



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:24 AM UTC

PDB ID : 6J2N / pdb_00006j2n
EMDB ID : EMD-9770
Title : yeast proteasome in substrate-processing state (C3-b)
Authors : Cong, Y.
Deposited on : 2019-01-02
Resolution : 7.50 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:

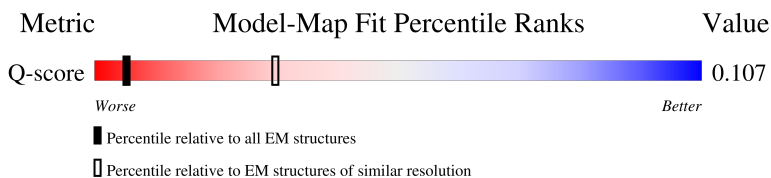
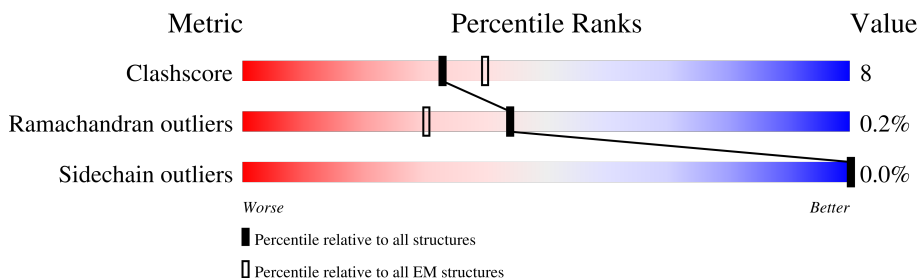
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 7.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (7.00 - 8.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	215	10% 68% 23% 9%
1	b	215	8% 74% 17% 9%
2	2	261	11% 64% 22% 13%
2	i	261	6% 69% 18% 13%

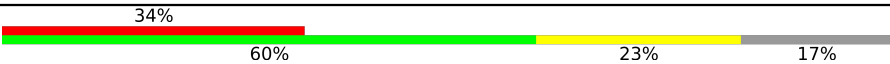
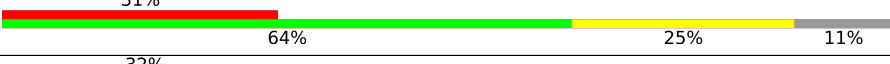
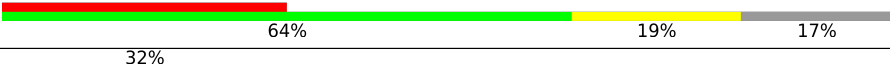
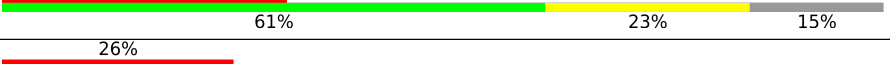
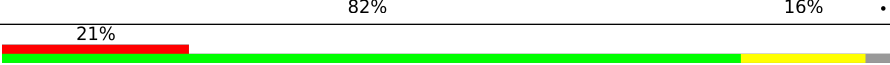
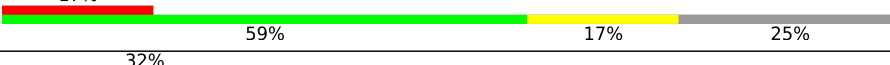
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Mol	Chain	Length	Quality of chain
3	3	205	
3	h	205	
4	4	198	
4	g	198	
5	5	287	
5	f	287	
6	6	241	
6	e	241	
7	7	266	
7	a	266	
8	A	252	
8	c	252	
9	B	250	
9	j	250	
10	C	258	
10	d	258	
11	D	254	
11	n	254	
12	E	260	
12	m	260	
13	F	234	
13	l	234	
14	G	288	
14	k	288	
15	H	467	

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Mol	Chain	Length	Quality of chain
16	I	437	
17	J	405	
18	K	428	
19	L	437	
20	M	434	
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106100 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 protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	359	Total	C	N	O	S	0	0
			2792	1755	499	523	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	363	Total	C	N	O	S	0	0
			2831	1779	472	565	15		

- Molecule 17 is a protein called 26S protease 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 protease 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 protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	361	Total	C	N	O	S	0	0
			2853	1798	507	536	12		

- Molecule 20 is a protein called 26S protease 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	255	Total	C	N	O	S	0	0
			2061	1312	352	391	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		

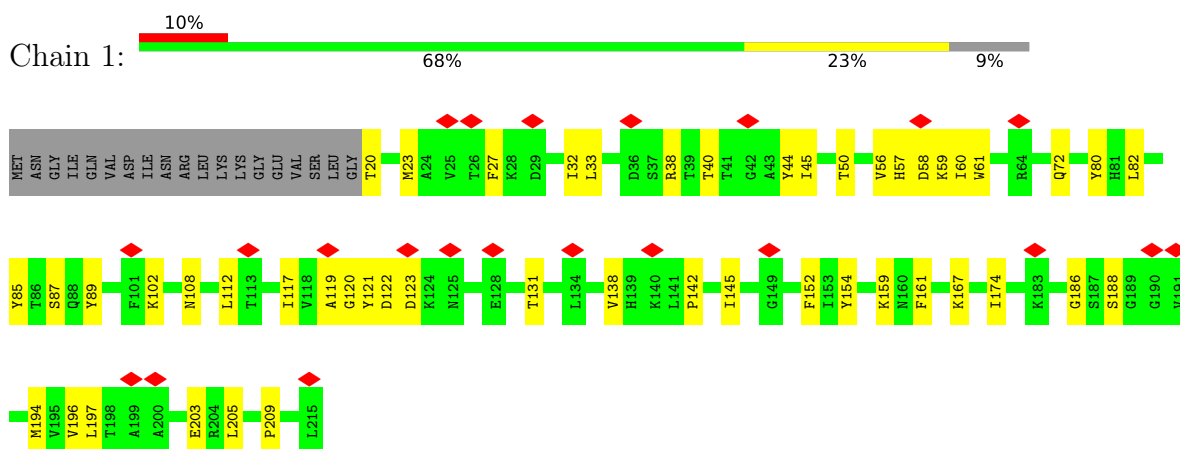
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

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

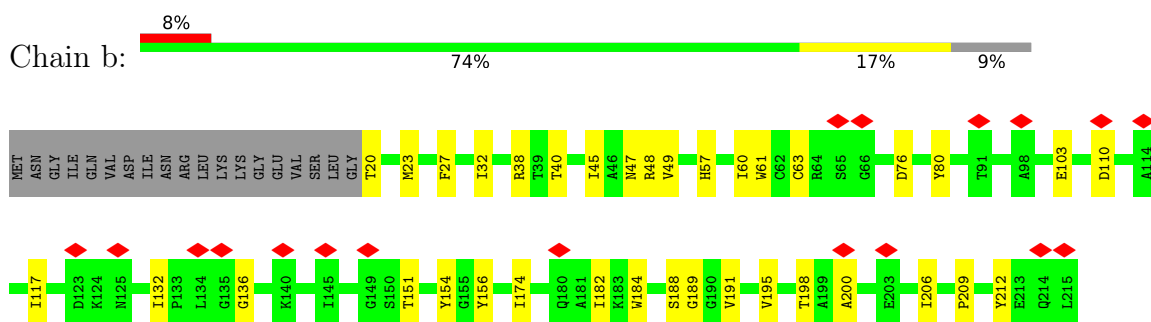
3 Residue-property plots

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.

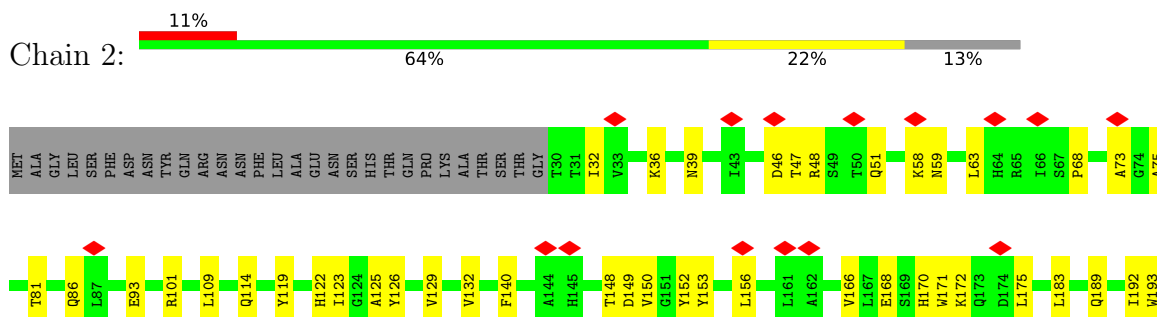
- Molecule 1: Proteasome subunit beta type-1

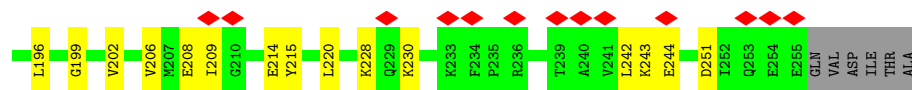


- Molecule 1: Proteasome subunit beta type-1



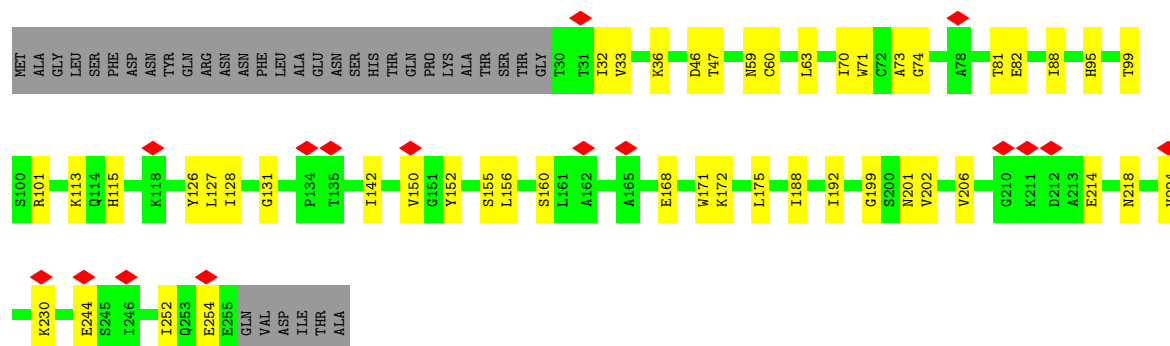
- Molecule 2: Proteasome subunit beta type-2





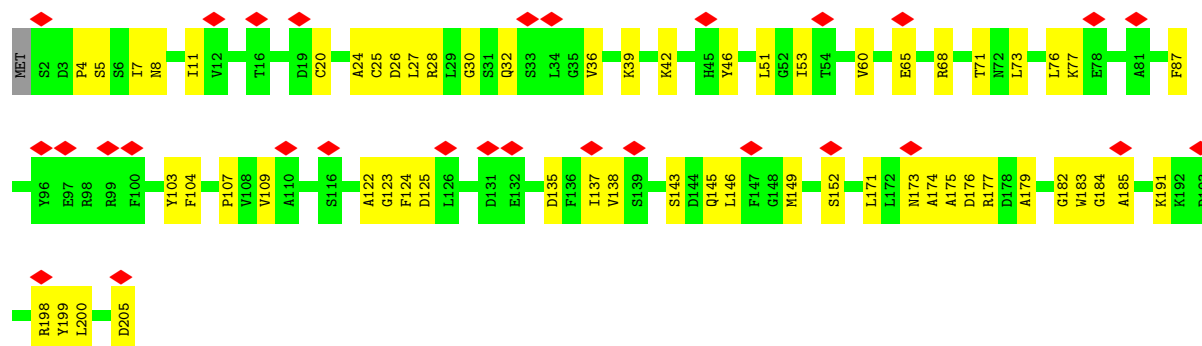
• Molecule 2: Proteasome subunit beta type-2

Chain i: 6% 69% 18% 13%



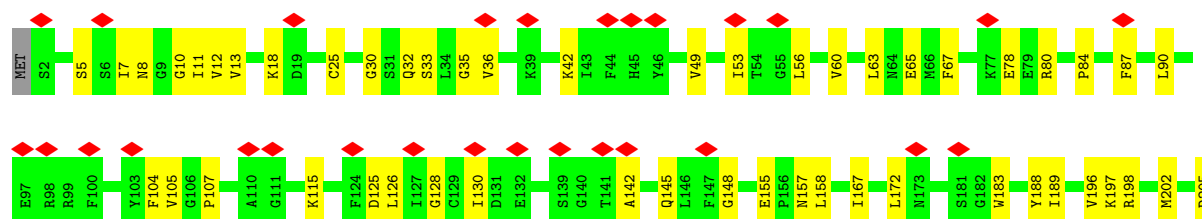
• Molecule 3: Proteasome subunit beta type-3

Chain 3: 14% 71% 29%



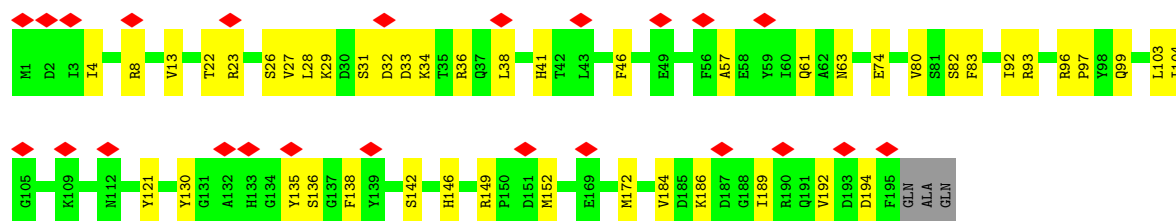
• Molecule 3: Proteasome subunit beta type-3

Chain h: 14% 75% 25%

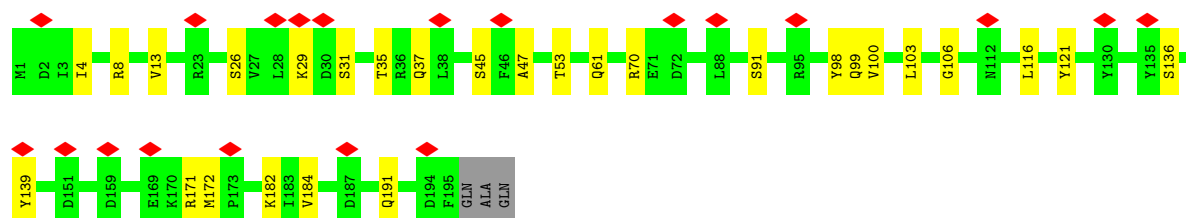
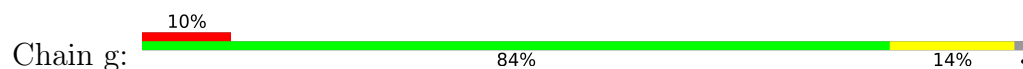


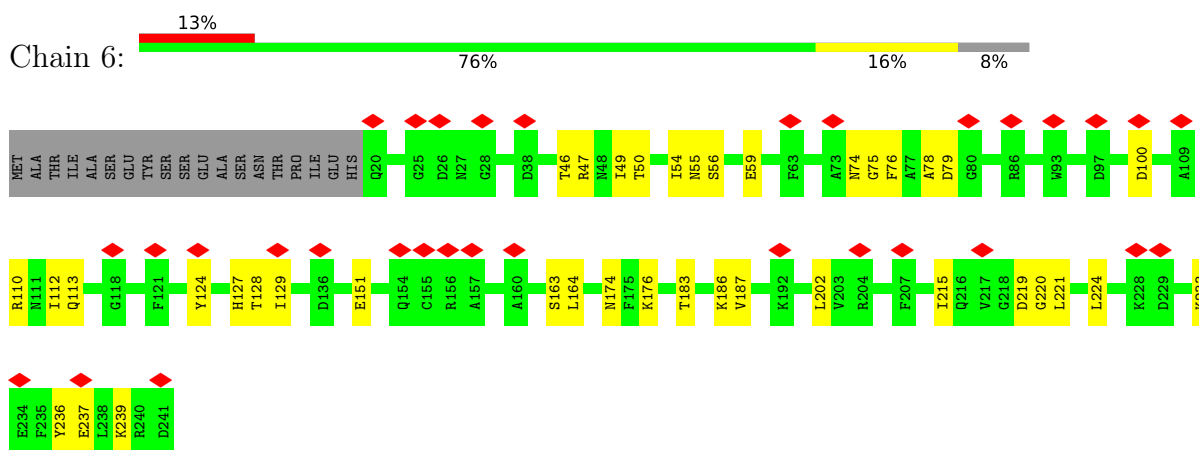
• Molecule 4: Proteasome subunit beta type-4

Chain 4: 12% 75% 23%

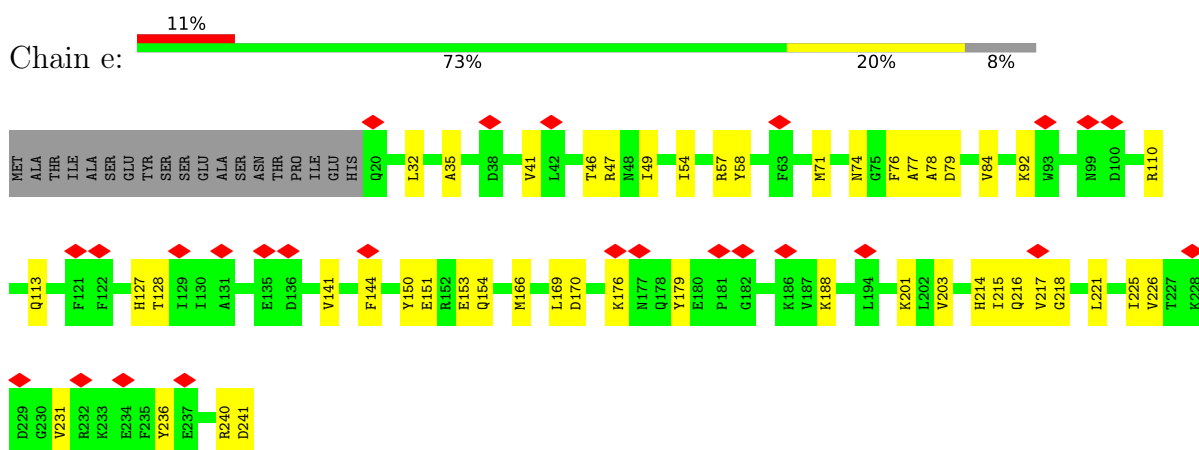


• Molecule 4: Proteasome subunit beta type-4

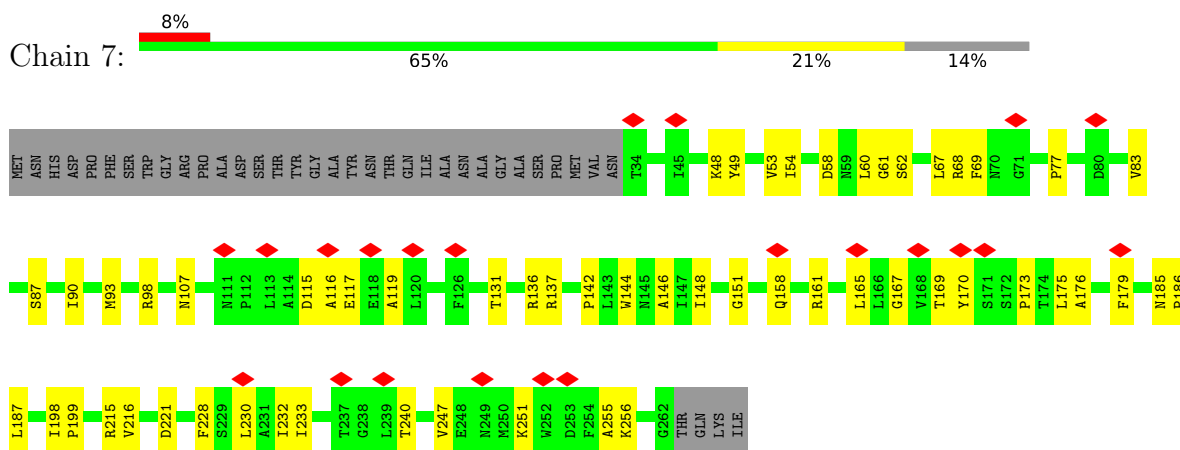




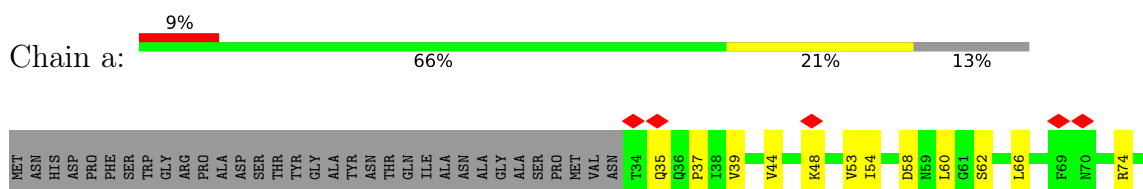
• Molecule 6: Proteasome subunit beta type-6

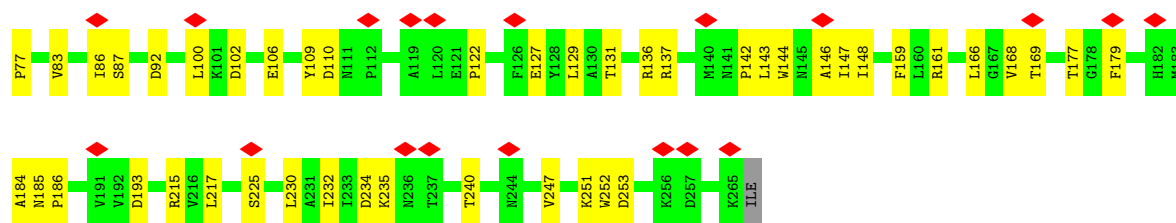


• Molecule 7: Proteasome subunit beta type-7

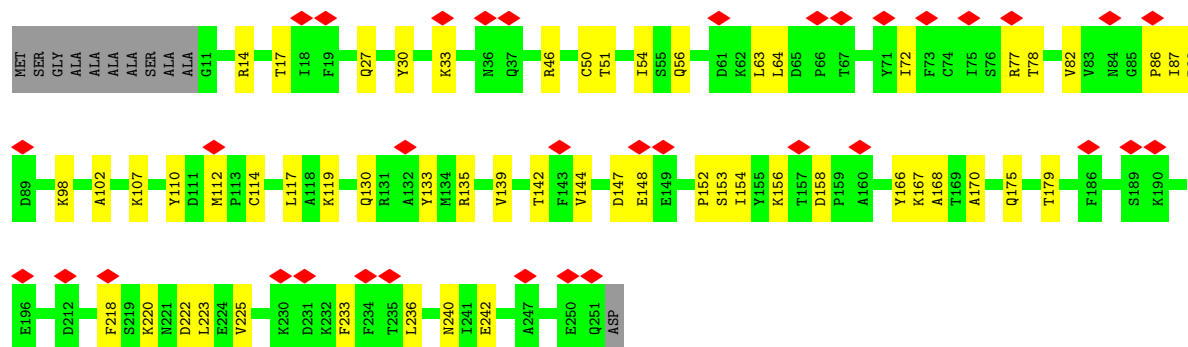
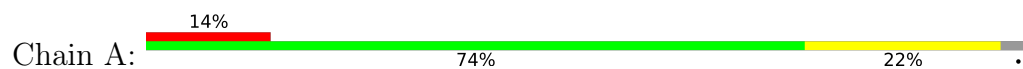


• Molecule 7: Proteasome subunit beta type-7

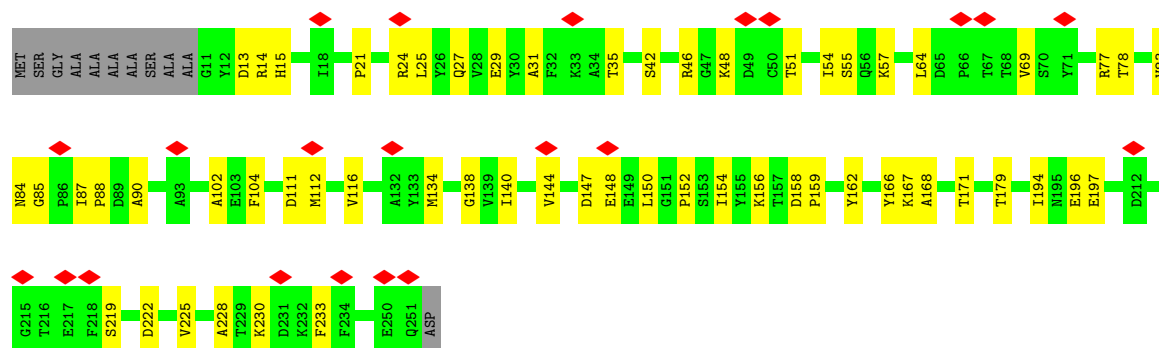
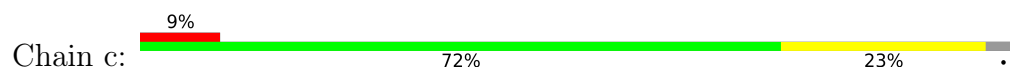




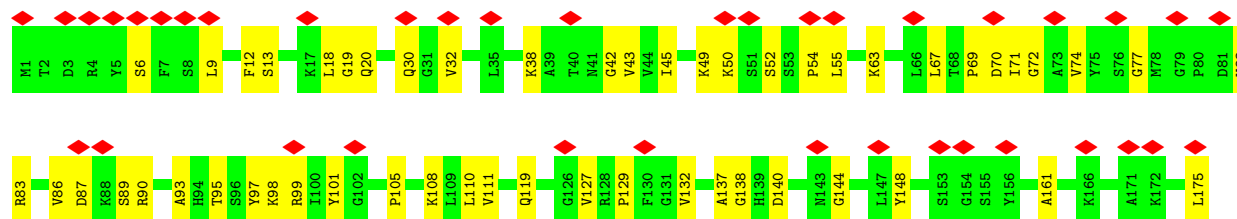
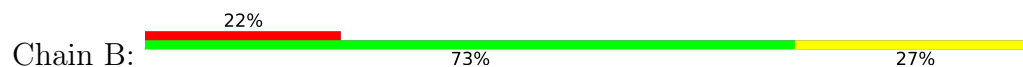
• Molecule 8: Proteasome subunit alpha type-1

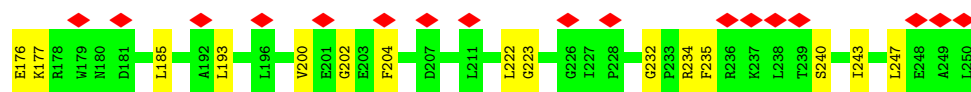


• Molecule 8: Proteasome subunit alpha type-1

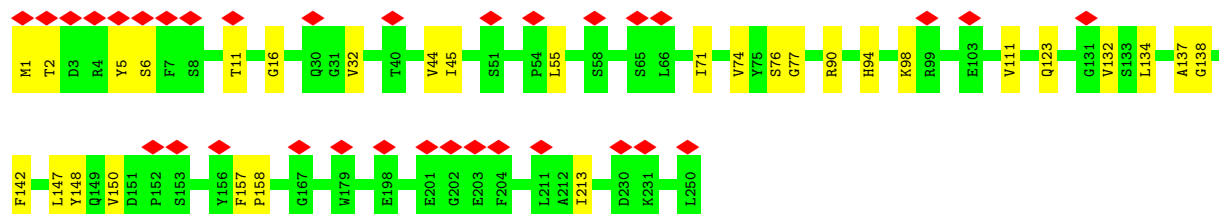
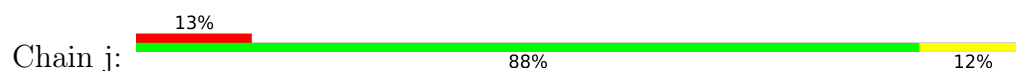


• Molecule 9: Proteasome subunit alpha type-2

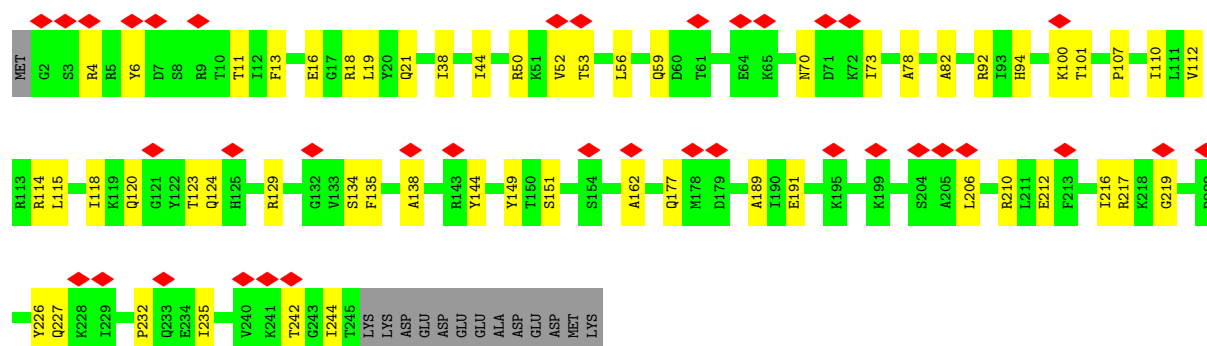
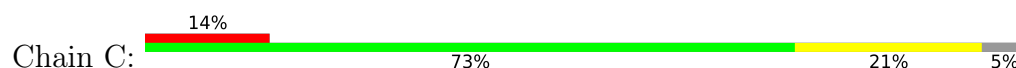




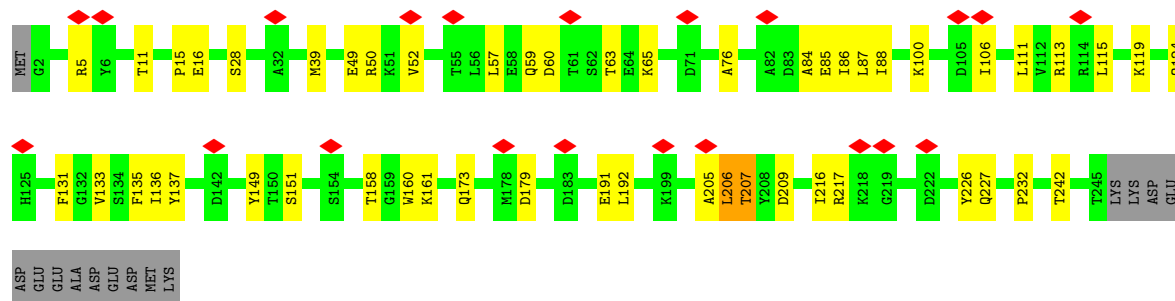
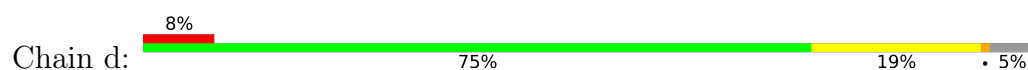
• Molecule 9: Proteasome subunit alpha type-2



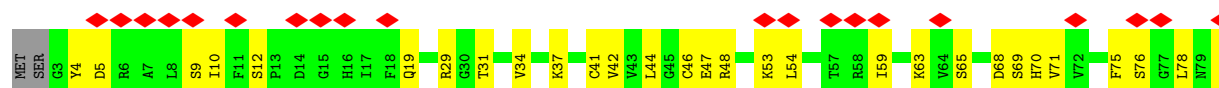
• Molecule 10: Proteasome subunit alpha type-3

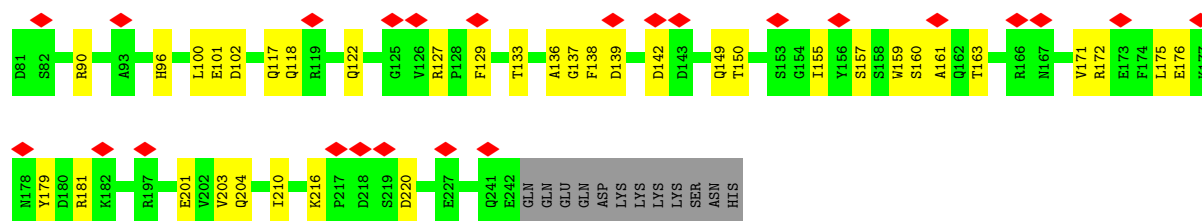


• Molecule 10: Proteasome subunit alpha type-3

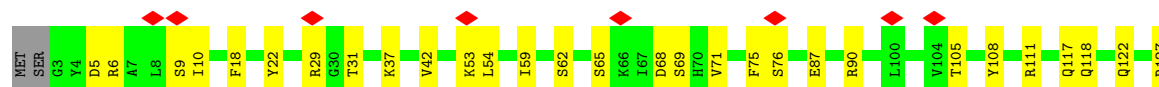
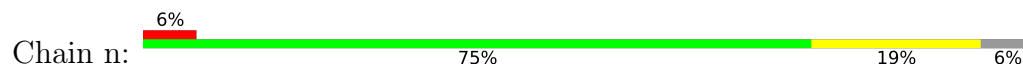


• Molecule 11: Proteasome subunit alpha type-4

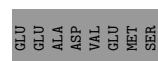
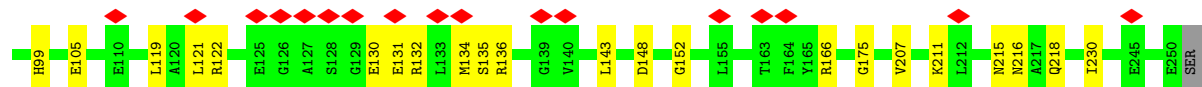
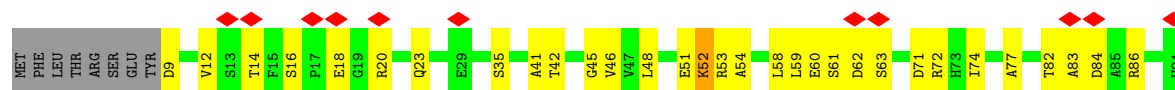




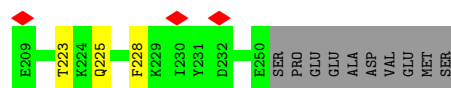
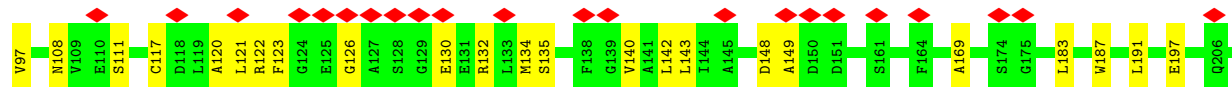
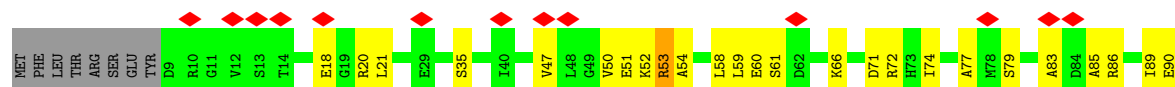
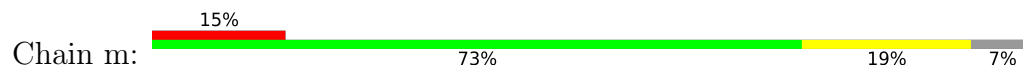
• Molecule 11: Proteasome subunit alpha type-4



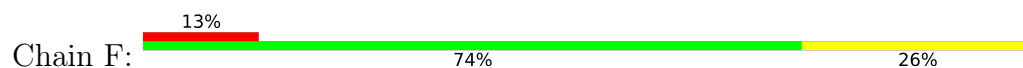
• Molecule 12: Proteasome subunit alpha type-5

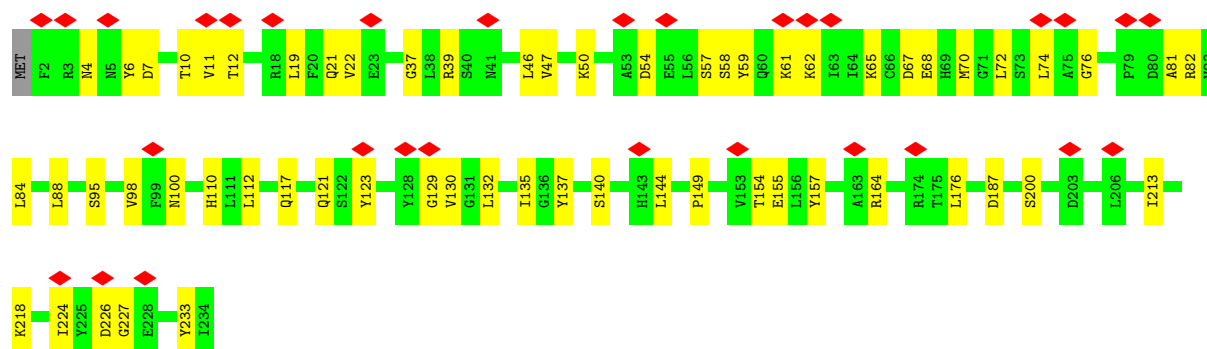


• Molecule 12: Proteasome subunit alpha type-5

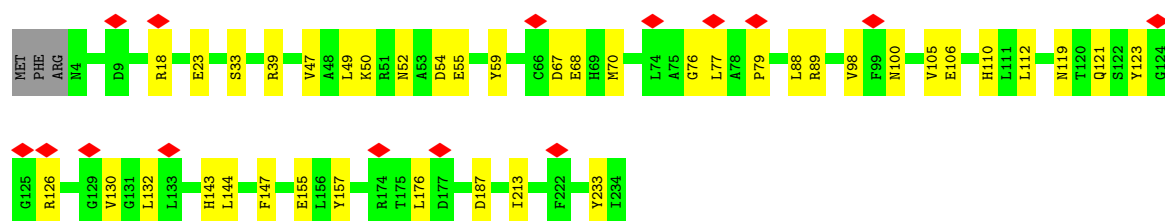
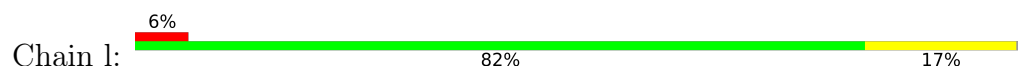


• Molecule 13: Proteasome subunit alpha type-6

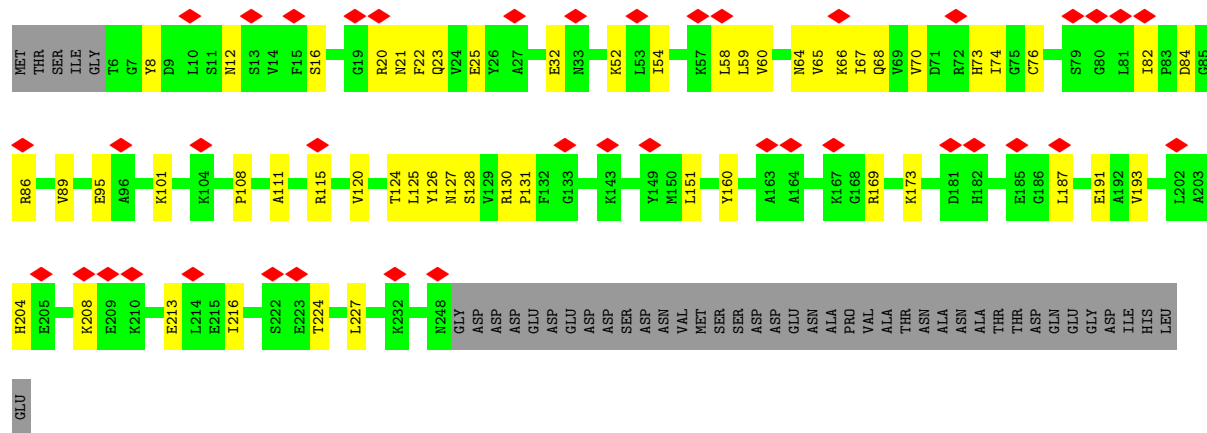




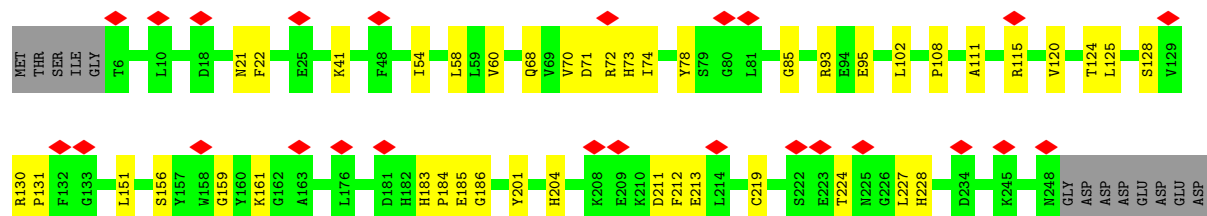
• Molecule 13: Proteasome subunit alpha type-6



• Molecule 14: Probable proteasome subunit alpha type-7



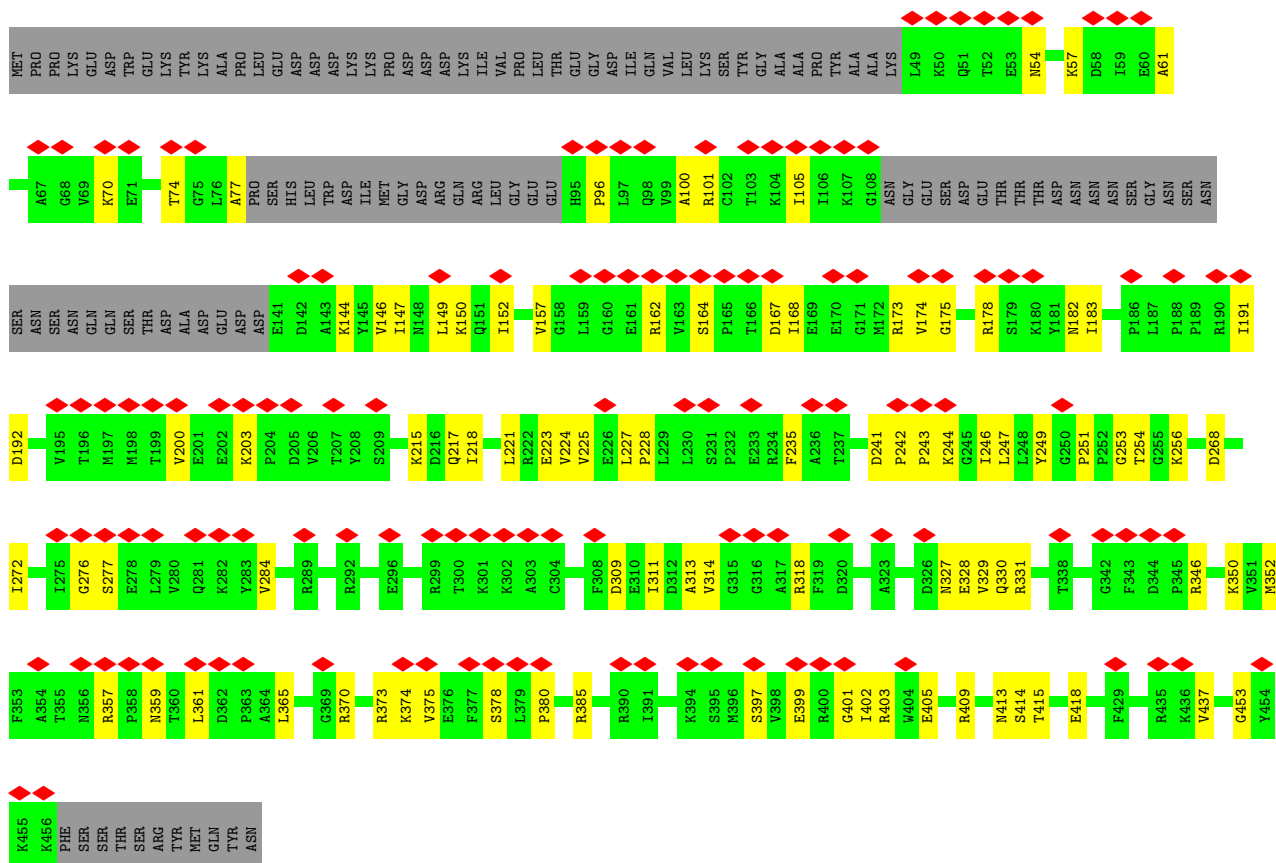
• Molecule 14: Probable proteasome subunit alpha type-7



ASP
SER
ASP
ASN
VAL
MET
SER
SER
ASP
ASP
GLU
ALA
ASN
PRO
VAL
ALA
THR
ASN
ALA
ASN
ALA
THR
THR
THR
ASP
GLN
GLU
GLY
ASP
PRO
ILE
HIS
LEU
GLU

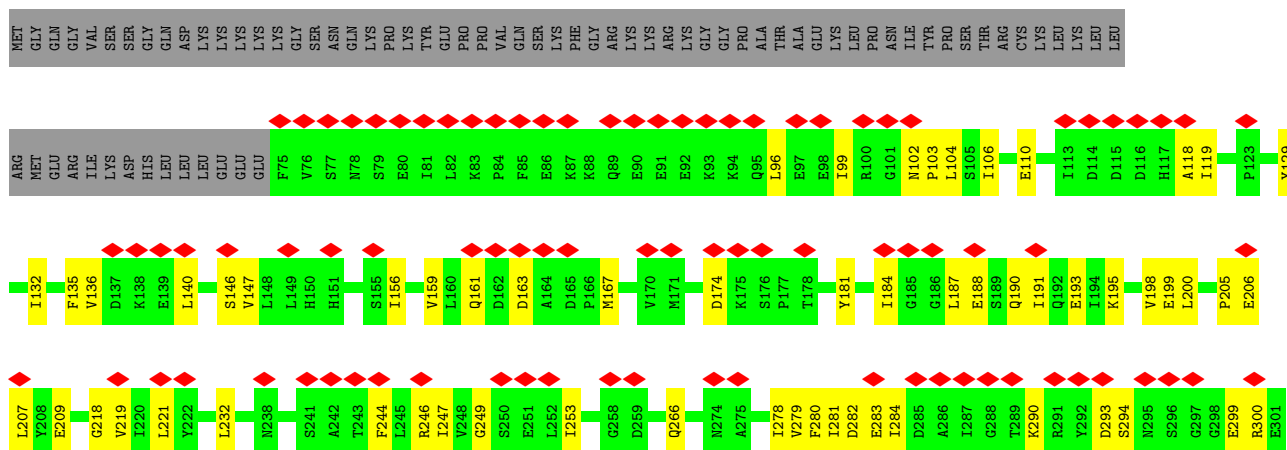
• Molecule 15: 26S protease regulatory subunit 7 homolog

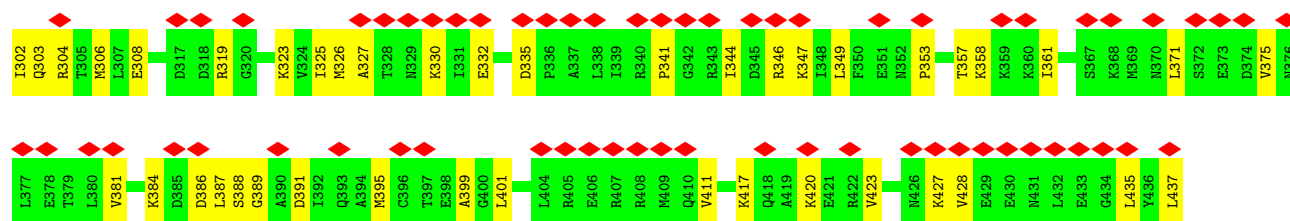
Chain H: 28% 57% 20% 23%



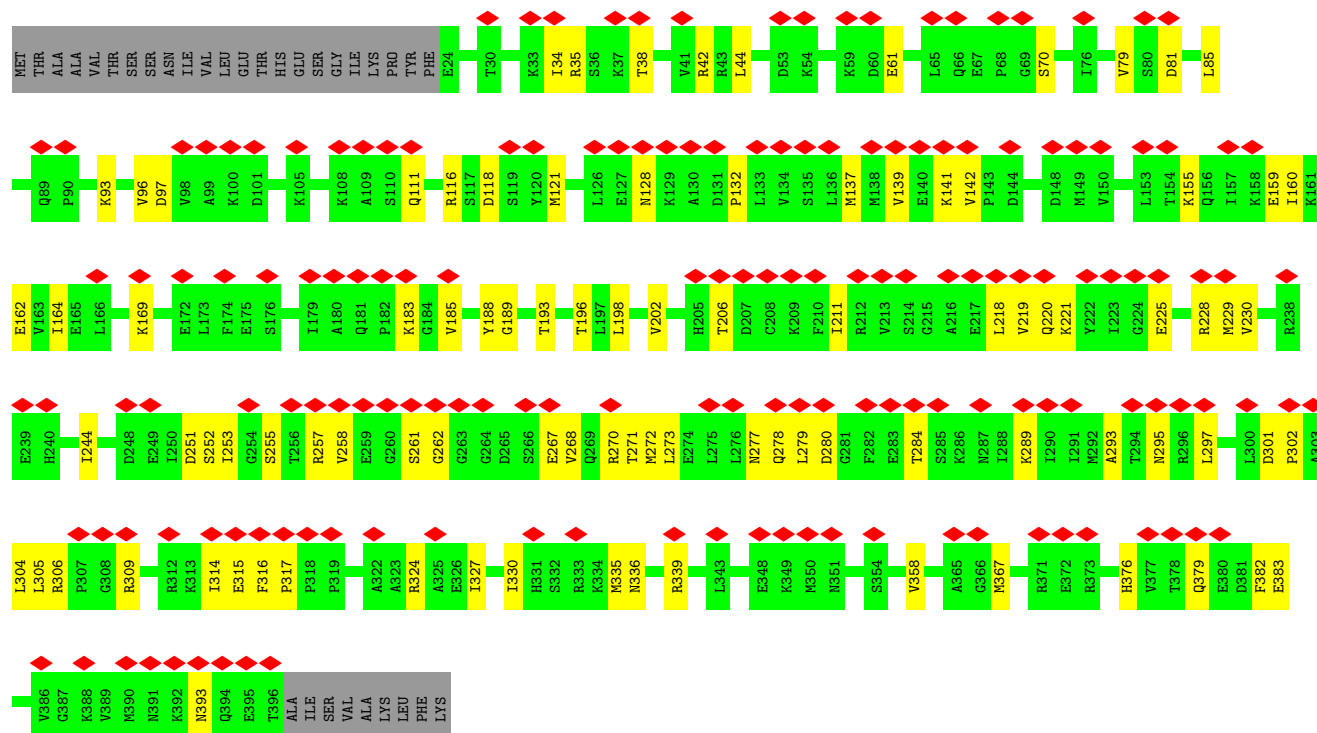
• Molecule 16: 26S protease regulatory subunit 4 homolog

Chain I: 34% 60% 23% 17%

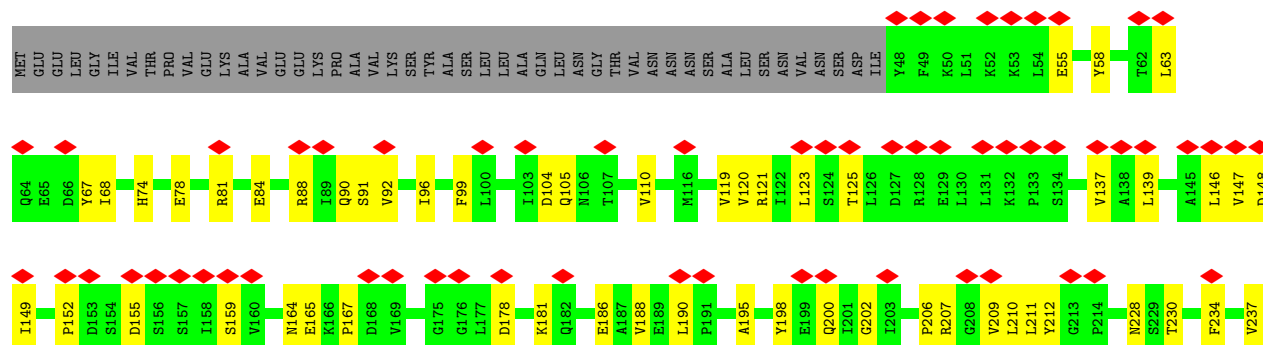


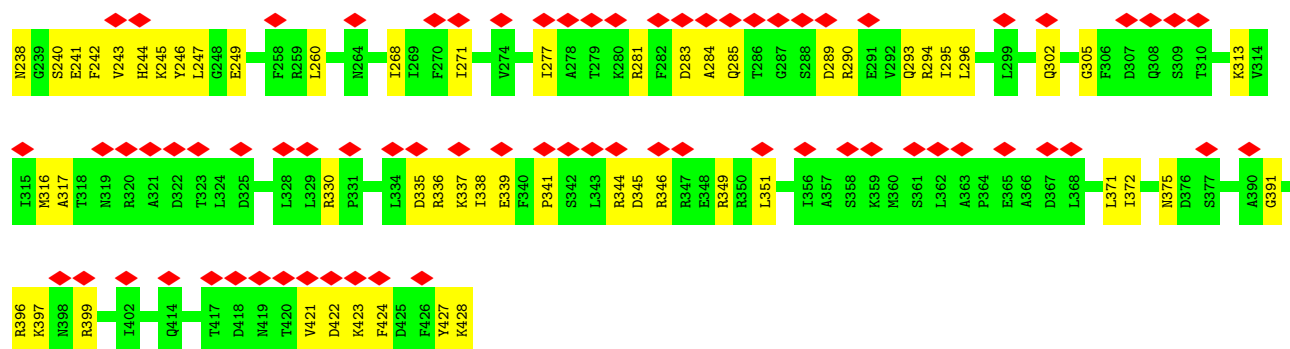


• Molecule 17: 26S protease regulatory subunit 8 homolog

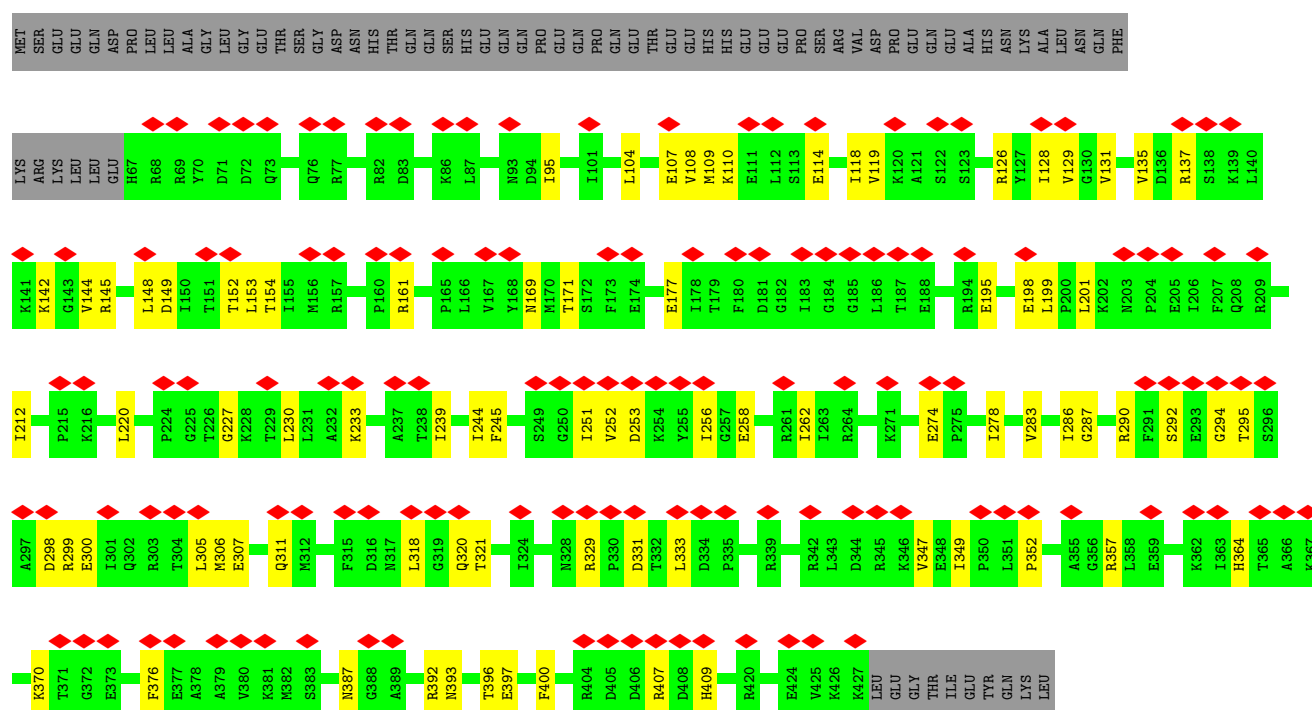


• Molecule 18: 26S protease regulatory subunit 6B homolog

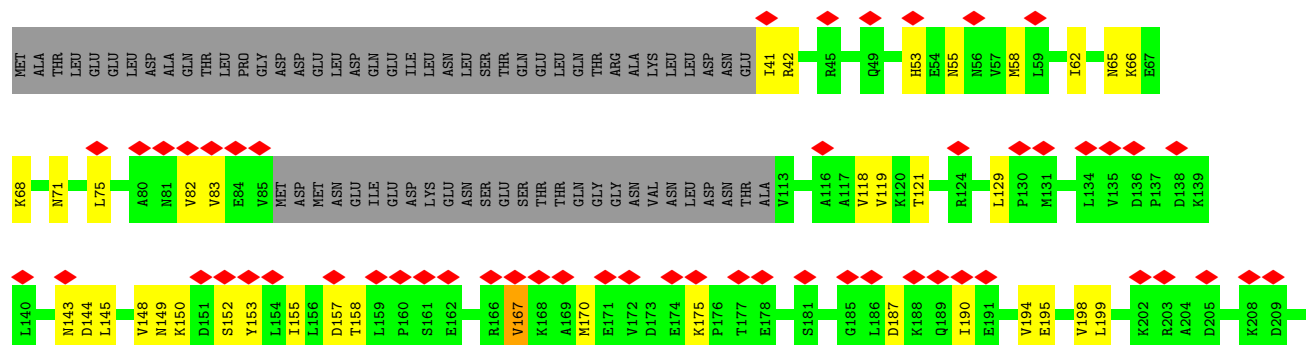


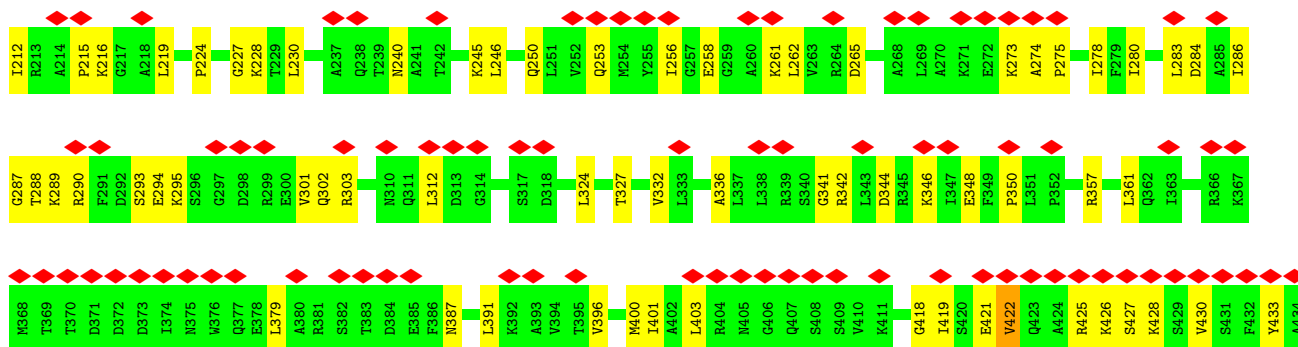


• Molecule 19: 26S protease subunit RPT4

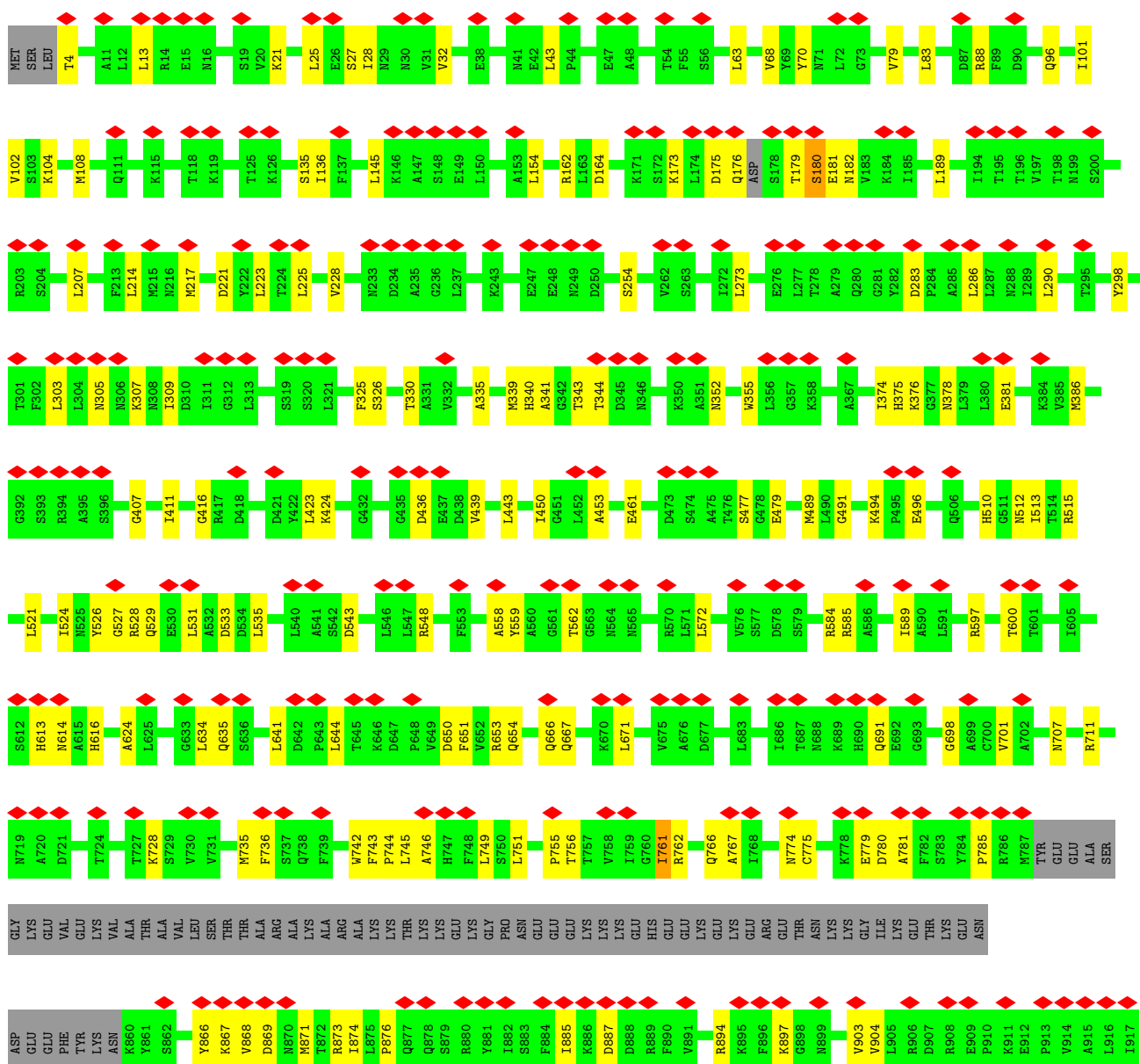


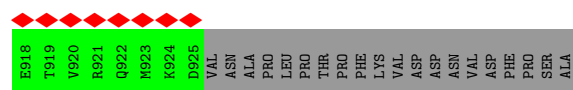
• Molecule 20: 26S protease regulatory subunit 6A



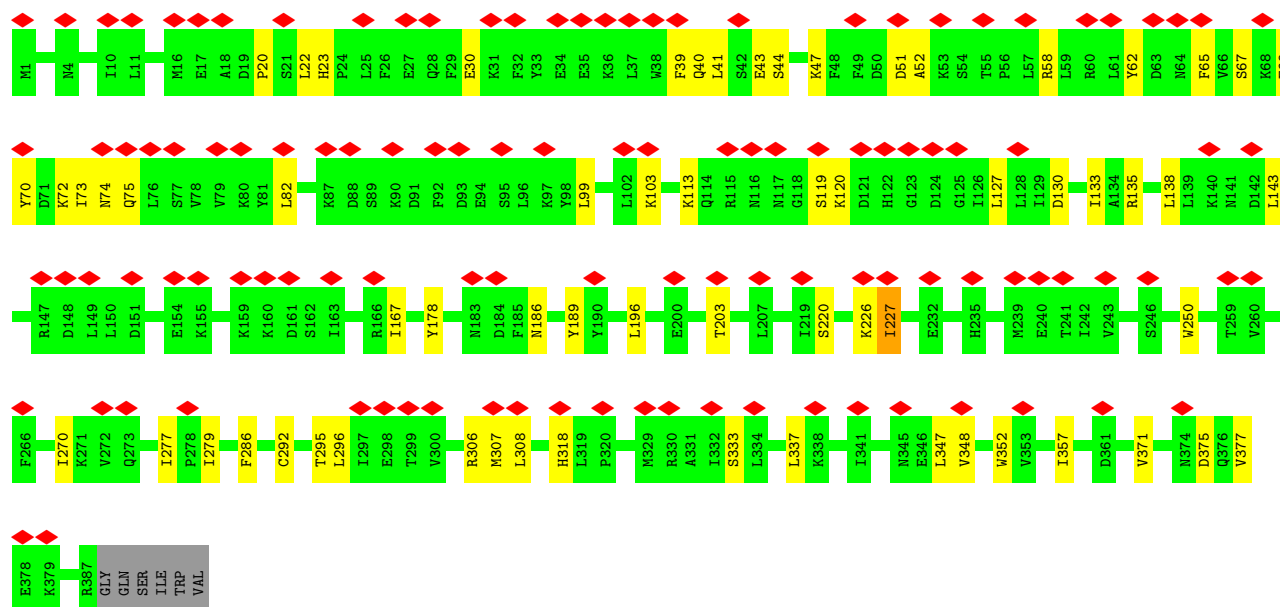
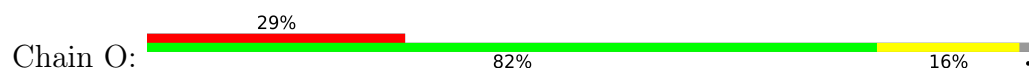


• Molecule 21: 26S proteasome regulatory subunit RPN2

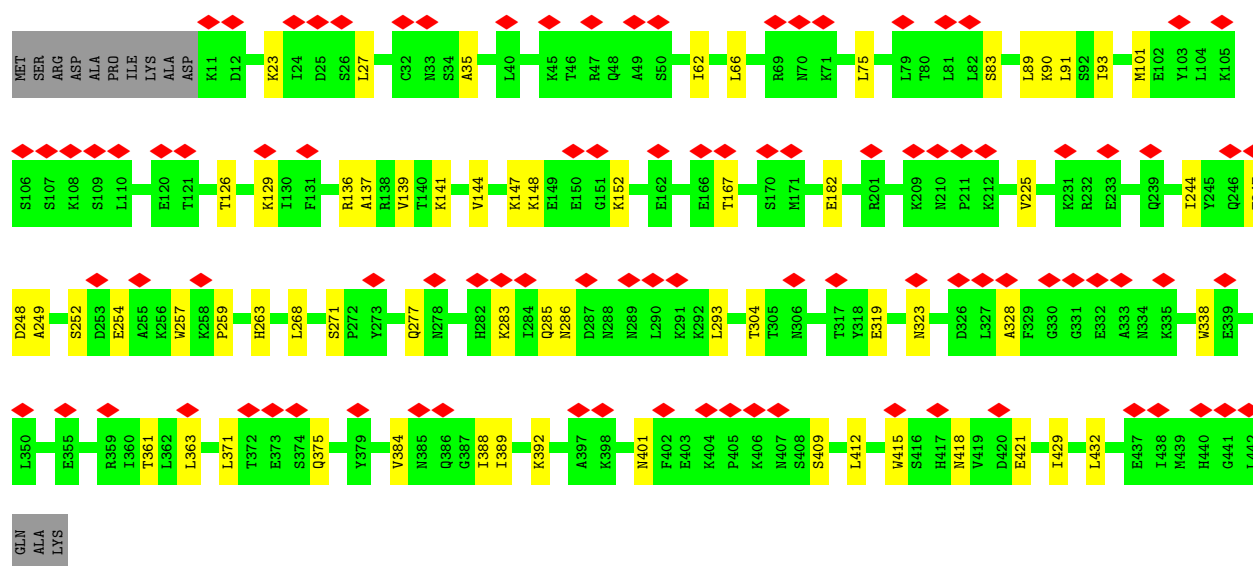
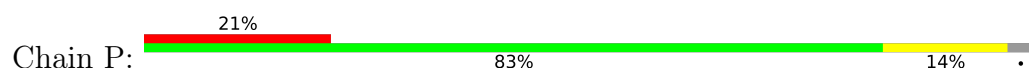




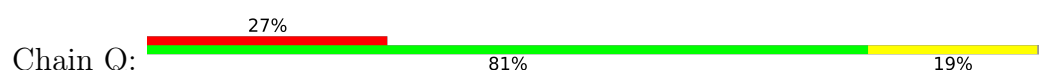
• Molecule 22: 26S proteasome regulatory subunit RPN9

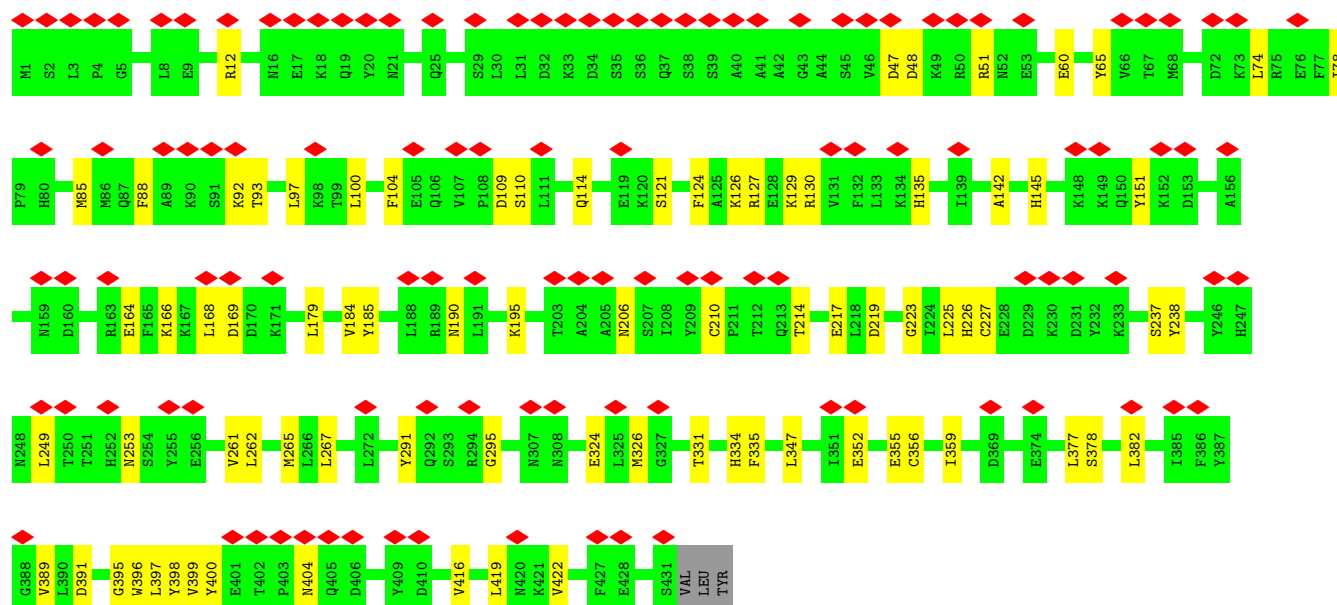


• Molecule 23: 26S proteasome regulatory subunit RPN5

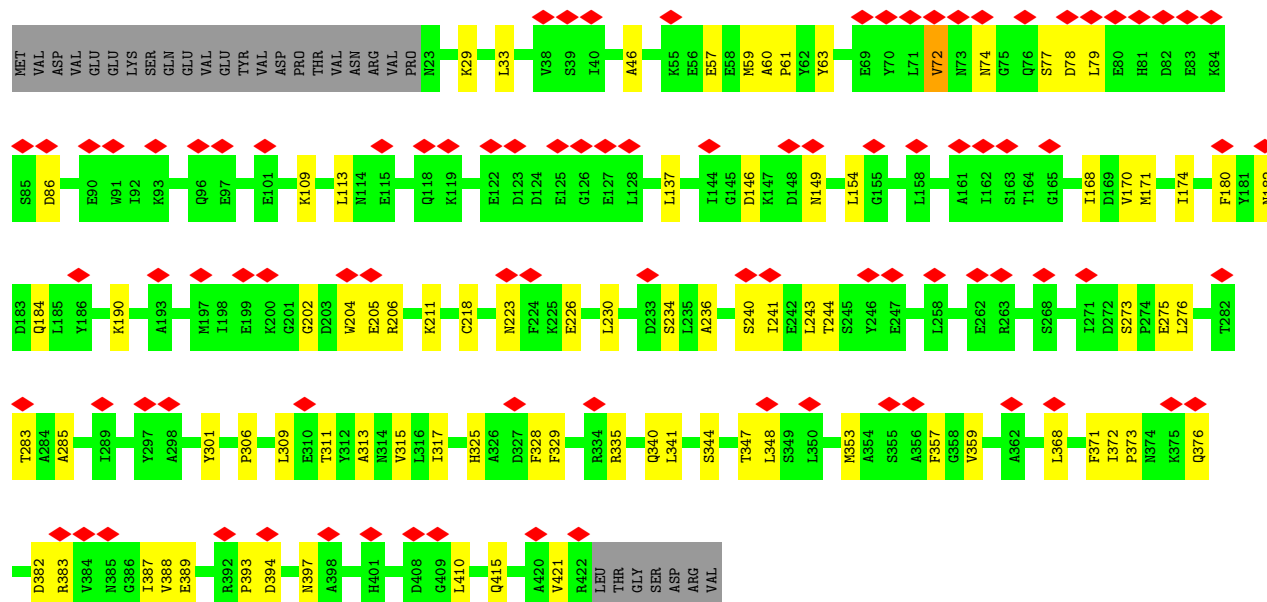
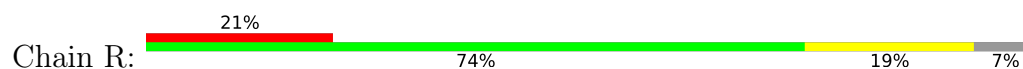


• Molecule 24: 26S proteasome regulatory subunit RPN6

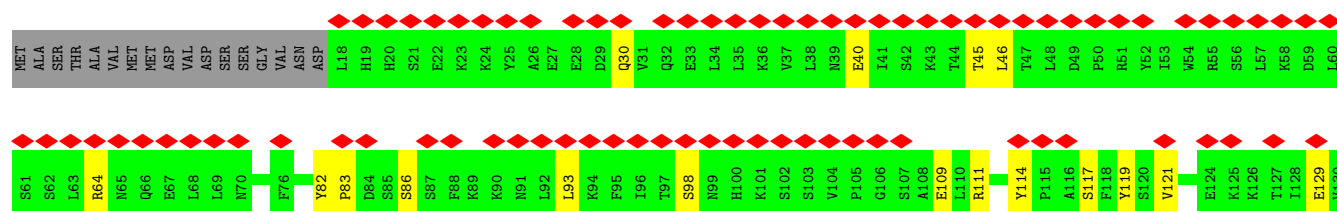
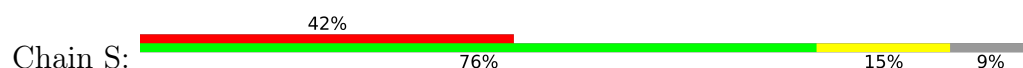


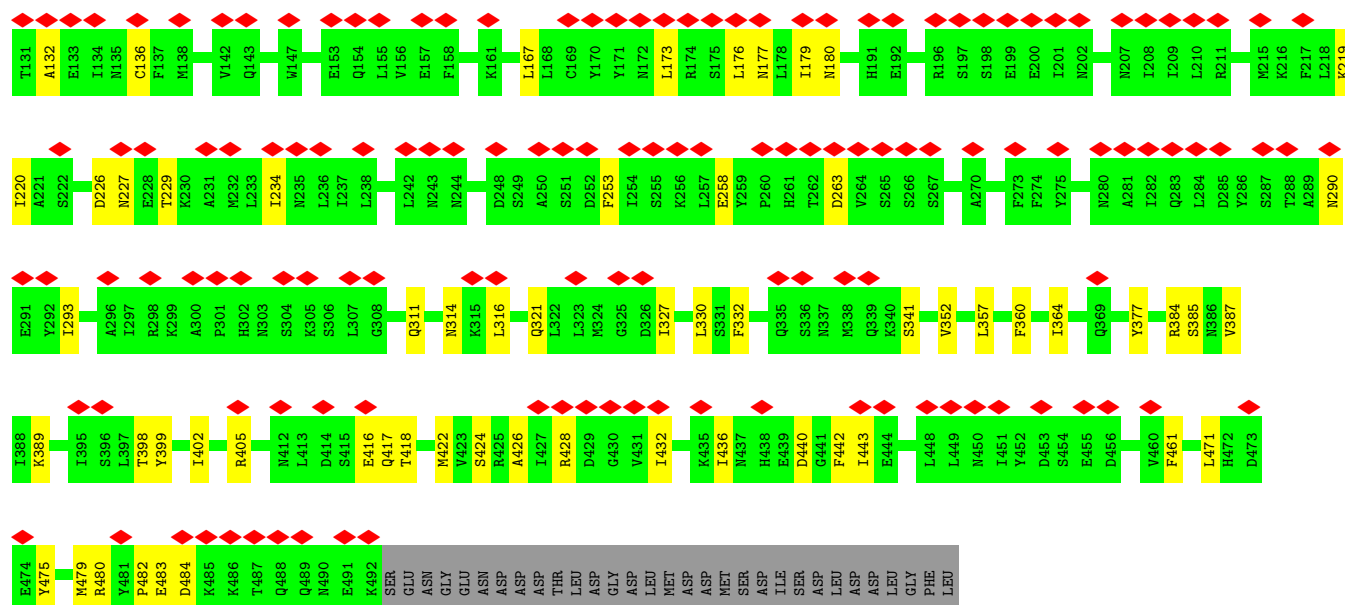


• Molecule 25: 26S proteasome regulatory subunit RPN7

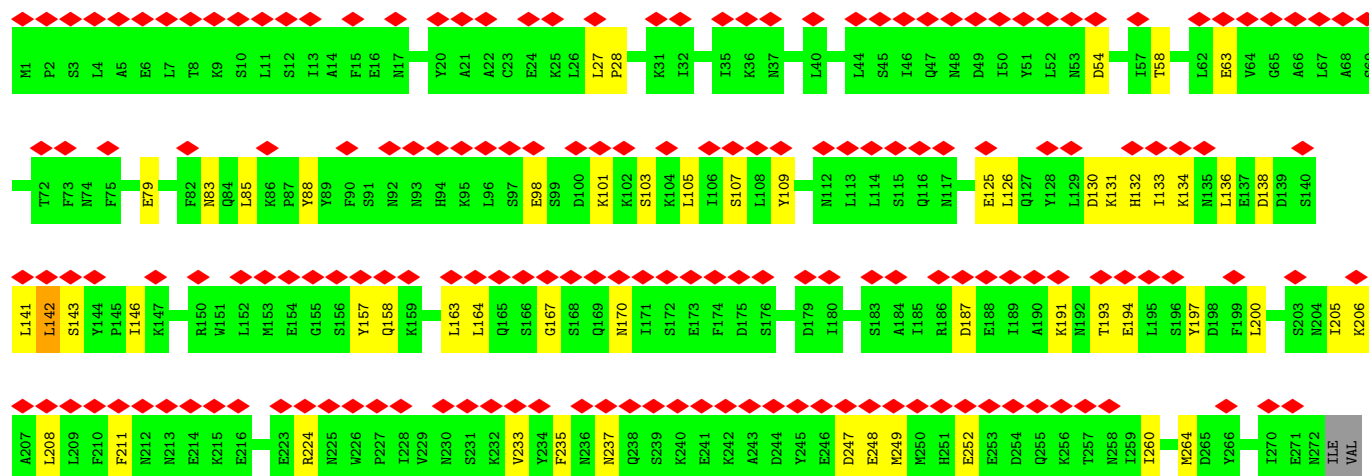
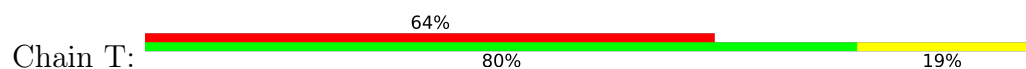


• Molecule 26: 26S proteasome regulatory subunit RPN3

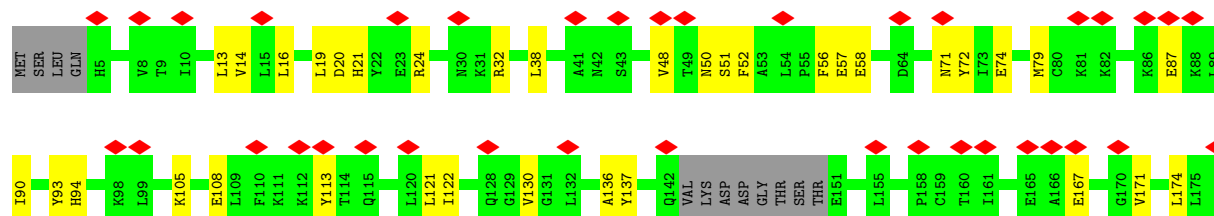


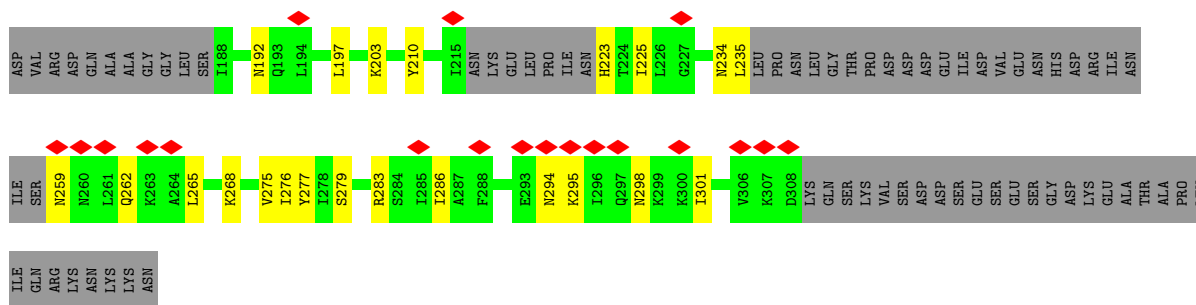


• Molecule 27: 26S proteasome regulatory subunit RPN12

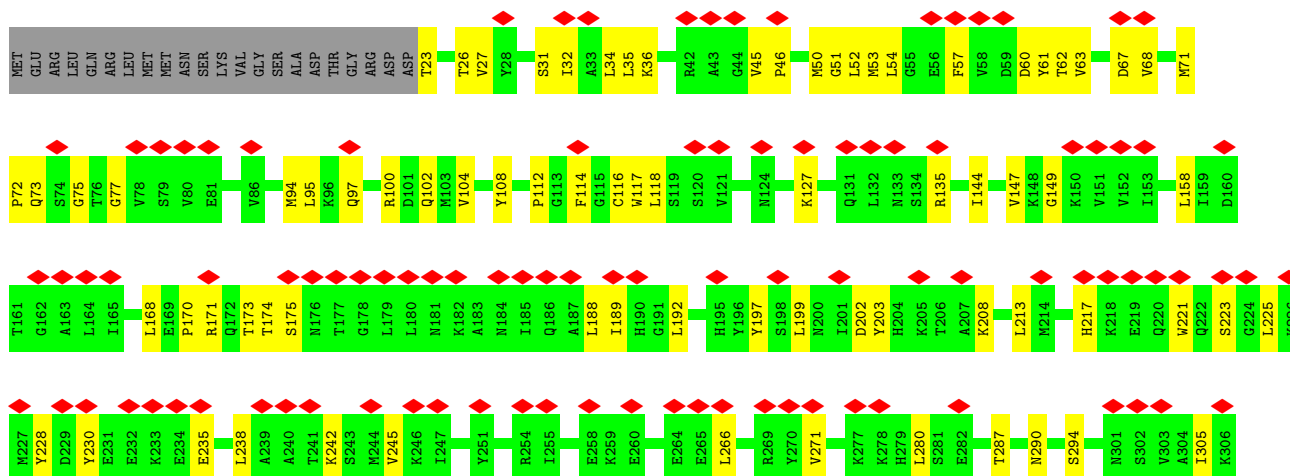


• Molecule 28: 26S proteasome regulatory subunit RPN8

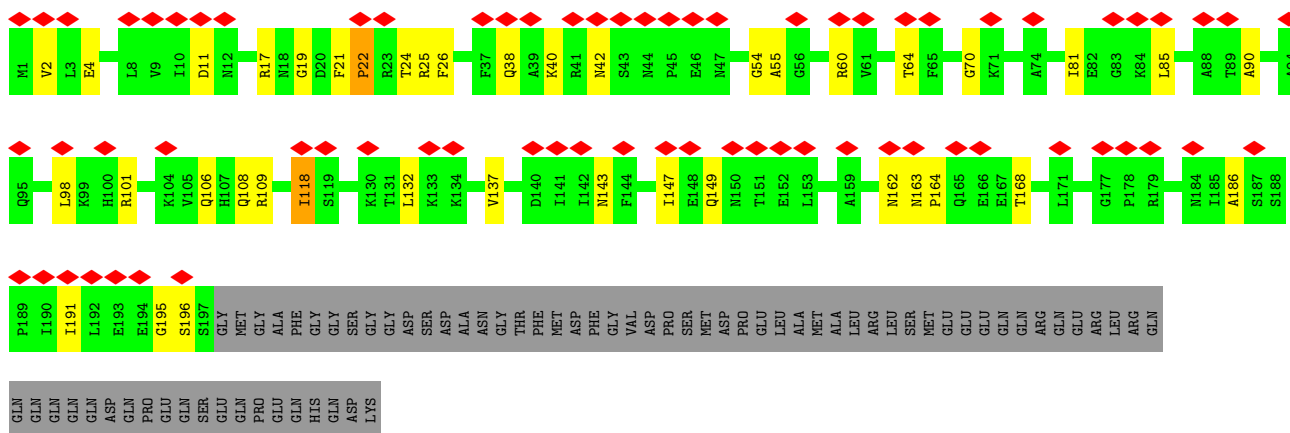




• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

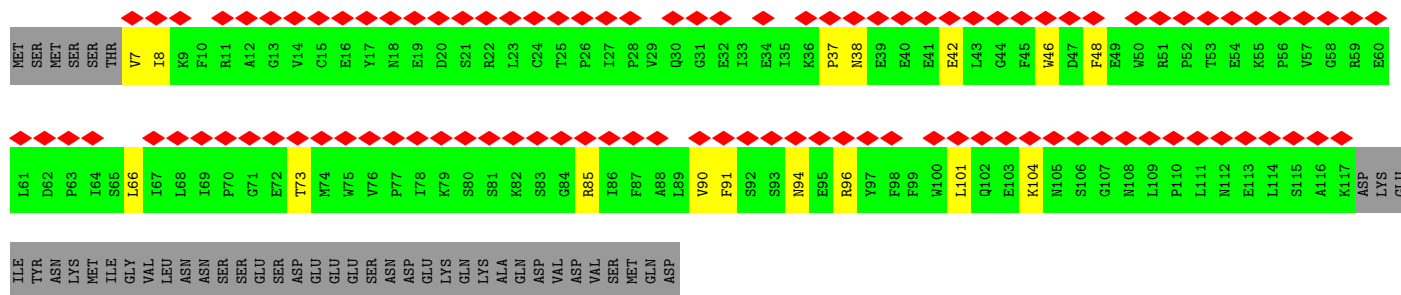


• Molecule 30: 26S proteasome regulatory subunit RPN10

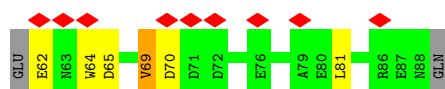
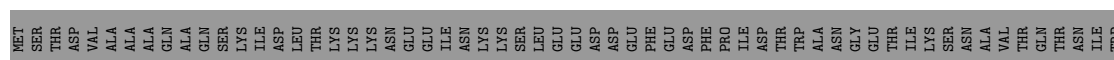


• Molecule 31: 26S proteasome regulatory subunit RPN13

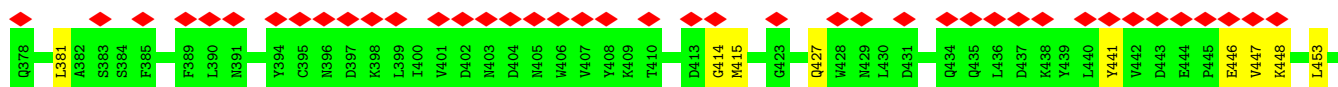
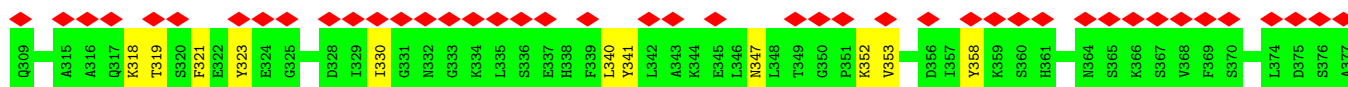
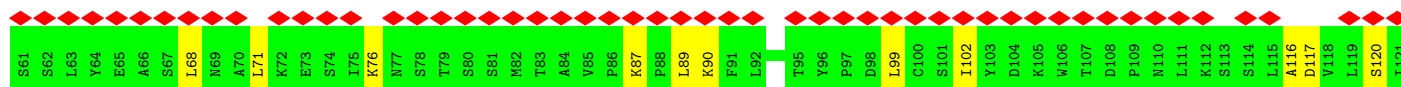
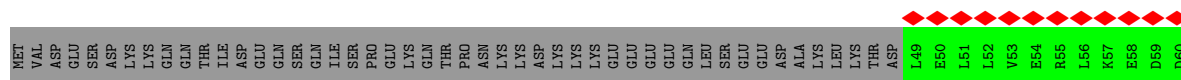


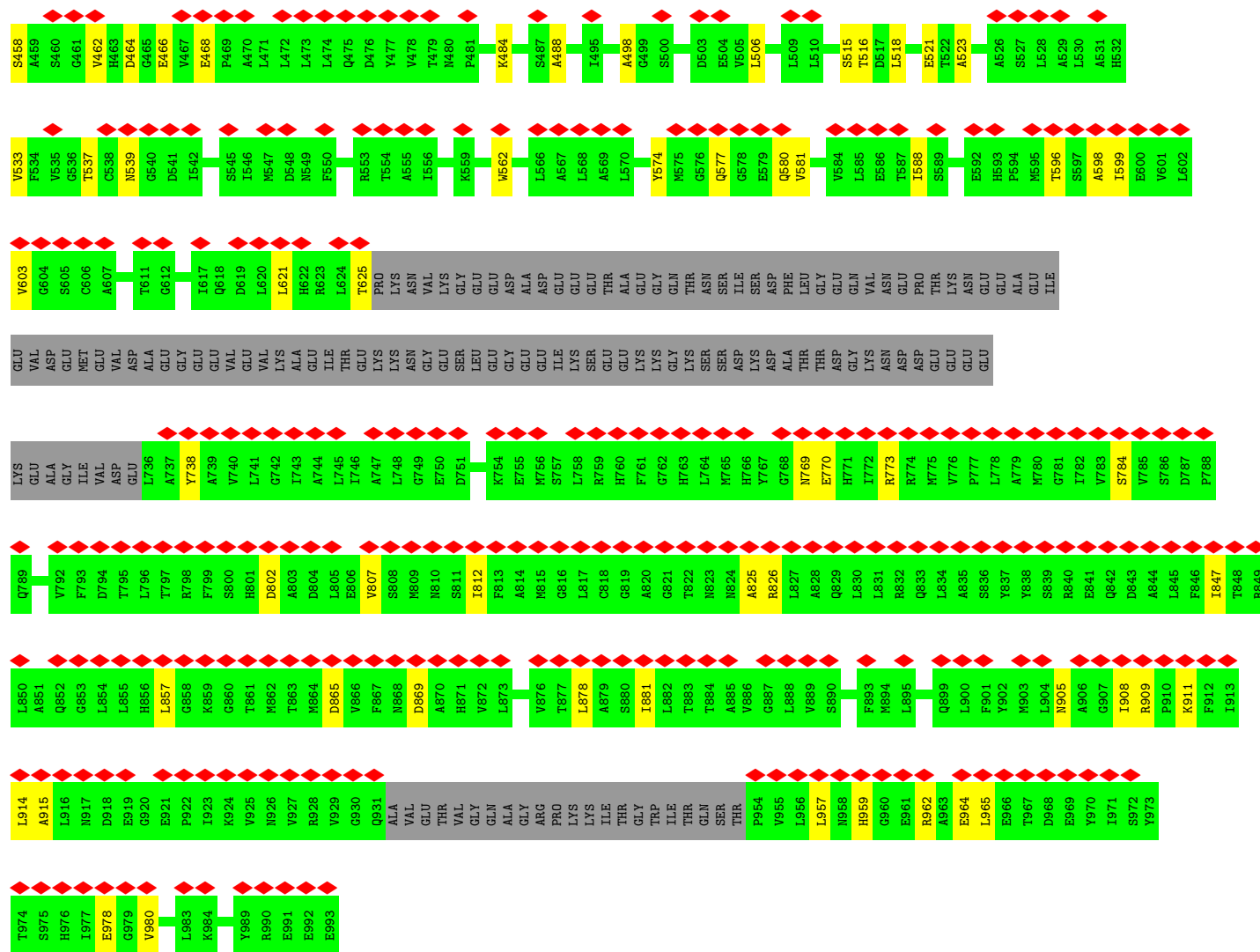


- Molecule 32: 26S proteasome complex subunit SEM1



- Molecule 33: 26S proteasome regulatory subunit RPN1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6171	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	2.295	Depositor
Minimum map value	-1.481	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.806	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	0.07	0/1541	0.21	0/2087
2	2	0.06	0/1750	0.20	0/2373
2	i	0.06	0/1750	0.22	0/2373
3	3	0.08	0/1611	0.24	0/2174
3	h	0.08	0/1611	0.24	0/2174
4	4	0.07	0/1589	0.23	0/2142
4	g	0.07	0/1589	0.22	0/2142
5	5	0.06	0/1681	0.21	0/2274
5	f	0.06	0/1681	0.21	0/2274
6	6	0.07	0/1795	0.22	0/2420
6	e	0.07	0/1795	0.25	0/2420
7	7	0.08	0/1821	0.25	0/2470
7	a	0.07	0/1846	0.24	0/2503
8	A	0.07	0/1945	0.24	0/2634
8	c	0.08	0/1945	0.27	0/2634
9	B	0.07	0/1952	0.22	0/2642
9	j	0.06	0/1952	0.20	0/2642
10	C	0.07	0/1934	0.22	0/2618
10	d	0.08	0/1934	0.26	0/2618
11	D	0.07	0/1910	0.24	0/2586
11	n	0.08	0/1910	0.26	0/2586
12	E	0.07	0/1886	0.26	0/2541
12	m	0.10	0/1886	0.22	0/2541
13	F	0.08	0/1823	0.28	0/2463
13	l	0.07	0/1800	0.22	0/2433
14	G	0.08	0/1932	0.22	0/2609
14	k	0.07	0/1932	0.22	0/2609
15	H	0.14	1/2831 (0.0%)	0.26	0/3808
16	I	0.12	0/2869	0.29	0/3867
17	J	0.08	0/2964	0.27	0/3981
18	K	0.09	0/3062	0.28	0/4132
19	L	0.09	0/2896	0.26	0/3895
20	M	0.10	0/2903	0.28	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	N	0.10	1/6670 (0.0%)	0.26	0/9023
22	O	0.07	0/3243	0.25	0/4374
23	P	0.07	0/3599	0.21	0/4854
24	Q	0.07	0/3527	0.23	0/4748
25	R	0.07	0/3272	0.23	0/4412
26	S	0.08	0/3966	0.25	0/5355
27	T	0.10	0/2279	0.28	0/3077
28	U	0.06	0/2087	0.22	0/2811
29	V	0.10	0/2271	0.31	0/3064
30	W	0.12	0/1557	0.32	0/2111
31	X	0.07	0/931	0.23	0/1262
32	Y	0.12	0/239	0.36	0/322
33	Z	0.12	1/6404 (0.0%)	0.25	0/8686
All	All	0.09	3/107912 (0.0%)	0.25	0/145760

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Z	468	GLU	C-N	7.03	1.50	1.33
15	H	192	ASP	C-N	5.34	1.46	1.33
21	N	217	MET	C-N	5.14	1.45	1.33

There are no bond angle outliers.

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	38	0
1	b	1512	0	1478	25	0
2	2	1719	0	1716	44	0
2	i	1719	0	1716	34	0
3	3	1581	0	1571	47	0
3	h	1581	0	1571	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	1561	0	1569	35	0
4	g	1561	0	1569	19	0
5	5	1644	0	1592	30	0
5	f	1644	0	1592	38	0
6	6	1757	0	1708	29	0
6	e	1757	0	1708	36	0
7	7	1790	0	1790	38	0
7	a	1815	0	1818	36	0
8	A	1907	0	1901	42	0
8	c	1907	0	1901	41	0
9	B	1915	0	1929	50	0
9	j	1915	0	1929	21	0
10	C	1904	0	1901	46	0
10	d	1904	0	1901	39	0
11	D	1881	0	1892	56	0
11	n	1881	0	1892	46	0
12	E	1861	0	1836	45	0
12	m	1861	0	1836	47	0
13	F	1795	0	1797	47	0
13	l	1773	0	1775	28	0
14	G	1892	0	1883	44	0
14	k	1892	0	1883	35	0
15	H	2792	0	2879	65	0
16	I	2831	0	2881	73	0
17	J	2928	0	3057	66	0
18	K	3019	0	3084	88	0
19	L	2853	0	2926	61	0
20	M	2866	0	2938	77	0
21	N	6562	0	6625	106	0
22	O	3182	0	3207	42	0
23	P	3545	0	3629	36	0
24	Q	3471	0	3495	49	0
25	R	3218	0	3216	54	0
26	S	3894	0	3938	57	0
27	T	2235	0	2207	37	0
28	U	2061	0	2116	55	0
29	V	2236	0	2242	66	0
30	W	1534	0	1542	30	0
31	X	906	0	888	10	0
32	Y	236	0	203	9	0
33	Z	6290	0	6236	83	0
All	All	106100	0	106441	1785	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 8.

All (1785) 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)
28:U:210:TYR:HH	28:U:223:HIS:N	1.59	0.99
21:N:510:HIS:HB3	21:N:513:ILE:HB	1.48	0.93
27:T:103:SER:HB2	27:T:142:LEU:HD23	1.53	0.89
21:N:742:TRP:CD1	29:V:61:TYR:HH	1.96	0.82
27:T:107:SER:HB3	27:T:142:LEU:HD13	1.62	0.81
27:T:141:LEU:O	27:T:142:LEU:HG	1.83	0.79
12:E:20:ARG:HG3	20:M:426:LYS:HD3	1.65	0.79
8:c:24:ARG:HH12	8:c:29:GLU:HB2	1.48	0.79
21:N:221:ASP:HA	21:N:894:ARG:HH22	1.49	0.77
8:c:64:LEU:HD12	8:c:69:VAL:HG13	1.67	0.77
12:E:60:GLU:OE1	12:E:63:SER:HB2	1.86	0.75
20:M:421:GLU:HG2	20:M:422:VAL:H	1.53	0.74
25:R:393:PRO:HB2	25:R:397:ASN:H	1.52	0.74
4:4:29:LYS:HD3	5:5:199:GLY:HA2	1.69	0.74
6:6:78:ALA:HB2	7:7:167:GLY:HA3	1.69	0.74
12:E:119:LEU:HG	12:E:134:MET:HE3	1.69	0.74
10:d:52:VAL:HG23	10:d:59:GLN:HE21	1.53	0.73
7:7:216:VAL:HG13	2:i:168:GLU:HG3	1.68	0.73
18:K:289:ASP:HA	19:L:299:ARG:HH21	1.53	0.72
10:d:205:ALA:C	10:d:206:LEU:HG	2.15	0.72
19:L:290:ARG:NH2	19:L:292:SER:OG	2.23	0.72
19:L:171:THR:HB	19:L:245:PHE:HB3	1.70	0.72
21:N:528:ARG:HB3	21:N:531:LEU:HB2	1.72	0.72
27:T:103:SER:HB2	27:T:142:LEU:CD2	2.20	0.71
10:d:206:LEU:HD12	10:d:206:LEU:O	1.90	0.71
25:R:359:VAL:HA	32:Y:81:LEU:HD22	1.73	0.71
18:K:244:HIS:O	19:L:299:ARG:NH1	2.24	0.71
30:W:162:ASN:HA	30:W:168:THR:HG21	1.73	0.70
17:J:79:VAL:HG12	17:J:81:ASP:H	1.56	0.70
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.73	0.70
11:D:37:LYS:HE2	11:D:160:SER:HA	1.73	0.70
21:N:512:ASN:ND2	29:V:61:TYR:CE2	2.60	0.70
3:h:5:SER:HB3	3:h:104:PHE:HB3	1.74	0.69
10:d:205:ALA:O	10:d:206:LEU:HG	1.92	0.69
33:Z:784:SER:O	33:Z:826:ARG:NH1	2.25	0.69
7:a:161:ARG:HD3	7:a:169:THR:HB	1.74	0.69
15:H:203:LYS:HE2	15:H:268:ASP:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:88:PRO:HD3	14:k:156:SER:HB3	1.73	0.69
11:n:118:GLN:NE2	12:m:83:ALA:O	2.25	0.69
18:K:188:VAL:HG22	18:K:313:LYS:HE2	1.73	0.69
21:N:666:GLN:HA	21:N:873:ARG:HH21	1.57	0.69
17:J:252:SER:HB2	17:J:295:ASN:H	1.56	0.69
11:D:5:ASP:O	11:D:19:GLN:NE2	2.26	0.69
33:Z:914:LEU:H	33:Z:980:VAL:HG22	1.58	0.68
1:1:40:THR:HG22	1:1:45:ILE:HG12	1.74	0.68
11:D:118:GLN:HE22	12:E:86:ARG:HB2	1.59	0.68
14:k:224:THR:HB	14:k:227:LEU:HB2	1.74	0.68
12:E:77:ALA:HB3	12:E:143:LEU:HB2	1.76	0.68
15:H:217:GLN:HE21	15:H:378:SER:H	1.41	0.68
29:V:188:LEU:HB3	29:V:192:LEU:HA	1.76	0.68
8:A:46:ARG:HH21	8:A:167:LYS:HA	1.58	0.68
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.76	0.68
1:1:20:THR:N	1:1:188:SER:HG	1.90	0.68
15:H:244:LYS:HZ1	15:H:346:ARG:HH11	1.42	0.68
1:1:80:TYR:HB2	8:A:102:ALA:HB1	1.76	0.67
12:m:52:LYS:NZ	12:m:61:SER:O	2.27	0.67
2:2:58:LYS:NZ	3:3:135:ASP:OD2	2.27	0.67
10:d:49:GLU:O	10:d:65:LYS:NZ	2.27	0.67
19:L:253:ASP:HB3	20:M:293:SER:HB2	1.76	0.67
2:i:63:LEU:HD11	2:i:71:TRP:HB3	1.77	0.67
12:m:52:LYS:O	12:m:53:ARG:HB2	1.94	0.67
17:J:164:ILE:HG12	17:J:289:LYS:HE2	1.76	0.67
22:O:357:ILE:HB	28:U:223:HIS:HB2	1.77	0.67
10:d:124:GLN:NE2	11:n:127:ARG:O	2.28	0.67
16:I:387:LEU:HD23	16:I:391:ASP:HB3	1.76	0.66
17:J:335:MET:HA	18:K:202:GLY:HA3	1.76	0.66
9:B:176:GLU:HA	10:C:56:LEU:HD21	1.76	0.66
11:D:181:ARG:HH12	12:E:60:GLU:HA	1.59	0.66
19:L:195:GLU:HA	19:L:199:LEU:HD13	1.77	0.66
25:R:348:LEU:HB2	25:R:388:VAL:HB	1.77	0.66
24:Q:85:MET:HG3	24:Q:126:LYS:HG2	1.76	0.66
31:X:38:ASN:HD22	31:X:42:GLU:H	1.43	0.66
12:E:18:GLU:OE1	20:M:426:LYS:NZ	2.23	0.66
33:Z:284:LEU:HB3	33:Z:293:MET:HB3	1.77	0.66
3:3:5:SER:HB2	3:3:104:PHE:HB3	1.78	0.66
1:b:182:ILE:HG12	1:b:189:GLY:HA2	1.77	0.66
18:K:246:TYR:HB2	19:L:256:ILE:HG12	1.77	0.66
21:N:711:ARG:NH2	21:N:781:ALA:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:40:THR:HG22	1:b:45:ILE:HG12	1.78	0.66
24:Q:93:THR:H	24:Q:129:LYS:HG2	1.61	0.66
17:J:132:PRO:HG2	17:J:137:MET:HE1	1.78	0.66
16:I:174:ASP:HB3	16:I:244:PHE:HB3	1.78	0.65
30:W:85:LEU:HD21	30:W:118:ILE:HG12	1.77	0.65
8:A:144:VAL:HG12	8:A:154:ILE:HG12	1.78	0.65
17:J:221:LYS:HB2	18:K:247:LEU:H	1.61	0.65
17:J:258:VAL:O	18:K:293:GLN:NE2	2.30	0.65
3:3:27:LEU:HB3	3:3:39:LYS:HA	1.77	0.65
21:N:207:LEU:HB3	21:N:228:VAL:HG13	1.78	0.65
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.77	0.65
31:X:91:PHE:H	31:X:96:ARG:HD3	1.61	0.65
6:6:174:ASN:HB3	6:6:176:LYS:HE2	1.79	0.65
19:L:129:VAL:HG12	19:L:153:LEU:HB3	1.78	0.65
16:I:294:SER:HB3	16:I:300:ARG:HG3	1.78	0.65
12:m:130:GLU:HB2	12:m:132:ARG:HH12	1.61	0.65
21:N:83:LEU:HD11	21:N:136:ILE:HG13	1.79	0.64
21:N:307:LYS:HD3	21:N:343:THR:HG21	1.78	0.64
28:U:105:LYS:O	30:W:60:ARG:NH2	2.29	0.64
2:i:70:ILE:HG12	2:i:131:GLY:HA3	1.79	0.64
16:I:218:GLY:HA3	16:I:344:ILE:HG12	1.78	0.64
26:S:173:LEU:O	26:S:177:ASN:ND2	2.31	0.64
28:U:283:ARG:HB2	29:V:287:THR:HG21	1.79	0.64
5:5:82:ARG:HH11	5:5:186:THR:HA	1.62	0.64
11:n:159:TRP:CE3	12:m:58:LEU:O	2.51	0.64
29:V:60:ASP:O	29:V:61:TYR:HB2	1.98	0.64
18:K:123:LEU:H	18:K:146:LEU:HD23	1.61	0.64
18:K:155:ASP:OD2	19:L:142:LYS:NZ	2.31	0.64
12:E:52:LYS:HE2	12:E:218:GLN:HB2	1.78	0.64
10:d:161:LYS:HB2	11:n:54:LEU:HB3	1.79	0.64
3:h:189:ILE:HB	3:h:196:VAL:HB	1.79	0.64
11:D:163:THR:HG21	11:D:171:VAL:HB	1.79	0.64
16:I:401:LEU:HD11	17:J:162:GLU:HB3	1.80	0.64
20:M:253:GLN:HG3	20:M:258:GLU:HG3	1.79	0.64
2:2:51:GLN:NE2	3:3:125:ASP:OD2	2.31	0.64
12:m:121:LEU:HB3	13:l:79:PRO:HB3	1.79	0.64
14:k:183:HIS:HD2	14:k:184:PRO:HD2	1.63	0.64
13:F:155:GLU:H	14:G:64:ASN:HD21	1.46	0.63
21:N:96:GLN:HG3	26:S:220:ILE:HG12	1.80	0.63
33:Z:865:ASP:O	33:Z:909:ARG:NH1	2.29	0.63
7:7:161:ARG:HE	7:7:169:THR:HB	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:397:LYS:HB3	18:K:399:ARG:HH11	1.63	0.63
19:L:407:ARG:HG2	19:L:409:HIS:H	1.63	0.63
3:3:175:ALA:HB1	3:3:182:GLY:HA2	1.80	0.63
8:A:119:LYS:HE3	9:B:83:ARG:HD2	1.80	0.63
13:F:67:ASP:HB3	13:F:70:MET:HB3	1.80	0.63
21:N:494:LYS:HE2	21:N:496:GLU:HB3	1.81	0.63
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.80	0.63
6:e:46:THR:HB	6:e:58:TYR:HA	1.80	0.63
10:C:18:ARG:NH1	16:I:435:LEU:O	2.29	0.63
12:m:51:GLU:O	12:m:53:ARG:HG2	1.98	0.63
17:J:189:GLY:HA3	17:J:316:PHE:HB3	1.79	0.63
27:T:194:GLU:OE1	27:T:224:ARG:NH2	2.31	0.63
5:f:251:ASN:ND2	5:f:265:ASN:OD1	2.32	0.63
18:K:244:HIS:CE1	18:K:249:GLU:HB3	2.34	0.63
20:M:219:LEU:HD23	20:M:346:LYS:HG2	1.81	0.63
25:R:373:PRO:HB2	32:Y:64:TRP:HZ3	1.64	0.63
22:O:186:ASN:HB3	22:O:226:LYS:HD2	1.80	0.62
21:N:654:GLN:HG3	21:N:698:GLY:HA3	1.81	0.62
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.81	0.62
11:D:10:ILE:HG22	11:D:12:SER:H	1.65	0.62
21:N:273:LEU:HB3	21:N:290:LEU:HD13	1.80	0.62
21:N:584:ARG:NH1	21:N:614:ASN:OD1	2.32	0.62
21:N:736:PHE:HB2	21:N:749:LEU:HD11	1.80	0.62
25:R:113:LEU:HD22	25:R:137:LEU:HD13	1.81	0.62
3:3:28:ARG:NH1	3:3:179:ALA:O	2.33	0.62
3:3:145:GLN:HE22	3:3:177:ARG:HB2	1.65	0.62
15:H:96:PRO:HB3	15:H:191:ILE:HG21	1.82	0.62
16:I:195:LYS:HG3	16:I:199:GLU:HB3	1.82	0.62
8:A:112:MET:HE2	8:A:117:LEU:HA	1.81	0.62
14:G:224:THR:HB	14:G:227:LEU:HB2	1.80	0.62
17:J:160:ILE:HG23	17:J:164:ILE:HD12	1.80	0.62
17:J:367:MET:HE1	18:K:336:ARG:HD3	1.81	0.62
21:N:562:THR:HA	21:N:597:ARG:HE	1.65	0.62
25:R:394:ASP:O	25:R:397:ASN:ND2	2.32	0.62
33:Z:577:GLN:HB3	33:Z:580:GLN:HB2	1.82	0.62
9:B:50:LYS:NZ	18:K:427:TYR:OH	2.33	0.62
16:I:198:VAL:HG13	16:I:323:LYS:HG3	1.81	0.62
19:L:352:PRO:O	19:L:357:ARG:NH1	2.32	0.62
22:O:73:ILE:HD12	30:W:17:ARG:HH11	1.64	0.62
25:R:168:ILE:HA	25:R:171:MET:HE3	1.81	0.62
5:5:94:ARG:NH1	5:5:244:ALA:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:246:LEU:HD12	20:M:280:ILE:HG12	1.80	0.62
6:e:49:ILE:HD11	6:e:216:GLN:HE21	1.64	0.62
4:g:8:ARG:HG3	4:g:13:VAL:HG22	1.82	0.62
10:C:4:ARG:NH2	10:C:6:TYR:OH	2.33	0.62
10:d:85:GLU:HA	10:d:88:ILE:HD12	1.82	0.62
21:N:510:HIS:CB	21:N:513:ILE:HD12	2.30	0.62
26:S:314:ASN:HB3	26:S:332:PHE:HZ	1.65	0.62
33:Z:802:ASP:HB3	33:Z:807:VAL:HG21	1.81	0.62
6:6:74:ASN:HB3	6:6:127:HIS:HB3	1.80	0.62
21:N:341:ALA:HA	21:N:374:ILE:HA	1.82	0.62
21:N:780:ASP:HB3	21:N:873:ARG:HD3	1.82	0.62
26:S:389:LYS:NZ	26:S:422:MET:O	2.32	0.62
8:A:72:ILE:HG12	8:A:82:VAL:HG22	1.82	0.61
27:T:193:THR:HA	27:T:197:TYR:HB3	1.82	0.61
1:l:145:ILE:HD11	1:l:154:TYR:HD1	1.65	0.61
7:a:137:ARG:HA	7:a:142:PRO:HG3	1.83	0.61
10:d:179:ASP:HB3	10:d:192:LEU:HD13	1.82	0.61
11:n:117:GLN:HE21	11:n:129:PHE:HB2	1.63	0.61
21:N:728:LYS:HB3	21:N:751:LEU:HB3	1.82	0.61
28:U:32:ARG:NH2	28:U:58:GLU:OE2	2.31	0.61
19:L:393:ASN:ND2	20:M:344:ASP:OD2	2.32	0.61
33:Z:539:ASN:H	33:Z:577:GLN:HE22	1.45	0.61
1:b:76:ASP:OD2	2:i:113:LYS:NZ	2.33	0.61
13:F:81:ALA:HB2	13:F:130:VAL:HG21	1.82	0.61
17:J:277:ASN:HB2	17:J:309:ARG:HE	1.64	0.61
7:7:107:ASN:HD21	7:7:119:ALA:HA	1.66	0.61
10:C:44:ILE:HB	10:C:216:ILE:HD12	1.81	0.61
11:n:181:ARG:NH2	12:m:60:GLU:CG	2.63	0.61
5:f:93:SER:HB3	5:f:249:SER:H	1.64	0.61
8:c:64:LEU:HD23	14:k:159:GLY:H	1.65	0.61
26:S:480:ARG:HD2	26:S:483:GLU:HB2	1.81	0.61
16:I:290:LYS:HD2	16:I:303:GLN:HG2	1.82	0.61
19:L:252:VAL:HG13	19:L:300:GLU:HB2	1.82	0.61
20:M:227:GLY:HA2	20:M:230:LEU:HB2	1.83	0.61
21:N:735:MET:HE3	21:N:745:LEU:HD13	1.83	0.61
22:O:30:GLU:OE2	22:O:58:ARG:NH1	2.34	0.61
10:C:124:GLN:NE2	11:D:127:ARG:O	2.34	0.61
6:e:35:ALA:HB2	6:e:141:VAL:HG23	1.83	0.61
7:a:131:THR:HG21	13:l:98:VAL:HG22	1.83	0.61
8:c:57:LYS:HE3	8:c:69:VAL:HB	1.83	0.61
15:H:225:VAL:HA	15:H:350:LYS:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:867:LYS:HG2	21:N:868:VAL:HG23	1.83	0.61
10:C:11:THR:HA	11:D:127:ARG:HB2	1.81	0.61
16:I:388:SER:OG	17:J:306:ARG:NH1	2.33	0.61
21:N:742:TRP:HD1	29:V:61:TYR:OH	1.83	0.61
27:T:142:LEU:HD12	27:T:142:LEU:O	2.01	0.61
17:J:297:LEU:HD21	17:J:302:PRO:HA	1.82	0.60
17:J:339:ARG:NH2	25:R:205:GLU:OE1	2.32	0.60
28:U:167:GLU:HG3	29:V:35:LEU:HD11	1.82	0.60
20:M:425:ARG:HG2	20:M:426:LYS:H	1.65	0.60
4:4:146:HIS:O	4:4:149:ARG:NH1	2.31	0.60
5:f:138:CYS:HB3	5:f:149:ILE:HG13	1.83	0.60
6:e:71:MET:HE3	6:e:84:VAL:HG22	1.84	0.60
14:G:52:LYS:HE3	14:G:59:LEU:HD21	1.84	0.60
8:c:168:ALA:HB3	9:j:55:LEU:HD13	1.84	0.60
22:O:74:ASN:OD1	22:O:75:GLN:N	2.35	0.60
33:Z:117:ASP:OD1	33:Z:138:ARG:NH1	2.34	0.60
2:i:46:ASP:HA	2:i:202:VAL:HA	1.82	0.60
22:O:70:TYR:HD1	22:O:75:GLN:HB3	1.67	0.60
33:Z:915:ALA:HB2	33:Z:957:LEU:HG	1.82	0.60
3:3:76:LEU:O	10:C:92:ARG:NH1	2.34	0.60
14:k:54:ILE:HD11	14:k:213:GLU:HB2	1.83	0.60
16:I:423:VAL:HA	16:I:427:LYS:HB2	1.83	0.60
23:P:90:LYS:HG3	23:P:129:LYS:HB3	1.84	0.60
27:T:164:LEU:O	27:T:170:ASN:ND2	2.34	0.60
9:B:93:ALA:HB1	9:B:105:PRO:HG2	1.82	0.60
10:d:16:GLU:O	11:n:29:ARG:NH1	2.35	0.60
17:J:336:ASN:ND2	18:K:200:GLN:O	2.35	0.60
11:D:68:ASP:HB3	11:D:71:VAL:HB	1.83	0.60
17:J:188:TYR:HB2	17:J:315:GLU:HA	1.83	0.60
21:N:742:TRP:CD1	29:V:61:TYR:OH	2.53	0.60
2:2:230:LYS:HB2	6:e:201:LYS:HD3	1.84	0.60
10:C:78:ALA:HB3	10:C:134:SER:HB3	1.83	0.60
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.83	0.60
23:P:141:LYS:HE2	23:P:182:GLU:HG3	1.83	0.60
24:Q:355:GLU:HB2	24:Q:399:VAL:HG22	1.82	0.60
2:2:192:ILE:HG12	2:2:199:GLY:HA2	1.84	0.60
3:3:46:TYR:HB3	3:3:71:THR:HG21	1.84	0.60
11:n:181:ARG:NH2	12:m:60:GLU:HG2	2.16	0.60
16:I:384:LYS:NZ	16:I:386:ASP:OD1	2.35	0.60
14:G:120:VAL:HG21	14:G:151:LEU:HD21	1.83	0.60
16:I:110:GLU:HB2	16:I:119:ILE:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:23:THR:HG21	29:V:171:ARG:HE	1.67	0.60
33:Z:133:ASP:OD1	33:Z:136:ARG:NH2	2.34	0.60
2:i:244:GLU:HG2	3:h:198:ARG:HG2	1.84	0.59
11:n:159:TRP:HE3	12:m:58:LEU:O	1.85	0.59
28:U:38:LEU:HB2	28:U:50:ASN:HB3	1.84	0.59
2:2:172:LYS:H	2:2:175:LEU:HD11	1.67	0.59
12:m:77:ALA:HB3	12:m:143:LEU:HB2	1.83	0.59
16:I:428:VAL:HG13	17:J:305:LEU:HD13	1.83	0.59
19:L:169:ASN:OD1	20:M:302:GLN:NE2	2.34	0.59
19:L:295:THR:OG1	19:L:298:ASP:O	2.20	0.59
4:4:29:LYS:HE3	4:4:31:SER:HB2	1.84	0.59
18:K:289:ASP:HA	19:L:299:ARG:NH2	2.16	0.59
33:Z:225:LEU:HD13	33:Z:256:LEU:HB2	1.84	0.59
3:3:138:VAL:HG11	3:3:146:LEU:HB2	1.85	0.59
10:C:44:ILE:H	10:C:216:ILE:HB	1.67	0.59
8:c:51:THR:HB	8:c:228:ALA:HB3	1.83	0.59
20:M:295:LYS:HB3	20:M:302:GLN:HB2	1.83	0.59
21:N:489:MET:HB3	21:N:524:ILE:HG13	1.84	0.59
22:O:40:GLN:O	22:O:58:ARG:NH2	2.29	0.59
4:4:149:ARG:HB2	4:4:152:MET:HG3	1.83	0.59
9:j:123:GLN:HE22	10:d:86:ILE:HG13	1.68	0.59
11:n:163:THR:HG21	11:n:171:VAL:HB	1.84	0.59
21:N:335:ALA:HB2	21:N:701:VAL:HA	1.85	0.59
25:R:33:LEU:O	25:R:74:ASN:ND2	2.35	0.59
25:R:306:PRO:HA	25:R:309:LEU:HD13	1.84	0.59
29:V:221:TRP:NE1	29:V:223:SER:OG	2.36	0.59
33:Z:574:TYR:HB2	33:Z:581:VAL:HG12	1.83	0.59
1:b:23:MET:HE2	1:b:174:ILE:HG12	1.84	0.59
8:A:46:ARG:HD3	8:A:154:ILE:HG13	1.84	0.59
11:D:161:ALA:HB1	11:D:175:LEU:HD23	1.85	0.59
26:S:327:ILE:HG21	32:Y:64:TRP:HE1	1.66	0.59
1:1:194:MET:HB2	1:1:205:LEU:HB2	1.85	0.59
5:5:82:ARG:NH2	5:5:199:GLY:O	2.36	0.59
10:C:216:ILE:HG12	10:C:227:GLN:HG2	1.85	0.59
11:D:149:GLN:NE2	11:D:157:SER:OG	2.36	0.59
14:G:68:GLN:HG3	14:G:89:VAL:HG11	1.85	0.59
6:e:47:ARG:NH1	6:e:215:ILE:O	2.36	0.59
7:a:127:GLU:HG2	13:l:100:ASN:HB2	1.83	0.59
7:a:215:ARG:HG2	7:a:247:VAL:HG13	1.85	0.59
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.85	0.59
18:K:90:GLN:HG2	18:K:147:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:392:LYS:HD2	23:P:401:ASN:HB2	1.85	0.59
16:I:147:VAL:HG12	16:I:159:VAL:HG23	1.85	0.59
24:Q:378:SER:HB2	25:R:344:SER:HB2	1.85	0.59
27:T:79:GLU:O	27:T:83:ASN:ND2	2.34	0.59
3:3:11:ILE:HD12	3:3:146:LEU:HD11	1.85	0.58
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.85	0.58
16:I:161:GLN:NE2	16:I:163:ASP:OD2	2.36	0.58
21:N:43:LEU:HD21	21:N:68:VAL:HG11	1.84	0.58
33:Z:257:PRO:HB2	33:Z:259:PRO:HD2	1.85	0.58
2:i:254:GLU:OE2	10:d:217:ARG:NH1	2.36	0.58
12:E:54:ALA:HA	12:E:59:LEU:HD23	1.85	0.58
10:d:119:LYS:HG2	10:d:131:PHE:HB2	1.85	0.58
25:R:218:CYS:HB3	25:R:223:ASN:HB2	1.85	0.58
7:a:232:ILE:HB	7:a:240:THR:HB	1.85	0.58
28:U:50:ASN:OD1	28:U:51:SER:N	2.36	0.58
33:Z:352:LYS:HB3	33:Z:466:GLU:HG3	1.83	0.58
3:3:109:VAL:HB	3:3:122:ALA:HB3	1.85	0.58
2:i:192:ILE:HG12	2:i:199:GLY:HA2	1.85	0.58
5:f:128:GLN:HB3	6:e:113:GLN:HE22	1.68	0.58
7:a:136:ARG:HB3	7:a:142:PRO:HA	1.86	0.58
10:C:217:ARG:HG2	10:C:219:GLY:H	1.68	0.58
11:D:155:ILE:HG22	12:E:82:THR:HB	1.84	0.58
13:l:18:ARG:NH2	13:l:23:GLU:OE2	2.29	0.58
15:H:168:ILE:HD12	15:H:174:VAL:HG11	1.85	0.58
23:P:66:LEU:HD13	23:P:75:LEU:HA	1.86	0.58
33:Z:116:ALA:HB3	33:Z:141:SER:HB2	1.84	0.58
6:6:74:ASN:OD1	6:6:75:GLY:N	2.35	0.58
6:e:214:HIS:HD2	6:e:217:VAL:HG23	1.66	0.58
8:c:42:SER:HA	8:c:55:SER:HA	1.84	0.58
9:j:134:LEU:HB2	9:j:150:VAL:HB	1.84	0.58
24:Q:142:ALA:HA	24:Q:145:HIS:HD2	1.68	0.58
25:R:347:THR:HG22	25:R:389:GLU:HG2	1.84	0.58
5:f:172:MET:H	5:f:192:SER:HB3	1.69	0.58
2:2:153:TYR:OH	2:2:168:GLU:OE1	2.22	0.58
4:g:37:GLN:O	4:g:61:GLN:NE2	2.37	0.58
9:B:87:ASP:OD1	9:B:90:ARG:NH2	2.37	0.58
3:3:77:LYS:O	9:B:108:LYS:NZ	2.34	0.58
7:7:131:THR:HG21	13:F:98:VAL:HG22	1.86	0.58
7:7:215:ARG:HG2	7:7:247:VAL:HG13	1.86	0.58
11:D:118:GLN:NE2	12:E:83:ALA:O	2.36	0.58
24:Q:92:LYS:HA	24:Q:129:LYS:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:223:ASN:HB3	25:R:226:GLU:HB2	1.86	0.58
32:Y:69:VAL:HG12	32:Y:70:ASP:H	1.69	0.58
2:i:74:GLY:HA3	2:i:81:THR:HG21	1.84	0.58
14:G:193:VAL:HG13	14:G:216:ILE:HG21	1.84	0.58
11:n:10:ILE:HD11	11:n:18:PHE:HD2	1.67	0.58
12:m:54:ALA:HA	12:m:59:LEU:HD23	1.86	0.58
20:M:195:GLU:HA	20:M:199:LEU:HD12	1.85	0.58
7:7:251:LYS:NZ	2:i:171:TRP:O	2.29	0.58
13:l:52:ASN:ND2	13:l:54:ASP:O	2.37	0.58
29:V:54:LEU:HB3	29:V:102:GLN:HB2	1.85	0.58
1:1:131:THR:HG21	7:7:68:ARG:HH21	1.67	0.57
1:b:198:THR:HG23	1:b:200:ALA:H	1.69	0.57
5:f:96:THR:HG22	5:f:101:VAL:HG22	1.84	0.57
10:C:177:GLN:HE22	11:D:53:LYS:HD3	1.69	0.57
17:J:196:THR:HG21	18:K:305:GLY:HA2	1.86	0.57
33:Z:76:LYS:NZ	33:Z:149:TRP:O	2.31	0.57
33:Z:87:LYS:HE2	33:Z:89:LEU:HB2	1.85	0.57
33:Z:330:ILE:HG22	33:Z:341:TYR:HB2	1.85	0.57
3:3:53:ILE:HG22	3:3:60:VAL:HG22	1.86	0.57
3:3:185:ALA:HB3	3:3:200:LEU:HB2	1.86	0.57
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.86	0.57
7:a:39:VAL:HG13	7:a:62:SER:H	1.70	0.57
19:L:149:ASP:OD2	19:L:152:THR:OG1	2.21	0.57
20:M:286:ILE:HG22	20:M:301:VAL:HG13	1.84	0.57
29:V:147:VAL:HG12	29:V:149:GLY:H	1.68	0.57
2:i:47:THR:HB	2:i:59:ASN:HA	1.85	0.57
5:f:82:ARG:HH21	5:f:185:PRO:HG2	1.68	0.57
6:e:47:ARG:NH2	6:e:218:GLY:HA3	2.19	0.57
9:B:119:GLN:NE2	10:C:82:ALA:O	2.37	0.57
10:d:76:ALA:HB3	10:d:136:ILE:HB	1.87	0.57
17:J:273:LEU:HD13	17:J:304:LEU:HD21	1.85	0.57
27:T:98:GLU:HB2	27:T:101:LYS:HG2	1.85	0.57
3:h:65:GLU:HB3	10:d:100:LYS:HG3	1.86	0.57
11:D:9:SER:HA	12:E:136:ARG:HD2	1.86	0.57
19:L:252:VAL:O	20:M:293:SER:N	2.35	0.57
3:3:173:ASN:ND2	6:e:176:LYS:O	2.36	0.57
9:B:32:VAL:HG21	9:B:63:LYS:HZ3	1.70	0.57
11:n:37:LYS:HG3	11:n:42:VAL:HG22	1.87	0.57
20:M:148:VAL:HG12	20:M:155:ILE:HA	1.84	0.57
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.34	0.57
6:6:50:THR:OG1	6:6:55:ASN:ND2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:170:ASP:HB3	6:e:176:LYS:HD2	1.86	0.57
11:D:159:TRP:CZ3	12:E:59:LEU:HB2	2.40	0.57
13:F:164:ARG:O	13:F:200:SER:OG	2.22	0.57
18:K:207:ARG:NH2	18:K:302:GLN:O	2.36	0.57
10:C:120:GLN:NE2	10:C:123:THR:OG1	2.37	0.57
14:G:68:GLN:O	14:G:76:CYS:N	2.35	0.57
16:I:319:ARG:NH2	33:Z:825:ALA:O	2.37	0.57
28:U:286:ILE:HG23	29:V:280:LEU:HG	1.87	0.57
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.87	0.57
16:I:249:GLY:HA3	16:I:284:ILE:HG12	1.87	0.57
33:Z:770:GLU:HG2	33:Z:773:ARG:HD2	1.86	0.57
1:1:38:ARG:HD2	1:1:45:ILE:HD13	1.86	0.57
2:2:123:ILE:HG22	2:2:125:ALA:H	1.70	0.57
7:7:232:ILE:HB	7:7:240:THR:HB	1.86	0.57
11:n:75:PHE:HB3	11:n:133:THR:HG22	1.86	0.57
21:N:589:ILE:HA	21:N:624:ALA:HB2	1.87	0.57
24:Q:185:TYR:HB3	24:Q:190:ASN:HB3	1.87	0.57
15:H:246:ILE:HB	15:H:352:MET:HG2	1.86	0.56
21:N:666:GLN:HG2	21:N:873:ARG:HE	1.70	0.56
30:W:21:PHE:HB2	30:W:22:PRO:HD3	1.87	0.56
2:2:196:LEU:HB3	6:e:215:ILE:HB	1.87	0.56
4:g:53:THR:HG22	4:g:100:VAL:HG22	1.86	0.56
10:C:50:ARG:HH21	10:C:212:GLU:HG2	1.71	0.56
25:R:240:SER:HB3	25:R:243:LEU:HB2	1.87	0.56
3:3:138:VAL:HG12	3:3:143:SER:HB2	1.86	0.56
5:5:76:THR:N	5:5:206:SER:HG	2.03	0.56
2:i:172:LYS:HB3	2:i:175:LEU:HD21	1.87	0.56
3:h:155:GLU:HB3	3:h:158:LEU:HD21	1.86	0.56
13:l:47:VAL:HG22	13:l:213:ILE:HG12	1.87	0.56
15:H:380:PRO:O	15:H:385:ARG:NH1	2.38	0.56
21:N:70:TYR:HE2	26:S:219:LYS:HD2	1.71	0.56
21:N:521:LEU:HB3	21:N:535:LEU:HD21	1.86	0.56
2:2:93:GLU:OE1	9:B:98:LYS:NZ	2.38	0.56
10:C:112:VAL:HG21	10:C:149:TYR:HD2	1.70	0.56
17:J:301:ASP:HB3	17:J:304:LEU:HG	1.86	0.56
20:M:421:GLU:HG2	20:M:422:VAL:N	2.19	0.56
26:S:417:GLN:HE22	27:T:208:LEU:HD23	1.69	0.56
2:2:129:VAL:HB	2:2:140:PHE:HB2	1.87	0.56
24:Q:164:GLU:HA	24:Q:168:LEU:HD12	1.86	0.56
26:S:227:ASN:HD22	26:S:263:ASP:HB2	1.69	0.56
33:Z:183:LYS:NZ	33:Z:292:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:156:LYS:NZ	8:A:158:ASP:OD1	2.38	0.56
14:G:54:ILE:HD11	14:G:213:GLU:HG3	1.87	0.56
14:k:183:HIS:ND1	14:k:186:GLY:O	2.38	0.56
15:H:453:GLY:O	16:I:347:LYS:NZ	2.37	0.56
22:O:352:TRP:HE1	28:U:235:LEU:HD13	1.69	0.56
26:S:389:LYS:HZ1	26:S:426:ALA:HB2	1.71	0.56
3:3:205:ASP:OD2	5:f:94:ARG:NH2	2.38	0.56
11:D:34:VAL:HG22	11:D:163:THR:HG23	1.88	0.56
17:J:70:SER:H	18:K:119:VAL:H	1.53	0.56
23:P:259:PRO:O	23:P:263:HIS:ND1	2.30	0.56
24:Q:97:LEU:HB3	24:Q:130:ARG:HH21	1.71	0.56
2:2:101:ARG:NH1	8:A:110:TYR:OH	2.35	0.56
7:a:77:PRO:HA	7:a:83:VAL:HA	1.87	0.56
9:B:111:VAL:HG21	9:B:148:TYR:HD2	1.70	0.56
11:n:159:TRP:CH2	12:m:59:LEU:HB2	2.39	0.56
23:P:225:VAL:HG11	23:P:328:ALA:HB1	1.88	0.56
29:V:52:LEU:HD21	29:V:104:VAL:HG22	1.88	0.56
11:D:122:GLN:HA	12:E:136:ARG:HE	1.70	0.56
11:n:139:ASP:HB3	11:n:142:ASP:HB3	1.88	0.56
15:H:247:LEU:HD23	15:H:374:LYS:HG2	1.87	0.56
3:3:28:ARG:HH21	3:3:183:TRP:CD1	2.24	0.55
21:N:543:ASP:OD1	21:N:548:ARG:NH2	2.39	0.55
23:P:126:THR:O	23:P:136:ARG:NH2	2.38	0.55
27:T:131:LYS:HD3	27:T:134:LYS:HB2	1.89	0.55
11:D:201:GLU:O	11:D:204:GLN:NE2	2.34	0.55
21:N:223:LEU:HD11	21:N:897:LYS:HE3	1.89	0.55
25:R:325:HIS:HB2	25:R:329:PHE:CE2	2.41	0.55
33:Z:769:ASN:OD1	33:Z:770:GLU:N	2.39	0.55
8:A:54:ILE:HG12	8:A:225:VAL:HG22	1.88	0.55
9:B:176:GLU:HB2	10:C:56:LEU:HD11	1.87	0.55
11:n:122:GLN:O	12:m:135:SER:N	2.38	0.55
17:J:267:GLU:OE1	18:K:290:ARG:NH1	2.39	0.55
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.70	0.55
9:B:13:SER:HB2	9:B:18:LEU:HD23	1.88	0.55
3:h:105:VAL:C	3:h:107:PRO:HD3	2.31	0.55
8:A:17:THR:HG23	8:A:27:GLN:HG3	1.89	0.55
10:d:216:ILE:HG12	10:d:227:GLN:HG2	1.88	0.55
12:m:20:ARG:HA	13:l:77:LEU:HD21	1.89	0.55
14:k:201:TYR:HA	14:k:204:HIS:HD2	1.72	0.55
19:L:290:ARG:HH21	19:L:294:GLY:H	1.53	0.55
23:P:137:ALA:HB2	23:P:167:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:260:ILE:HG22	27:T:264:MET:HE2	1.89	0.55
1:1:38:ARG:NH2	1:1:186:GLY:O	2.40	0.55
3:3:73:LEU:HD23	3:3:76:LEU:HD12	1.88	0.55
1:b:61:TRP:HZ3	1:b:195:VAL:HG11	1.72	0.55
8:A:78:THR:H	8:A:233:PHE:HB2	1.72	0.55
11:n:68:ASP:HB3	11:n:71:VAL:HB	1.89	0.55
12:m:18:GLU:OE1	12:m:20:ARG:NH2	2.40	0.55
17:J:185:VAL:HB	17:J:289:LYS:HZ1	1.72	0.55
19:L:109:MET:N	19:L:118:ILE:O	2.40	0.55
29:V:170:PRO:HB3	29:V:175:SER:OG	2.07	0.55
10:d:50:ARG:NH2	10:d:63:THR:OG1	2.40	0.55
24:Q:223:GLY:HA2	24:Q:226:HIS:HD2	1.72	0.55
30:W:40:LYS:HE3	30:W:191:ILE:HG12	1.88	0.55
33:Z:225:LEU:HD21	33:Z:253:VAL:HA	1.89	0.55
33:Z:266:LYS:NZ	33:Z:290:GLU:OE1	2.40	0.55
14:G:73:HIS:ND1	14:G:74:ILE:HG13	2.22	0.55
13:l:50:LYS:HB3	13:l:59:TYR:HB3	1.89	0.55
18:K:84:GLU:HB3	18:K:88:ARG:HH12	1.72	0.55
18:K:209:VAL:HG23	18:K:336:ARG:HB2	1.89	0.55
19:L:329:ARG:HG2	19:L:331:ASP:H	1.71	0.55
24:Q:78:ILE:HG12	24:Q:100:LEU:HD13	1.88	0.55
7:7:187:LEU:HD11	7:7:216:VAL:HG11	1.90	0.54
20:M:82:VAL:HA	20:M:119:VAL:HA	1.88	0.54
11:D:44:LEU:HD11	11:D:136:ALA:HB3	1.89	0.54
8:c:140:ILE:HG12	8:c:159:PRO:HD3	1.89	0.54
9:j:45:ILE:HD12	9:j:74:VAL:HB	1.89	0.54
10:d:84:ALA:HB2	10:d:133:VAL:HG21	1.88	0.54
30:W:11:ASP:HA	30:W:55:ALA:HB3	1.88	0.54
1:1:117:ILE:HG12	1:1:131:THR:HG23	1.90	0.54
2:2:228:LYS:NZ	3:3:152:SER:O	2.39	0.54
1:b:151:THR:HA	1:b:154:TYR:HE2	1.71	0.54
2:i:155:SER:HG	2:i:160:SER:HG	1.55	0.54
21:N:512:ASN:OD1	21:N:515:ARG:NH2	2.33	0.54
26:S:475:TYR:OH	28:U:295:LYS:N	2.41	0.54
5:f:250:VAL:N	5:f:266:HIS:O	2.38	0.54
10:C:206:LEU:HD23	10:C:244:ILE:HG21	1.88	0.54
10:d:137:TYR:HE2	10:d:151:SER:HB2	1.71	0.54
7:a:100:LEU:HD21	7:a:129:LEU:HD11	1.89	0.54
10:d:191:GLU:HG2	10:d:242:THR:HG22	1.89	0.54
13:l:67:ASP:HB3	13:l:70:MET:HB3	1.89	0.54
16:I:209:GLU:OE2	16:I:319:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:312:LEU:HD13	20:M:342:ARG:HG2	1.90	0.54
22:O:306:ARG:NH2	28:U:234:ASN:OD1	2.41	0.54
25:R:325:HIS:HB3	25:R:328:PHE:HB2	1.88	0.54
25:R:382:ASP:HB3	25:R:387:ILE:H	1.73	0.54
6:6:47:ARG:NH1	6:6:215:ILE:O	2.35	0.54
11:D:41:CYS:HA	11:D:138:PHE:HZ	1.73	0.54
19:L:230:LEU:HD11	19:L:387:ASN:HB2	1.89	0.54
20:M:62:ILE:HG13	20:M:66:LYS:HG3	1.88	0.54
21:N:154:LEU:HD22	21:N:189:LEU:HD21	1.88	0.54
15:H:318:ARG:NH2	15:H:328:GLU:OE1	2.39	0.54
15:H:330:GLN:NE2	20:M:250:GLN:OE1	2.41	0.54
17:J:61:GLU:OE2	18:K:121:ARG:NH2	2.40	0.54
22:O:189:TYR:HE2	22:O:227:ILE:HB	1.72	0.54
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.73	0.54
28:U:210:TYR:OH	28:U:223:HIS:N	2.34	0.54
8:A:133:TYR:HD1	14:G:127:ASN:HB3	1.73	0.54
2:2:109:LEU:HD21	2:2:148:THR:HB	1.89	0.54
2:2:166:VAL:O	2:2:170:HIS:ND1	2.37	0.54
7:7:48:LYS:HG2	7:7:53:VAL:HG12	1.89	0.54
2:i:101:ARG:HE	8:c:150:LEU:HD11	1.72	0.54
6:e:35:ALA:O	6:e:154:GLN:NE2	2.39	0.54
9:B:177:LYS:NZ	24:Q:206:ASN:O	2.41	0.54
14:G:124:THR:HG22	14:G:131:PRO:HB3	1.89	0.54
12:m:126:GLY:HA2	12:m:132:ARG:HG3	1.88	0.54
17:J:225:GLU:OE2	17:J:228:ARG:NH2	2.40	0.54
6:e:49:ILE:HG22	6:e:54:ILE:HA	1.89	0.54
13:F:72:LEU:HD13	13:F:132:LEU:HD22	1.89	0.54
14:G:124:THR:HA	14:G:131:PRO:HG3	1.89	0.54
21:N:378:ASN:HD21	21:N:381:GLU:HB2	1.72	0.54
7:7:49:TYR:O	7:7:158:GLN:NE2	2.32	0.53
21:N:83:LEU:HD13	21:N:135:SER:HB3	1.90	0.53
21:N:653:ARG:NH1	21:N:691:GLN:OE1	2.41	0.53
25:R:240:SER:HB2	25:R:244:THR:HG22	1.90	0.53
28:U:13:LEU:HD21	29:V:36:LYS:HG2	1.90	0.53
8:c:15:HIS:O	8:c:27:GLN:NE2	2.41	0.53
8:c:64:LEU:N	14:k:159:GLY:O	2.41	0.53
22:O:377:VAL:HG13	28:U:197:LEU:HD22	1.90	0.53
25:R:57:GLU:OE1	25:R:109:LYS:NZ	2.34	0.53
1:b:63:CYS:HB2	1:b:117:ILE:HB	1.91	0.53
5:f:106:VAL:HA	6:e:151:GLU:HG2	1.91	0.53
11:n:62:SER:OG	11:n:211:GLU:OE2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:85:ALA:HB2	12:m:140:VAL:HG21	1.90	0.53
15:H:223:GLU:HG2	20:M:403:LEU:HD23	1.89	0.53
18:K:188:VAL:HG12	18:K:230:THR:HG21	1.91	0.53
23:P:432:LEU:HD13	28:U:225:ILE:HG13	1.89	0.53
24:Q:51:ARG:HD2	24:Q:88:PHE:HA	1.91	0.53
24:Q:227:CYS:HB3	24:Q:334:HIS:HE2	1.72	0.53
33:Z:68:LEU:HD23	33:Z:71:LEU:HD12	1.91	0.53
1:l:87:SER:O	8:A:98:LYS:NZ	2.38	0.53
11:D:4:TYR:HD1	11:D:10:ILE:HG21	1.72	0.53
18:K:211:LEU:HB2	18:K:317:ALA:HA	1.91	0.53
22:O:286:PHE:HE1	22:O:337:LEU:HD23	1.73	0.53
23:P:248:ASP:HA	23:P:252:SER:HB3	1.90	0.53
25:R:182:ASN:OD1	25:R:184:GLN:NE2	2.42	0.53
25:R:204:TRP:HE1	25:R:234:SER:HA	1.74	0.53
3:3:28:ARG:HB2	3:3:183:TRP:HB2	1.90	0.53
12:m:71:ASP:OD1	12:m:72:ARG:N	2.41	0.53
15:H:313:ALA:HA	16:I:304:ARG:HE	1.72	0.53
25:R:359:VAL:HG12	32:Y:81:LEU:HD13	1.90	0.53
33:Z:301:THR:O	33:Z:307:HIS:NE2	2.38	0.53
1:b:20:THR:N	1:b:188:SER:HG	2.06	0.53
4:g:29:LYS:HG3	4:g:31:SER:H	1.74	0.53
20:M:53:HIS:CE1	30:W:70:GLY:HA3	2.44	0.53
29:V:57:PHE:HB2	29:V:63:VAL:HA	1.90	0.53
1:l:27:PHE:HE2	1:l:32:ILE:HG13	1.73	0.53
3:3:8:ASN:ND2	3:3:30:GLY:O	2.32	0.53
15:H:314:VAL:HG13	15:H:329:VAL:HG22	1.91	0.53
20:M:175:LYS:HE2	20:M:240:ASN:HB3	1.90	0.53
22:O:143:LEU:HD13	22:O:178:TYR:HA	1.88	0.53
24:Q:404:ASN:O	25:R:397:ASN:ND2	2.42	0.53
11:D:78:LEU:HG	11:D:80:ALA:H	1.73	0.53
28:U:38:LEU:HD13	28:U:87:GLU:HB3	1.91	0.53
33:Z:441:TYR:HA	33:Z:448:LYS:HE2	1.89	0.53
1:b:80:TYR:HB2	8:c:102:ALA:HB1	1.91	0.53
1:b:103:GLU:HG3	14:k:102:LEU:HA	1.90	0.53
15:H:164:SER:OG	15:H:167:ASP:O	2.27	0.53
15:H:277:SER:OG	16:I:308:GLU:OE1	2.26	0.53
15:H:418:GLU:HG2	16:I:341:PRO:HG2	1.90	0.53
16:I:294:SER:HA	16:I:299:GLU:HA	1.91	0.53
20:M:216:LYS:HD3	20:M:341:GLY:HA2	1.90	0.53
26:S:311:GLN:NE2	26:S:341:SER:OG	2.42	0.53
26:S:482:PRO:HG2	28:U:301:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:4:ILE:HD13	4:g:45:SER:HB3	1.90	0.53
5:f:108:LYS:HB3	5:f:120:MET:HB3	1.91	0.53
6:e:41:VAL:HG12	6:e:225:ILE:HA	1.90	0.53
9:B:45:ILE:HD12	9:B:74:VAL:HB	1.90	0.53
11:D:159:TRP:CH2	12:E:59:LEU:HB2	2.44	0.53
18:K:99:PHE:HA	18:K:110:VAL:HG12	1.91	0.53
21:N:742:TRP:CE3	21:N:743:PHE:HB3	2.44	0.53
24:Q:104:PHE:HB3	24:Q:114:GLN:HE21	1.73	0.53
26:S:136:CYS:HB3	26:S:179:ILE:HG21	1.91	0.53
4:4:8:ARG:HG3	4:4:13:VAL:HG22	1.91	0.52
2:i:252:ILE:HD11	10:d:226:TYR:HB2	1.90	0.52
10:C:50:ARG:NH1	10:C:59:GLN:O	2.37	0.52
11:D:122:GLN:O	12:E:135:SER:OG	2.27	0.52
8:c:144:VAL:HG12	8:c:154:ILE:HG12	1.91	0.52
17:J:183:LYS:NZ	17:J:280:ASP:OD1	2.34	0.52
24:Q:12:ARG:HH22	24:Q:60:GLU:HG3	1.74	0.52
1:b:63:CYS:N	1:b:117:ILE:O	2.39	0.52
7:a:48:LYS:HG2	7:a:53:VAL:HG12	1.91	0.52
12:E:122:ARG:NH1	12:E:131:GLU:O	2.42	0.52
16:I:330:LYS:HG2	16:I:332:GLU:H	1.74	0.52
20:M:284:ASP:O	20:M:288:THR:OG1	2.21	0.52
29:V:116:CYS:HG	29:V:117:TRP:CD1	2.27	0.52
1:1:59:LYS:HD3	1:1:121:TYR:HD2	1.74	0.52
12:E:71:ASP:OD1	12:E:72:ARG:N	2.43	0.52
8:c:148:GLU:HG2	8:c:230:LYS:HE3	1.90	0.52
19:L:118:ILE:HG12	19:L:128:ILE:HG12	1.92	0.52
21:N:145:LEU:O	21:N:173:LYS:NZ	2.38	0.52
21:N:176:GLN:HG2	21:N:182:ASN:ND2	2.24	0.52
3:3:65:GLU:OE2	3:3:68:ARG:NH1	2.42	0.52
13:F:176:LEU:HD13	14:G:58:LEU:HD23	1.91	0.52
20:M:290:ARG:NH2	20:M:294:GLU:OE2	2.39	0.52
2:2:48:ARG:NH2	6:e:241:ASP:OD2	2.43	0.52
9:B:95:THR:HA	9:B:99:ARG:HD2	1.92	0.52
10:C:18:ARG:HH22	16:I:437:LEU:HD22	1.74	0.52
11:n:31:THR:O	11:n:76:SER:OG	2.28	0.52
12:m:50:VAL:HG21	12:m:66:LYS:HB2	1.91	0.52
15:H:385:ARG:NH1	15:H:413:ASN:OD1	2.42	0.52
1:1:89:TYR:HD1	14:G:111:ALA:HB1	1.74	0.52
2:2:206:VAL:HB	2:2:214:GLU:HB2	1.92	0.52
7:7:137:ARG:HA	7:7:142:PRO:HG3	1.92	0.52
10:C:162:ALA:HB3	11:D:54:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:67:ASP:OD1	13:F:68:GLU:N	2.43	0.52
13:F:154:THR:OG1	14:G:64:ASN:ND2	2.42	0.52
14:G:68:GLN:HB2	14:G:76:CYS:HB3	1.92	0.52
18:K:396:ARG:HA	19:L:195:GLU:HG3	1.92	0.52
24:Q:127:ARG:HA	24:Q:130:ARG:HB2	1.91	0.52
28:U:48:VAL:HG22	28:U:90:ILE:HD11	1.90	0.52
4:4:63:ASN:HD22	4:4:83:PHE:HZ	1.56	0.52
9:B:30:GLN:HG2	18:K:428:LYS:HA	1.92	0.52
9:B:50:LYS:HE3	18:K:424:PHE:CG	2.45	0.52
15:H:276:GLY:N	15:H:309:ASP:O	2.40	0.52
33:Z:588:ILE:HG12	33:Z:596:THR:HB	1.92	0.52
3:3:28:ARG:HG3	3:3:183:TRP:CE3	2.45	0.52
3:3:65:GLU:HB3	10:C:100:LYS:HG3	1.91	0.52
8:c:14:ARG:HE	8:c:21:PRO:HD2	1.74	0.52
13:l:132:LEU:HB2	13:l:147:PHE:HB3	1.91	0.52
16:I:181:TYR:HB3	16:I:191:ILE:HD13	1.91	0.52
21:N:175:ASP:O	21:N:176:GLN:C	2.53	0.52
21:N:491:GLY:H	21:N:526:TYR:HB3	1.74	0.52
24:Q:416:VAL:HA	25:R:410:LEU:HD21	1.91	0.52
3:3:177:ARG:HH12	6:e:166:MET:HE3	1.74	0.52
5:f:76:THR:N	5:f:245:TYR:O	2.43	0.52
11:n:117:GLN:NE2	11:n:129:PHE:O	2.43	0.52
16:I:102:ASN:N	16:I:103:PRO:CD	2.73	0.52
16:I:293:ASP:OD1	16:I:294:SER:N	2.41	0.52
19:L:144:VAL:HA	19:L:161:ARG:HG2	1.91	0.52
19:L:177:GLU:HB2	19:L:233:LYS:HD3	1.92	0.52
22:O:67:SER:HA	22:O:113:LYS:HE3	1.92	0.52
7:a:110:ASP:OD1	14:k:93:ARG:NH1	2.42	0.52
10:C:44:ILE:HG21	10:C:138:ALA:HB1	1.92	0.52
13:F:121:GLN:NE2	14:G:84:ASP:OD1	2.43	0.52
24:Q:391:ASP:OD1	25:R:347:THR:OG1	2.27	0.52
28:U:94:HIS:CE1	28:U:122:ILE:HG12	2.45	0.52
29:V:27:VAL:HA	29:V:63:VAL:HG11	1.92	0.52
31:X:48:PHE:HB2	31:X:66:LEU:HB3	1.92	0.52
11:D:172:ARG:NH1	11:D:176:GLU:OE2	2.43	0.51
20:M:62:ILE:HD12	20:M:65:ASN:HB2	1.93	0.51
23:P:361:THR:HG22	23:P:363:LEU:H	1.75	0.51
26:S:418:THR:OG1	27:T:158:GLN:OE1	2.26	0.51
2:2:46:ASP:HA	2:2:202:VAL:HA	1.90	0.51
4:g:26:SER:OG	5:f:208:GLN:NE2	2.44	0.51
11:D:216:LYS:HB2	11:D:220:ASP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:187:TRP:HA	12:m:191:LEU:HD11	1.91	0.51
20:M:144:ASP:OD1	20:M:145:LEU:N	2.44	0.51
25:R:273:SER:HB3	25:R:276:LEU:HB2	1.92	0.51
29:V:73:GLN:HE21	29:V:77:GLY:HA2	1.74	0.51
2:2:119:TYR:HB3	2:2:122:HIS:HB3	1.90	0.51
7:a:58:ASP:O	7:a:74:ARG:NH2	2.43	0.51
9:B:200:VAL:HG22	9:B:202:GLY:H	1.75	0.51
13:l:143:HIS:ND1	13:l:155:GLU:OE2	2.40	0.51
15:H:253:GLY:HA2	15:H:256:LYS:HE2	1.92	0.51
15:H:327:ASN:O	15:H:331:ARG:NH2	2.43	0.51
18:K:123:LEU:HG	18:K:125:THR:H	1.74	0.51
22:O:43:GLU:HA	22:O:82:LEU:HD21	1.93	0.51
26:S:417:GLN:HE22	27:T:208:LEU:HA	1.74	0.51
6:6:55:ASN:HB3	7:7:170:TYR:CZ	2.45	0.51
8:A:14:ARG:NE	14:G:8:TYR:OH	2.30	0.51
11:n:157:SER:OG	11:n:159:TRP:NE1	2.41	0.51
13:l:88:LEU:HD11	13:l:112:LEU:HD11	1.93	0.51
18:K:120:VAL:HG11	18:K:139:LEU:HD22	1.92	0.51
24:Q:419:LEU:HD22	25:R:410:LEU:HD23	1.93	0.51
30:W:132:LEU:HB3	30:W:137:VAL:HB	1.92	0.51
33:Z:964:GLU:HG3	33:Z:965:LEU:HG	1.91	0.51
18:K:104:ASP:OD1	18:K:105:GLN:N	2.42	0.51
18:K:195:ALA:HA	18:K:198:TYR:HD2	1.74	0.51
20:M:278:ILE:O	20:M:324:LEU:N	2.38	0.51
25:R:202:GLY:HA3	25:R:206:ARG:HD2	1.93	0.51
26:S:330:LEU:HD12	32:Y:65:ASP:H	1.75	0.51
33:Z:139:LEU:HD21	33:Z:161:ILE:HG21	1.92	0.51
2:2:149:ASP:OD1	2:2:150:VAL:N	2.43	0.51
6:6:220:GLY:HA2	6:6:237:GLU:HA	1.93	0.51
5:f:188:TYR:HE1	5:f:198:LYS:HG3	1.76	0.51
16:I:219:VAL:HB	16:I:325:ILE:HG12	1.91	0.51
16:I:282:ASP:OD1	16:I:283:GLU:N	2.44	0.51
17:J:85:LEU:HD11	17:J:93:LYS:HB3	1.93	0.51
18:K:210:LEU:HD12	18:K:337:LYS:HG2	1.93	0.51
24:Q:121:SER:HB3	24:Q:126:LYS:HD2	1.93	0.51
29:V:50:MET:HG3	29:V:71:MET:HB2	1.93	0.51
1:1:61:TRP:HD1	1:1:197:LEU:HD11	1.76	0.51
1:1:154:TYR:HE2	1:b:184:TRP:HB3	1.76	0.51
4:4:146:HIS:HA	5:f:281:SER:HB2	1.92	0.51
12:E:35:SER:OG	12:E:51:GLU:O	2.21	0.51
14:G:70:VAL:N	14:G:74:ILE:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:159:TRP:CZ3	12:m:59:LEU:HB2	2.46	0.51
17:J:336:ASN:HB3	17:J:376:HIS:ND1	2.25	0.51
19:L:107:GLU:HB2	19:L:145:ARG:HD3	1.93	0.51
19:L:227:GLY:HA3	19:L:349:ILE:HG21	1.92	0.51
20:M:262:LEU:HA	20:M:265:ASP:HB2	1.93	0.51
20:M:274:ALA:HB3	20:M:275:PRO:HD3	1.92	0.51
4:4:130:TYR:OH	5:f:242:ARG:NH2	2.38	0.51
6:e:74:ASN:O	6:e:127:HIS:N	2.41	0.51
8:A:218:PHE:HB3	8:A:222:ASP:HB2	1.93	0.51
12:m:71:ASP:HB3	12:m:74:ILE:HB	1.91	0.51
20:M:149:ASN:OD1	20:M:150:LYS:N	2.43	0.51
21:N:635:GLN:NE2	21:N:667:GLN:OE1	2.29	0.51
22:O:75:GLN:NE2	22:O:119:SER:O	2.43	0.51
5:5:252:LEU:HB2	5:5:263:HIS:HB2	1.93	0.51
1:b:47:ASN:OD1	1:b:49:VAL:HG22	2.11	0.51
8:A:135:ARG:HB2	14:G:125:LEU:HD22	1.92	0.51
16:I:136:VAL:HB	16:I:140:LEU:HD12	1.92	0.51
17:J:116:ARG:HG2	17:J:118:ASP:H	1.76	0.51
17:J:251:ASP:OD1	17:J:253:ILE:HG12	2.10	0.51
28:U:265:LEU:HB3	28:U:268:LYS:HE2	1.93	0.51
1:1:196:VAL:HB	1:1:203:GLU:HB3	1.91	0.51
15:H:227:LEU:HD22	20:M:403:LEU:HD22	1.93	0.51
20:M:71:ASN:HB3	29:V:75:GLY:HA3	1.93	0.51
26:S:129:GLU:OE2	26:S:132:ALA:N	2.44	0.51
26:S:167:LEU:HD13	26:S:180:ASN:HD22	1.76	0.51
29:V:27:VAL:HA	29:V:63:VAL:CG1	2.41	0.51
2:2:63:LEU:HD12	2:2:215:TYR:HE1	1.75	0.50
4:4:92:ILE:HA	4:4:97:PRO:HB3	1.93	0.50
1:b:38:ARG:HA	1:b:48:ARG:HA	1.93	0.50
1:b:57:HIS:HB3	1:b:60:ILE:HB	1.92	0.50
10:C:19:LEU:HG	10:C:21:GLN:H	1.76	0.50
12:E:48:LEU:HD23	12:E:77:ALA:HB2	1.92	0.50
11:n:181:ARG:NH2	12:m:60:GLU:HG3	2.25	0.50
11:n:200:LEU:O	11:n:204:GLN:NE2	2.44	0.50
15:H:147:ILE:HD11	15:H:157:VAL:HG23	1.93	0.50
15:H:217:GLN:NE2	15:H:378:SER:OG	2.44	0.50
19:L:131:VAL:HB	19:L:135:VAL:HG21	1.93	0.50
25:R:33:LEU:HB3	25:R:74:ASN:HD22	1.76	0.50
29:V:57:PHE:CB	29:V:63:VAL:HA	2.40	0.50
12:m:122:ARG:HG3	12:m:134:MET:HG3	1.92	0.50
15:H:57:LYS:HA	15:H:61:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:205:PRO:HD2	33:Z:826:ARG:HH21	1.77	0.50
16:I:347:LYS:HE2	16:I:349:LEU:HD21	1.94	0.50
18:K:152:PRO:HG2	18:K:260:LEU:HB2	1.93	0.50
18:K:423:LYS:HE3	18:K:424:PHE:CE2	2.47	0.50
7:7:77:PRO:HA	7:7:83:VAL:HA	1.94	0.50
12:E:166:ARG:HB3	13:F:58:SER:HB3	1.94	0.50
13:l:67:ASP:OD1	13:l:68:GLU:N	2.43	0.50
14:k:70:VAL:N	14:k:74:ILE:O	2.41	0.50
23:P:388:ILE:HG22	23:P:389:ILE:HG23	1.94	0.50
28:U:276:ILE:HD13	29:V:294:SER:HB2	1.94	0.50
2:i:36:LYS:HD3	2:i:152:TYR:HA	1.93	0.50
4:g:4:ILE:HG22	4:g:103:LEU:HD12	1.93	0.50
8:A:220:LYS:HD3	8:A:242:GLU:HB2	1.93	0.50
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.93	0.50
15:H:54:ASN:HB2	16:I:96:LEU:HD23	1.92	0.50
18:K:148:ASP:OD1	18:K:149:ILE:N	2.45	0.50
23:P:271:SER:OG	23:P:277:GLN:NE2	2.41	0.50
27:T:206:LYS:HG3	27:T:211:PHE:HB2	1.94	0.50
11:D:65:SER:HB3	11:D:90:ARG:HH21	1.76	0.50
10:d:5:ARG:NH2	11:n:9:SER:O	2.36	0.50
11:n:118:GLN:HE22	12:m:86:ARG:HB3	1.77	0.50
33:Z:169:VAL:HG22	33:Z:195:PHE:HD1	1.75	0.50
2:2:114:GLN:HE22	8:A:107:LYS:HA	1.76	0.50
1:b:132:ILE:HG23	1:b:136:GLY:HA2	1.93	0.50
5:f:273:TRP:HA	5:f:276:LYS:HE2	1.94	0.50
8:c:84:ASN:OD1	8:c:85:GLY:N	2.45	0.50
33:Z:446:GLU:HG2	33:Z:484:LYS:HG3	1.93	0.50
9:B:70:ASP:HA	9:B:234:ARG:HB2	1.94	0.50
13:F:226:ASP:OD1	13:F:227:GLY:N	2.45	0.50
11:n:68:ASP:OD1	11:n:69:SER:N	2.43	0.50
18:K:295:ILE:HG13	18:K:296:LEU:HD12	1.93	0.50
27:T:200:LEU:HB2	27:T:233:VAL:HB	1.94	0.50
4:4:29:LYS:HE3	4:4:32:ASP:H	1.76	0.50
5:f:87:ILE:O	5:f:254:HIS:ND1	2.40	0.50
13:F:76:GLY:HA3	13:F:130:VAL:HA	1.94	0.50
11:n:111:ARG:NH2	12:m:90:GLU:OE2	2.45	0.50
11:n:181:ARG:HH22	12:m:60:GLU:HG2	1.76	0.50
13:l:54:ASP:OD1	13:l:55:GLU:N	2.45	0.50
16:I:132:ILE:HG12	16:I:156:ILE:HD12	1.94	0.50
18:K:371:LEU:O	18:K:375:ASN:ND2	2.34	0.50
20:M:41:ILE:HG23	20:M:42:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:303:LEU:HD21	21:N:755:PRO:HB3	1.94	0.50
23:P:89:LEU:HG	23:P:91:LEU:H	1.77	0.50
27:T:85:LEU:HD23	27:T:88:TYR:HD2	1.77	0.50
7:7:151:GLY:HA2	7:7:233:ILE:HG21	1.94	0.50
3:h:35:GLY:HA3	3:h:183:TRP:HH2	1.77	0.50
3:h:115:LYS:HG3	9:j:142:PHE:HE1	1.76	0.50
10:C:52:VAL:HG23	10:C:59:GLN:HE21	1.77	0.50
17:J:139:VAL:HG22	17:J:211:ILE:HG12	1.94	0.50
18:K:63:LEU:HG	21:N:572:LEU:HD22	1.94	0.50
18:K:391:GLY:HA3	19:L:212:ILE:HG21	1.93	0.50
26:S:290:ASN:OD1	26:S:321:GLN:NE2	2.45	0.50
28:U:19:LEU:HG	29:V:208:LYS:HD3	1.93	0.50
33:Z:812:ILE:HD12	33:Z:847:ILE:HG22	1.93	0.50
3:3:25:CYS:HB2	3:3:42:LYS:NZ	2.27	0.49
4:4:96:ARG:HH12	5:5:164:GLN:HA	1.77	0.49
5:f:183:GLU:OE2	11:n:141:ARG:NH1	2.40	0.49
5:f:233:LYS:HB3	5:f:271:LEU:HD21	1.93	0.49
15:H:157:VAL:O	15:H:182:ASN:ND2	2.45	0.49
18:K:423:LYS:HE3	18:K:424:PHE:HE2	1.76	0.49
22:O:23:HIS:HB2	22:O:65:PHE:HZ	1.77	0.49
26:S:357:LEU:HA	26:S:384:ARG:HH22	1.77	0.49
30:W:2:VAL:HG13	30:W:196:SER:HB2	1.93	0.49
31:X:85:ARG:HD2	31:X:101:LEU:HD12	1.94	0.49
33:Z:515:SER:OG	33:Z:521:GLU:OE1	2.30	0.49
4:4:33:ASP:OD1	4:4:34:LYS:N	2.45	0.49
6:e:110:ARG:NE	6:e:150:TYR:OH	2.32	0.49
9:B:6:SER:HB3	9:B:19:GLY:H	1.77	0.49
8:c:158:ASP:OD1	8:c:162:TYR:N	2.45	0.49
15:H:254:THR:HG21	15:H:415:THR:HB	1.93	0.49
18:K:283:ASP:OD1	18:K:284:ALA:N	2.44	0.49
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.45	0.49
27:T:205:ILE:HD13	27:T:208:LEU:HD12	1.93	0.49
2:2:39:ASN:HB3	2:2:208:GLU:HG3	1.93	0.49
6:6:100:ASP:OD2	13:F:65:LYS:NZ	2.31	0.49
5:f:105:THR:OG1	6:e:153:GLU:OE1	2.29	0.49
24:Q:295:GLY:N	24:Q:324:GLU:OE1	2.44	0.49
27:T:126:LEU:O	27:T:130:ASP:N	2.44	0.49
11:D:96:HIS:HE1	11:D:102:ASP:HB2	1.77	0.49
15:H:365:LEU:HA	15:H:370:ARG:HH21	1.78	0.49
17:J:169:LYS:HE3	17:J:206:THR:HG22	1.95	0.49
22:O:196:LEU:HB2	22:O:203:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:47:ASP:OD1	24:Q:48:ASP:N	2.46	0.49
25:R:61:PRO:HG2	25:R:180:PHE:HZ	1.77	0.49
27:T:247:ASP:H	27:T:249:MET:HE3	1.78	0.49
33:Z:347:ASN:HB3	33:Z:353:VAL:HG23	1.93	0.49
5:f:82:ARG:NE	5:f:185:PRO:O	2.46	0.49
13:F:123:TYR:HB2	14:G:128:SER:HA	1.94	0.49
8:c:54:ILE:HG12	8:c:225:VAL:HG22	1.95	0.49
10:d:60:ASP:HA	10:d:232:PRO:HG2	1.95	0.49
11:n:5:ASP:OD1	11:n:6:ARG:NH1	2.46	0.49
18:K:397:LYS:HB3	18:K:399:ARG:NH1	2.27	0.49
21:N:510:HIS:CD2	29:V:62:THR:OG1	2.66	0.49
23:P:409:SER:HB3	23:P:412:LEU:HD12	1.94	0.49
24:Q:356:CYS:HA	24:Q:397:LEU:HB3	1.95	0.49
7:7:48:LYS:HD2	7:7:173:PRO:HA	1.95	0.49
17:J:160:ILE:HD11	17:J:198:LEU:HD21	1.94	0.49
17:J:230:VAL:HG11	17:J:272:MET:HA	1.93	0.49
18:K:244:HIS:HE1	18:K:249:GLU:HB3	1.76	0.49
18:K:245:LYS:HA	19:L:299:ARG:NH1	2.27	0.49
5:5:82:ARG:HH21	5:5:200:ASP:HA	1.77	0.49
17:J:220:GLN:HB2	17:J:225:GLU:HG3	1.95	0.49
3:h:30:GLY:HA2	3:h:36:VAL:HG23	1.94	0.49
4:g:70:ARG:HH21	10:d:113:ARG:HD2	1.77	0.49
11:D:46:CYS:SG	11:D:47:GLU:N	2.85	0.49
12:m:54:ALA:HA	12:m:59:LEU:CD2	2.43	0.49
18:K:167:PRO:O	18:K:228:ASN:ND2	2.42	0.49
33:Z:323:TYR:HB3	33:Z:537:THR:HG22	1.95	0.49
1:1:44:TYR:HD1	7:a:179:PHE:HZ	1.59	0.49
1:1:102:LYS:HD3	1:1:138:VAL:HG23	1.94	0.49
5:5:82:ARG:HG2	5:5:87:ILE:HG12	1.94	0.49
6:6:79:ASP:HB3	6:6:124:TYR:HB3	1.94	0.49
7:a:234:ASP:OD1	7:a:235:LYS:N	2.46	0.49
10:C:191:GLU:HG2	10:C:242:THR:HG22	1.94	0.49
12:E:14:THR:HA	13:F:21:GLN:HE22	1.78	0.49
12:E:99:HIS:HE1	12:E:105:GLU:HB3	1.77	0.49
15:H:57:LYS:HD3	16:I:99:ILE:HG22	1.94	0.49
15:H:414:SER:HB3	15:H:418:GLU:HB2	1.94	0.49
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.95	0.49
20:M:283:LEU:H	20:M:327:THR:HB	1.78	0.49
22:O:296:LEU:HD11	22:O:308:LEU:HB2	1.95	0.49
23:P:147:LYS:HB3	23:P:152:LYS:HB2	1.93	0.49
25:R:154:LEU:HD11	25:R:170:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:301:TYR:HE2	25:R:341:LEU:HB2	1.77	0.49
26:S:293:ILE:HD13	26:S:316:LEU:HD23	1.95	0.49
28:U:108:GLU:HB2	30:W:60:ARG:HH22	1.78	0.49
29:V:26:THR:O	29:V:63:VAL:HB	2.12	0.49
10:C:53:THR:HA	10:C:210:ARG:HE	1.78	0.49
13:F:46:LEU:HG	13:F:135:ILE:HD13	1.93	0.49
8:c:87:ILE:N	8:c:88:PRO:HD2	2.28	0.49
15:H:228:PRO:HB3	15:H:242:PRO:HG2	1.94	0.49
18:K:211:LEU:HD23	18:K:338:ILE:HB	1.95	0.49
23:P:323:ASN:OD1	23:P:338:TRP:NE1	2.46	0.49
24:Q:135:HIS:ND1	24:Q:169:ASP:OD2	2.45	0.48
25:R:372:ILE:HB	26:S:398:THR:HG22	1.94	0.48
25:R:415:GLN:HE21	26:S:471:LEU:HD21	1.78	0.48
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.94	0.48
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.61	0.48
6:6:76:PHE:CE2	6:6:78:ALA:HB3	2.48	0.48
7:a:77:PRO:HB3	7:a:83:VAL:HG22	1.95	0.48
15:H:70:LYS:O	15:H:74:THR:OG1	2.26	0.48
17:J:42:ARG:NE	26:S:484:ASP:OD2	2.46	0.48
6:6:221:LEU:N	6:6:236:TYR:O	2.40	0.48
7:a:148:ILE:HD11	7:a:177:THR:HG23	1.95	0.48
14:G:32:GLU:OE2	14:G:169:ARG:NH2	2.45	0.48
14:G:187:LEU:HD23	14:G:191:GLU:HB3	1.95	0.48
8:c:35:THR:HA	8:c:85:GLY:HA2	1.95	0.48
13:l:121:GLN:NE2	14:k:130:ARG:O	2.34	0.48
15:H:235:PHE:HE1	20:M:400:MET:HE1	1.77	0.48
17:J:279:LEU:O	17:J:284:THR:N	2.45	0.48
28:U:259:ASN:HA	28:U:262:GLN:HB2	1.96	0.48
33:Z:857:LEU:HD11	33:Z:908:ILE:HD11	1.95	0.48
1:1:72:GLN:HE22	2:2:148:THR:H	1.61	0.48
10:C:144:TYR:HB3	11:D:59:ILE:HG22	1.95	0.48
12:E:41:ALA:HA	12:E:46:VAL:HG22	1.96	0.48
9:j:137:ALA:HB2	9:j:147:LEU:HD13	1.96	0.48
13:l:123:TYR:N	14:k:128:SER:O	2.45	0.48
15:H:311:ILE:HG23	15:H:361:LEU:HD21	1.94	0.48
17:J:193:THR:OG1	17:J:255:SER:OG	2.31	0.48
23:P:429:ILE:HD11	28:U:203:LYS:HG2	1.94	0.48
30:W:109:ARG:HH22	30:W:195:GLY:HA3	1.78	0.48
33:Z:621:LEU:O	33:Z:625:THR:OG1	2.29	0.48
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.95	0.48
11:D:68:ASP:OD1	11:D:69:SER:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:90:ARG:O	9:j:94:HIS:ND1	2.35	0.48
11:n:181:ARG:HH12	12:m:60:GLU:HA	1.78	0.48
14:k:95:GLU:OE1	14:k:115:ARG:NH2	2.40	0.48
18:K:212:TYR:HB2	18:K:339:GLU:HA	1.96	0.48
19:L:307:GLU:OE2	19:L:311:GLN:NE2	2.46	0.48
20:M:215:PRO:HA	20:M:341:GLY:H	1.79	0.48
20:M:401:ILE:HD11	20:M:422:VAL:HG21	1.96	0.48
21:N:774:ASN:ND2	21:N:866:TYR:O	2.37	0.48
21:N:885:ILE:HG12	21:N:887:ASP:H	1.79	0.48
23:P:286:ASN:HA	23:P:293:LEU:HD11	1.96	0.48
26:S:364:ILE:HB	26:S:377:TYR:HE1	1.77	0.48
27:T:143:SER:HA	27:T:146:ILE:HB	1.94	0.48
29:V:45:VAL:HA	29:V:144:ILE:HG21	1.95	0.48
29:V:61:TYR:O	29:V:62:THR:HB	2.13	0.48
33:Z:144:SER:HB3	33:Z:154:ILE:HG12	1.94	0.48
6:e:57:ARG:HH12	7:a:193:ASP:HB3	1.78	0.48
12:E:211:LYS:O	12:E:216:ASN:ND2	2.41	0.48
13:l:119:ASN:HB3	13:l:126:ARG:H	1.78	0.48
14:k:41:LYS:HB3	14:k:161:LYS:HA	1.94	0.48
16:I:106:ILE:HD11	16:I:146:SER:HB3	1.93	0.48
16:I:358:LYS:HD3	16:I:381:VAL:HG12	1.93	0.48
2:2:101:ARG:NH2	8:A:147:ASP:OD2	2.47	0.48
3:3:51:LEU:HD22	3:3:87:PHE:HZ	1.77	0.48
7:7:176:ALA:HB3	7:7:185:ASN:HB2	1.95	0.48
2:i:81:THR:HG23	2:i:127:LEU:HD11	1.94	0.48
8:A:14:ARG:HE	14:G:8:TYR:HH	1.59	0.48
9:B:161:ALA:HB1	9:B:175:LEU:HB3	1.96	0.48
13:F:39:ARG:HD3	13:F:144:LEU:HB2	1.94	0.48
28:U:298:ASN:HA	28:U:301:ILE:HD12	1.95	0.48
5:5:78:THR:OG1	5:5:204:VAL:O	2.22	0.48
9:j:32:VAL:O	9:j:76:SER:OG	2.30	0.48
11:n:65:SER:HB3	11:n:90:ARG:HH21	1.79	0.48
11:n:105:THR:HB	11:n:108:TYR:HB3	1.96	0.48
16:I:188:GLU:HA	16:I:191:ILE:HD12	1.96	0.48
16:I:395:MET:HA	16:I:423:VAL:HG21	1.96	0.48
18:K:341:PRO:O	18:K:344:ARG:NH1	2.39	0.48
3:h:53:ILE:HG22	3:h:60:VAL:HG22	1.95	0.48
15:H:162:ARG:H	15:H:183:ILE:HG21	1.79	0.48
15:H:397:SER:HB3	15:H:437:VAL:HG12	1.96	0.48
27:T:163:LEU:O	27:T:167:GLY:N	2.46	0.48
28:U:57:GLU:OE2	29:V:97:GLN:NE2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:171:VAL:HG11	29:V:217:HIS:HB3	1.95	0.48
4:4:36:ARG:HG2	4:4:46:PHE:HE2	1.78	0.48
6:6:112:ILE:HD13	6:6:128:THR:HG21	1.96	0.48
7:7:256:LYS:HG2	1:b:206:ILE:HG21	1.95	0.48
12:E:218:GLN:HE21	12:E:230:ILE:HG21	1.79	0.48
17:J:96:VAL:HB	17:J:121:MET:HA	1.95	0.48
19:L:318:LEU:HB3	19:L:321:THR:HB	1.96	0.48
20:M:143:ASN:HB3	20:M:261:LYS:HD3	1.96	0.48
21:N:533:ASP:OD1	21:N:559:TYR:OH	2.32	0.48
22:O:196:LEU:HD13	22:O:203:THR:HB	1.96	0.48
24:Q:179:LEU:HD21	24:Q:217:GLU:HG2	1.95	0.48
33:Z:256:LEU:HB3	33:Z:257:PRO:HD3	1.96	0.48
33:Z:498:ALA:HA	33:Z:533:VAL:HA	1.96	0.48
33:Z:596:THR:HA	33:Z:599:ILE:HD12	1.96	0.48
4:4:27:VAL:O	4:g:171:ARG:NH1	2.47	0.47
11:n:181:ARG:HH22	12:m:60:GLU:CG	2.27	0.47
16:I:246:ARG:HE	17:J:278:GLN:HE21	1.62	0.47
21:N:179:THR:O	21:N:180:SER:HB3	2.13	0.47
21:N:762:ARG:NE	21:N:767:ALA:HB2	2.29	0.47
23:P:384:VAL:HG12	24:Q:352:GLU:HG3	1.94	0.47
1:1:82:LEU:HA	1:1:85:TYR:HB3	1.96	0.47
2:i:88:ILE:HB	2:i:115:HIS:HE1	1.79	0.47
6:e:32:LEU:HD21	6:e:169:LEU:HD11	1.95	0.47
9:B:42:GLY:HA3	9:B:185:LEU:HD22	1.96	0.47
10:C:16:GLU:O	11:D:29:ARG:NH2	2.36	0.47
12:E:52:LYS:HZ2	12:E:216:ASN:C	2.21	0.47
14:k:183:HIS:CE1	14:k:185:GLU:HB2	2.49	0.47
14:k:211:ASP:OD1	14:k:212:PHE:N	2.47	0.47
18:K:152:PRO:HD2	18:K:260:LEU:HD13	1.96	0.47
10:C:135:PHE:HB2	10:C:151:SER:HB3	1.96	0.47
11:D:37:LYS:HB3	11:D:42:VAL:HG23	1.96	0.47
12:E:61:SER:HB2	12:E:215:ASN:O	2.14	0.47
16:I:102:ASN:HB3	17:J:97:ASP:OD1	2.14	0.47
17:J:261:SER:HA	18:K:293:GLN:HG3	1.96	0.47
17:J:270:ARG:HG3	17:J:271:THR:HG23	1.95	0.47
17:J:379:GLN:HA	17:J:382:PHE:HD2	1.79	0.47
21:N:104:LYS:HG3	21:N:108:MET:HE2	1.97	0.47
21:N:527:GLY:H	21:N:558:ALA:HA	1.79	0.47
32:Y:69:VAL:HG12	32:Y:70:ASP:N	2.29	0.47
33:Z:151:HIS:HB3	33:Z:153:TYR:HD2	1.78	0.47
1:1:58:ASP:OD2	8:A:77:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:54:ILE:HD11	7:7:230:LEU:HD21	1.96	0.47
9:B:49:LYS:HA	9:B:63:LYS:NZ	2.29	0.47
11:D:139:ASP:HB2	11:D:142:ASP:HB3	1.96	0.47
13:F:7:ASP:H	13:F:12:THR:HG21	1.79	0.47
8:c:25:LEU:HG	8:c:27:GLN:H	1.79	0.47
19:L:149:ASP:HB3	19:L:154:THR:H	1.79	0.47
19:L:396:THR:HA	20:M:212:ILE:HD12	1.95	0.47
21:N:707:ASN:HD21	21:N:785:PRO:HG2	1.80	0.47
23:P:101:MET:HG3	23:P:139:VAL:HG12	1.96	0.47
24:Q:359:ILE:HD12	24:Q:395:GLY:HA2	1.97	0.47
29:V:225:LEU:HB3	29:V:228:TYR:HB2	1.95	0.47
2:i:33:VAL:HG22	2:i:188:ILE:HD11	1.95	0.47
4:g:99:GLN:HB3	4:g:121:TYR:HB2	1.97	0.47
12:E:52:LYS:NZ	12:E:215:ASN:O	2.46	0.47
17:J:383:GLU:OE1	24:Q:166:LYS:NZ	2.34	0.47
20:M:194:VAL:HG13	20:M:198:VAL:HB	1.97	0.47
20:M:427:SER:OG	20:M:428:LYS:N	2.40	0.47
25:R:60:ALA:HA	25:R:63:TYR:HB3	1.96	0.47
33:Z:914:LEU:HD22	33:Z:959:HIS:CD2	2.49	0.47
1:1:56:VAL:HB	1:1:82:LEU:HD12	1.95	0.47
7:7:90:ILE:HG23	7:7:93:MET:HE2	1.96	0.47
11:D:117:GLN:HE21	11:D:129:PHE:HB2	1.79	0.47
15:H:100:ALA:HB3	15:H:149:LEU:HD13	1.96	0.47
21:N:479:GLU:HB2	21:N:512:ASN:HB3	1.97	0.47
21:N:512:ASN:ND2	29:V:61:TYR:CD2	2.82	0.47
26:S:475:TYR:CZ	28:U:294:ASN:HB2	2.50	0.47
28:U:14:VAL:HG21	28:U:48:VAL:HG12	1.95	0.47
29:V:173:THR:HG22	29:V:174:THR:HG23	1.96	0.47
30:W:54:GLY:HA3	30:W:90:ALA:HB2	1.95	0.47
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.96	0.47
2:2:126:TYR:HB3	2:2:156:LEU:HD21	1.97	0.47
7:7:77:PRO:HB3	7:7:83:VAL:HG22	1.97	0.47
2:i:99:THR:HG22	8:c:116:VAL:HG21	1.97	0.47
3:h:7:ILE:HG23	3:h:32:GLN:HG3	1.97	0.47
7:a:184:ALA:HB2	7:a:217:LEU:HD21	1.97	0.47
9:B:240:SER:HA	9:B:243:ILE:HD12	1.97	0.47
8:c:156:LYS:HB3	8:c:166:TYR:HE2	1.78	0.47
15:H:77:ALA:HA	15:H:101:ARG:HE	1.80	0.47
15:H:178:ARG:HG2	15:H:284:VAL:HB	1.96	0.47
16:I:353:PRO:HB3	16:I:357:THR:HG21	1.97	0.47
17:J:34:ILE:O	17:J:38:THR:OG1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:155:LYS:HD3	17:J:317:PRO:HG3	1.95	0.47
18:K:186:GLU:HA	18:K:190:LEU:HD13	1.97	0.47
19:L:370:LYS:HE3	19:L:376:PHE:HZ	1.78	0.47
24:Q:326:MET:HA	24:Q:335:PHE:HE2	1.80	0.47
26:S:119:TYR:CE2	26:S:121:VAL:HB	2.49	0.47
29:V:53:MET:HA	29:V:68:VAL:HG12	1.95	0.47
7:7:136:ARG:HB3	7:7:142:PRO:HA	1.97	0.47
1:b:209:PRO:HA	1:b:212:TYR:CE2	2.50	0.47
8:A:170:ALA:HB3	8:A:175:GLN:HG3	1.96	0.47
13:F:22:VAL:HG13	13:F:149:PRO:HG2	1.95	0.47
14:G:20:ARG:HH21	14:G:25:GLU:HG2	1.80	0.47
8:c:31:ALA:HB1	8:c:138:GLY:HA2	1.96	0.47
8:c:147:ASP:OD1	8:c:148:GLU:N	2.47	0.47
18:K:91:SER:OG	18:K:92:VAL:N	2.45	0.47
21:N:756:THR:HG21	21:N:876:PRO:HG3	1.96	0.47
26:S:173:LEU:H	26:S:176:LEU:HD12	1.78	0.47
29:V:62:THR:HG22	29:V:62:THR:O	2.14	0.47
8:c:77:ARG:HG2	8:c:78:THR:HG23	1.97	0.47
18:K:238:ASN:HB2	18:K:241:GLU:HG3	1.96	0.47
18:K:240:SER:HB2	19:L:306:MET:HB2	1.96	0.47
22:O:292:CYS:O	22:O:295:THR:OG1	2.24	0.47
23:P:144:VAL:HG12	23:P:148:LYS:HE3	1.97	0.47
33:Z:516:THR:HB	33:Z:562:TRP:HE3	1.80	0.47
7:7:144:TRP:HE3	7:7:165:LEU:HD21	1.79	0.47
11:D:48:ARG:HG3	11:D:63:LYS:HE2	1.96	0.47
12:E:42:THR:OG1	12:E:45:GLY:O	2.26	0.47
15:H:399:GLU:HG2	15:H:401:GLY:H	1.80	0.47
18:K:277:ILE:HG12	18:K:295:ILE:HD12	1.96	0.47
21:N:510:HIS:HB3	21:N:513:ILE:CB	2.32	0.47
21:N:779:GLU:HG2	21:N:866:TYR:CE1	2.50	0.47
30:W:101:ARG:HE	30:W:108:GLN:HE21	1.60	0.47
33:Z:358:TYR:HE1	33:Z:962:ARG:HB2	1.80	0.47
8:A:147:ASP:OD1	8:A:148:GLU:N	2.48	0.46
11:D:70:HIS:ND1	11:D:71:VAL:HG23	2.30	0.46
9:j:5:TYR:O	9:j:11:THR:OG1	2.34	0.46
12:m:72:ARG:O	12:m:228:PHE:N	2.48	0.46
14:k:201:TYR:HA	14:k:204:HIS:CD2	2.50	0.46
15:H:224:VAL:HG21	15:H:373:ARG:HG3	1.96	0.46
18:K:345:ASP:OD1	18:K:346:ARG:N	2.48	0.46
21:N:436:ASP:HB2	21:N:439:VAL:HG23	1.97	0.46
21:N:529:GLN:H	21:N:558:ALA:HB1	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:418:THR:O	27:T:157:TYR:OH	2.32	0.46
28:U:174:LEU:HD13	29:V:31:SER:HB3	1.96	0.46
6:6:164:LEU:HD11	3:h:148:GLY:H	1.79	0.46
1:b:110:ASP:OD2	7:a:35:GLN:NE2	2.48	0.46
12:E:16:SER:C	12:E:18:GLU:H	2.24	0.46
14:k:108:PRO:HG2	14:k:111:ALA:HB3	1.97	0.46
21:N:298:TYR:OH	21:N:766:GLN:NE2	2.45	0.46
28:U:276:ILE:HG23	29:V:290:ASN:HB3	1.98	0.46
3:3:7:ILE:HG23	3:3:32:GLN:HG3	1.96	0.46
3:3:30:GLY:HA2	3:3:36:VAL:HG23	1.95	0.46
5:f:136:SER:HB3	12:m:97:VAL:HB	1.97	0.46
11:D:161:ALA:HB3	12:E:58:LEU:HD13	1.97	0.46
12:E:130:GLU:HB3	12:E:132:ARG:HH12	1.79	0.46
14:G:12:ASN:ND2	14:G:126:TYR:O	2.41	0.46
21:N:424:LYS:NZ	21:N:461:GLU:OE1	2.48	0.46
21:N:667:GLN:O	21:N:671:LEU:HB2	2.16	0.46
23:P:249:ALA:HB1	23:P:285:GLN:HG3	1.97	0.46
24:Q:382:LEU:HD11	25:R:340:GLN:HB3	1.97	0.46
27:T:187:ASP:O	27:T:191:LYS:HG3	2.15	0.46
5:f:120:MET:HG3	5:f:127:CYS:HB2	1.98	0.46
14:k:120:VAL:HG21	14:k:151:LEU:HD21	1.98	0.46
15:H:77:ALA:O	15:H:101:ARG:NH2	2.47	0.46
16:I:187:LEU:HD13	16:I:232:LEU:HD21	1.98	0.46
17:J:111:GLN:HE22	17:J:128:ASN:HB2	1.79	0.46
21:N:309:ILE:HG22	21:N:339:MET:HB3	1.96	0.46
26:S:82:TYR:CD2	26:S:86:SER:HB3	2.49	0.46
33:Z:151:HIS:HB3	33:Z:153:TYR:CD2	2.50	0.46
33:Z:228:GLU:HG2	33:Z:264:PHE:HZ	1.81	0.46
2:2:129:VAL:N	2:2:140:PHE:O	2.48	0.46
9:B:86:VAL:HA	9:B:89:SER:HB3	1.96	0.46
13:F:110:HIS:HB2	14:G:86:ARG:HH21	1.81	0.46
18:K:96:ILE:HD12	19:L:126:ARG:HB3	1.97	0.46
18:K:241:GLU:O	18:K:243:VAL:HG23	2.14	0.46
20:M:348:GLU:HG2	20:M:350:PRO:HD3	1.98	0.46
24:Q:151:TYR:HB3	24:Q:184:VAL:HG13	1.97	0.46
28:U:74:GLU:OE2	28:U:113:TYR:OH	2.33	0.46
1:1:23:MET:HE2	1:1:174:ILE:HG12	1.97	0.46
1:1:89:TYR:CD1	14:G:111:ALA:HB1	2.51	0.46
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.97	0.46
9:B:97:TYR:O	9:B:101:TYR:N	2.46	0.46
11:D:175:LEU:HA	11:D:179:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:187:ASP:OD1	13:F:233:TYR:OH	2.33	0.46
10:d:149:TYR:OH	11:n:59:ILE:O	2.23	0.46
14:k:70:VAL:HB	14:k:74:ILE:HB	1.97	0.46
16:I:247:ILE:HD13	16:I:279:VAL:HG13	1.98	0.46
18:K:421:VAL:HG12	18:K:422:ASP:O	2.16	0.46
21:N:283:ASP:HB3	21:N:286:LEU:HB2	1.97	0.46
21:N:352:ASN:HB3	21:N:355:TRP:CE3	2.51	0.46
6:e:179:TYR:HA	6:e:188:LYS:HA	1.96	0.46
8:c:48:LYS:HD3	8:c:197:GLU:HG2	1.98	0.46
19:L:258:GLU:O	19:L:262:ILE:HG12	2.16	0.46
30:W:25:ARG:HH11	30:W:26:PHE:H	1.63	0.46
31:X:73:THR:HG23	31:X:90:VAL:H	1.81	0.46
6:6:202:LEU:HD21	2:i:230:LYS:HD3	1.97	0.46
9:B:13:SER:HB2	9:B:18:LEU:HA	1.98	0.46
13:F:50:LYS:HB3	13:F:59:TYR:HB3	1.98	0.46
19:L:244:ILE:HB	19:L:278:ILE:HA	1.97	0.46
21:N:305:ASN:HD22	21:N:871:MET:HE1	1.81	0.46
24:Q:121:SER:HA	24:Q:124:PHE:HD2	1.80	0.46
33:Z:506:LEU:HD22	33:Z:539:ASN:HD21	1.80	0.46
2:2:202:VAL:HB	2:2:220:LEU:HB3	1.97	0.46
3:3:20:CYS:HB3	3:3:191:LYS:HG2	1.98	0.46
5:f:237:LEU:HD11	5:f:272:PHE:HD1	1.80	0.46
8:A:156:LYS:HB3	8:A:166:TYR:HE2	1.81	0.46
13:F:4:ASN:C	13:F:6:TYR:H	2.22	0.46
8:c:194:ILE:HG22	8:c:196:GLU:H	1.81	0.46
18:K:244:HIS:C	19:L:299:ARG:HH11	2.23	0.46
30:W:186:ALA:HA	30:W:191:ILE:HD12	1.98	0.46
1:1:33:LEU:HD21	1:1:119:ALA:HB3	1.98	0.46
4:4:34:LYS:HB3	4:4:46:PHE:CE1	2.51	0.46
5:5:156:LYS:NZ	11:D:101:GLU:OE1	2.47	0.46
8:c:179:THR:HG23	9:j:55:LEU:HD12	1.98	0.46
20:M:55:ASN:HA	20:M:58:MET:HE3	1.97	0.46
21:N:775:CYS:N	21:N:869:ASP:OD2	2.44	0.46
27:T:235:PHE:CZ	27:T:237:ASN:HB2	2.51	0.46
5:5:162:VAL:HG11	5:5:192:SER:HA	1.97	0.45
6:e:221:LEU:HB3	6:e:236:TYR:HB3	1.98	0.45
9:B:193:LEU:HD13	9:B:247:LEU:HD23	1.97	0.45
13:F:10:THR:HG22	13:F:21:GLN:HG3	1.97	0.45
10:d:15:PRO:HA	11:n:22:TYR:CZ	2.51	0.45
15:H:149:LEU:HD21	15:H:175:GLY:HA3	1.97	0.45
15:H:173:ARG:NH2	16:I:129:TYR:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:200:LEU:HD11	16:I:207:LEU:HD22	1.98	0.45
13:l:187:ASP:HA	13:l:233:TYR:HE1	1.81	0.45
15:H:150:LYS:HG2	15:H:152:ILE:H	1.82	0.45
25:R:368:LEU:HD23	25:R:371:PHE:HD2	1.80	0.45
26:S:93:LEU:O	26:S:98:SER:OG	2.29	0.45
26:S:352:VAL:HG13	26:S:387:VAL:HA	1.99	0.45
5:5:76:THR:O	5:5:206:SER:N	2.49	0.45
3:h:63:LEU:HD12	3:h:105:VAL:HG11	1.97	0.45
10:C:13:PHE:CD2	11:D:19:GLN:HB3	2.52	0.45
10:C:94:HIS:CD2	10:C:114:ARG:HG2	2.52	0.45
10:d:11:THR:HB	11:n:127:ARG:HB3	1.96	0.45
12:m:21:LEU:HD13	12:m:123:PHE:HZ	1.82	0.45
16:I:205:PRO:HD2	33:Z:826:ARG:NH2	2.30	0.45
33:Z:516:THR:HA	33:Z:523:ALA:HB3	1.99	0.45
33:Z:905:ASN:HA	33:Z:908:ILE:HD12	1.98	0.45
3:3:76:LEU:HB3	10:C:92:ARG:HD3	1.98	0.45
6:6:110:ARG:NH1	6:6:113:GLN:OE1	2.50	0.45
6:6:183:THR:HB	6:6:186:LYS:HB3	1.99	0.45
3:h:13:VAL:HG13	3:h:167:ILE:HD11	1.99	0.45
3:h:78:GLU:HG3	3:h:80:ARG:HG2	1.99	0.45
4:g:91:SER:HB3	4:g:98:TYR:HB2	1.98	0.45
13:F:54:ASP:H	13:F:57:SER:HB3	1.81	0.45
12:m:52:LYS:NZ	12:m:61:SER:HB2	2.31	0.45
15:H:241:ASP:HB2	15:H:346:ARG:HH21	1.82	0.45
17:J:251:ASP:HA	17:J:293:ALA:O	2.17	0.45
18:K:74:HIS:NE2	18:K:78:GLU:OE2	2.49	0.45
28:U:16:LEU:HG	29:V:32:ILE:HG12	1.99	0.45
33:Z:145:ASP:OD1	33:Z:146:PHE:N	2.49	0.45
1:1:60:ILE:HA	1:1:120:GLY:HA2	1.99	0.45
4:4:80:VAL:HG12	4:4:104:ILE:HD13	1.98	0.45
6:6:239:LYS:HE2	2:i:224:VAL:H	1.80	0.45
1:b:151:THR:HA	1:b:154:TYR:CE2	2.51	0.45
2:i:206:VAL:HB	2:i:214:GLU:HB2	1.99	0.45
3:h:12:VAL:HG22	3:h:25:CYS:HB3	1.97	0.45
3:h:188:TYR:HE1	3:h:197:LYS:HG3	1.82	0.45
6:e:128:THR:HB	6:e:144:PHE:HB2	1.97	0.45
9:B:38:LYS:HA	9:B:43:VAL:HG22	1.98	0.45
10:C:232:PRO:HA	10:C:235:ILE:HD12	1.98	0.45
17:J:193:THR:HG1	17:J:255:SER:HG	1.60	0.45
17:J:202:VAL:HG12	17:J:244:ILE:HD13	1.98	0.45
18:K:351:LEU:HD21	24:Q:237:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:307:MET:HG3	22:O:347:LEU:HD22	1.99	0.45
23:P:254:GLU:HA	23:P:257:TRP:HB3	1.99	0.45
30:W:143:ASN:HD21	30:W:149:GLN:H	1.64	0.45
3:3:107:PRO:HG2	3:3:124:PHE:HB2	1.98	0.45
5:5:84:GLN:OE1	5:5:221:TRP:NE1	2.47	0.45
5:5:106:VAL:HA	6:6:151:GLU:HG2	1.99	0.45
11:D:31:THR:O	11:D:76:SER:OG	2.33	0.45
11:D:75:PHE:HB3	11:D:133:THR:HG22	1.99	0.45
13:l:105:VAL:HG11	13:l:143:HIS:HB2	1.98	0.45
14:k:73:HIS:CD2	14:k:74:ILE:HG13	2.51	0.45
24:Q:422:VAL:HG13	29:V:266:LEU:HD11	1.99	0.45
26:S:234:ILE:HD11	26:S:258:GLU:HG2	1.98	0.45
26:S:352:VAL:HG22	26:S:387:VAL:HG22	1.98	0.45
31:X:48:PHE:HD2	31:X:66:LEU:HD23	1.82	0.45
2:2:132:VAL:HG11	2:2:209:ILE:HA	1.98	0.45
4:4:135:TYR:HA	4:4:138:PHE:HE2	1.81	0.45
8:c:51:THR:OG1	8:c:152:PRO:HB3	2.17	0.45
19:L:104:LEU:HB2	19:L:148:LEU:HB2	1.98	0.45
19:L:114:GLU:OE1	19:L:137:ARG:NH1	2.50	0.45
21:N:179:THR:O	21:N:179:THR:OG1	2.31	0.45
21:N:309:ILE:HG21	21:N:340:HIS:CE1	2.51	0.45
21:N:386:MET:HE3	21:N:407:GLY:HA3	1.97	0.45
23:P:415:TRP:CH2	29:V:235:GLU:HB3	2.52	0.45
24:Q:262:LEU:HD13	24:Q:291:TYR:HB2	1.98	0.45
28:U:276:ILE:O	28:U:279:SER:OG	2.28	0.45
1:1:50:THR:OG1	2:2:149:ASP:OD2	2.34	0.45
2:2:86:GLN:NE2	9:B:98:LYS:O	2.42	0.45
5:5:112:ILE:HD11	5:5:131:GLU:HB3	1.98	0.45
6:e:214:HIS:NE2	6:e:216:GLN:HB2	2.32	0.45
13:F:19:LEU:HG	13:F:21:GLN:H	1.82	0.45
13:F:37:GLY:HA3	13:F:46:LEU:HD23	1.97	0.45
16:I:184:ILE:HD11	16:I:191:ILE:HD11	1.98	0.45
18:K:281:ARG:HH22	18:K:285:GLN:H	1.63	0.45
18:K:281:ARG:NH2	18:K:285:GLN:H	2.15	0.45
20:M:167:VAL:HB	20:M:262:LEU:HD21	1.98	0.45
20:M:175:LYS:HE3	20:M:273:LYS:HZ1	1.81	0.45
6:6:163:SER:O	3:h:145:GLN:HG2	2.16	0.45
3:h:125:ASP:OD1	3:h:128:GLY:N	2.50	0.45
13:F:84:LEU:HD13	13:F:112:LEU:HD11	1.98	0.45
14:G:65:VAL:HG12	14:G:67:ILE:H	1.82	0.45
18:K:206:PRO:HB3	18:K:335:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:201:LEU:HD12	19:L:239:ILE:HD13	1.98	0.45
23:P:23:LYS:HA	23:P:27:LEU:HD11	1.99	0.45
24:Q:195:LYS:HG2	24:Q:225:LEU:HD13	1.99	0.45
28:U:52:PHE:O	28:U:93:TYR:OH	2.28	0.45
1:l:122:ASP:OD1	1:l:123:ASP:N	2.49	0.45
4:g:26:SER:OG	4:g:139:TYR:OH	2.30	0.45
6:6:183:THR:HG21	6:6:187:VAL:HB	1.99	0.45
8:A:114:CYS:SG	8:A:153:SER:OG	2.74	0.45
8:A:130:GLN:HG3	9:B:127:VAL:HG13	1.98	0.45
8:A:236:LEU:HD22	8:A:240:ASN:HB3	1.99	0.45
8:c:84:ASN:HD22	8:c:171:THR:HB	1.81	0.45
9:j:16:GLY:O	10:d:28:SER:OG	2.35	0.45
10:d:158:THR:OG1	10:d:160:TRP:NE1	2.50	0.45
18:K:178:ASP:HA	18:K:181:LYS:HD3	1.99	0.45
1:l:159:LYS:HG2	1:b:156:TYR:HE1	1.82	0.44
3:h:10:GLY:HA3	3:h:42:LYS:HE2	1.99	0.44
5:f:113:ASN:OD1	5:f:116:LEU:N	2.50	0.44
15:H:215:LYS:HA	15:H:218:ILE:HD12	1.99	0.44
18:K:245:LYS:NZ	19:L:253:ASP:O	2.38	0.44
21:N:510:HIS:CG	21:N:513:ILE:HD12	2.52	0.44
24:Q:261:VAL:HG12	24:Q:265:MET:HE2	1.99	0.44
29:V:127:LYS:HA	29:V:158:LEU:HD22	1.97	0.44
10:d:207:THR:OG1	10:d:209:ASP:OD1	2.33	0.44
17:J:252:SER:HA	17:J:257:ARG:HG3	1.99	0.44
24:Q:249:LEU:HB2	24:Q:253:ASN:HB2	2.00	0.44
30:W:4:GLU:CD	30:W:109:ARG:HE	2.25	0.44
31:X:85:ARG:HH22	31:X:104:LYS:HG3	1.81	0.44
5:5:94:ARG:NH2	3:h:205:ASP:OD2	2.40	0.44
6:e:76:PHE:CZ	7:a:166:LEU:HB3	2.53	0.44
13:F:7:ASP:HA	13:F:12:THR:HB	1.99	0.44
8:c:78:THR:HA	8:c:233:PHE:HB2	1.99	0.44
13:l:106:GLU:OE2	13:l:110:HIS:NE2	2.50	0.44
18:K:268:ILE:HG12	18:K:313:LYS:HB3	1.99	0.44
21:N:254:SER:HB2	21:N:286:LEU:HD11	1.98	0.44
21:N:585:ARG:HB2	21:N:616:HIS:HB3	1.99	0.44
25:R:174:ILE:HD13	25:R:190:LYS:HB3	1.99	0.44
27:T:109:TYR:HE2	27:T:125:GLU:HG2	1.82	0.44
27:T:143:SER:HA	27:T:146:ILE:HD12	1.98	0.44
28:U:275:VAL:HG11	29:V:245:VAL:HG13	2.00	0.44
29:V:46:PRO:HA	29:V:112:PRO:HG3	1.98	0.44
30:W:143:ASN:ND2	30:W:149:GLN:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:352:LYS:HG2	33:Z:462:VAL:HG23	1.98	0.44
10:C:70:ASN:OD1	10:C:73:ILE:N	2.50	0.44
12:m:47:VAL:HG11	12:m:197:GLU:HA	2.00	0.44
15:H:100:ALA:HA	15:H:173:ARG:HB3	1.99	0.44
22:O:130:ASP:HA	22:O:133:ILE:HD12	1.99	0.44
33:Z:381:LEU:HD13	33:Z:414:GLY:HA2	1.99	0.44
4:g:8:ARG:HH11	4:g:116:LEU:HB3	1.82	0.44
4:g:136:SER:HA	4:g:172:MET:HE1	1.99	0.44
5:f:191:ASP:OD1	5:f:192:SER:N	2.51	0.44
10:C:107:PRO:HD2	10:C:110:ILE:HD12	1.99	0.44
9:j:157:PHE:HB3	10:d:57:LEU:HD11	1.98	0.44
15:H:251:PRO:HG2	15:H:254:THR:HB	1.99	0.44
16:I:184:ILE:HB	16:I:187:LEU:HD12	1.99	0.44
17:J:159:GLU:HB3	17:J:314:ILE:HG12	2.00	0.44
21:N:25:LEU:HD23	21:N:28:ILE:HD12	1.99	0.44
27:T:134:LYS:HA	27:T:138:ASP:HB3	1.99	0.44
3:3:176:ASP:HB3	5:f:104:GLN:HE22	1.82	0.44
4:4:82:SER:OG	10:C:101:THR:O	2.23	0.44
6:6:127:HIS:HE1	6:6:129:ILE:HD11	1.83	0.44
1:b:27:PHE:CE2	1:b:32:ILE:HG13	2.53	0.44
5:f:139:ARG:HH12	12:m:72:ARG:HE	1.65	0.44
12:E:148:ASP:OD1	12:E:152:GLY:N	2.50	0.44
13:F:95:SER:O	13:F:100:ASN:N	2.50	0.44
14:G:95:GLU:HB3	14:G:115:ARG:HD3	2.00	0.44
14:G:204:HIS:NE2	14:G:208:LYS:HA	2.33	0.44
10:d:173:GLN:HB3	11:n:53:LYS:HB2	1.99	0.44
16:I:253:ILE:HG13	16:I:302:ILE:HG12	2.00	0.44
21:N:600:THR:HA	21:N:634:LEU:HD22	1.98	0.44
23:P:35:ALA:HB1	23:P:62:ILE:HG12	2.00	0.44
26:S:360:PHE:CD2	26:S:384:ARG:HD3	2.53	0.44
29:V:57:PHE:HE1	29:V:135:ARG:HD2	1.83	0.44
33:Z:120:SER:HB3	33:Z:138:ARG:NH2	2.32	0.44
33:Z:427:GLN:HA	33:Z:458:SER:HA	2.00	0.44
1:1:27:PHE:CE2	1:1:32:ILE:HG13	2.52	0.44
1:1:59:LYS:HB3	1:1:121:TYR:HB3	1.99	0.44
1:b:47:ASN:ND2	2:i:150:VAL:O	2.51	0.44
9:B:50:LYS:HE2	9:B:52:SER:HB2	2.00	0.44
10:C:13:PHE:HD2	11:D:19:GLN:HB3	1.83	0.44
9:j:44:VAL:HG23	9:j:213:ILE:HG22	1.99	0.44
16:I:167:MET:HB3	16:I:266:GLN:HB3	1.98	0.44
18:K:81:ARG:HH12	21:N:613:HIS:CD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:110:LYS:HA	19:L:142:LYS:HE2	1.99	0.44
23:P:83:SER:HB3	23:P:93:ILE:HG13	1.99	0.44
25:R:211:LYS:HD3	25:R:230:LEU:HD22	2.00	0.44
29:V:51:GLY:HA3	29:V:108:TYR:CZ	2.52	0.44
33:Z:134:SER:HA	33:Z:137:TYR:CD2	2.53	0.44
33:Z:295:ARG:HD3	33:Z:321:PHE:HZ	1.81	0.44
5:5:233:LYS:HG3	5:5:252:LEU:HD21	1.99	0.44
2:i:32:ILE:HB	2:i:156:LEU:HB3	1.99	0.44
4:g:106:GLY:HA2	4:g:184:VAL:HG11	2.00	0.44
13:l:76:GLY:HA3	13:l:130:VAL:HG23	2.00	0.44
15:H:144:LYS:HE3	20:M:75:LEU:HG	1.99	0.44
16:I:118:ALA:HB2	16:I:132:ILE:HD11	1.99	0.44
17:J:327:ILE:HG22	17:J:358:VAL:HG11	1.98	0.44
20:M:157:ASP:OD1	20:M:158:THR:N	2.50	0.44
24:Q:400:TYR:OH	24:Q:404:ASN:ND2	2.33	0.44
27:T:248:GLU:H	27:T:252:GLU:HG3	1.83	0.44
10:d:135:PHE:H	10:d:151:SER:HB3	1.83	0.44
12:m:223:THR:HG22	12:m:225:GLN:H	1.82	0.44
15:H:105:ILE:HB	15:H:146:VAL:HG22	2.00	0.44
16:I:281:ILE:HB	16:I:326:MET:HG2	1.99	0.44
20:M:336:ALA:O	20:M:342:ARG:NH1	2.51	0.44
28:U:122:ILE:HD12	28:U:137:TYR:HE2	1.82	0.44
33:Z:181:GLY:HA2	33:Z:230:ILE:HD13	2.00	0.44
2:2:243:LYS:HE3	5:f:286:ILE:HG21	1.99	0.43
4:4:136:SER:HB3	4:4:172:MET:HE2	1.98	0.43
5:5:114:PRO:HA	5:5:260:TRP:CD1	2.52	0.43
12:E:207:VAL:HG12	15:H:409:ARG:HH12	1.82	0.43
13:F:76:GLY:O	20:M:433:TYR:OH	2.34	0.43
13:F:117:GLN:HE21	13:F:121:GLN:HG3	1.82	0.43
12:m:117:CYS:HA	12:m:120:ALA:HB3	1.99	0.43
12:m:169:ALA:HB1	12:m:183:LEU:HD22	1.99	0.43
20:M:119:VAL:HB	20:M:155:ILE:HD11	2.00	0.43
20:M:289:LYS:HG2	20:M:332:VAL:HG11	2.00	0.43
22:O:189:TYR:HB2	22:O:220:SER:HB2	1.99	0.43
25:R:236:ALA:HB3	25:R:275:GLU:HB3	2.00	0.43
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.33	0.43
26:S:327:ILE:HG13	32:Y:64:TRP:HZ2	1.83	0.43
28:U:122:ILE:HD12	28:U:137:TYR:CE2	2.53	0.43
5:5:266:HIS:HB3	5:5:271:LEU:HD11	2.00	0.43
2:i:128:ILE:HG13	2:i:156:LEU:HD22	1.99	0.43
5:f:113:ASN:HD21	5:f:116:LEU:HD13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:46:ARG:HH11	8:A:152:PRO:HB2	1.82	0.43
9:B:9:LEU:HD11	9:B:129:PRO:HD3	1.99	0.43
12:E:61:SER:O	12:E:62:ASP:OD1	2.36	0.43
12:E:175:GLY:HA2	15:H:409:ARG:NH2	2.33	0.43
14:G:54:ILE:HG12	14:G:59:LEU:HD23	1.99	0.43
8:c:111:ASP:OD1	8:c:112:MET:N	2.52	0.43
10:d:106:ILE:HD13	10:d:111:LEU:HD13	2.01	0.43
14:k:183:HIS:CD2	14:k:184:PRO:HD2	2.48	0.43
15:H:221:LEU:O	15:H:225:VAL:HB	2.19	0.43
16:I:193:GLU:HB3	16:I:346:ARG:NH1	2.34	0.43
17:J:327:ILE:HA	17:J:330:ILE:HD12	1.99	0.43
21:N:762:ARG:NH2	21:N:766:GLN:O	2.50	0.43
22:O:250:TRP:CE2	22:O:270:ILE:HG22	2.53	0.43
31:X:37:PRO:HB3	31:X:46:TRP:HD1	1.83	0.43
33:Z:262:VAL:HG11	33:Z:287:ARG:HD3	2.00	0.43
33:Z:415:MET:HG2	33:Z:447:VAL:HA	1.99	0.43
3:h:172:LEU:HD22	3:h:202:MET:HB3	2.00	0.43
11:n:142:ASP:OD1	11:n:143:ASP:N	2.52	0.43
13:l:176:LEU:HD22	14:k:58:LEU:HD23	1.99	0.43
14:k:219:CYS:HB2	14:k:228:HIS:CD2	2.53	0.43
15:H:399:GLU:HB3	15:H:402:ILE:HG23	2.00	0.43
16:I:135:PHE:CD2	16:I:136:VAL:HG13	2.53	0.43
16:I:399:ALA:HB1	16:I:411:VAL:HG11	2.00	0.43
17:J:262:GLY:H	18:K:281:ARG:HD3	1.82	0.43
19:L:198:GLU:HG3	19:L:239:ILE:HG12	2.00	0.43
19:L:397:GLU:HA	19:L:400:PHE:HD2	1.83	0.43
20:M:167:VAL:HG11	20:M:262:LEU:HD11	2.00	0.43
3:3:149:MET:HG3	3:3:174:ALA:HB2	2.00	0.43
5:5:243:ASP:OD1	3:h:33:SER:OG	2.36	0.43
7:7:198:ILE:HB	7:7:199:PRO:HD3	2.00	0.43
4:g:35:THR:HA	4:g:45:SER:HA	2.00	0.43
11:D:10:ILE:HG12	12:E:23:GLN:HE22	1.84	0.43
14:G:108:PRO:HG2	14:G:111:ALA:HB3	1.99	0.43
15:H:200:VAL:HG22	15:H:272:ILE:HG12	2.01	0.43
16:I:190:GLN:NE2	16:I:349:LEU:O	2.51	0.43
16:I:278:ILE:HG23	16:I:323:LYS:H	1.84	0.43
16:I:371:LEU:HD22	16:I:375:VAL:HG11	2.00	0.43
20:M:224:PRO:HA	20:M:228:LYS:HE2	1.99	0.43
30:W:163:ASN:HB3	30:W:164:PRO:HD3	2.01	0.43
2:i:32:ILE:O	2:i:156:LEU:N	2.51	0.43
8:A:63:LEU:HD11	14:G:173:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:96:HIS:ND1	11:D:102:ASP:O	2.48	0.43
13:F:65:LYS:HE3	13:F:224:ILE:HD12	2.01	0.43
13:F:88:LEU:HD21	13:F:112:LEU:HB2	1.99	0.43
12:m:148:ASP:OD1	12:m:149:ALA:N	2.51	0.43
13:l:157:TYR:CE2	14:k:60:VAL:HG22	2.53	0.43
14:k:21:ASN:OD1	14:k:22:PHE:N	2.51	0.43
19:L:119:VAL:HG21	19:L:148:LEU:HD21	2.01	0.43
21:N:175:ASP:HB2	21:N:181:GLU:HB2	2.00	0.43
26:S:40:GLU:HA	26:S:46:LEU:HD12	2.01	0.43
26:S:426:ALA:HB1	26:S:432:ILE:HG12	2.00	0.43
27:T:27:LEU:HB2	27:T:28:PRO:HD3	2.01	0.43
29:V:71:MET:HE3	29:V:72:PRO:HD2	2.00	0.43
33:Z:99:LEU:HD23	33:Z:102:ILE:HD12	1.99	0.43
6:6:56:SER:HB2	7:7:170:TYR:CD1	2.53	0.43
2:i:32:ILE:HD13	2:i:73:ALA:HB1	2.00	0.43
3:h:104:PHE:HA	3:h:126:LEU:HD22	2.01	0.43
7:a:185:ASN:HB2	7:a:186:PRO:HD3	2.00	0.43
8:A:56:GLN:HA	8:A:223:LEU:HD23	2.00	0.43
8:A:179:THR:HG21	9:B:54:PRO:HD2	2.00	0.43
9:B:140:ASP:OD1	9:B:144:GLY:N	2.52	0.43
10:C:59:GLN:HE22	10:C:210:ARG:HG2	1.84	0.43
11:D:122:GLN:HE21	12:E:84:ASP:HA	1.82	0.43
11:D:175:LEU:HA	11:D:179:TYR:CD2	2.54	0.43
17:J:218:LEU:HG	17:J:229:MET:HB3	2.00	0.43
33:Z:295:ARG:HD3	33:Z:321:PHE:CZ	2.53	0.43
4:4:41:HIS:NE2	4:4:186:LYS:O	2.52	0.43
8:A:82:VAL:HB	8:A:142:THR:HB	2.01	0.43
8:c:13:ASP:HB2	9:j:2:THR:HG22	2.01	0.43
13:l:33:SER:OG	13:l:49:LEU:O	2.29	0.43
22:O:51:ASP:OD1	22:O:52:ALA:N	2.51	0.43
29:V:95:LEU:HB3	29:V:100:ARG:HB2	1.99	0.43
13:F:137:TYR:CZ	13:F:218:LYS:HG2	2.54	0.43
10:d:39:MET:HE2	10:d:161:LYS:HA	2.01	0.43
10:d:113:ARG:NH1	11:n:87:GLU:OE2	2.52	0.43
22:O:135:ARG:HA	22:O:138:LEU:HD12	2.01	0.43
25:R:59:MET:O	25:R:63:TYR:N	2.39	0.43
28:U:192:ASN:HB2	29:V:230:TYR:HD2	1.83	0.43
29:V:202:ASP:OD1	29:V:203:TYR:N	2.52	0.43
30:W:21:PHE:H	30:W:25:ARG:HB2	1.84	0.43
33:Z:518:LEU:HB2	33:Z:562:TRP:HH2	1.84	0.43
2:2:75:ALA:HB3	2:2:126:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:177:ARG:NH2	5:f:102:ALA:O	2.52	0.43
2:i:82:GLU:HG2	3:h:130:ILE:HD12	2.01	0.43
8:c:134:MET:HE3	14:k:125:LEU:HD13	1.99	0.43
9:j:158:PRO:O	10:d:57:LEU:HG	2.19	0.43
11:n:216:LYS:HB2	11:n:220:ASP:HB3	2.00	0.43
21:N:326:SER:N	29:V:168:LEU:HD11	2.34	0.43
21:N:746:ALA:HA	21:N:749:LEU:HD13	2.00	0.43
21:N:761:ILE:HG13	21:N:904:VAL:HG22	2.01	0.43
29:V:114:PHE:H	29:V:118:LEU:HD23	1.83	0.43
33:Z:318:LYS:C	33:Z:319:THR:HG1	2.26	0.43
2:2:68:PRO:HB3	9:B:223:GLY:HA3	2.00	0.43
6:6:224:LEU:HG	6:6:233:LYS:HG2	2.00	0.43
7:7:148:ILE:HG23	7:7:175:LEU:HD23	2.00	0.43
5:f:93:SER:OG	5:f:104:GLN:O	2.28	0.43
6:e:203:VAL:HG12	6:e:221:LEU:HD21	2.00	0.43
7:a:54:ILE:HD11	7:a:230:LEU:HD21	2.00	0.43
16:I:280:PHE:CE1	16:I:325:ILE:HD12	2.54	0.43
16:I:395:MET:HE2	16:I:420:LYS:HA	2.01	0.43
20:M:357:ARG:HD2	20:M:391:LEU:HD21	2.00	0.43
24:Q:267:LEU:HD13	24:Q:331:THR:HG22	2.01	0.43
26:S:114:TYR:HB2	26:S:117:SER:HB2	2.00	0.43
26:S:330:LEU:N	32:Y:62:GLU:O	2.52	0.43
26:S:399:TYR:CD2	26:S:402:ILE:HD12	2.54	0.43
7:7:60:LEU:HD11	7:7:62:SER:HB3	2.01	0.42
2:i:47:THR:O	2:i:60:CYS:N	2.49	0.42
5:f:94:ARG:NH1	5:f:244:ALA:O	2.52	0.42
5:f:249:SER:HA	5:f:267:ASP:HA	2.01	0.42
7:a:102:ASP:O	7:a:106:GLU:N	2.42	0.42
8:A:64:LEU:HG	14:G:160:TYR:CE1	2.54	0.42
10:C:115:LEU:HD23	10:C:118:ILE:HD12	2.01	0.42
11:D:37:LYS:HA	11:D:42:VAL:HA	2.00	0.42
13:l:39:ARG:HD3	13:l:144:LEU:HB2	2.00	0.42
16:I:391:ASP:OD2	17:J:306:ARG:NH1	2.52	0.42
17:J:35:ARG:HH22	26:S:45:THR:HG21	1.84	0.42
21:N:443:LEU:HD22	21:N:477:SER:HB2	2.00	0.42
24:Q:65:TYR:HD2	24:Q:74:LEU:HD13	1.84	0.42
25:R:283:THR:HG22	25:R:285:ALA:H	1.83	0.42
27:T:191:LYS:HG2	27:T:224:ARG:HH22	1.83	0.42
3:3:103:TYR:OH	4:4:93:ARG:NH1	2.42	0.42
4:4:135:TYR:HA	4:4:138:PHE:CE2	2.54	0.42
7:7:62:SER:HB3	7:7:67:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:56:LEU:O	3:h:60:VAL:HG23	2.18	0.42
9:B:12:PHE:HB3	10:C:21:GLN:HG2	2.01	0.42
12:E:121:LEU:HB2	13:F:82:ARG:HH21	1.84	0.42
12:m:85:ALA:O	12:m:89:ILE:HG12	2.18	0.42
17:J:141:LYS:HG2	17:J:142:VAL:HG22	2.00	0.42
20:M:379:LEU:HD22	20:M:419:ILE:HD12	2.01	0.42
23:P:371:LEU:HD22	23:P:375:GLN:HB3	2.01	0.42
26:S:405:ARG:HG2	26:S:416:GLU:HG2	2.02	0.42
4:4:99:GLN:HB3	4:4:121:TYR:HB2	2.01	0.42
6:6:46:THR:HB	6:6:59:GLU:H	1.84	0.42
6:e:76:PHE:HE2	6:e:78:ALA:HB3	1.84	0.42
6:e:226:VAL:HG22	6:e:231:VAL:HG22	2.02	0.42
7:a:44:VAL:HG12	7:a:148:ILE:HD12	2.01	0.42
8:A:156:LYS:HE3	8:A:166:TYR:HE2	1.84	0.42
9:B:9:LEU:HD21	9:B:20:GLN:HG2	2.00	0.42
9:B:67:LEU:HD13	9:B:110:LEU:HD21	2.00	0.42
14:k:124:THR:HA	14:k:131:PRO:HG3	2.01	0.42
17:J:324:ARG:HA	17:J:327:ILE:HD12	2.00	0.42
23:P:319:GLU:OE1	23:P:323:ASN:HB3	2.19	0.42
24:Q:210:CYS:HB3	24:Q:214:THR:HB	2.01	0.42
26:S:234:ILE:HG23	26:S:253:PHE:HE2	1.84	0.42
31:X:7:VAL:HG12	31:X:8:ILE:HG13	2.00	0.42
3:3:24:ALA:HB1	3:3:171:LEU:HD22	2.02	0.42
4:4:22:THR:HA	4:4:27:VAL:HA	2.02	0.42
5:5:109:VAL:HG21	5:5:253:TYR:HE2	1.84	0.42
13:F:62:LYS:O	13:F:74:LEU:N	2.51	0.42
8:c:46:ARG:HH21	8:c:167:LYS:HG2	1.84	0.42
9:j:1:MET:HE3	9:j:6:SER:HB3	2.00	0.42
15:H:249:TYR:N	15:H:375:VAL:O	2.52	0.42
16:I:221:LEU:HD12	16:I:327:ALA:HB2	2.01	0.42
20:M:361:LEU:HD21	20:M:391:LEU:HD22	2.00	0.42
23:P:244:ILE:HD12	23:P:247:THR:HB	2.01	0.42
28:U:72:TYR:HB3	29:V:94:MET:SD	2.60	0.42
28:U:174:LEU:HD21	29:V:34:LEU:HD23	2.02	0.42
2:2:244:GLU:HG3	3:3:198:ARG:HG2	2.00	0.42
4:4:192:VAL:HG12	4:4:194:ASP:H	1.83	0.42
6:e:76:PHE:HD2	6:e:79:ASP:H	1.66	0.42
13:F:157:TYR:CZ	14:G:60:VAL:HG22	2.54	0.42
18:K:349:ARG:NH2	18:K:372:ILE:O	2.49	0.42
25:R:29:LYS:HB3	25:R:46:ALA:HB1	2.02	0.42
27:T:63:GLU:HG3	27:T:105:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:22:PRO:HD2	30:W:24:THR:O	2.20	0.42
33:Z:307:HIS:CE1	33:Z:340:LEU:HD12	2.54	0.42
1:1:61:TRP:CD1	1:1:197:LEU:HD21	2.55	0.42
3:3:123:GLY:HA3	3:3:137:ILE:HG21	2.01	0.42
4:4:4:ILE:HG12	4:4:103:LEU:HD12	2.00	0.42
4:4:38:LEU:HD23	4:4:61:GLN:HG3	2.02	0.42
7:7:58:ASP:HA	7:7:228:PHE:HA	2.02	0.42
8:A:156:LYS:HE3	8:A:166:TYR:CE2	2.55	0.42
13:F:39:ARG:NH2	13:F:155:GLU:OE2	2.52	0.42
9:j:77:GLY:HA3	9:j:132:VAL:HG12	2.01	0.42
11:n:132:SER:OG	11:n:150:THR:O	2.32	0.42
14:k:71:ASP:CG	14:k:72:ARG:H	2.26	0.42
15:H:244:LYS:NZ	15:H:346:ARG:HD3	2.33	0.42
16:I:174:ASP:O	16:I:244:PHE:N	2.44	0.42
19:L:251:ILE:N	20:M:293:SER:OG	2.53	0.42
19:L:274:GLU:HB3	19:L:320:GLN:HG3	2.01	0.42
20:M:83:VAL:N	20:M:118:VAL:O	2.52	0.42
23:P:421:GLU:HB2	28:U:235:LEU:HD23	2.00	0.42
33:Z:878:LEU:HD23	33:Z:881:ILE:HD12	2.01	0.42
4:4:28:LEU:HA	4:g:171:ARG:HH12	1.84	0.42
5:5:113:ASN:OD1	5:5:116:LEU:N	2.53	0.42
7:7:185:ASN:HB3	7:7:186:PRO:HD3	2.02	0.42
2:i:126:TYR:HB3	2:i:156:LEU:HD11	2.02	0.42
11:D:71:VAL:HG22	11:D:137:GLY:HA3	2.01	0.42
11:D:117:GLN:HG2	11:D:129:PHE:HB2	2.00	0.42
13:F:12:THR:HG23	14:G:23:GLN:HE21	1.84	0.42
15:H:173:ARG:NE	16:I:129:TYR:HB3	2.35	0.42
15:H:357:ARG:HG2	15:H:359:ASN:H	1.85	0.42
16:I:193:GLU:HB3	16:I:346:ARG:HH12	1.83	0.42
20:M:175:LYS:HE3	20:M:273:LYS:NZ	2.35	0.42
20:M:187:ASP:HA	20:M:190:ILE:HB	2.01	0.42
26:S:440:ASP:HB3	26:S:442:PHE:CE2	2.54	0.42
28:U:121:LEU:HD23	28:U:136:ALA:HA	2.00	0.42
30:W:25:ARG:HG3	30:W:26:PHE:CD2	2.54	0.42
33:Z:352:LYS:NZ	33:Z:464:ASP:OD1	2.41	0.42
2:2:75:ALA:H	2:2:81:THR:HG21	1.85	0.42
7:7:117:GLU:HG2	13:F:140:SER:HA	2.01	0.42
3:h:87:PHE:HA	3:h:90:LEU:HD12	2.01	0.42
11:D:133:THR:H	11:D:150:THR:HG1	1.67	0.42
12:m:85:ALA:HB1	12:m:142:LEU:HD21	2.01	0.42
18:K:190:LEU:O	18:K:195:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:96:GLN:HB2	26:S:219:LYS:HE3	2.01	0.42
21:N:761:ILE:HG23	21:N:767:ALA:H	1.85	0.42
26:S:479:MET:O	26:S:482:PRO:HD2	2.20	0.42
28:U:171:VAL:HB	29:V:217:HIS:HD2	1.85	0.42
29:V:238:LEU:HD22	29:V:242:LYS:HB2	2.01	0.42
33:Z:911:LYS:HE3	33:Z:964:GLU:HB3	2.00	0.42
2:2:242:LEU:N	3:3:199:TYR:O	2.46	0.42
4:4:22:THR:HB	4:4:27:VAL:HG22	2.00	0.42
5:f:86:GLY:HA3	5:f:254:HIS:HE1	1.84	0.42
8:c:14:ARG:HH21	8:c:21:PRO:HG2	1.85	0.42
9:j:111:VAL:HG21	9:j:148:TYR:HD2	1.85	0.42
13:l:121:GLN:HG3	14:k:130:ARG:HB3	2.02	0.42
17:J:393:ASN:OD1	18:K:330:ARG:NH1	2.35	0.42
19:L:290:ARG:HH21	19:L:294:GLY:N	2.16	0.42
29:V:67:ASP:OD1	29:V:68:VAL:N	2.52	0.42
29:V:197:TYR:CE2	29:V:199:LEU:HB2	2.54	0.42
33:Z:598:ALA:HB3	33:Z:738:TYR:HB3	2.02	0.42
4:4:142:SER:HB2	5:f:214:VAL:HG23	2.01	0.42
5:5:265:ASN:OD1	5:5:266:HIS:N	2.53	0.42
7:7:61:GLY:HA3	7:7:69:PHE:HB2	2.02	0.42
3:h:18:LYS:HB2	3:h:157:ASN:HA	2.02	0.42
9:B:77:GLY:HA3	9:B:132:VAL:HG12	2.02	0.42
12:m:108:ASN:HB3	12:m:111:SER:HB2	2.02	0.42
18:K:137:VAL:HG12	18:K:149:ILE:HA	2.02	0.42
21:N:102:VAL:HA	21:N:136:ILE:HG21	2.02	0.42
22:O:41:LEU:O	22:O:43:GLU:HG3	2.20	0.42
22:O:44:SER:O	22:O:47:LYS:N	2.53	0.42
25:R:211:LYS:HB3	25:R:230:LEU:HB3	2.02	0.42
28:U:16:LEU:HD22	29:V:213:LEU:HD21	2.01	0.42
2:2:251:ASP:HB3	10:C:226:TYR:CE1	2.55	0.41
7:7:179:PHE:CE2	7:7:221:ASP:HB2	2.55	0.41
9:B:72:GLY:N	9:B:137:ALA:O	2.43	0.41
18:K:237:VAL:O	18:K:271:ILE:HA	2.19	0.41
21:N:325:PHE:HB3	29:V:168:LEU:HD11	2.02	0.41
23:P:268:LEU:HD11	23:P:277:GLN:HG2	2.02	0.41
28:U:71:ASN:ND2	30:W:64:THR:OG1	2.53	0.41
1:1:142:PRO:HB2	1:1:161:PHE:CZ	2.55	0.41
5:5:130:TRP:O	5:5:134:LEU:N	2.49	0.41
7:a:60:LEU:HD22	7:a:225:SER:HB3	2.02	0.41
9:B:69:PRO:O	9:B:235:PHE:N	2.52	0.41
13:F:11:VAL:HA	14:G:130:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:129:GLY:HA2	13:F:149:PRO:HB3	2.01	0.41
17:J:44:LEU:HD21	18:K:67:TYR:HD2	1.85	0.41
18:K:159:SER:HA	18:K:242:PHE:HA	2.03	0.41
19:L:220:LEU:HD23	19:L:347:VAL:HB	2.02	0.41
21:N:330:THR:HG21	21:N:744:PRO:HG2	2.03	0.41
25:R:78:ASP:OD1	25:R:79:LEU:N	2.53	0.41
26:S:385:SER:O	26:S:389:LYS:HG2	2.20	0.41
30:W:98:LEU:HB3	30:W:108:GLN:NE2	2.35	0.41
33:Z:277:GLU:HG3	33:Z:279:THR:H	1.85	0.41
2:i:127:LEU:HD13	2:i:142:ILE:HD11	2.00	0.41
3:h:8:ASN:HA	3:h:30:GLY:O	2.20	0.41
4:g:4:ILE:HD12	4:g:47:ALA:HB2	2.02	0.41
11:D:100:LEU:C	11:D:102:ASP:H	2.28	0.41
18:K:164:ASN:HB3	18:K:234:PHE:HD2	1.85	0.41
19:L:108:VAL:HA	19:L:119:VAL:HG12	2.02	0.41
20:M:149:ASN:ND2	20:M:152:SER:OG	2.54	0.41
20:M:418:GLY:HA2	20:M:422:VAL:HG11	2.03	0.41
21:N:79:VAL:HG22	21:N:101:ILE:HG23	2.02	0.41
22:O:20:PRO:HD2	22:O:22:LEU:HG	2.01	0.41
23:P:418:ASN:HA	28:U:235:LEU:HD21	2.03	0.41
33:Z:146:PHE:HD2	33:Z:147:GLU:HG3	1.85	0.41
33:Z:869:ASP:OD2	33:Z:978:GLU:N	2.52	0.41
7:7:115:ASP:OD1	7:7:116:ALA:N	2.53	0.41
2:i:201:ASN:ND2	2:i:218:ASN:OD1	2.53	0.41
13:F:50:LYS:HG2	13:F:61:LYS:HA	2.02	0.41
11:n:132:SER:HB2	11:n:152:PRO:HD3	2.02	0.41
12:m:122:ARG:HA	13:l:126:ARG:NH1	2.34	0.41
20:M:224:PRO:O	20:M:387:ASN:ND2	2.54	0.41
21:N:63:LEU:HD22	21:N:88:ARG:HG2	2.02	0.41
22:O:127:LEU:HB2	22:O:167:ILE:HG12	2.01	0.41
22:O:308:LEU:HB3	22:O:348:VAL:HB	2.01	0.41
26:S:377:TYR:CE2	27:T:133:ILE:HG21	2.55	0.41
27:T:54:ASP:O	27:T:58:THR:HG23	2.21	0.41
30:W:101:ARG:HH22	30:W:106:GLN:HB2	1.86	0.41
10:C:38:ILE:HG21	10:C:189:ALA:HB1	2.03	0.41
11:D:203:VAL:HG21	11:D:210:ILE:HG12	2.02	0.41
12:E:20:ARG:HG2	20:M:430:VAL:HB	2.03	0.41
11:n:71:VAL:HG22	11:n:137:GLY:HA3	2.02	0.41
15:H:403:ARG:HE	15:H:405:GLU:HB2	1.86	0.41
16:I:306:MET:HE1	16:I:335:ASP:H	1.84	0.41
18:K:55:GLU:HA	18:K:58:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:159:SER:HG	18:K:244:HIS:HE2	1.68	0.41
18:K:290:ARG:HB3	18:K:294:ARG:HH12	1.84	0.41
25:R:77:SER:OG	25:R:86:ASP:N	2.54	0.41
26:S:424:SER:O	26:S:428:ARG:HG2	2.20	0.41
3:3:25:CYS:HB2	3:3:42:LYS:HZ3	1.85	0.41
7:7:255:ALA:HB1	1:b:191:VAL:HG21	2.02	0.41
9:B:32:VAL:HG21	9:B:63:LYS:NZ	2.34	0.41
8:c:83:VAL:HG11	8:c:90:ALA:HB2	2.02	0.41
11:n:181:ARG:HH22	12:m:60:GLU:HA	1.85	0.41
19:L:129:VAL:HG11	19:L:148:LEU:HD22	2.02	0.41
19:L:252:VAL:HG23	19:L:286:ILE:HG22	2.03	0.41
20:M:170:MET:HG3	20:M:245:LYS:O	2.21	0.41
25:R:311:THR:O	25:R:315:VAL:HB	2.21	0.41
27:T:132:HIS:O	27:T:136:LEU:HB3	2.19	0.41
33:Z:87:LYS:HD3	33:Z:90:LYS:HG3	2.02	0.41
6:e:77:ALA:HB3	7:a:168:VAL:HA	2.03	0.41
7:a:122:PRO:HB2	7:a:159:PHE:HB3	2.02	0.41
8:A:30:TYR:HD1	8:A:33:LYS:HD2	1.86	0.41
8:A:168:ALA:HB3	9:B:55:LEU:HD13	2.01	0.41
14:G:12:ASN:HB3	14:G:127:ASN:HA	2.02	0.41
15:H:243:PRO:HG3	20:M:396:VAL:HG11	2.03	0.41
19:L:95:ILE:HD13	20:M:68:LYS:HE3	2.02	0.41
20:M:290:ARG:H	20:M:332:VAL:HG21	1.86	0.41
21:N:376:LYS:HA	21:N:411:ILE:HG12	2.02	0.41
21:N:641:LEU:HD23	21:N:644:LEU:HD12	2.03	0.41
25:R:335:ARG:CZ	25:R:376:GLN:HB3	2.50	0.41
28:U:192:ASN:HB2	29:V:230:TYR:CD2	2.56	0.41
30:W:19:GLY:C	30:W:25:ARG:HB3	2.45	0.41
33:Z:599:ILE:O	33:Z:603:VAL:HG13	2.20	0.41
33:Z:911:LYS:HG3	33:Z:964:GLU:HB2	2.02	0.41
3:3:27:LEU:HD12	3:3:184:GLY:HA3	2.02	0.41
2:i:95:HIS:NE2	8:c:104:PHE:HE1	2.19	0.41
3:h:11:ILE:HG21	3:h:142:ALA:HB3	2.02	0.41
6:e:92:LYS:HB3	13:l:89:ARG:HH22	1.85	0.41
8:A:50:CYS:SG	8:A:51:THR:N	2.94	0.41
8:A:135:ARG:HD3	14:G:125:LEU:HA	2.03	0.41
9:B:82:TYR:CZ	9:B:86:VAL:HG21	2.56	0.41
14:G:21:ASN:OD1	14:G:22:PHE:N	2.53	0.41
8:c:219:SER:H	8:c:222:ASP:HB2	1.85	0.41
16:I:103:PRO:C	16:I:104:LEU:HD12	2.45	0.41
16:I:361:ILE:HG13	16:I:389:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:271:ILE:HD12	18:K:316:MET:HG2	2.03	0.41
20:M:256:ILE:HG21	20:M:303:ARG:NH1	2.35	0.41
21:N:162:ARG:HE	21:N:164:ASP:HB3	1.86	0.41
22:O:72:LYS:HG2	22:O:73:ILE:HG12	2.03	0.41
22:O:333:SER:HB2	23:P:304:THR:HG22	2.03	0.41
26:S:461:PHE:HB3	28:U:277:TYR:CE1	2.56	0.41
1:1:108:ASN:O	1:1:112:LEU:N	2.54	0.41
2:2:36:LYS:HD2	2:2:152:TYR:HA	2.03	0.41
2:2:171:TRP:HB2	2:2:183:LEU:HD21	2.02	0.41
2:2:193:TRP:CD1	6:e:240:ARG:HD2	2.55	0.41
3:3:4:PRO:HA	3:3:7:ILE:HD12	2.01	0.41
4:4:23:ARG:NH2	5:5:191:ASP:OD2	2.54	0.41
5:5:181:ARG:HE	5:5:257:GLU:CD	2.29	0.41
5:5:271:LEU:HD23	5:5:274:LYS:HD2	2.03	0.41
3:h:49:VAL:HG22	3:h:84:PRO:HG3	2.03	0.41
7:a:86:ILE:HG12	7:a:147:ILE:HG12	2.02	0.41
7:a:109:TYR:HB3	14:k:93:ARG:NH1	2.36	0.41
8:A:87:ILE:N	8:A:88:PRO:HD2	2.36	0.41
9:B:71:ILE:HA	9:B:138:GLY:HA2	2.02	0.41
9:B:204:PHE:HD1	9:B:247:LEU:HD13	1.85	0.41
12:E:9:ASP:CG	13:F:4:ASN:HD21	2.28	0.41
12:E:52:LYS:O	12:E:53:ARG:HB2	2.21	0.41
10:d:87:LEU:HD22	10:d:115:LEU:HD22	2.03	0.41
12:m:35:SER:O	12:m:79:SER:OG	2.23	0.41
14:k:68:GLN:OE1	14:k:93:ARG:NH2	2.54	0.41
17:J:219:VAL:HG22	17:J:268:VAL:HG11	2.02	0.41
18:K:164:ASN:OD1	18:K:165:GLU:N	2.54	0.41
18:K:238:ASN:HB3	19:L:306:MET:HE3	2.03	0.41
20:M:129:LEU:HD11	20:M:155:ILE:HD12	2.02	0.41
21:N:214:LEU:HB2	21:N:225:LEU:HD21	2.02	0.41
22:O:39:PHE:HB2	22:O:52:ALA:HB2	2.01	0.41
22:O:62:TYR:HB2	22:O:69:PHE:HZ	1.85	0.41
22:O:120:LYS:HG2	30:W:81:ILE:HB	2.02	0.41
22:O:318:HIS:ND1	22:O:318:HIS:O	2.54	0.41
22:O:371:VAL:O	22:O:375:ASP:N	2.49	0.41
24:Q:347:LEU:HD22	24:Q:377:LEU:HD13	2.03	0.41
26:S:30:GLN:OE1	26:S:64:ARG:NH2	2.54	0.41
28:U:56:PHE:CE2	28:U:58:GLU:HB2	2.56	0.41
33:Z:181:GLY:HA3	33:Z:266:LYS:HG3	2.03	0.41
33:Z:211:PHE:CG	33:Z:220:ALA:HB2	2.56	0.41
2:2:206:VAL:N	2:2:214:GLU:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:26:ASP:OD1	3:3:42:LYS:NZ	2.54	0.41
10:C:70:ASN:HD21	10:C:73:ILE:HD12	1.85	0.41
9:j:123:GLN:NE2	10:d:86:ILE:HG13	2.36	0.41
18:K:290:ARG:CB	18:K:294:ARG:HH12	2.34	0.41
19:L:364:HIS:CD2	19:L:392:ARG:HE	2.38	0.41
21:N:339:MET:HE2	21:N:707:ASN:HB2	2.03	0.41
21:N:510:HIS:CE1	29:V:61:TYR:HB3	2.56	0.41
22:O:41:LEU:HD22	22:O:82:LEU:HA	2.03	0.41
23:P:283:LYS:HD2	23:P:286:ASN:HD21	1.85	0.41
25:R:72:VAL:HG12	25:R:72:VAL:O	2.20	0.41
25:R:146:ASP:OD2	25:R:149:ASN:ND2	2.36	0.41
25:R:382:ASP:OD1	25:R:383:ARG:N	2.53	0.41
28:U:21:HIS:NE2	29:V:100:ARG:HD2	2.35	0.41
28:U:79:MET:HG3	29:V:72:PRO:HD3	2.03	0.41
2:2:32:ILE:HD13	2:2:73:ALA:HB1	2.02	0.40
4:4:41:HIS:HB2	4:4:74:GLU:OE2	2.21	0.40
7:a:37:PRO:HB3	7:a:144:TRP:CD1	2.57	0.40
14:G:66:LYS:HE2	14:G:82:ILE:HG12	2.02	0.40
9:j:71:ILE:HG12	9:j:138:GLY:HA3	2.03	0.40
14:k:54:ILE:HB	14:k:211:ASP:HB3	2.03	0.40
14:k:78:TYR:CE2	14:k:85:GLY:HA3	2.57	0.40
19:L:283:VAL:HG23	19:L:333:LEU:HD21	2.02	0.40
19:L:287:GLY:HA2	19:L:305:LEU:HD21	2.03	0.40
21:N:28:ILE:O	21:N:32:VAL:HG13	2.21	0.40
22:O:99:LEU:O	22:O:103:LYS:HB3	2.21	0.40
26:S:417:GLN:NE2	27:T:208:LEU:HA	2.35	0.40
29:V:57:PHE:CG	29:V:63:VAL:HA	2.55	0.40
30:W:38:GLN:HG3	30:W:42:ASN:HD22	1.86	0.40
33:Z:290:GLU:HB3	33:Z:293:MET:HG3	2.02	0.40
1:1:152:PHE:CZ	7:a:66:LEU:HD13	2.56	0.40
6:6:46:THR:OG1	6:6:219:ASP:O	2.39	0.40
12:E:18:GLU:HB3	20:M:426:LYS:HD2	2.03	0.40
21:N:416:GLY:HA3	21:N:453:ALA:HB1	2.03	0.40
24:Q:389:VAL:HG23	24:Q:398:TYR:HB2	2.03	0.40
33:Z:217:GLU:HA	33:Z:220:ALA:HB3	2.02	0.40
1:1:167:LYS:HD2	1:1:196:VAL:HG11	2.02	0.40
2:2:47:THR:HB	2:2:59:ASN:HA	2.03	0.40
3:3:76:LEU:HD13	10:C:92:ARG:HD3	2.04	0.40
4:g:182:LYS:HE2	4:g:191:GLN:HE21	1.86	0.40
7:a:92:ASP:CG	7:a:143:LEU:HD22	2.45	0.40
8:A:86:PRO:HD2	8:A:139:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:16:SER:OG	14:G:20:ARG:O	2.37	0.40
20:M:246:LEU:HD22	20:M:262:LEU:HD13	2.03	0.40
21:N:4:THR:HG22	21:N:27:SER:HB3	2.04	0.40
21:N:650:ASP:OD1	21:N:651:PHE:N	2.53	0.40
22:O:277:ILE:HG22	22:O:279:ILE:H	1.85	0.40
25:R:353:MET:HA	25:R:357:PHE:CD2	2.56	0.40
5:5:106:VAL:HG22	6:6:151:GLU:HG2	2.03	0.40
3:h:63:LEU:O	3:h:67:PHE:N	2.37	0.40
5:f:234:ARG:HA	5:f:237:LEU:HB3	2.03	0.40
7:a:251:LYS:HE3	7:a:253:ASP:HB2	2.03	0.40
15:H:357:ARG:HH21	15:H:359:ASN:HD22	1.67	0.40
16:I:206:GLU:HA	16:I:209:GLU:HB2	2.02	0.40
20:M:283:LEU:O	20:M:287:GLY:N	2.53	0.40
21:N:13:LEU:HA	21:N:21:LYS:HE2	2.03	0.40
21:N:344:THR:HG22	21:N:375:HIS:HA	2.03	0.40
24:Q:219:ASP:HB3	24:Q:238:TYR:HB3	2.03	0.40
1:1:209:PRO:HG2	7:a:252:TRP:CZ2	2.56	0.40
2:2:189:GLN:HB2	2:2:220:LEU:HD21	2.02	0.40
6:e:74:ASN:HB3	6:e:127:HIS:HB3	2.03	0.40
7:a:87:SER:OG	7:a:146:ALA:HB3	2.21	0.40
9:B:9:LEU:O	10:C:129:ARG:HD3	2.22	0.40
9:j:94:HIS:HA	9:j:98:LYS:HB3	2.04	0.40
17:J:44:LEU:HD13	18:K:68:ILE:HG12	2.03	0.40
20:M:121:THR:HG21	20:M:153:TYR:HD1	1.86	0.40
21:N:423:LEU:HB2	21:N:450:ILE:HD13	2.04	0.40
28:U:20:ASP:OD2	28:U:24:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
1	b	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
2	2	224/261 (86%)	215 (96%)	9 (4%)	0	100	100
2	i	224/261 (86%)	217 (97%)	7 (3%)	0	100	100
3	3	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
3	h	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
4	4	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
4	g	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
5	5	210/287 (73%)	205 (98%)	5 (2%)	0	100	100
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
6	6	220/241 (91%)	212 (96%)	8 (4%)	0	100	100
6	e	220/241 (91%)	211 (96%)	9 (4%)	0	100	100
7	7	227/266 (85%)	218 (96%)	9 (4%)	0	100	100
7	a	230/266 (86%)	221 (96%)	9 (4%)	0	100	100
8	A	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
8	c	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
9	B	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
9	j	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
10	C	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
10	d	242/258 (94%)	231 (96%)	10 (4%)	1 (0%)	30	67
11	D	238/254 (94%)	226 (95%)	12 (5%)	0	100	100
11	n	238/254 (94%)	228 (96%)	10 (4%)	0	100	100
12	E	240/260 (92%)	226 (94%)	13 (5%)	1 (0%)	30	67
12	m	240/260 (92%)	230 (96%)	9 (4%)	1 (0%)	30	67
13	F	231/234 (99%)	218 (94%)	13 (6%)	0	100	100
13	l	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
14	G	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
14	k	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
15	H	353/467 (76%)	316 (90%)	37 (10%)	0	100	100
16	I	361/437 (83%)	333 (92%)	28 (8%)	0	100	100
17	J	371/405 (92%)	351 (95%)	20 (5%)	0	100	100
18	K	379/428 (89%)	347 (92%)	32 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	L	359/437 (82%)	334 (93%)	25 (7%)	0	100	100
20	M	363/434 (84%)	332 (92%)	29 (8%)	2 (1%)	21	59
21	N	843/945 (89%)	793 (94%)	46 (6%)	4 (0%)	24	63
22	O	385/393 (98%)	342 (89%)	42 (11%)	1 (0%)	36	72
23	P	430/445 (97%)	391 (91%)	39 (9%)	0	100	100
24	Q	429/434 (99%)	397 (92%)	32 (8%)	0	100	100
25	R	398/429 (93%)	357 (90%)	38 (10%)	3 (1%)	16	54
26	S	473/523 (90%)	451 (95%)	21 (4%)	1 (0%)	43	78
27	T	270/274 (98%)	238 (88%)	32 (12%)	0	100	100
28	U	245/338 (72%)	242 (99%)	2 (1%)	1 (0%)	30	67
29	V	282/306 (92%)	242 (86%)	37 (13%)	3 (1%)	11	46
30	W	195/268 (73%)	176 (90%)	16 (8%)	3 (2%)	8	40
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100	100
32	Y	25/89 (28%)	18 (72%)	6 (24%)	1 (4%)	2	18
33	Z	807/993 (81%)	740 (92%)	67 (8%)	0	100	100
All	All	13376/15139 (88%)	12565 (94%)	789 (6%)	22 (0%)	44	78

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	N	180	SER
21	N	874	ILE
28	U	130	VAL
30	W	22	PRO
10	d	207	THR
12	m	53	ARG
32	Y	69	VAL
12	E	12	VAL
21	N	761	ILE
21	N	903	VAL
25	R	241	ILE
25	R	421	VAL
29	V	189	ILE
29	V	305	ILE
30	W	147	ILE
20	M	167	VAL
25	R	72	VAL

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Mol	Chain	Res	Type
26	S	83	PRO
20	M	422	VAL
22	O	227	ILE
29	V	271	VAL
30	W	118	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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%)	203 (100%)	0	100	100
10	d	203/216 (94%)	202 (100%)	1 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	197 (100%)	1 (0%)	81	83
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	320/385 (83%)	320 (100%)	0	100	100
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	308/377 (82%)	308 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
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%)	447 (100%)	0	100	100
27	T	254/256 (99%)	253 (100%)	1 (0%)	84	84
28	U	234/308 (76%)	234 (100%)	0	100	100
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	11624/13054 (89%)	11621 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	E	52	LYS

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Mol	Chain	Res	Type
10	d	206	LEU
27	T	142	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	47	ASN
2	2	95	HIS
2	2	143	HIS
2	2	201	ASN
3	3	145	GLN
3	3	169	GLN
3	3	204	GLN
4	4	63	ASN
5	5	251	ASN
5	5	283	ASN
6	6	27	ASN
6	6	55	ASN
6	6	98	HIS
6	6	127	HIS
6	6	216	GLN
7	7	95	HIS
7	7	107	ASN
1	b	72	GLN
1	b	180	GLN
2	i	114	GLN
2	i	115	HIS
2	i	122	HIS
2	i	170	HIS
3	h	145	GLN
3	h	169	GLN
3	h	173	ASN
4	g	55	GLN
4	g	61	GLN
4	g	86	GLN
4	g	147	HIS
4	g	191	GLN
5	f	104	GLN
5	f	128	GLN
5	f	208	GLN
6	e	113	GLN
6	e	114	HIS

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Mol	Chain	Res	Type
6	e	127	HIS
6	e	171	ASN
6	e	177	ASN
7	a	70	ASN
7	a	145	ASN
8	A	37	GLN
10	C	59	GLN
10	C	120	GLN
10	C	147	GLN
10	C	227	GLN
11	D	79	ASN
11	D	94	GLN
11	D	117	GLN
12	E	23	GLN
12	E	180	GLN
12	E	218	GLN
13	F	4	ASN
13	F	21	GLN
13	F	117	GLN
13	F	143	HIS
13	F	152	ASN
14	G	23	GLN
14	G	64	ASN
14	G	68	GLN
14	G	182	HIS
14	G	183	HIS
8	c	185	HIS
9	j	123	GLN
10	d	103	ASN
11	n	96	HIS
11	n	117	GLN
11	n	118	GLN
11	n	122	GLN
11	n	204	GLN
13	l	43	HIS
14	k	73	HIS
14	k	147	HIS
14	k	204	HIS
14	k	244	GLN
15	H	217	GLN
16	I	204	HIS
17	J	66	GLN

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Mol	Chain	Res	Type
17	J	111	GLN
17	J	170	HIS
17	J	181	GLN
17	J	278	GLN
17	J	295	ASN
18	K	64	GLN
18	K	106	ASN
19	L	67	HIS
19	L	302	GLN
20	M	53	HIS
20	M	74	GLN
21	N	300	ASN
21	N	308	ASN
21	N	329	HIS
21	N	340	HIS
21	N	360	GLN
21	N	375	HIS
21	N	499	HIS
21	N	707	ASN
21	N	738	GLN
21	N	772	GLN
22	O	4	ASN
22	O	122	HIS
22	O	253	GLN
22	O	326	HIS
22	O	354	GLN
23	P	76	ASN
23	P	98	GLN
23	P	286	ASN
23	P	337	HIS
23	P	401	ASN
24	Q	145	HIS
24	Q	178	HIS
24	Q	186	HIS
24	Q	226	HIS
24	Q	361	HIS
24	Q	404	ASN
24	Q	425	GLN
25	R	397	ASN
25	R	406	GLN
25	R	415	GLN
26	S	32	GLN

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Mol	Chain	Res	Type
26	S	135	ASN
26	S	139	HIS
26	S	191	HIS
26	S	227	ASN
26	S	261	HIS
26	S	290	ASN
26	S	311	GLN
26	S	312	GLN
26	S	321	GLN
26	S	334	HIS
26	S	347	HIS
26	S	369	GLN
26	S	417	GLN
26	S	470	GLN
26	S	472	HIS
27	T	127	GLN
27	T	236	ASN
28	U	94	HIS
28	U	156	HIS
29	V	73	GLN
29	V	111	HIS
29	V	186	GLN
30	W	92	GLN
30	W	170	HIS
31	X	38	ASN
31	X	94	ASN
33	Z	214	HIS
33	Z	338	HIS
33	Z	361	HIS
33	Z	577	GLN
33	Z	899	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

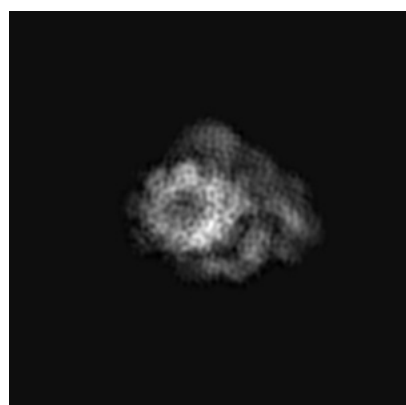
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9770. These allow visual inspection of the internal detail of the map and identification of artifacts.

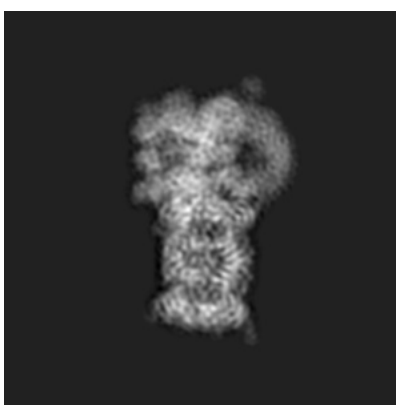
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

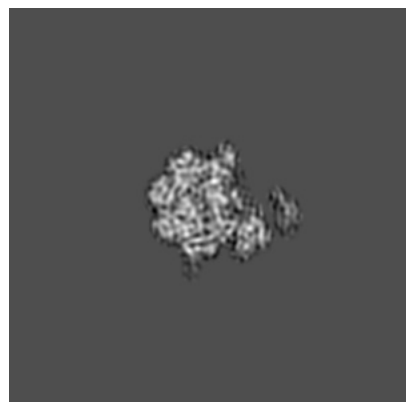


Z

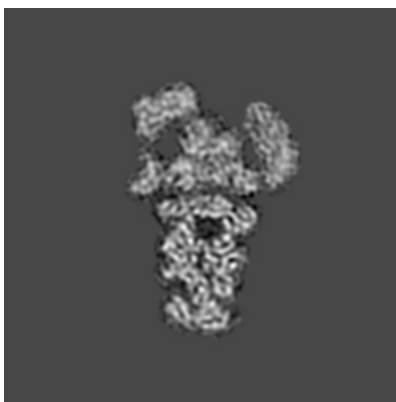
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180

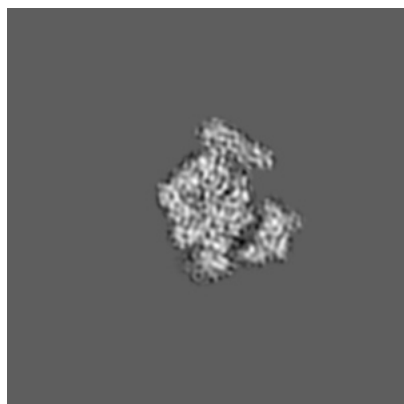


Z Index: 180

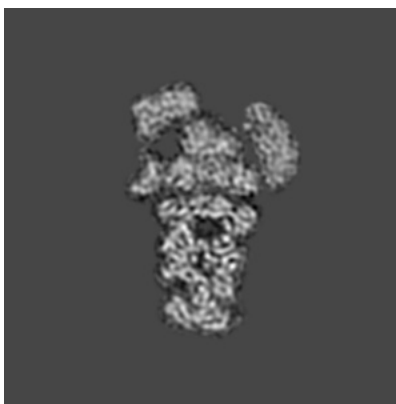
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

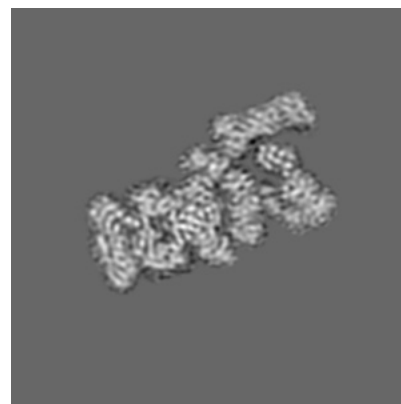
6.3.1 Primary map



X Index: 206



Y Index: 179

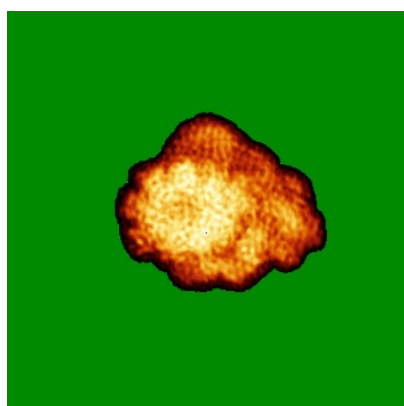


Z Index: 162

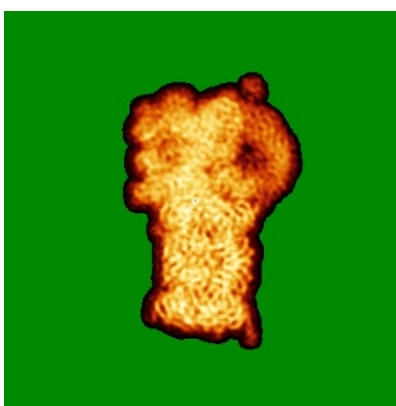
The images above show the largest variance slices of the map in three orthogonal directions.

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

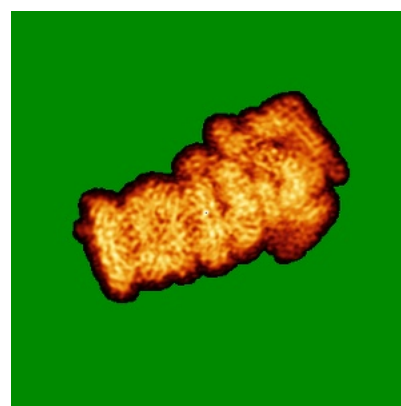
6.4.1 Primary map



X



Y

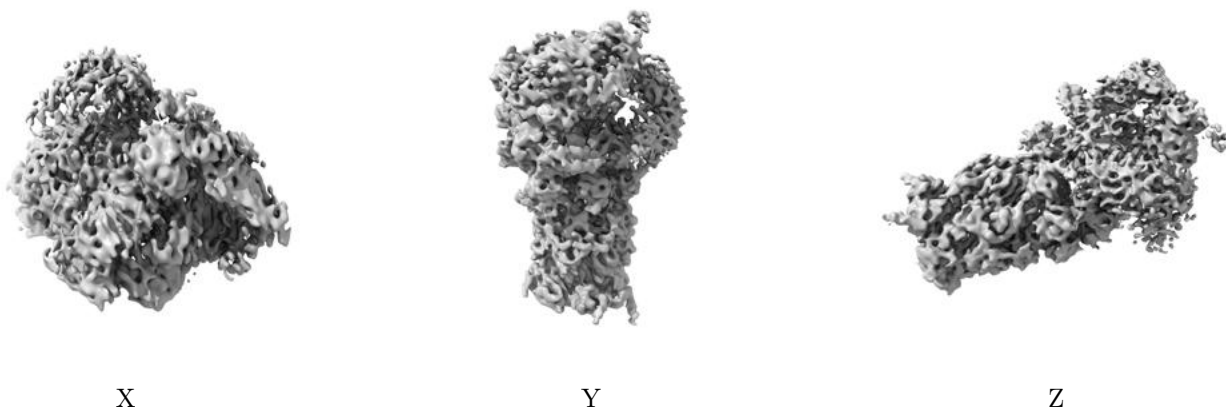


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.806. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

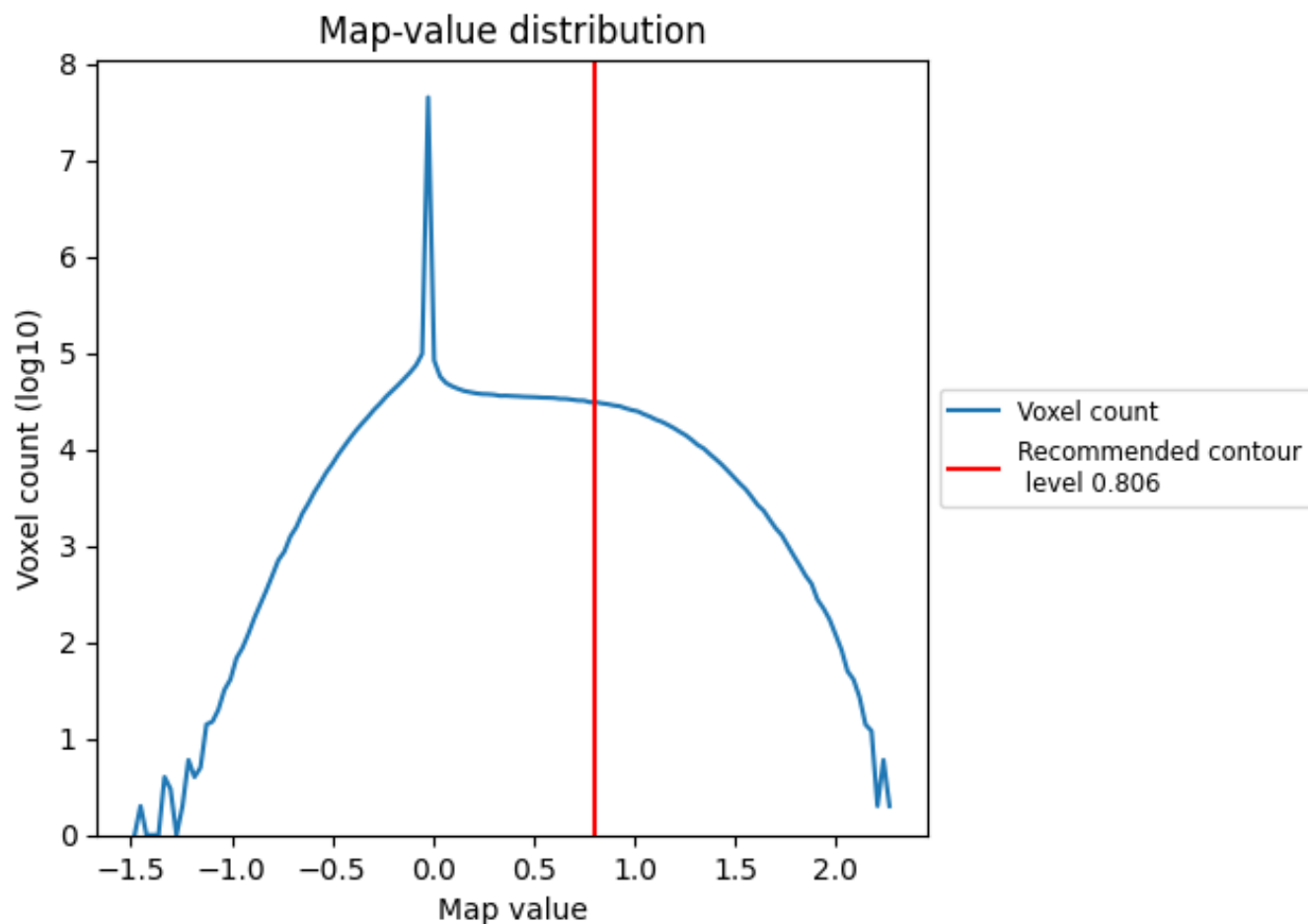
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

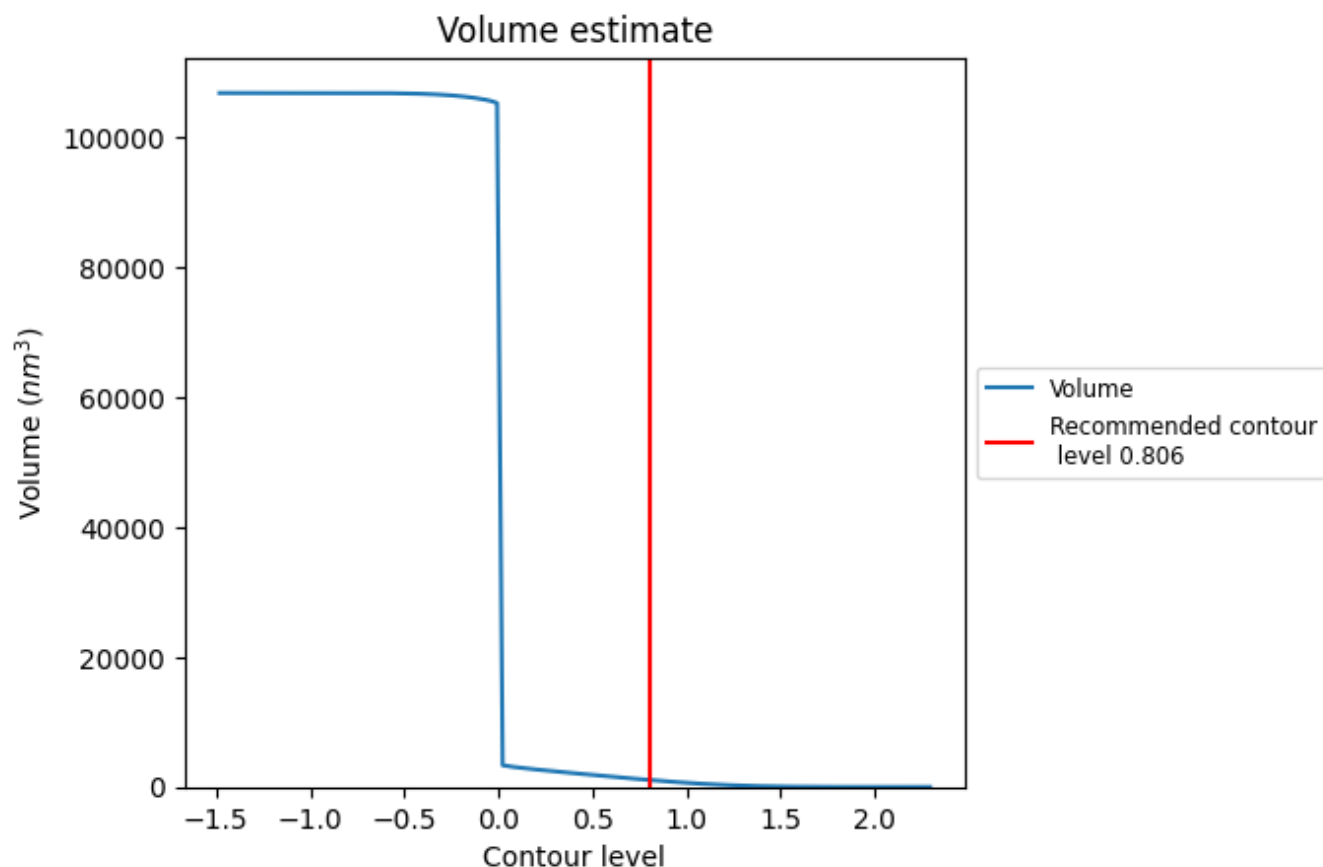
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

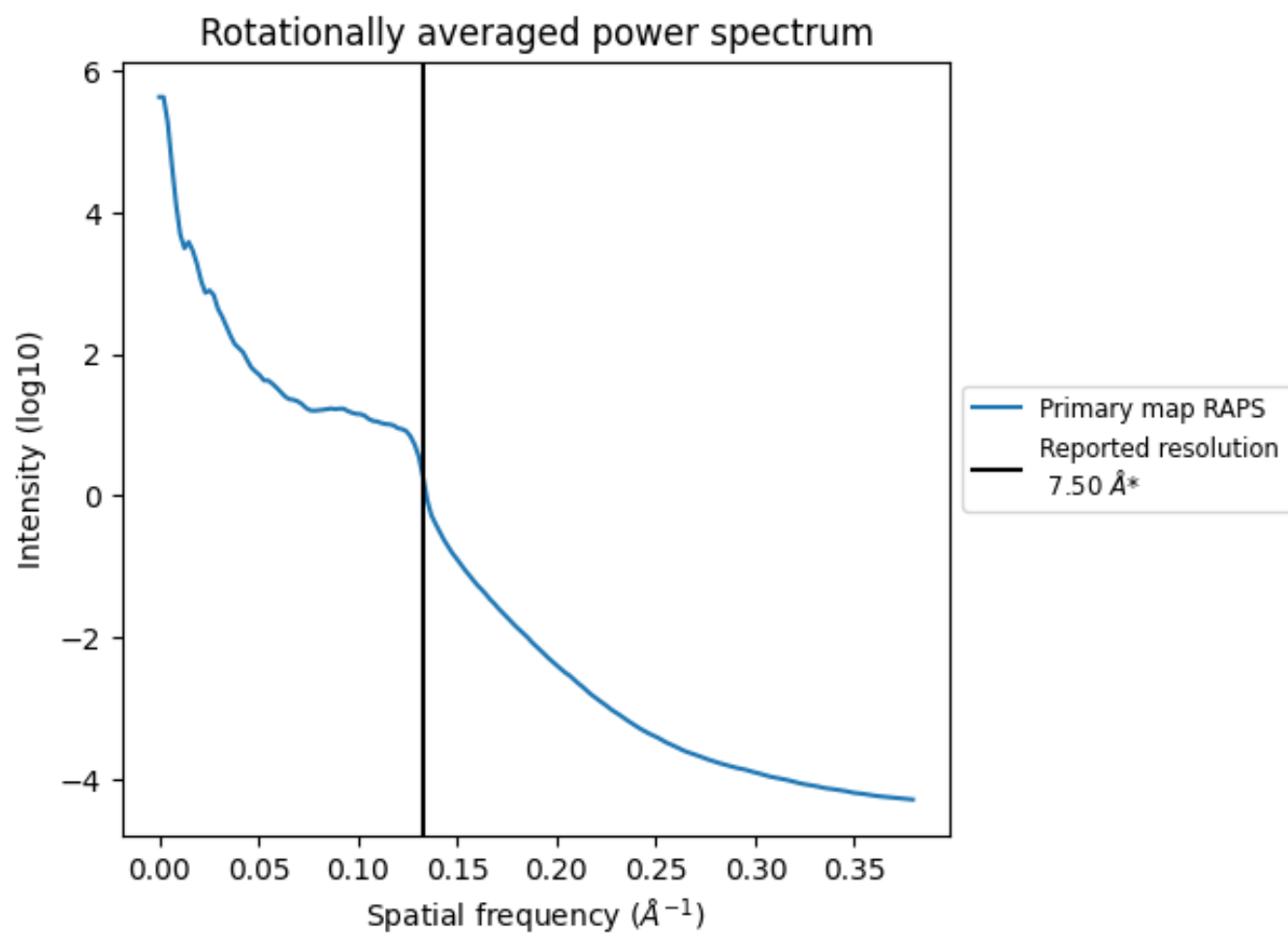
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1070 nm³; this corresponds to an approximate mass of 966 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

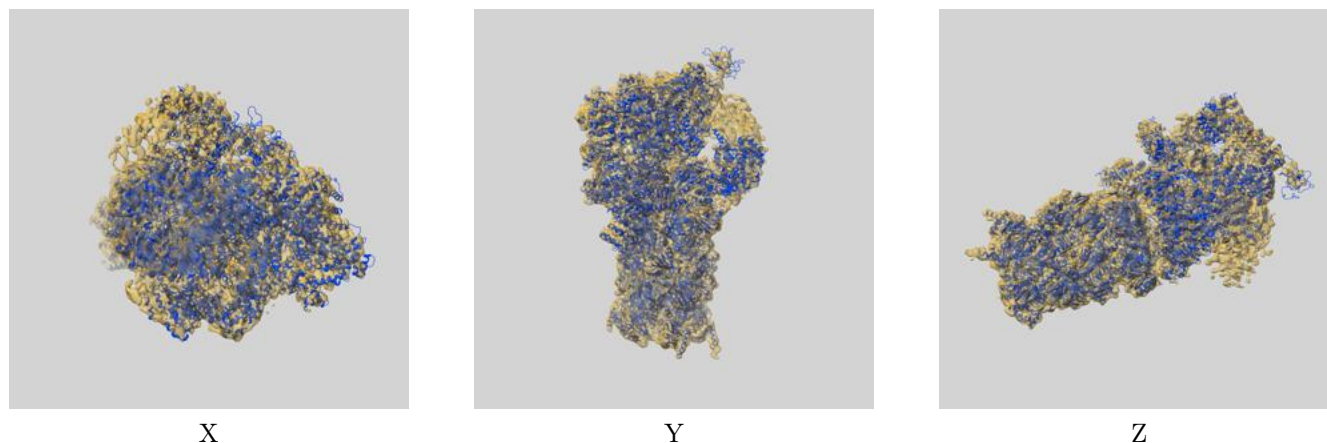
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9770 and PDB model 6J2N. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



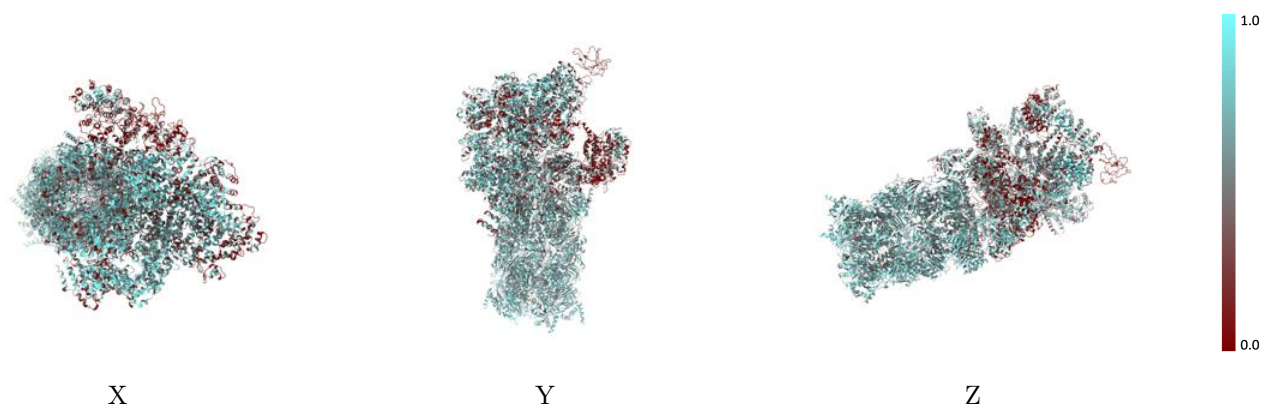
The images above show the 3D surface view of the map at the recommended contour level 0.806 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



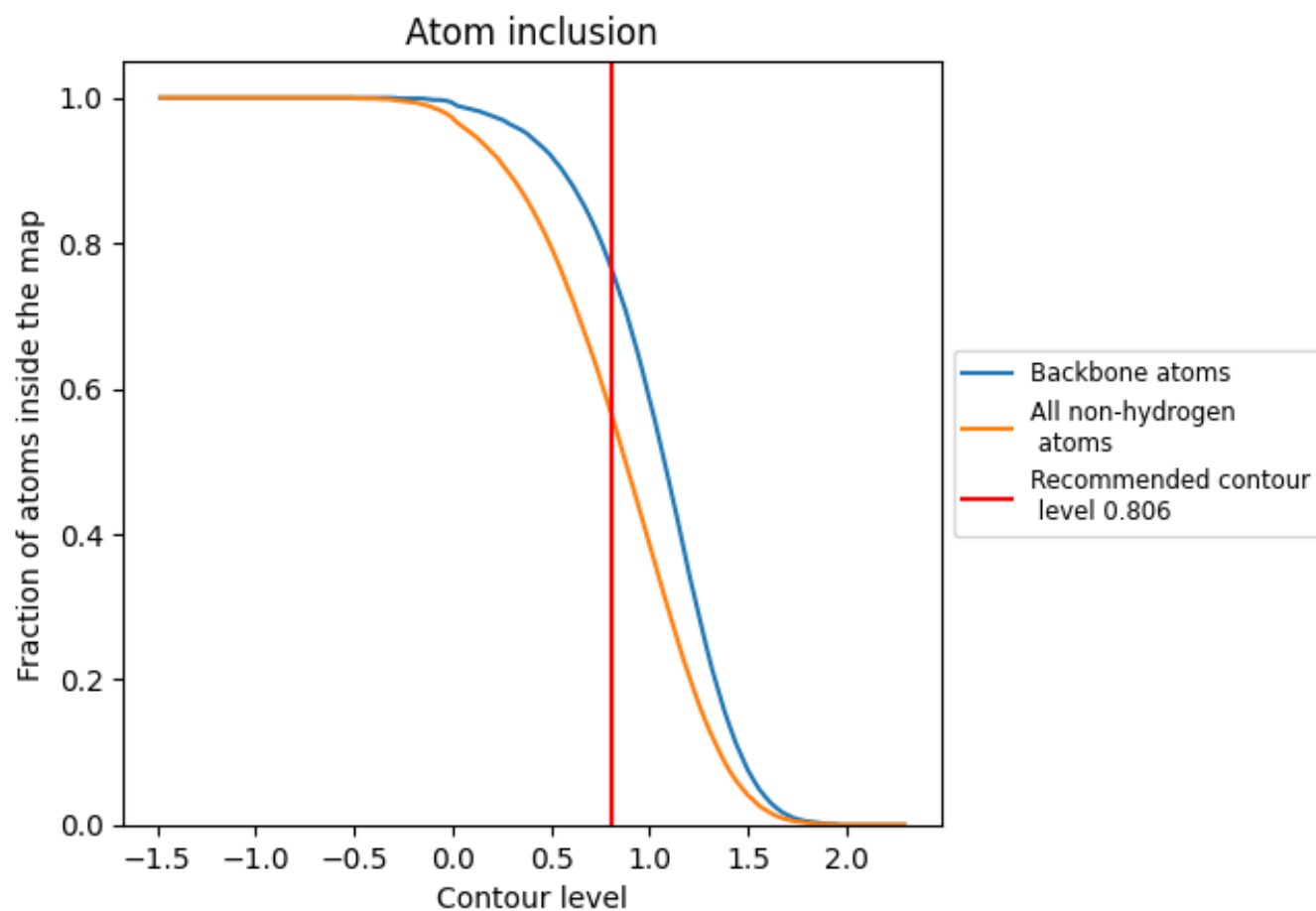
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.806).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 57% 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 (0.806) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5660	 0.1070
1	 0.6310	 0.1370
2	 0.6500	 0.1370
3	 0.6260	 0.1230
4	 0.6370	 0.1330
5	 0.6660	 0.1350
6	 0.6500	 0.1340
7	 0.6500	 0.1420
A	 0.6050	 0.1390
B	 0.5830	 0.1250
C	 0.6260	 0.1360
D	 0.6150	 0.1230
E	 0.6390	 0.1420
F	 0.6270	 0.1300
G	 0.6380	 0.1300
H	 0.5170	 0.0750
I	 0.4530	 0.0800
J	 0.4380	 0.0910
K	 0.5240	 0.1080
L	 0.5060	 0.0800
M	 0.5220	 0.0770
N	 0.6110	 0.0870
O	 0.5750	 0.0980
P	 0.6190	 0.1120
Q	 0.5780	 0.1130
R	 0.5880	 0.1040
S	 0.4610	 0.0870
T	 0.3120	 0.0680
U	 0.6080	 0.1140
V	 0.5440	 0.0880
W	 0.5520	 0.0730
X	 0.0860	 -0.0100
Y	 0.5430	 0.0780
Z	 0.2480	 0.0380
a	 0.6450	 0.1360



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Chain	Atom inclusion	Q-score
b	 0.6510	 0.1350
c	 0.6800	 0.1310
d	 0.6780	 0.1420
e	 0.6560	 0.1390
f	 0.6670	 0.1350
g	 0.6440	 0.1400
h	 0.6480	 0.1270
i	 0.6580	 0.1380
j	 0.6580	 0.1200
k	 0.6780	 0.1440
l	 0.7030	 0.1430
m	 0.6400	 0.1230
n	 0.6920	 0.1320