)	13 (6%)	0	100	100
7	a	230/266 (86%)	223 (97%)	7 (3%)	0	100	100
8	A	239/252 (95%)	230 (96%)	9 (4%)	0	100	100
8	c	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
9	B	248/250 (99%)	237 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	248/250 (99%)	232 (94%)	16 (6%)	0	100	100
10	C	242/258 (94%)	231 (96%)	11 (4%)	0	100	100
10	d	242/258 (94%)	229 (95%)	13 (5%)	0	100	100
11	D	238/254 (94%)	225 (94%)	11 (5%)	2 (1%)	16	54
11	n	238/254 (94%)	227 (95%)	11 (5%)	0	100	100
12	E	240/260 (92%)	229 (95%)	9 (4%)	2 (1%)	16	54
12	m	240/260 (92%)	228 (95%)	12 (5%)	0	100	100
13	F	231/234 (99%)	217 (94%)	14 (6%)	0	100	100
13	l	229/234 (98%)	227 (99%)	2 (1%)	0	100	100
14	G	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
14	k	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
15	H	351/467 (75%)	313 (89%)	38 (11%)	0	100	100
16	I	360/437 (82%)	324 (90%)	36 (10%)	0	100	100
17	J	371/405 (92%)	350 (94%)	19 (5%)	2 (0%)	25	64
18	K	379/428 (89%)	336 (89%)	40 (11%)	3 (1%)	16	54
19	L	369/437 (84%)	338 (92%)	31 (8%)	0	100	100
20	M	363/434 (84%)	329 (91%)	32 (9%)	2 (1%)	22	60
21	N	843/945 (89%)	783 (93%)	56 (7%)	4 (0%)	25	64
22	O	385/393 (98%)	345 (90%)	40 (10%)	0	100	100
23	P	430/445 (97%)	381 (89%)	49 (11%)	0	100	100
24	Q	429/434 (99%)	394 (92%)	35 (8%)	0	100	100
25	R	398/429 (93%)	354 (89%)	41 (10%)	3 (1%)	16	54
26	S	473/523 (90%)	454 (96%)	18 (4%)	1 (0%)	44	78
27	T	270/274 (98%)	228 (84%)	42 (16%)	0	100	100
28	U	254/338 (75%)	244 (96%)	8 (3%)	2 (1%)	16	54
29	V	282/306 (92%)	239 (85%)	36 (13%)	7 (2%)	4	27
30	W	195/268 (73%)	177 (91%)	14 (7%)	4 (2%)	5	30
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100	100
32	Y	25/89 (28%)	20 (80%)	5 (20%)	0	100	100
33	Z	807/993 (81%)	747 (93%)	60 (7%)	0	100	100
All	All	13392/15139 (88%)	12503 (93%)	855 (6%)	34 (0%)	38	72

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	7	ALA
11	D	10	ILE
18	K	292	VAL
18	K	421	VAL
21	N	903	VAL
25	R	241	ILE
18	K	188	VAL
21	N	724	THR
21	N	874	ILE
29	V	60	ASP
29	V	61	TYR
30	W	22	PRO
12	E	134	MET
28	U	130	VAL
3	3	105	VAL
12	E	135	SER
17	J	134	VAL
20	M	167	VAL
25	R	421	VAL
29	V	144	ILE
29	V	172	GLN
29	V	189	ILE
30	W	147	ILE
20	M	422	VAL
3	h	105	VAL
25	R	72	VAL
21	N	761	ILE
26	S	83	PRO
29	V	303	VAL
30	W	21	PHE
17	J	258	VAL
28	U	215	ILE
29	V	165	ILE
30	W	118	ILE

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	162/178 (91%)	162 (100%)	0	100	100
1	b	162/178 (91%)	162 (100%)	0	100	100
2	2	185/214 (86%)	185 (100%)	0	100	100
2	i	185/214 (86%)	185 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	173/175 (99%)	173 (100%)	0	100	100
4	g	173/175 (99%)	173 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
5	f	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	195/224 (87%)	195 (100%)	0	100	100
7	a	198/224 (88%)	198 (100%)	0	100	100
8	A	206/210 (98%)	206 (100%)	0	100	100
8	c	206/210 (98%)	206 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	j	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	202 (100%)	1 (0%)	86	89
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	212/226 (94%)	212 (100%)	0	100	100
11	n	212/226 (94%)	212 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	190/193 (98%)	190 (100%)	0	100	100
14	G	201/239 (84%)	201 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	319/385 (83%)	317 (99%)	2 (1%)	84	88
17	J	325/352 (92%)	325 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	317/377 (84%)	317 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	710 (100%)	3 (0%)	89	90
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	447/489 (91%)	446 (100%)	1 (0%)	92	93
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	241/308 (78%)	240 (100%)	1 (0%)	89	90
29	V	249/268 (93%)	249 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	101/144 (70%)	101 (100%)	0	100	100
32	Y	26/81 (32%)	26 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	11639/13054 (89%)	11631 (100%)	8 (0%)	92	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	C	18	ARG
16	I	435	LEU
16	I	436	TYR
21	N	231	ASN
21	N	510	HIS
21	N	512	ASN
26	S	477	VAL
28	U	151	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	180	GLN
2	2	115	HIS

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Mol	Chain	Res	Type
2	2	138	HIS
2	2	143	HIS
3	3	89	GLN
3	3	169	GLN
4	4	55	GLN
4	4	86	GLN
4	4	112	ASN
4	4	133	HIS
4	4	146	HIS
4	4	147	HIS
5	5	104	GLN
5	5	251	ASN
5	5	266	HIS
5	5	284	ASN
6	6	127	HIS
6	6	172	GLN
6	6	178	GLN
7	7	35	GLN
7	7	153	GLN
7	7	249	ASN
1	b	79	GLN
2	i	64	HIS
2	i	110	GLN
2	i	114	GLN
2	i	143	HIS
2	i	223	ASN
3	h	204	GLN
4	g	86	GLN
5	f	104	GLN
5	f	137	GLN
5	f	141	HIS
6	e	98	HIS
6	e	111	ASN
6	e	174	ASN
6	e	216	GLN
7	a	70	ASN
8	A	15	HIS
8	A	126	GLN
8	A	181	ASN
9	B	143	ASN
10	C	21	GLN
10	C	120	GLN

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Mol	Chain	Res	Type
11	D	19	GLN
11	D	94	GLN
11	D	122	GLN
11	D	178	ASN
12	E	147	HIS
13	F	43	HIS
13	F	60	GLN
13	F	121	GLN
14	G	62	GLN
14	G	64	ASN
14	G	73	HIS
14	G	121	GLN
14	G	183	HIS
14	G	195	GLN
14	G	207	ASN
14	G	228	HIS
14	G	244	GLN
8	c	208	HIS
9	j	20	GLN
10	d	59	GLN
10	d	120	GLN
10	d	125	HIS
10	d	168	ASN
11	n	19	GLN
11	n	117	GLN
11	n	118	GLN
11	n	167	ASN
11	n	209	ASN
12	m	99	HIS
12	m	157	HIS
13	l	43	HIS
13	l	210	ASN
14	k	121	GLN
14	k	147	HIS
15	H	95	HIS
15	H	98	GLN
15	H	265	ASN
17	J	25	GLN
17	J	28	GLN
17	J	156	GLN
17	J	240	HIS
18	K	180	GLN

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Mol	Chain	Res	Type
18	K	388	GLN
19	L	99	GLN
19	L	203	ASN
19	L	273	HIS
19	L	302	GLN
19	L	328	ASN
20	M	240	ASN
20	M	364	HIS
21	N	116	GLN
21	N	176	GLN
21	N	300	ASN
21	N	375	HIS
21	N	525	ASN
22	O	75	GLN
22	O	117	ASN
22	O	177	GLN
22	O	235	HIS
22	O	304	ASN
22	O	326	HIS
22	O	354	GLN
23	P	30	ASN
23	P	183	GLN
23	P	401	ASN
24	Q	19	GLN
24	Q	145	HIS
24	Q	178	HIS
24	Q	226	HIS
24	Q	379	GLN
24	Q	418	GLN
24	Q	425	GLN
25	R	325	HIS
25	R	399	GLN
26	S	19	HIS
26	S	20	HIS
26	S	32	GLN
26	S	135	ASN
26	S	191	HIS
26	S	207	ASN
26	S	235	ASN
26	S	311	GLN
26	S	314	ASN
26	S	321	GLN

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Mol	Chain	Res	Type
26	S	369	GLN
26	S	437	ASN
26	S	438	HIS
26	S	450	ASN
27	T	74	ASN
27	T	93	ASN
27	T	192	ASN
28	U	71	ASN
28	U	127	GLN
28	U	128	GLN
28	U	142	GLN
28	U	173	HIS
29	V	172	GLN
29	V	186	GLN
29	V	193	ASN
29	V	195	HIS
29	V	217	HIS
30	W	29	GLN
30	W	42	ASN
30	W	106	GLN
30	W	107	HIS
30	W	136	ASN
31	X	38	ASN
31	X	94	ASN
33	Z	132	HIS
33	Z	276	ASN
33	Z	379	GLN
33	Z	577	GLN
33	Z	760	HIS
33	Z	766	HIS
33	Z	801	HIS
33	Z	810	ASN
33	Z	897	HIS
33	Z	959	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

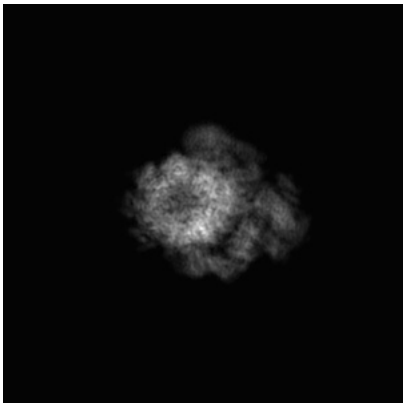
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9773. These allow visual inspection of the internal detail of the map and identification of artifacts.

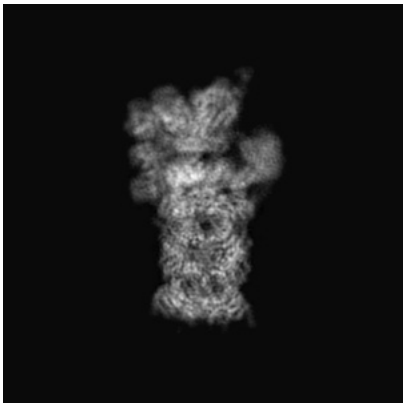
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

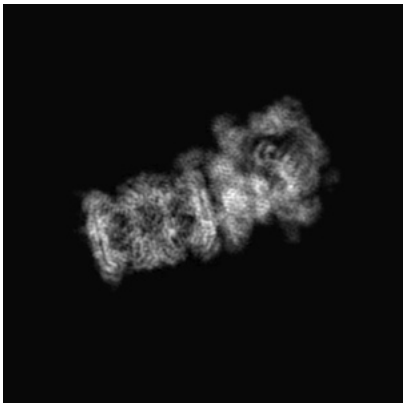
6.1.1 Primary map



X



Y

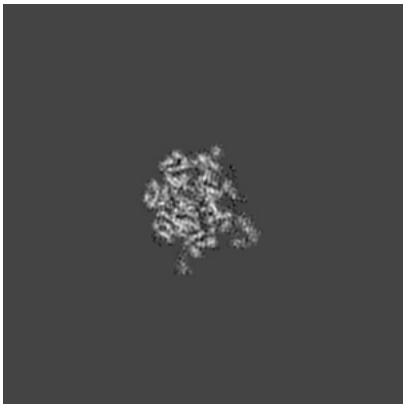


Z

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

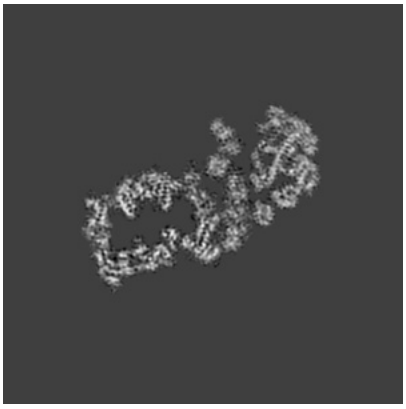
6.2 Central slices

6.2.1 Primary map



X Index: 180

Y Index: 180

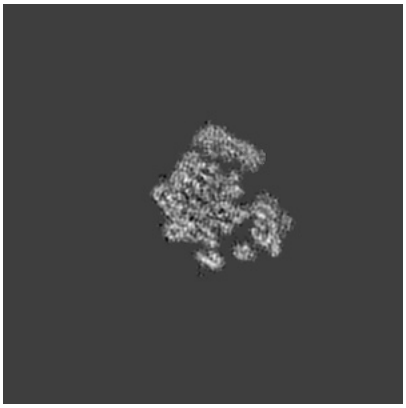


Z Index: 180

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 206

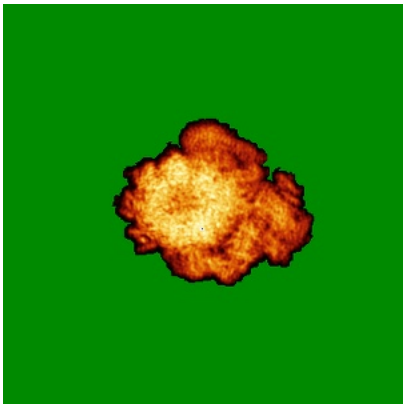
Y Index: 178

Z Index: 159

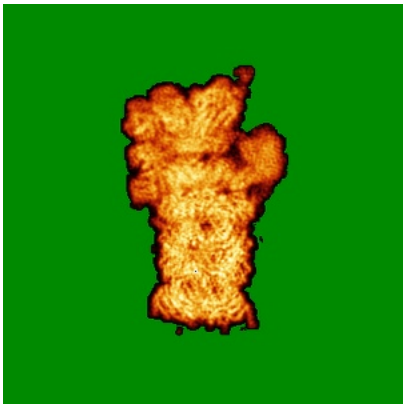
The images above show the largest variance slices of the map in three orthogonal directions.

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

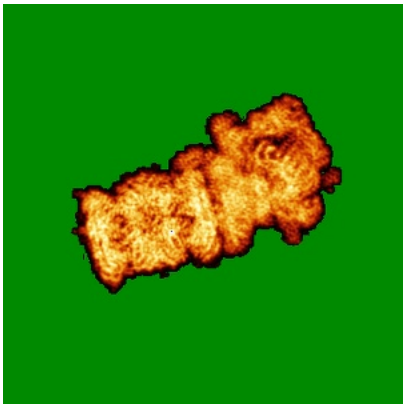
6.4.1 Primary map



X



Y

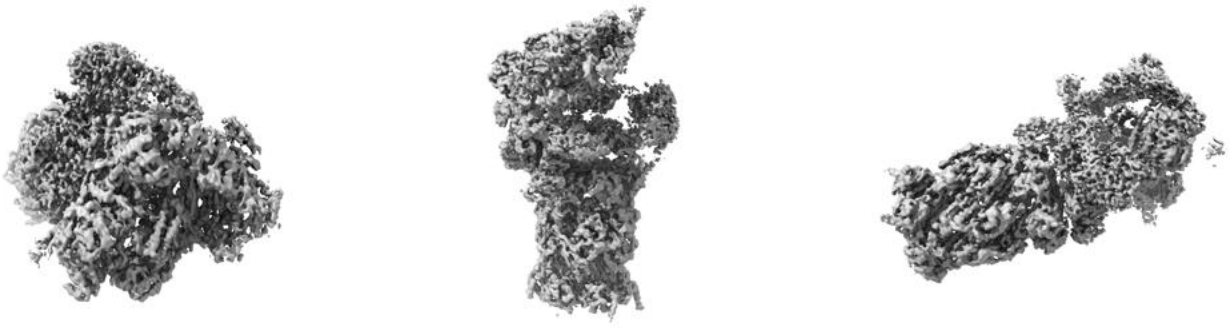


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.686. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

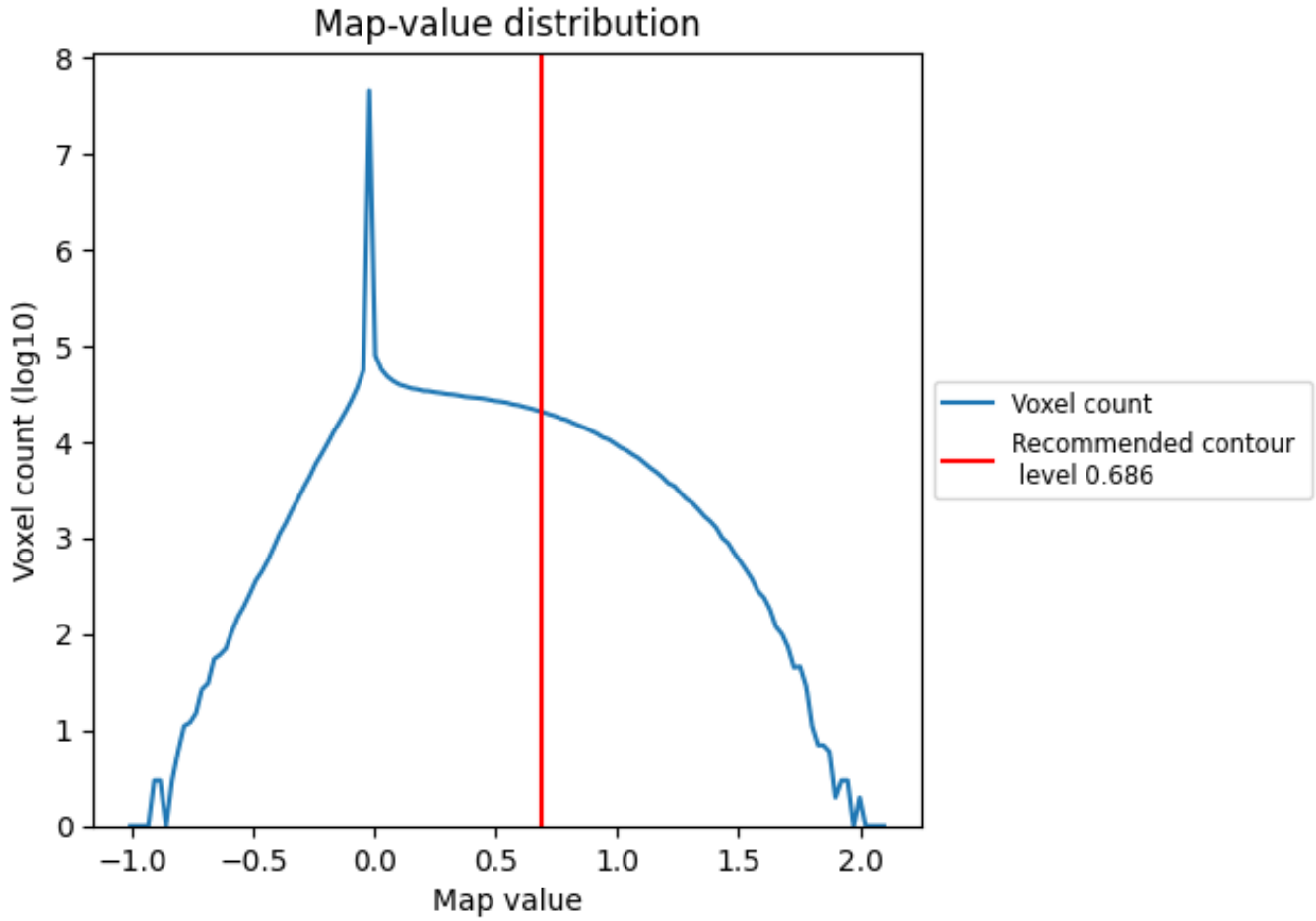
6.6 Mask visualisation (i)

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

7 Map analysis

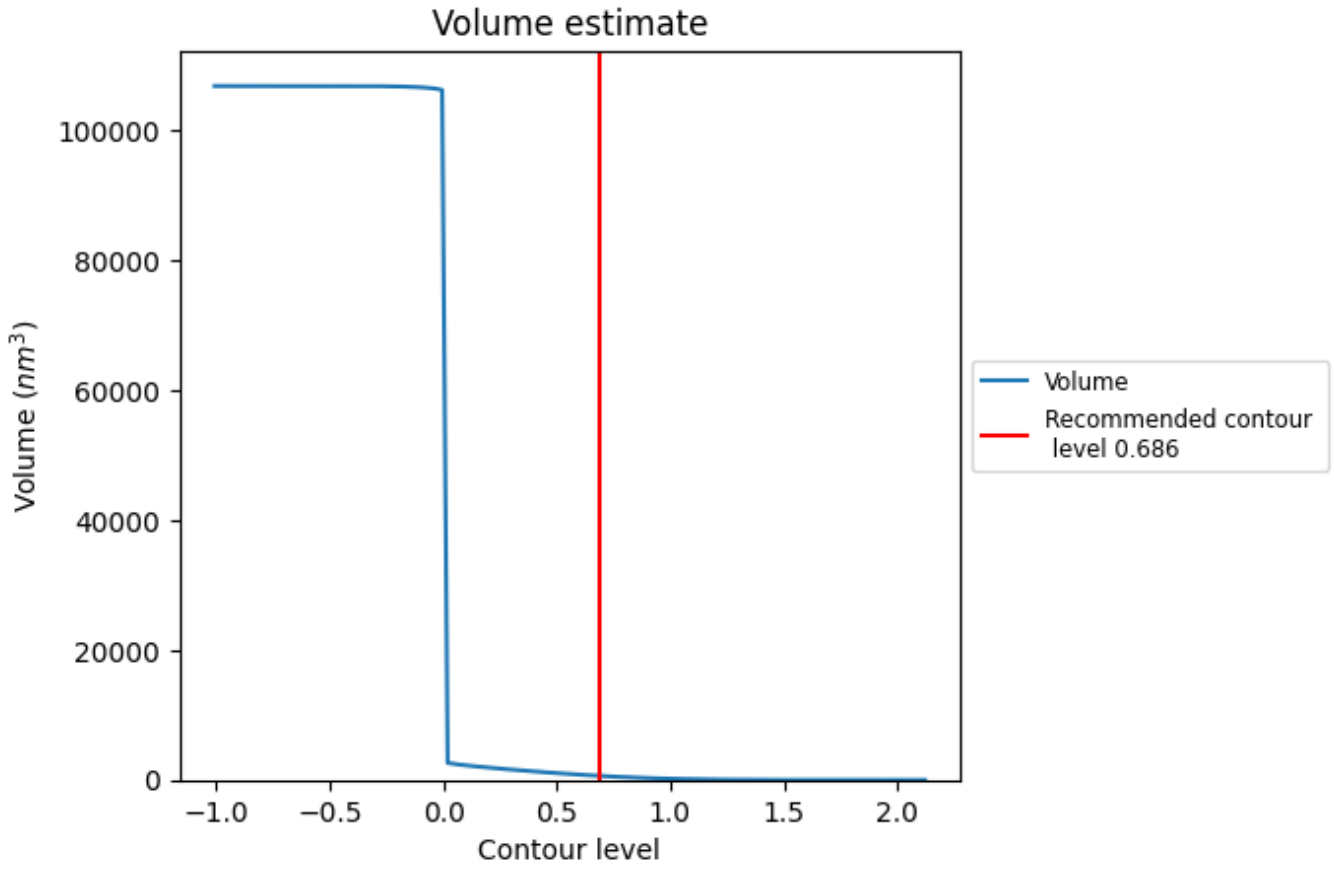
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

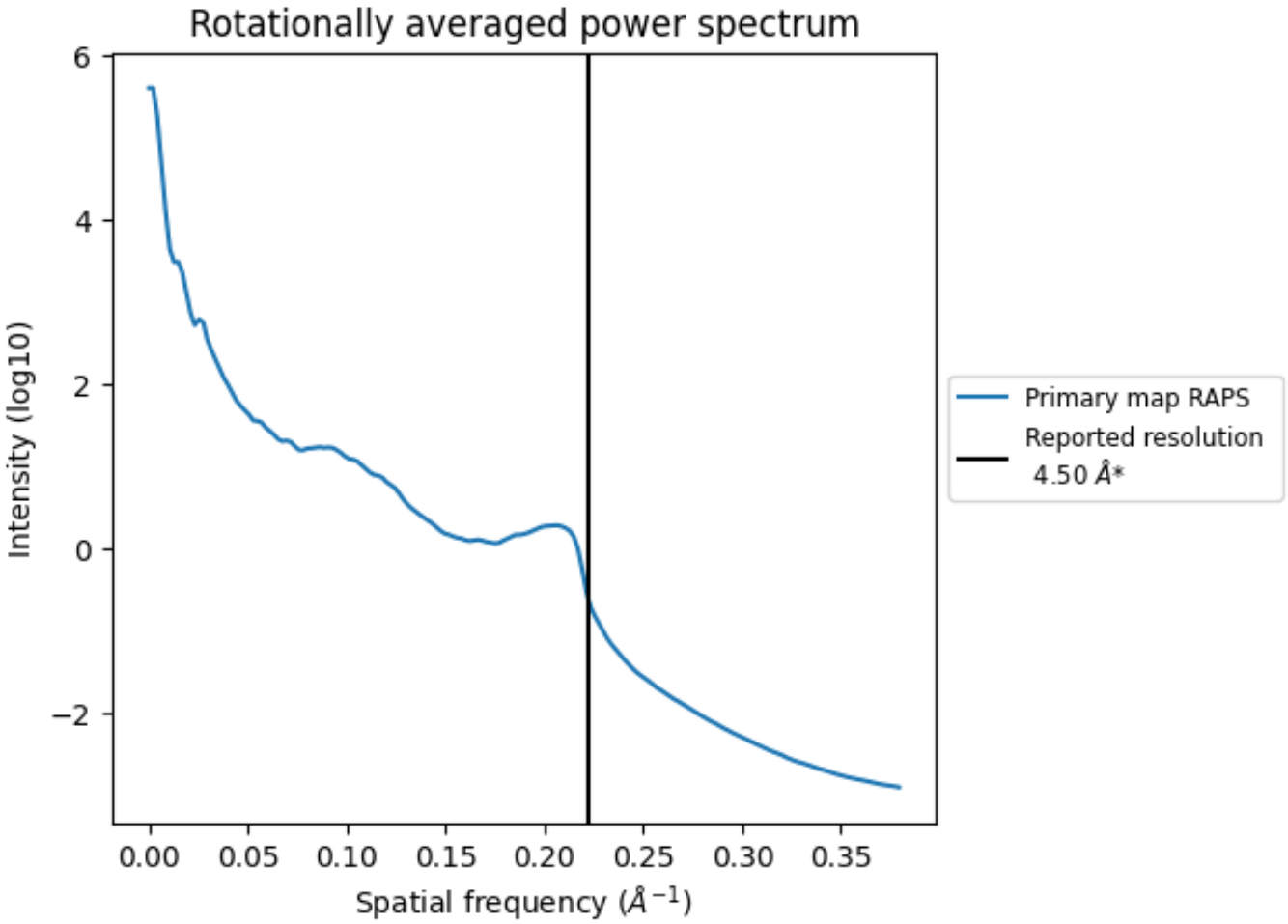
7.2 Volume estimate



The volume at the recommended contour level is 636 nm^3; this corresponds to an approximate mass of 574 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

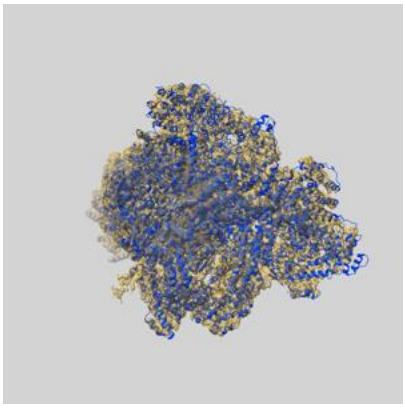
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

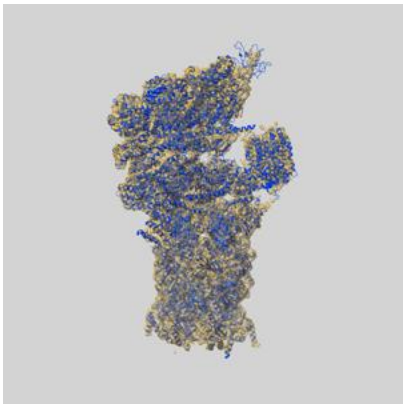
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9773 and PDB model 6J30. Per-residue inclusion information can be found in section 3 on page 11.

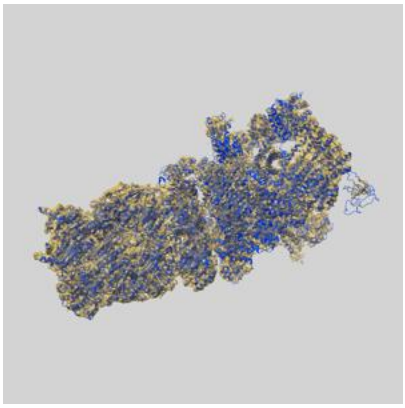
9.1 Map-model overlay



X



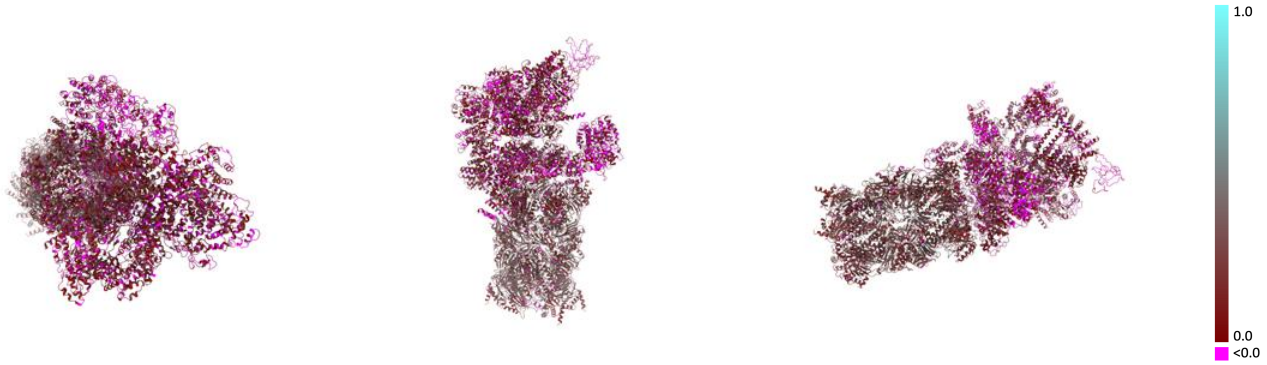
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.686 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.

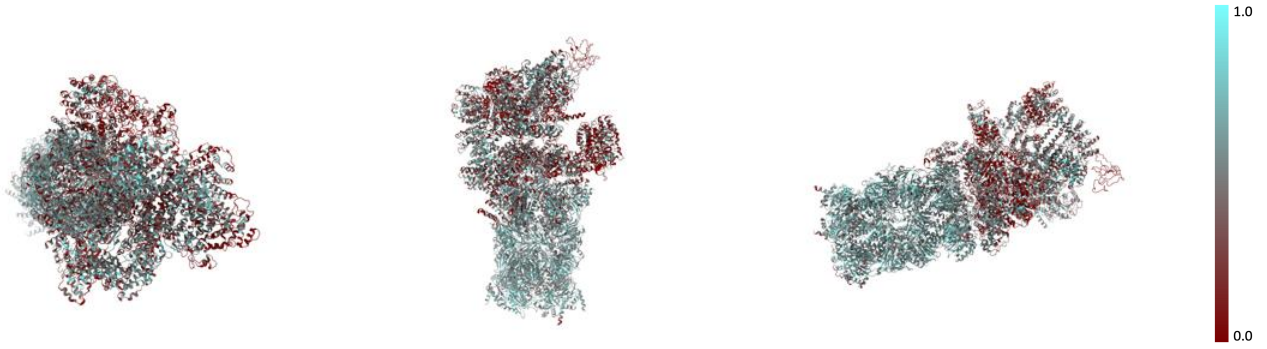
9.2 Q-score mapped to coordinate model



X Y Z

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

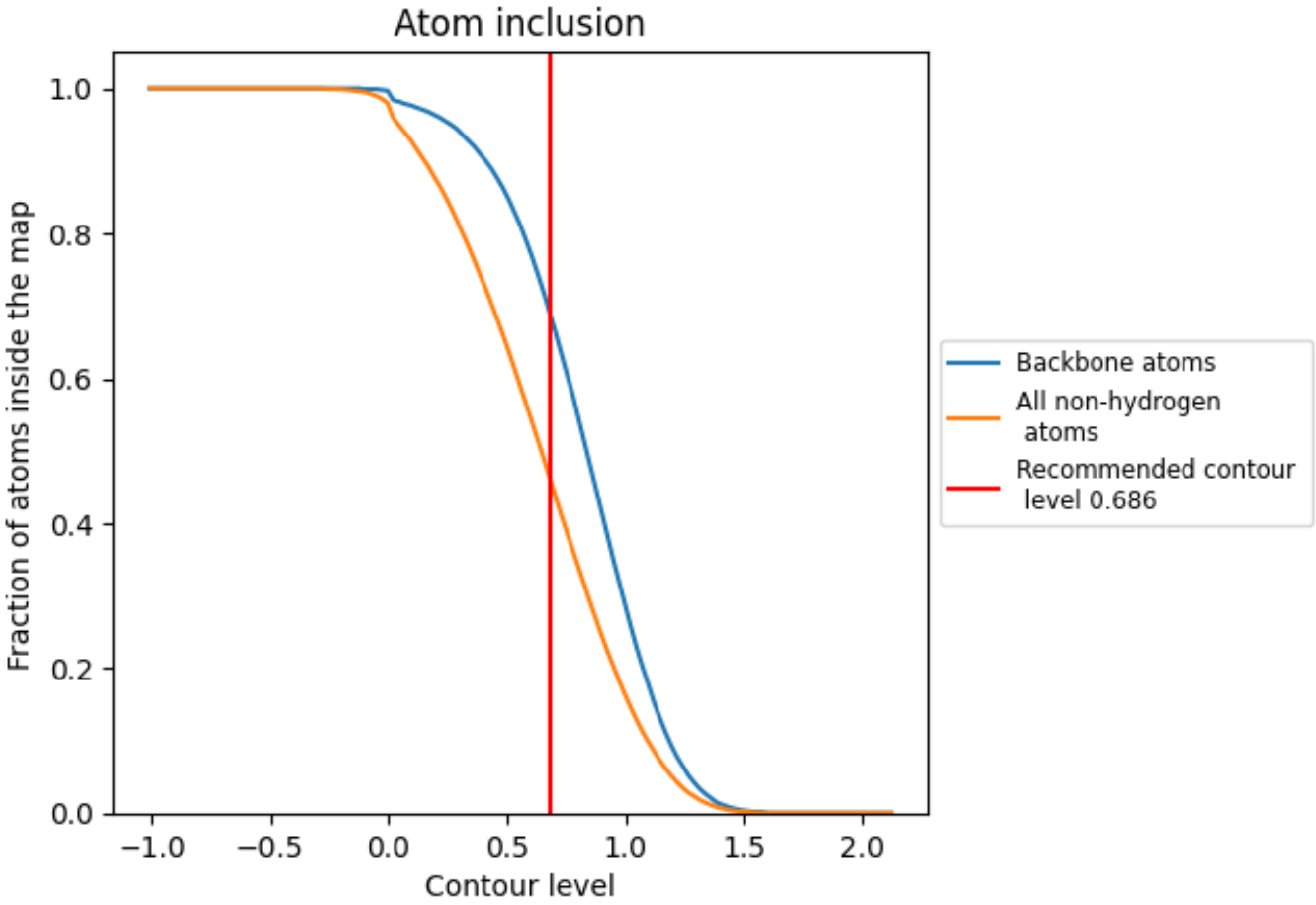
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.686).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 46% 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 (0.686) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4570	0.1710
1	0.6120	0.2860
2	0.5980	0.2640
3	0.5810	0.2540
4	0.6020	0.2560
5	0.6020	0.2670
6	0.6060	0.2690
7	0.6100	0.2740
A	0.5450	0.2310
B	0.4860	0.2040
C	0.5090	0.1880
D	0.5520	0.2190
E	0.5460	0.2210
F	0.5650	0.2210
G	0.5700	0.2380
H	0.3540	0.1410
I	0.3080	0.1030
J	0.2950	0.1080
K	0.3320	0.1150
L	0.3820	0.1520
M	0.3840	0.1380
N	0.4490	0.1330
O	0.4020	0.1020
P	0.4490	0.1250
Q	0.3680	0.1110
R	0.3890	0.0980
S	0.3390	0.1080
T	0.2080	0.0490
U	0.4530	0.1550
V	0.3640	0.1150
W	0.3950	0.0980
X	0.0290	-0.0280
Y	0.5000	0.1450
Z	0.2140	0.0320
a	0.6110	0.2860

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Chain	Atom inclusion	Q-score
b	0.6070	0.2680
c	0.5950	0.2280
d	0.5640	0.2290
e	0.5980	0.2550
f	0.6230	0.2740
g	0.6050	0.2700
h	0.5840	0.2840
i	0.5960	0.2760
j	0.5500	0.2170
k	0.5990	0.2380
l	0.6180	0.2470
m	0.5550	0.2150
n	0.5830	0.2290