



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:51 PM UTC

PDB ID : 6J2C / pdb_00006j2c
EMDB ID : EMD-9769
Title : Yeast proteasome in translocation competent state (C3-a)
Authors : Cong, Y.
Deposited on : 2019-01-01
Resolution : 7.00 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

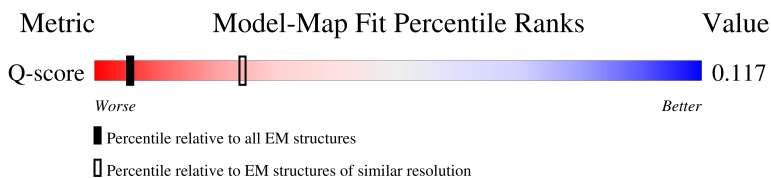
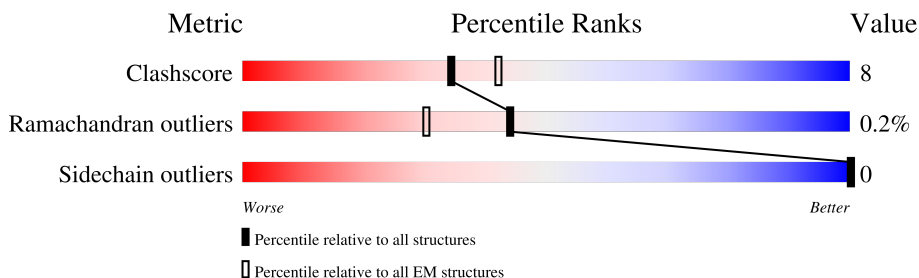
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 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	483 (6.50 - 7.50)

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	
1	b	215	
2	2	261	
2	i	261	

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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 106149 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	243	Total	C	N	O	S	0	0
			1921	1221	322	370	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	241	Total	C	N	O	S	0	0
			1890	1181	331	374	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	233	Total	C	N	O	S	0	0
			1795	1129	312	350	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	244	Total	C	N	O	S	0	0
			1896	1205	330	357	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		

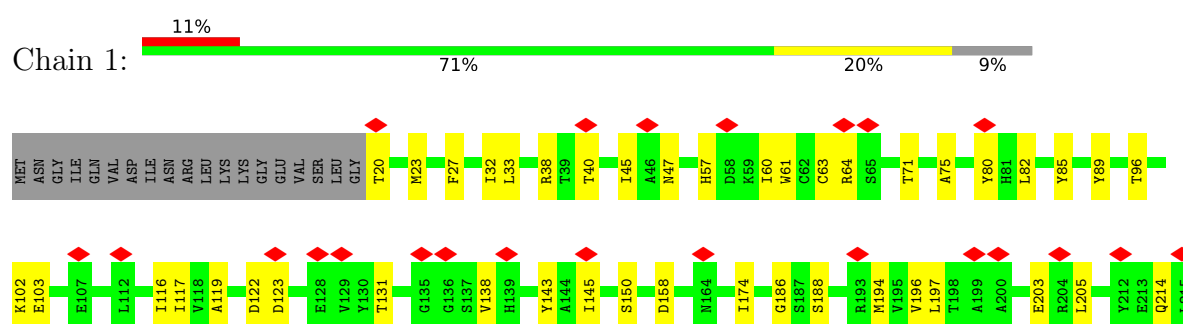
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

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

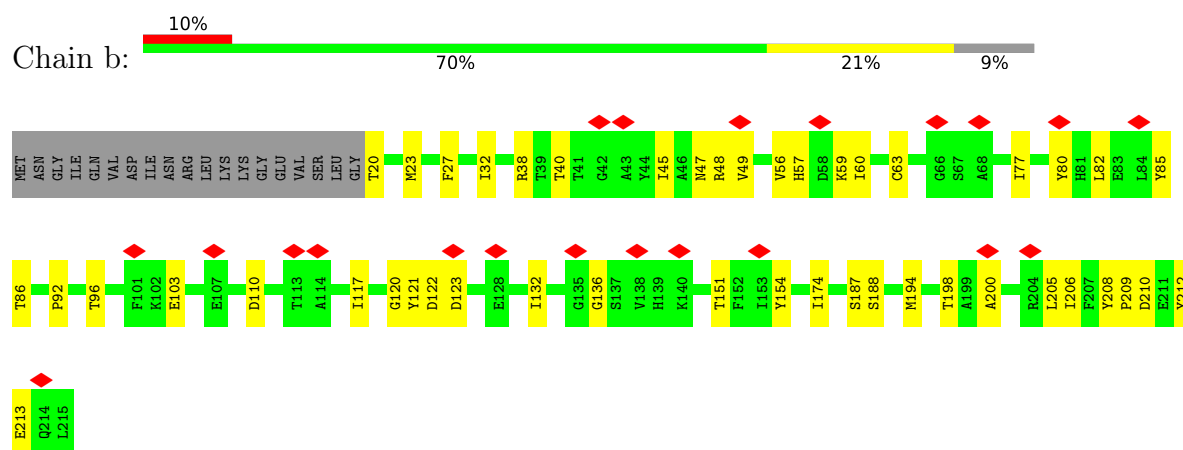
3 Residue-property plots

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.

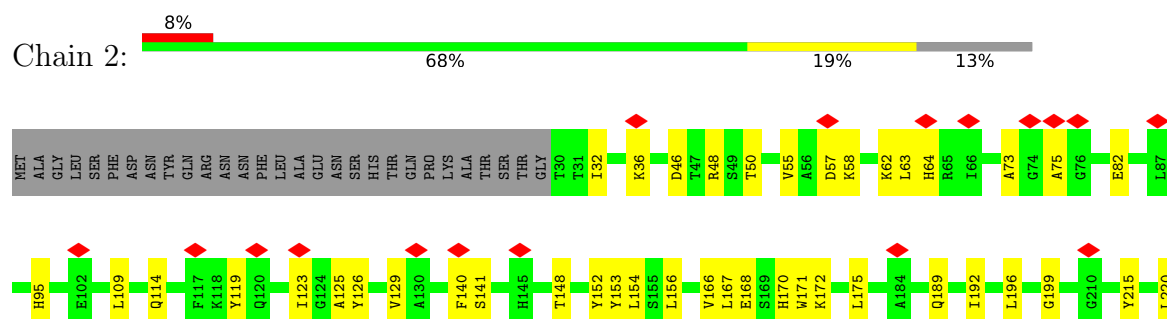
- Molecule 1: Proteasome subunit beta type-1

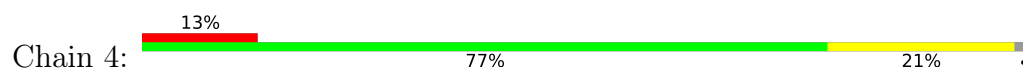


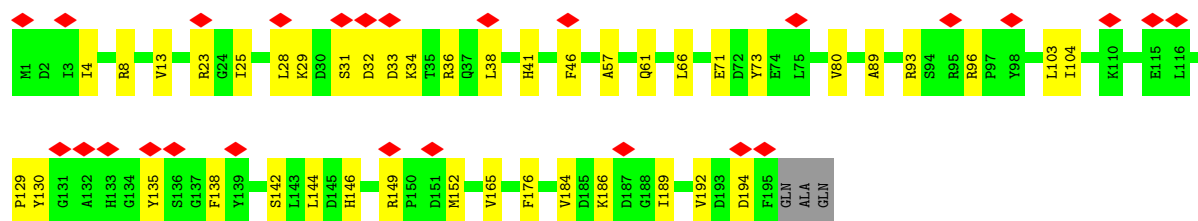
- Molecule 1: Proteasome subunit beta type-1



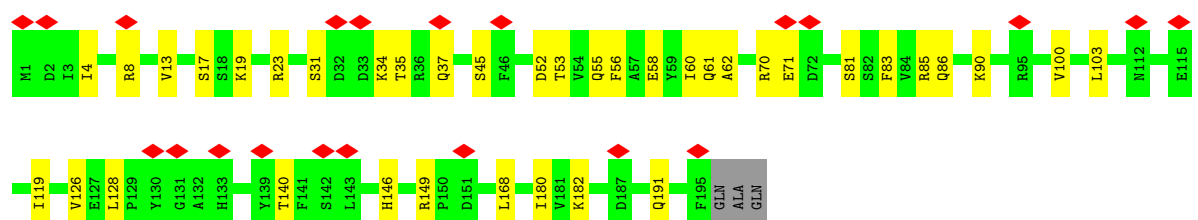
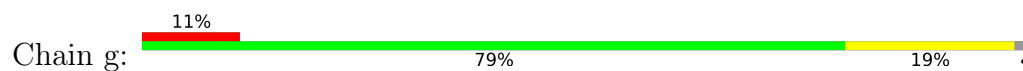
- Molecule 2: Proteasome subunit beta type-2



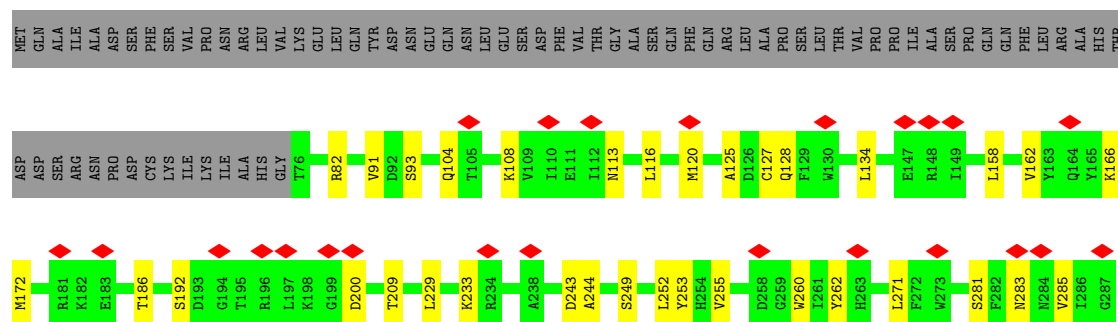




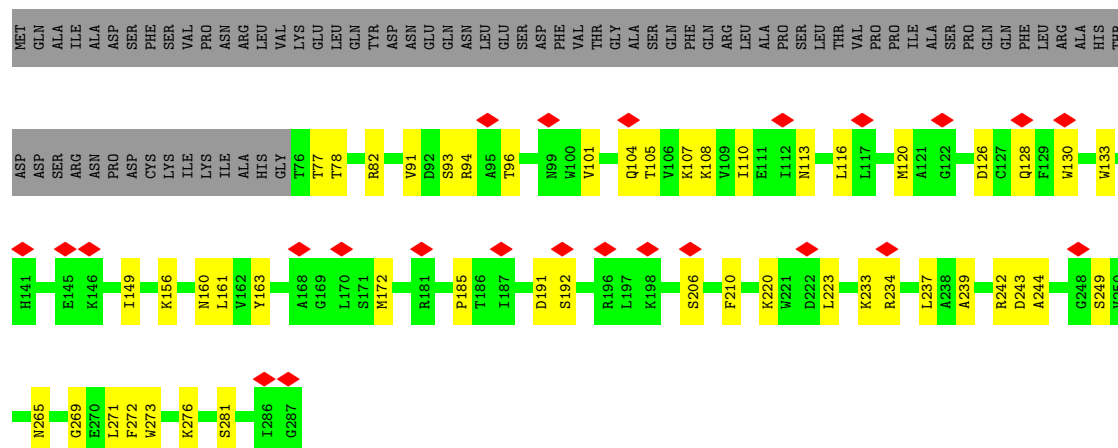
• Molecule 4: Proteasome subunit beta type-4



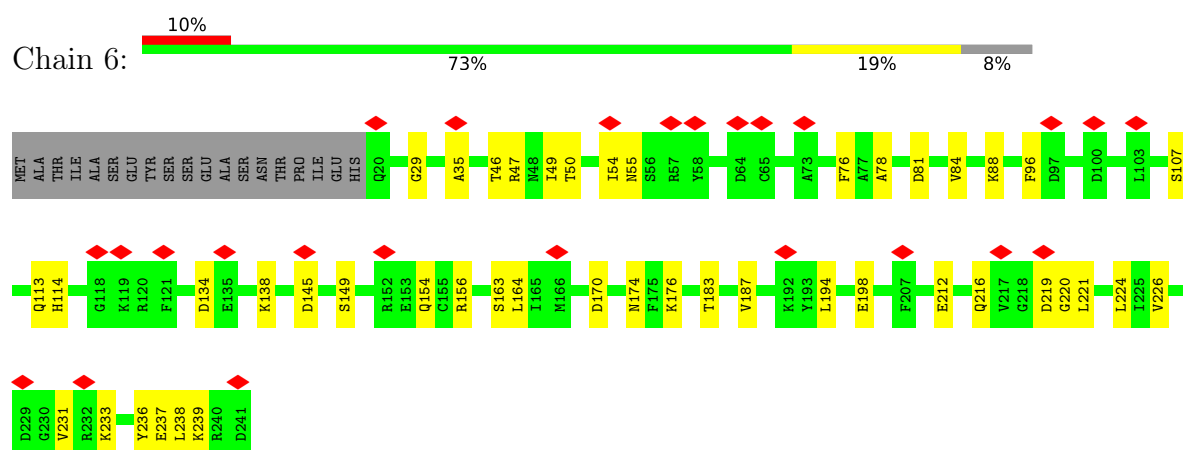
• Molecule 5: Proteasome subunit beta type-5



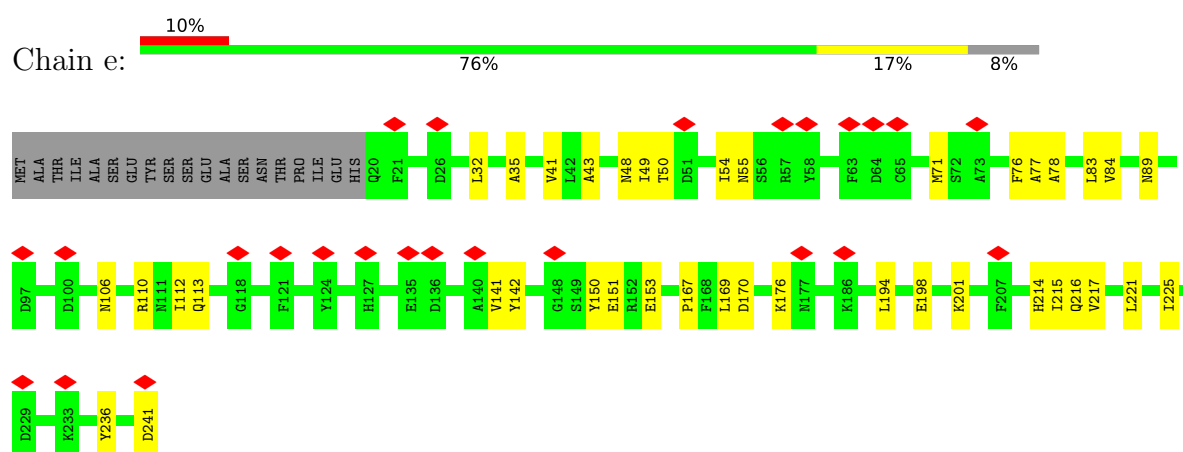
• Molecule 5: Proteasome subunit beta type-5



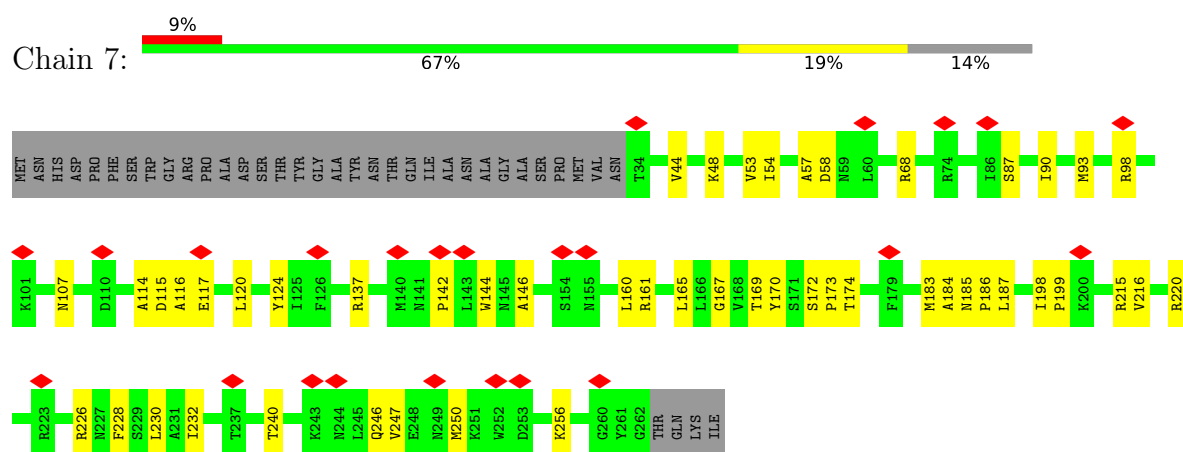
• Molecule 6: Proteasome subunit beta type-6



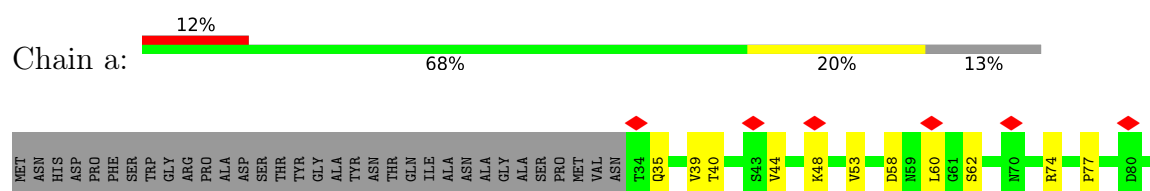
• Molecule 6: Proteasome subunit beta type-6

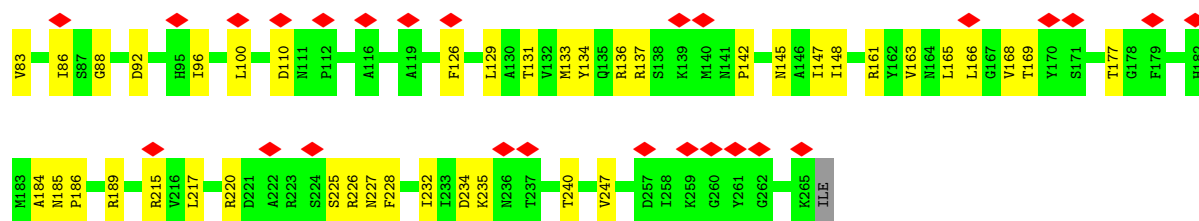


• Molecule 7: Proteasome subunit beta type-7



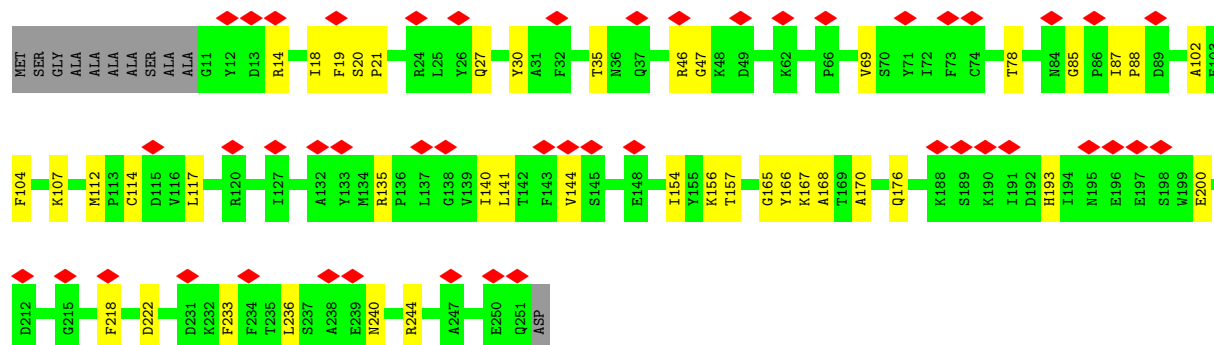
• Molecule 7: Proteasome subunit beta type-7





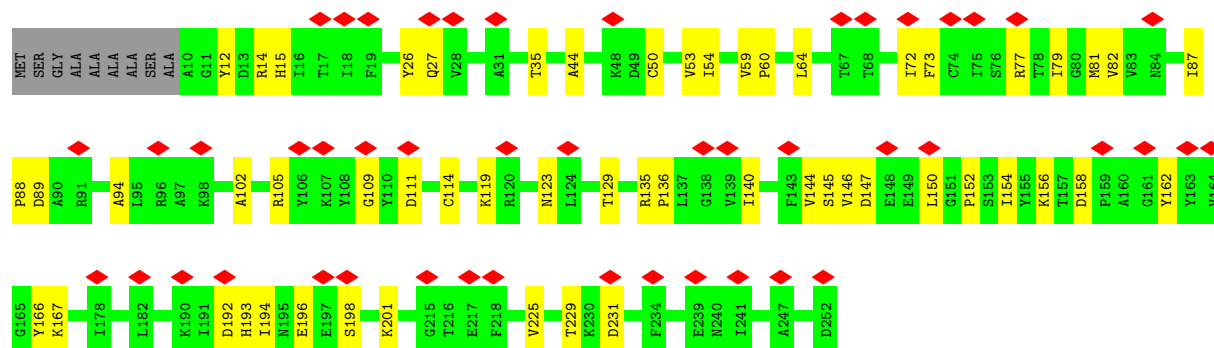
• Molecule 8: Proteasome subunit alpha type-1

Chain A: 19% 79% 17%



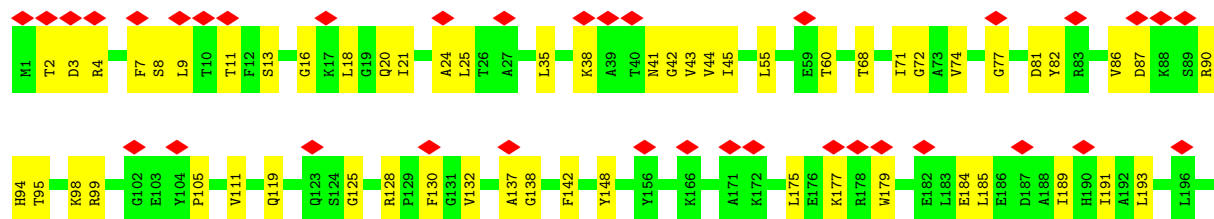
• Molecule 8: Proteasome subunit alpha type-1

Chain c: 19% 75% 22%



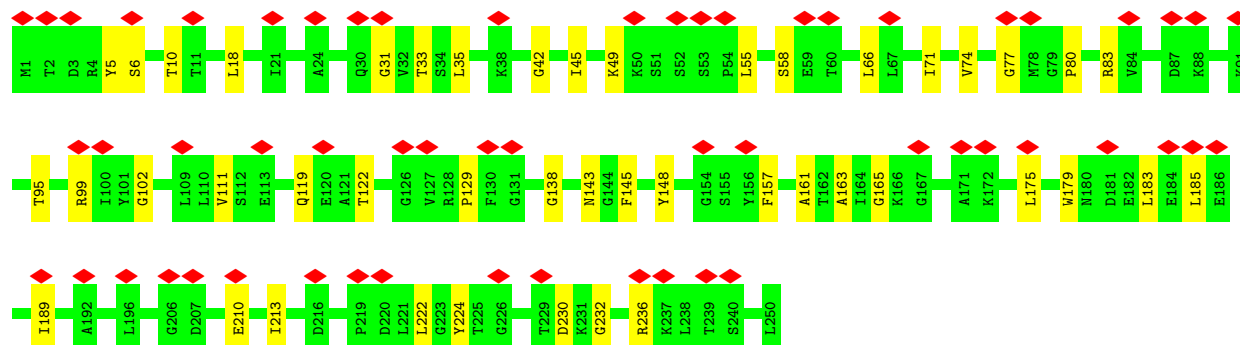
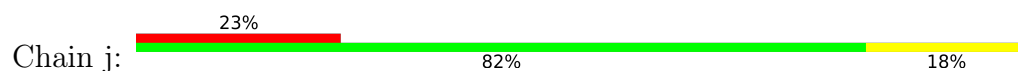
• Molecule 9: Proteasome subunit alpha type-2

Chain B: 19% 73% 27%

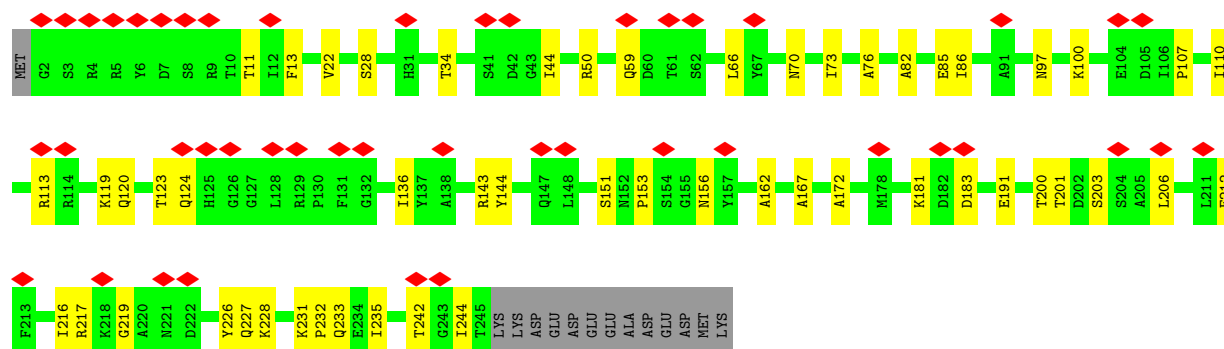
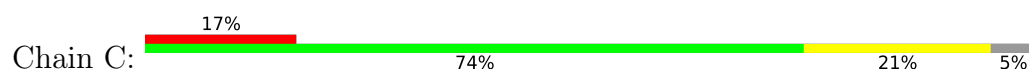




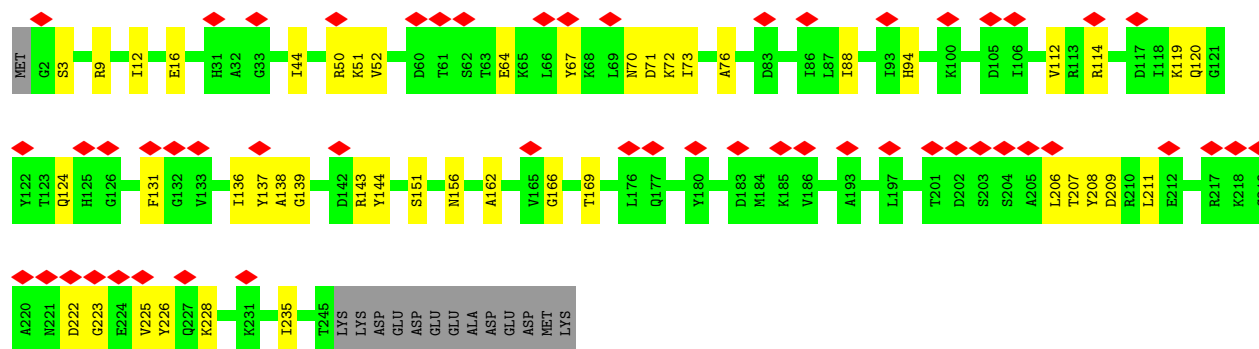
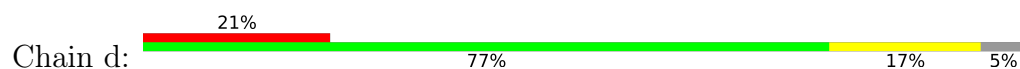
• Molecule 9: Proteasome subunit alpha type-2



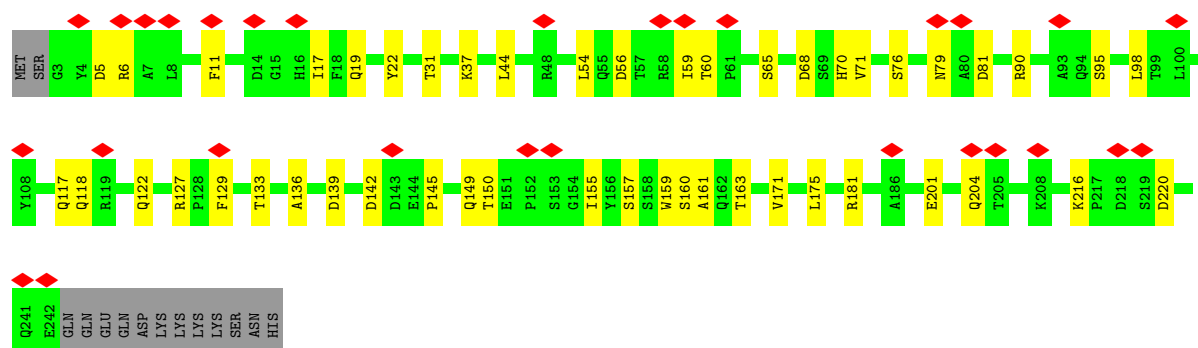
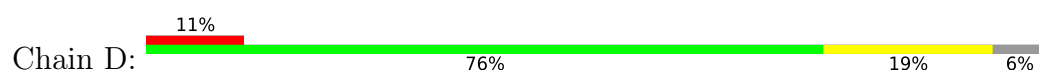
• Molecule 10: Proteasome subunit alpha type-3



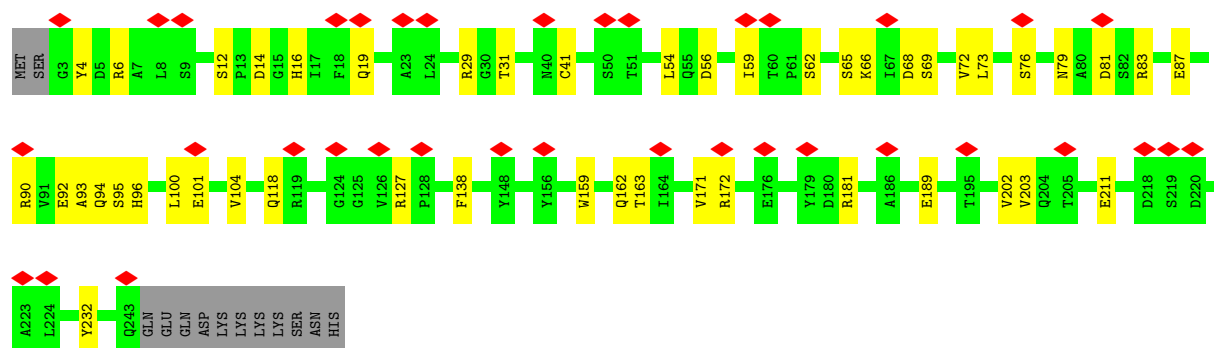
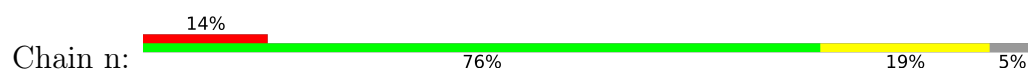
• Molecule 10: Proteasome subunit alpha type-3



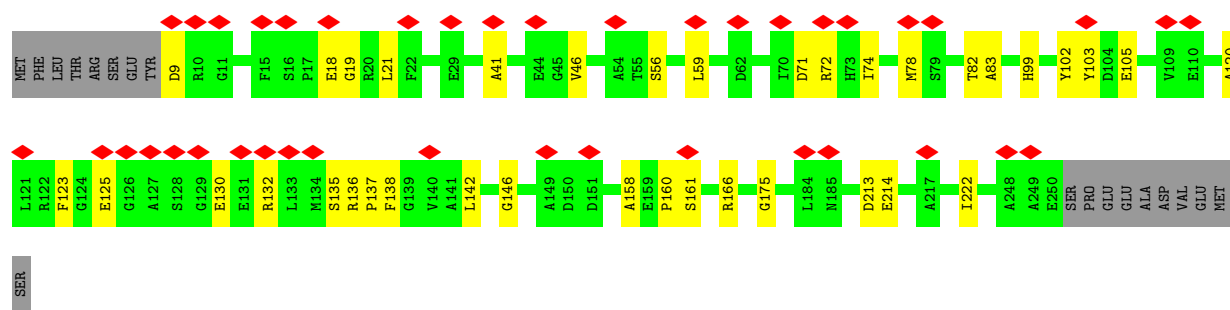
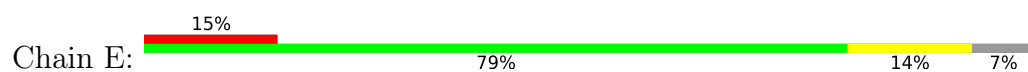
• Molecule 11: Proteasome subunit alpha type-4



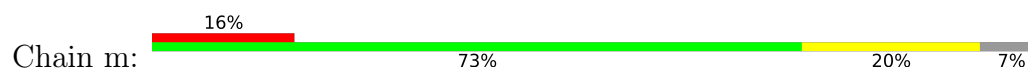
• Molecule 11: Proteasome subunit alpha type-4

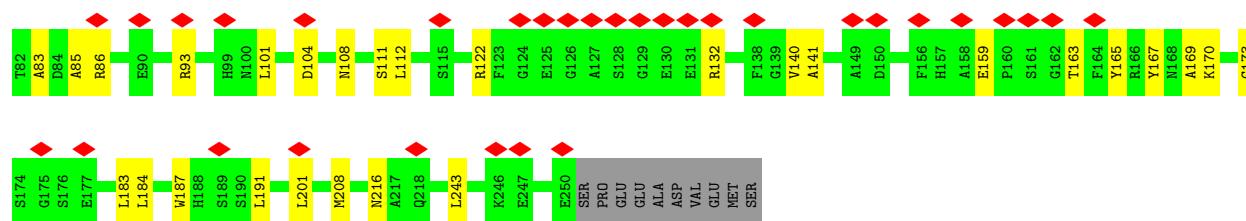


• Molecule 12: Proteasome subunit alpha type-5

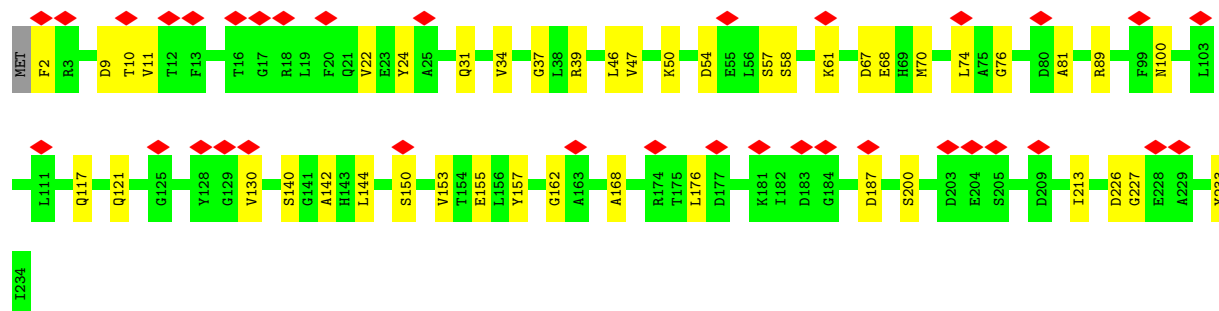
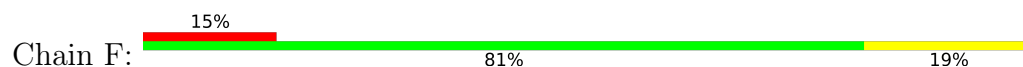


• Molecule 12: Proteasome subunit alpha type-5

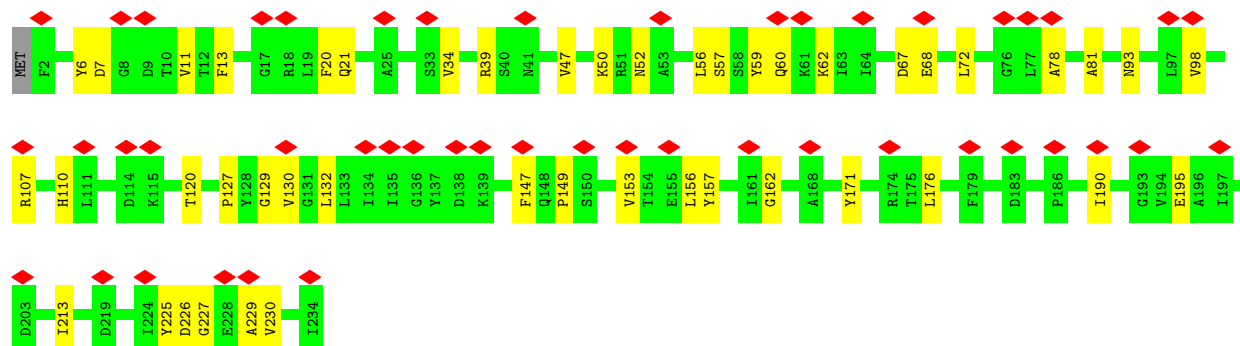
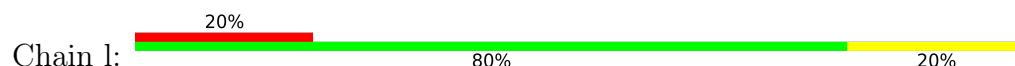




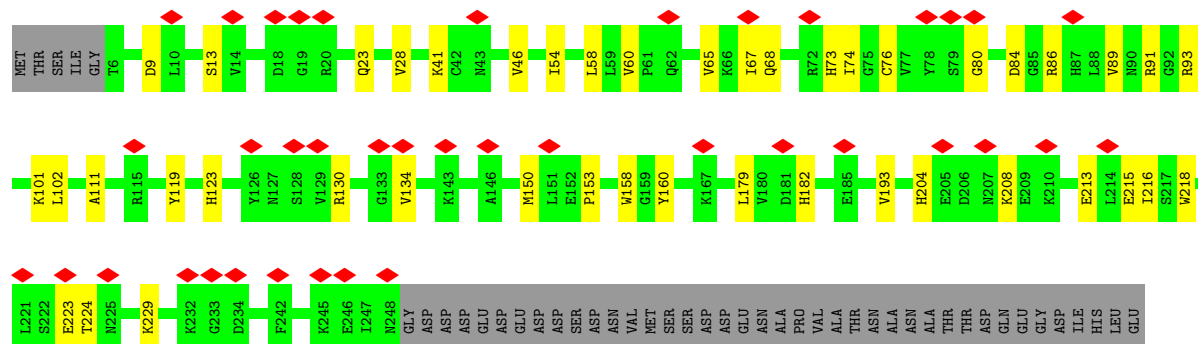
• Molecule 13: Proteasome subunit alpha type-6



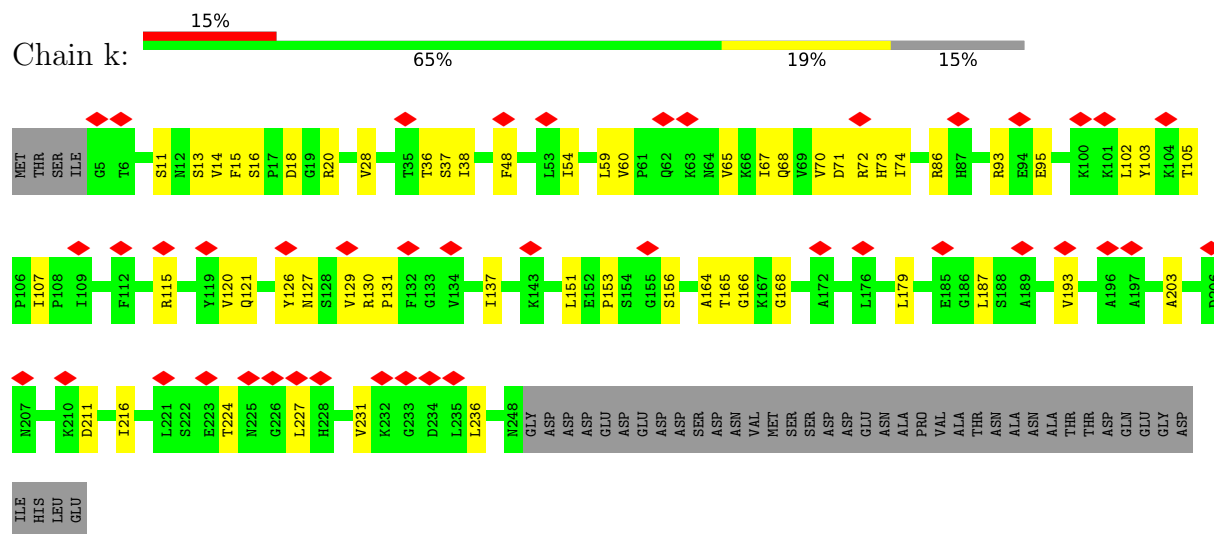
• Molecule 13: Proteasome subunit alpha type-6



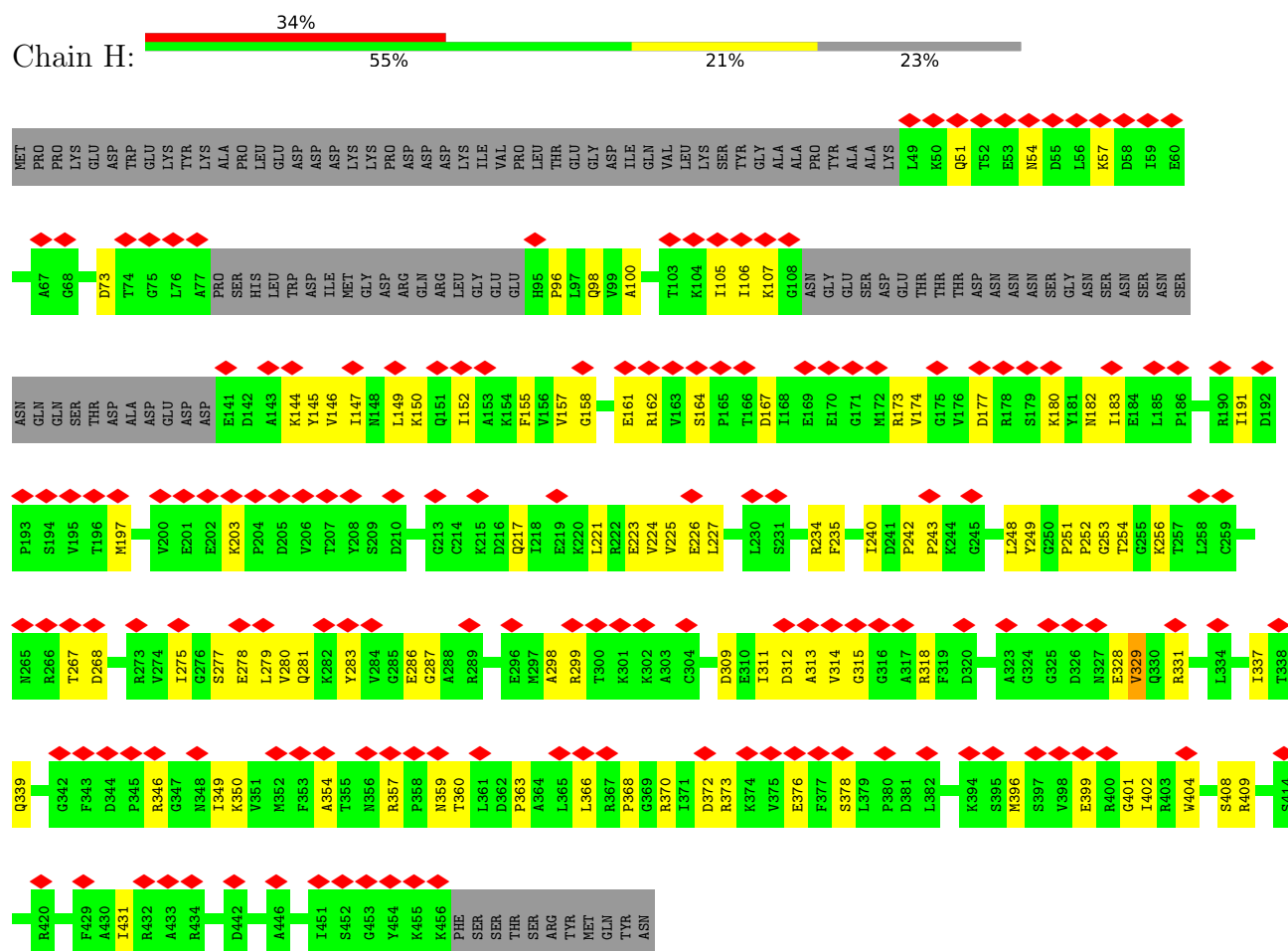
• Molecule 14: Probable proteasome subunit alpha type-7



- Molecule 14: Probable proteasome subunit alpha type-7

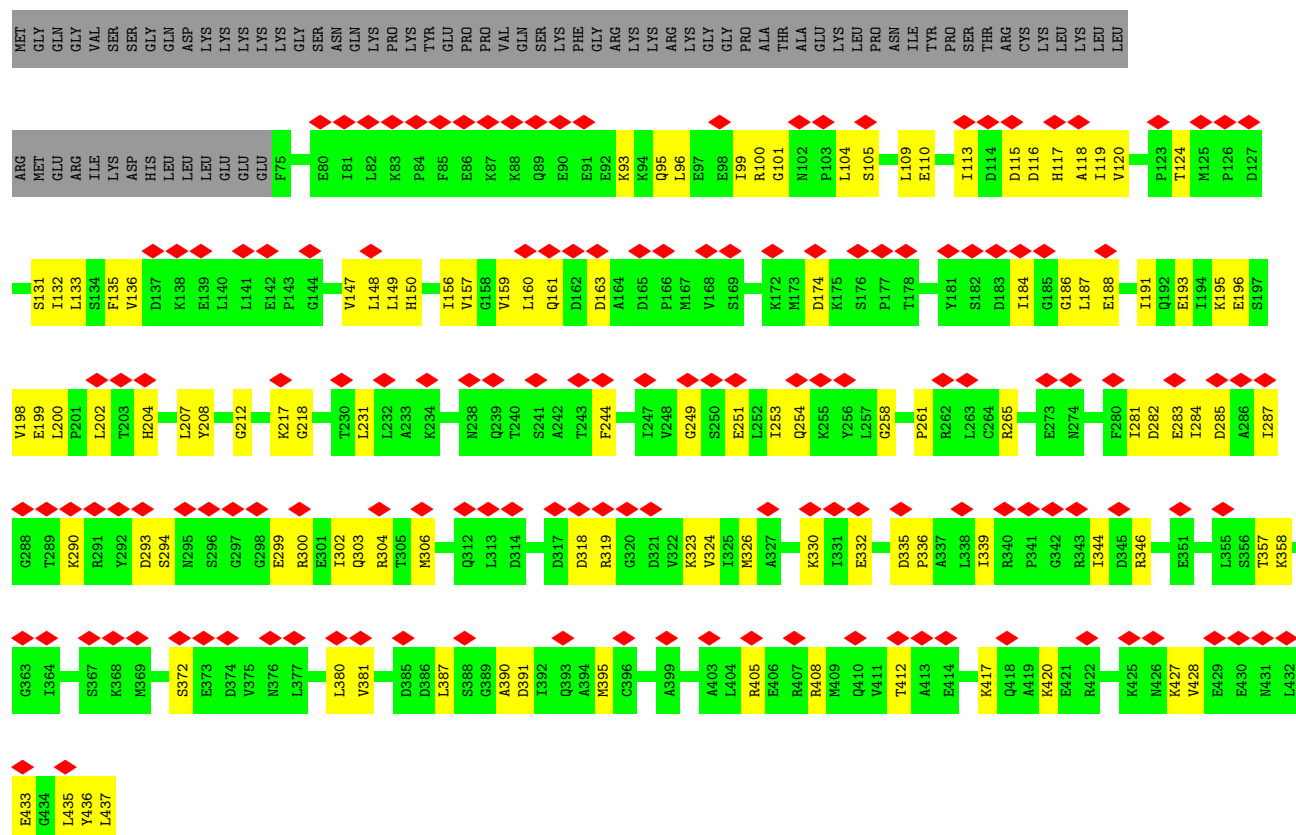


- Molecule 15: 26S protease regulatory subunit 7 homolog

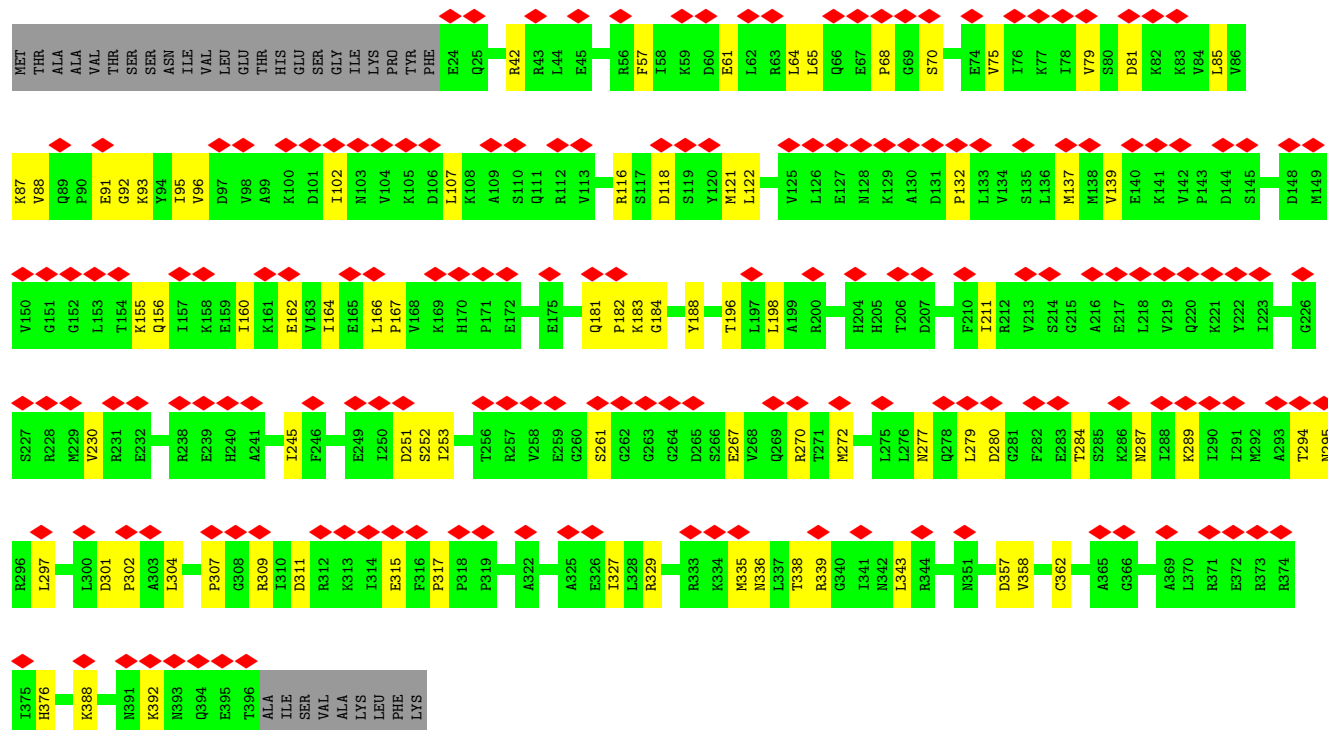
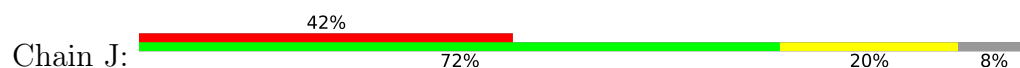


- Molecule 16: 26S protease regulatory subunit 4 homolog



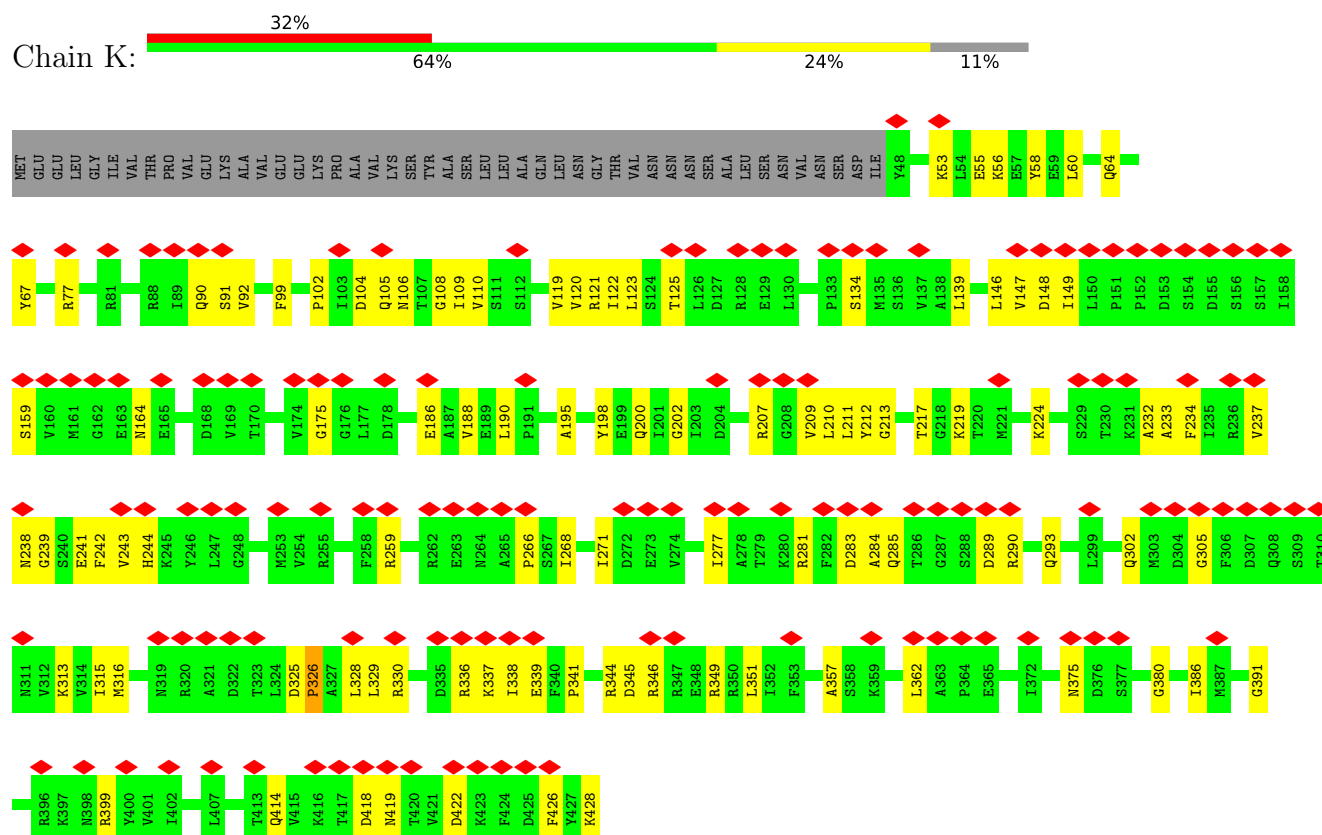


- Molecule 17: 26S protease regulatory subunit 8 homolog



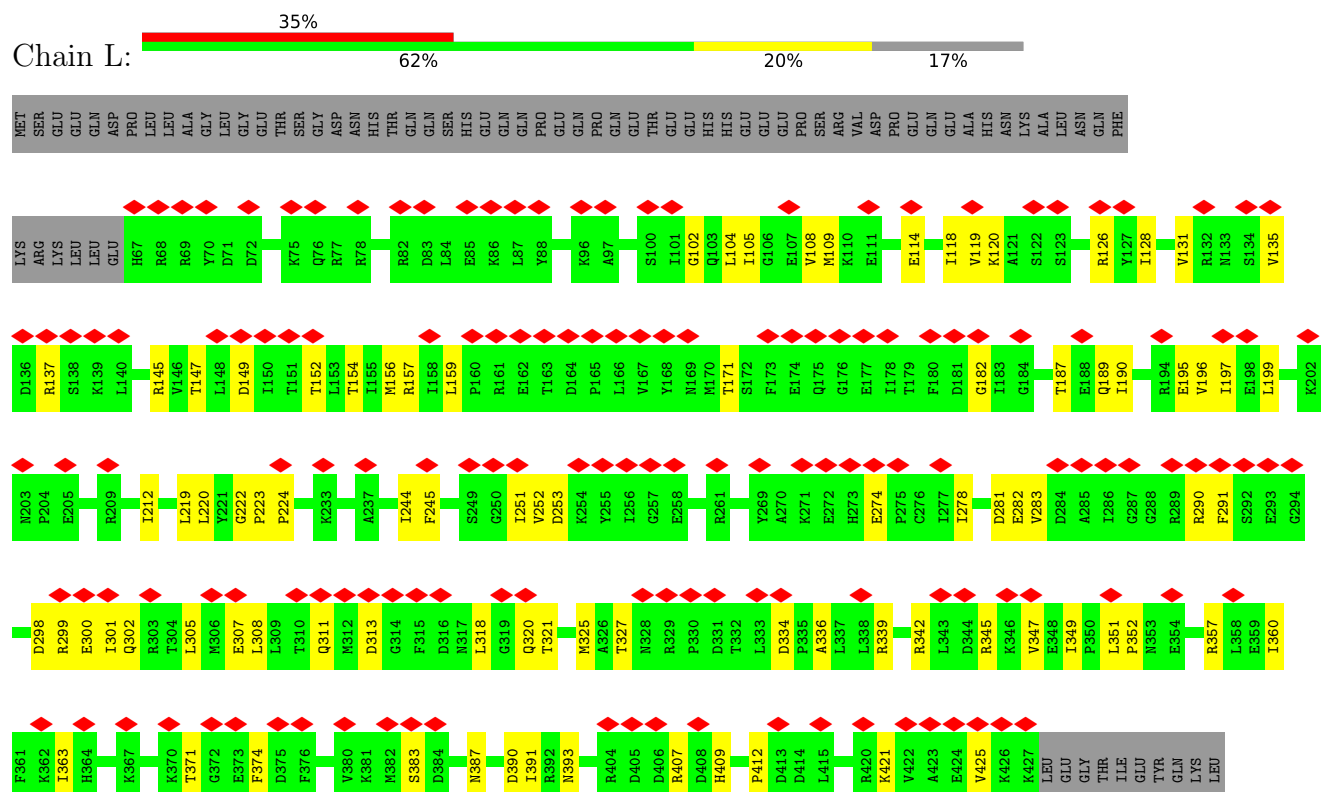
• Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K:

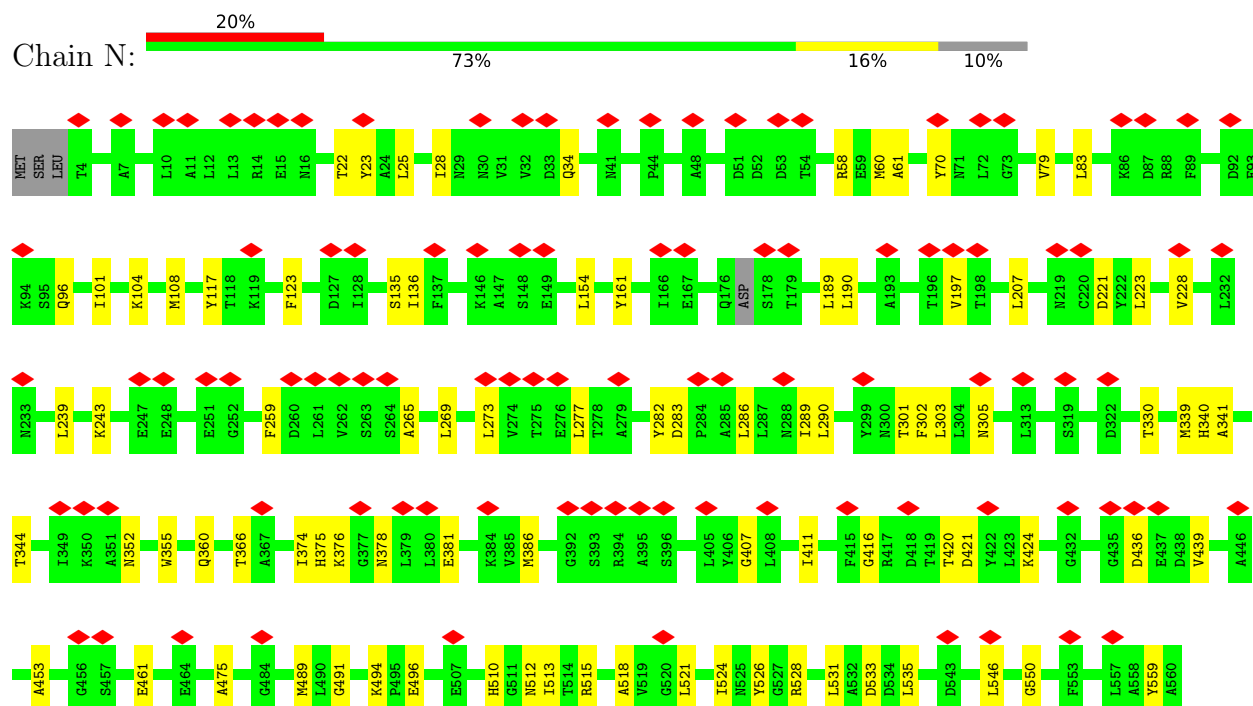


• Molecule 19: 26S protease subunit RPT4

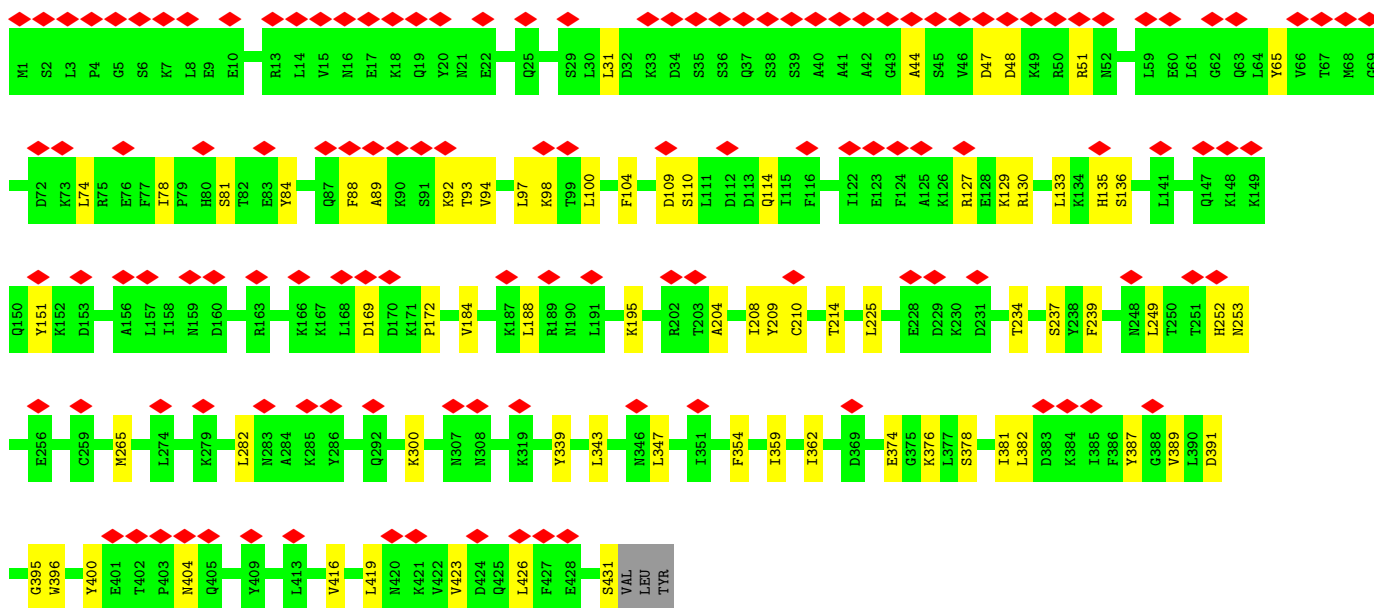
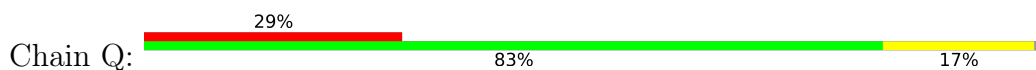
Chain L:



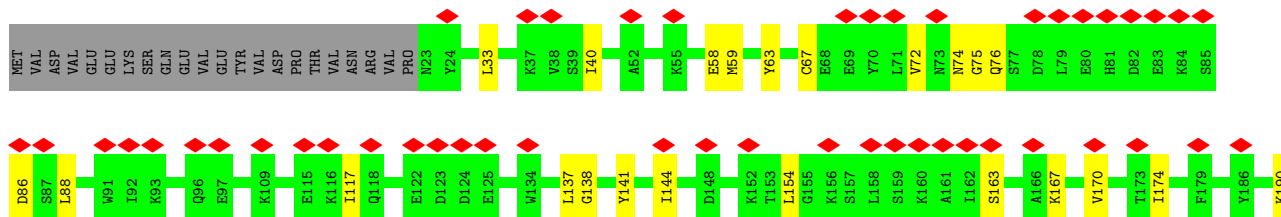
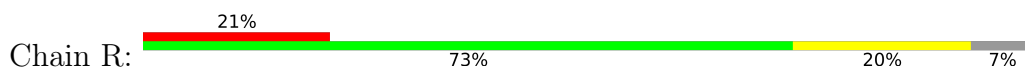
Chain M: 36% 63% 21% 15%

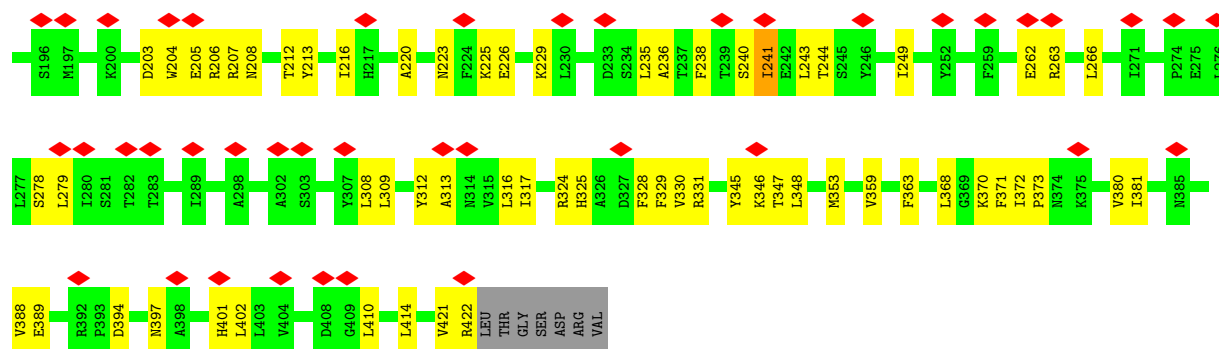


- Molecule 24: 26S proteasome regulatory subunit RPN6



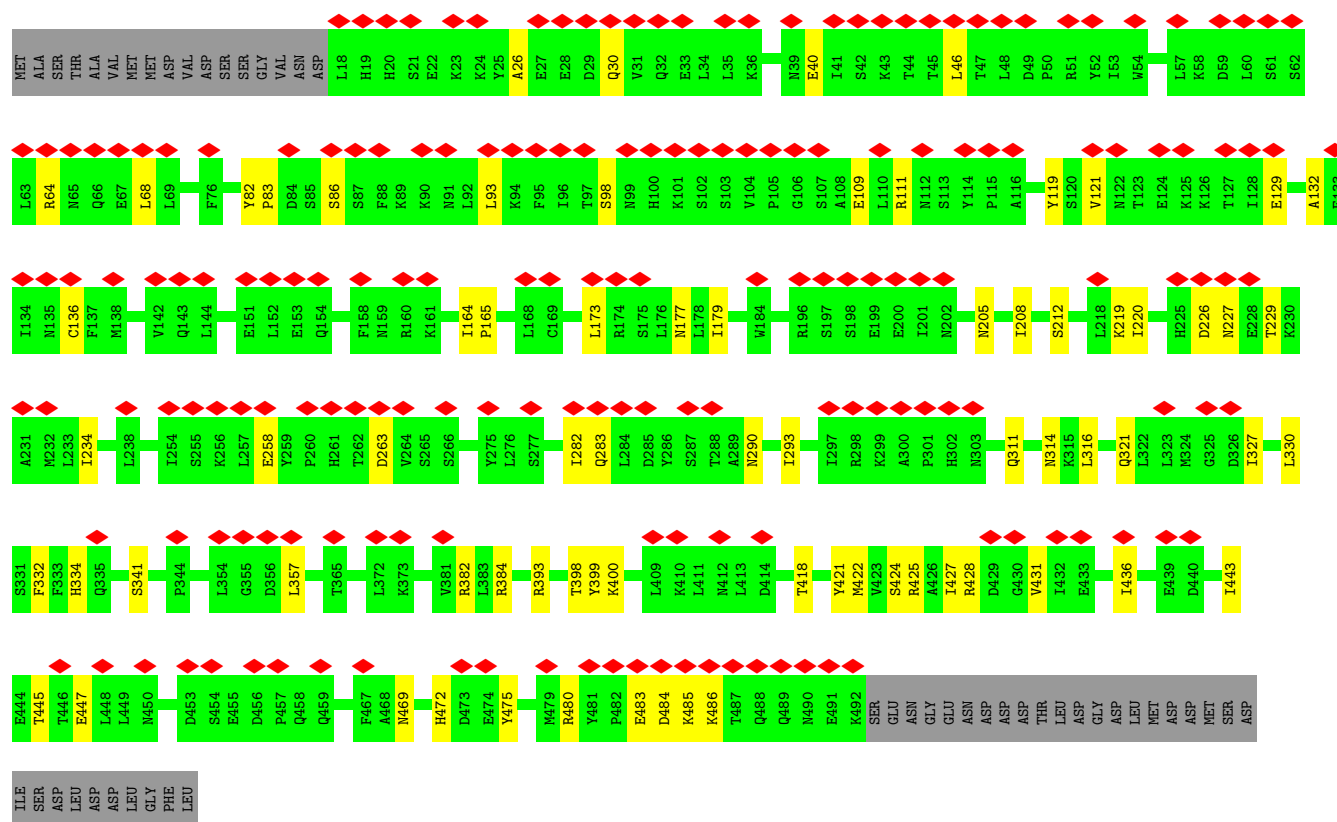
- Molecule 25: 26S proteasome regulatory subunit RPN7





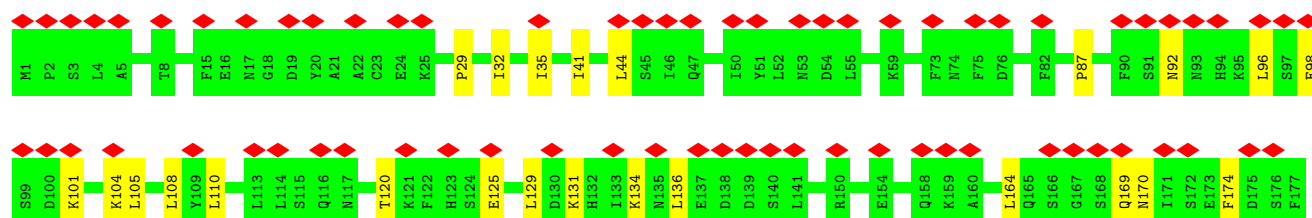
• Molecule 26: 26S proteasome regulatory subunit RPN3

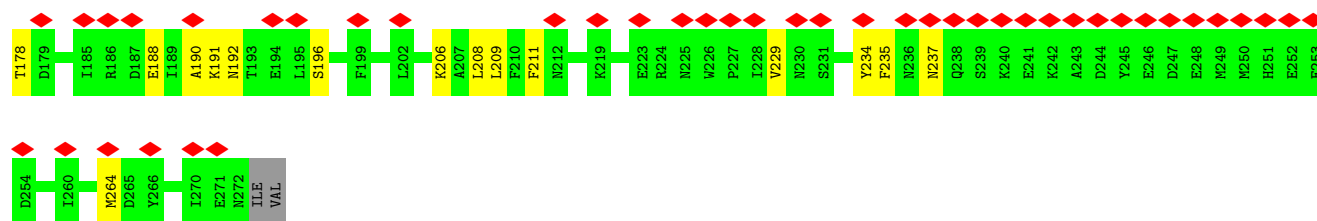
Chain S: 35% 77% 14% 9%



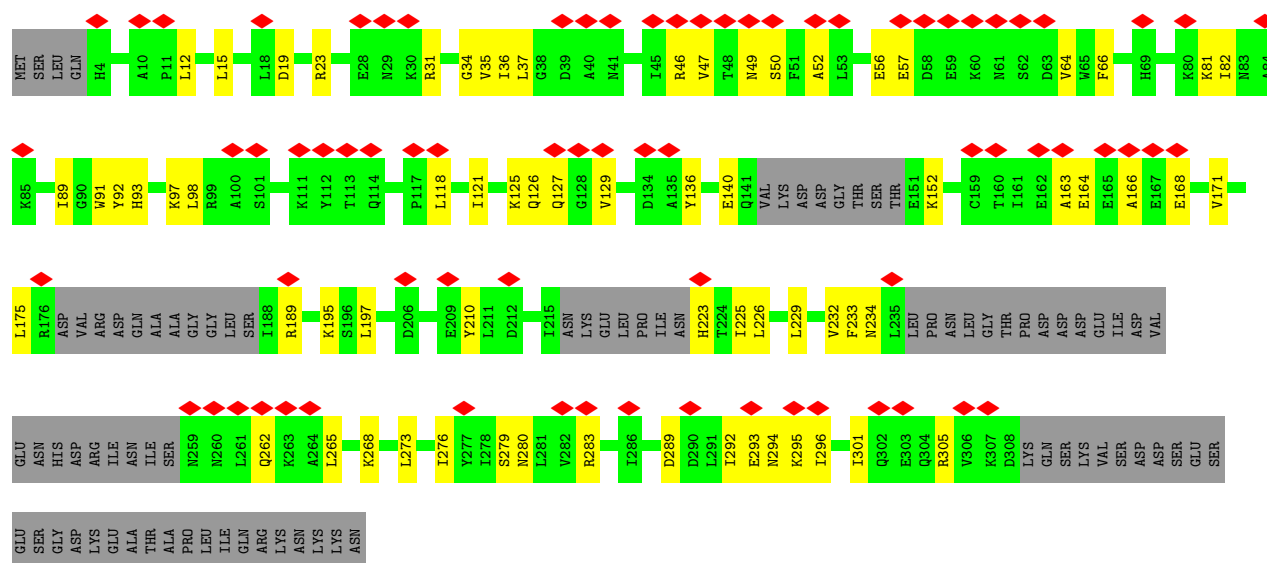
• Molecule 27: 26S proteasome regulatory subunit RPN12

Chain T: 41% 85% 14%

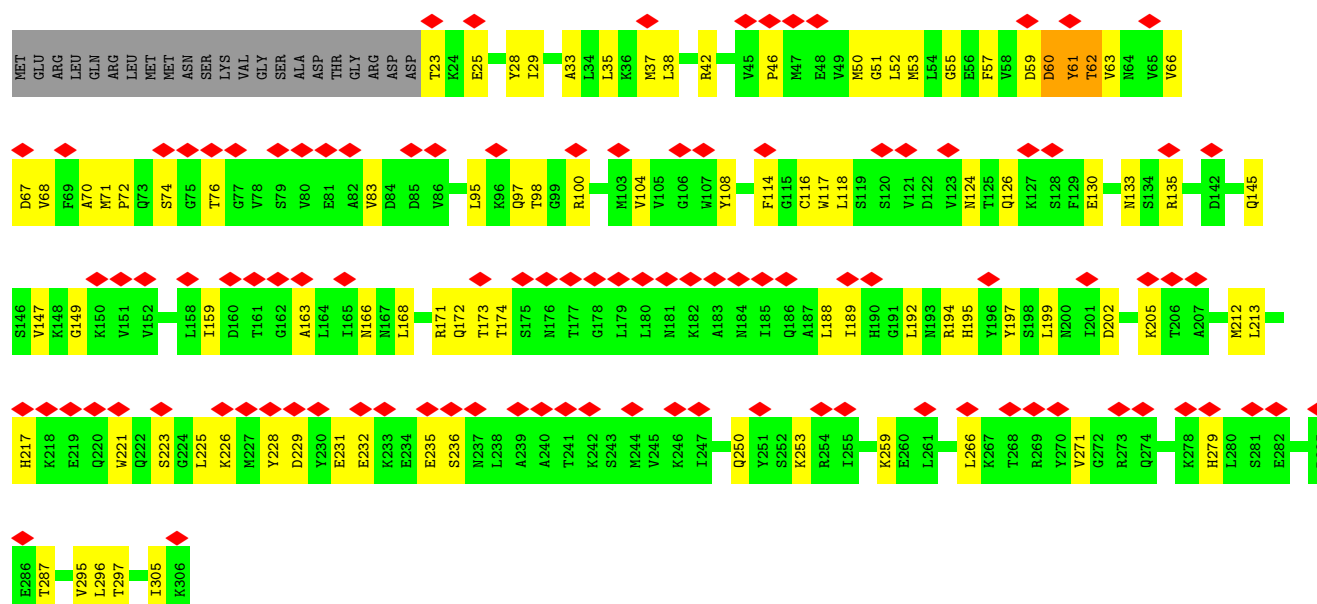




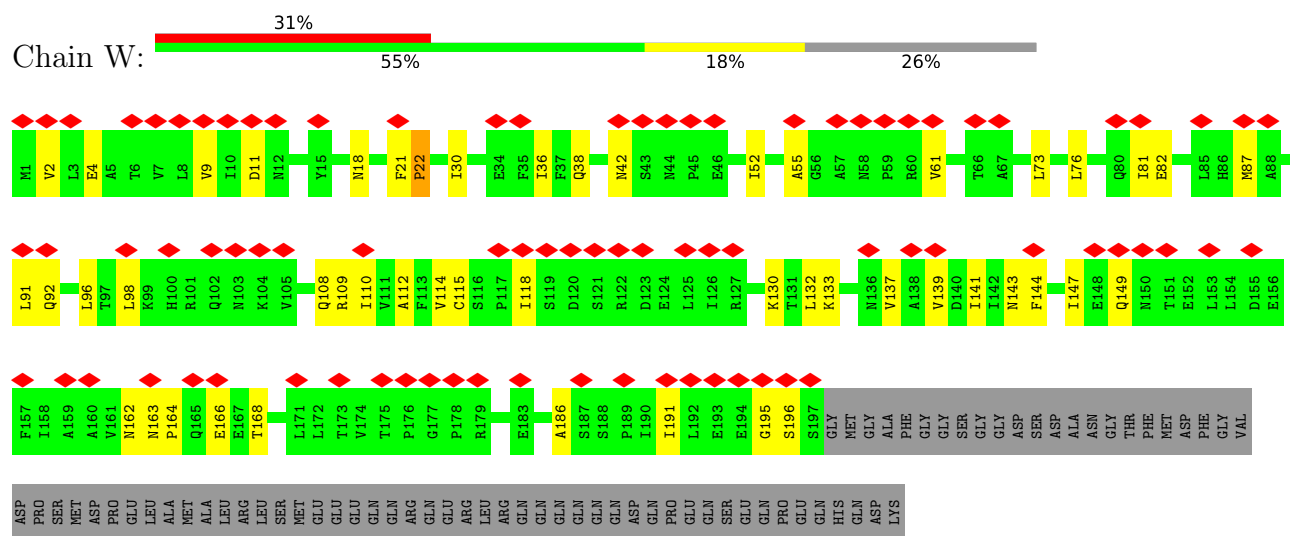
• Molecule 28: 26S proteasome regulatory subunit RPN8



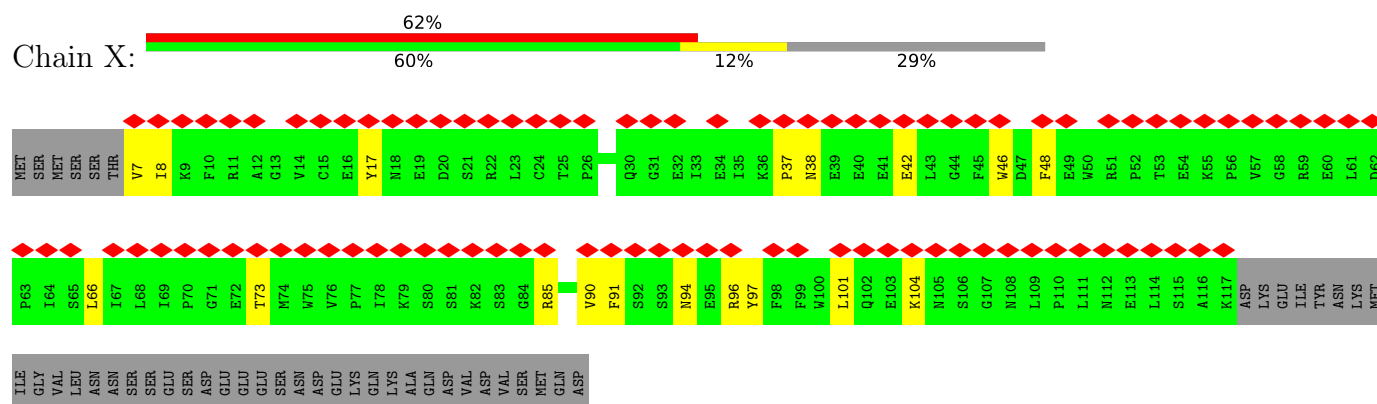
• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11



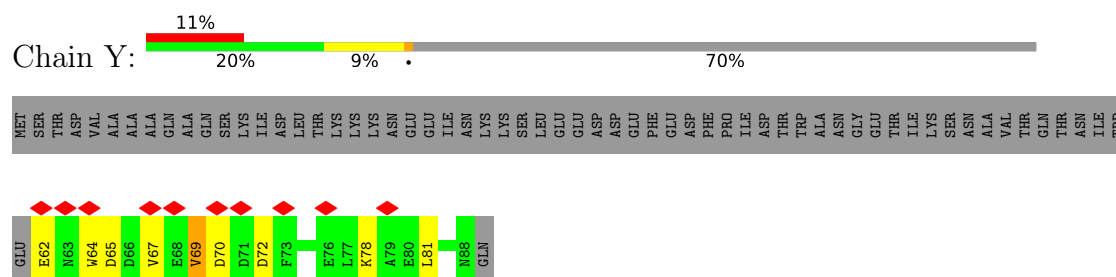
- Molecule 30: 26S proteasome regulatory subunit RPN10



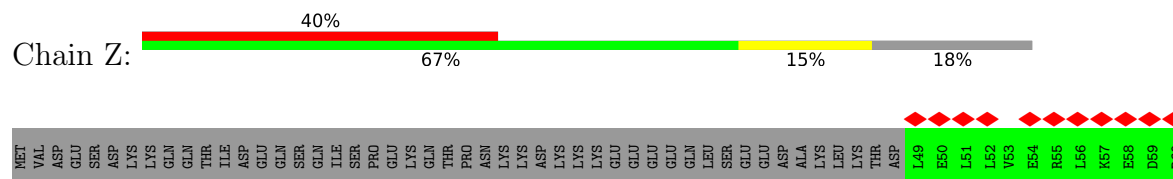
- Molecule 31: 26S proteasome regulatory subunit RPN13



- 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	8320	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	2.100	Depositor
Minimum map value	-1.052	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.657	Depositor
Map size ($\text{\AA}$)	474.47998, 474.47998, 474.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.07	0/1541	0.21	0/2087
1	b	0.07	0/1541	0.22	0/2087
2	2	0.07	0/1750	0.21	0/2373
2	i	0.06	0/1750	0.21	0/2373
3	3	0.07	0/1611	0.24	0/2174
3	h	0.07	0/1611	0.25	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	0.07	0/1681	0.22	0/2274
6	6	0.07	0/1795	0.22	0/2420
6	e	0.07	0/1795	0.24	0/2420
7	7	0.08	0/1821	0.24	0/2470
7	a	0.07	0/1846	0.24	0/2503
8	A	0.07	0/1945	0.23	0/2634
8	c	0.07	0/1959	0.23	0/2652
9	B	0.07	0/1952	0.24	0/2642
9	j	0.06	0/1952	0.20	0/2642
10	C	0.07	0/1934	0.23	0/2618
10	d	0.07	0/1934	0.22	0/2618
11	D	0.07	0/1910	0.24	0/2586
11	n	0.08	0/1919	0.24	0/2598
12	E	0.06	0/1886	0.21	0/2541
12	m	0.06	0/1886	0.19	0/2541
13	F	0.08	0/1823	0.25	0/2463
13	l	0.07	0/1823	0.22	0/2463
14	G	0.07	0/1932	0.23	0/2609
14	k	0.07	0/1936	0.23	0/2614
15	H	0.10	0/2831	0.28	0/3808
16	I	0.10	0/2869	0.29	0/3867
17	J	0.09	0/2964	0.28	0/3981
18	K	0.09	0/3062	0.28	0/4132
19	L	0.08	0/2896	0.25	0/3895
20	M	0.19	1/2903 (0.0%)	0.29	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	N	0.09	0/6670	0.24	0/9023
22	O	0.08	0/3243	0.24	0/4374
23	P	0.07	0/3599	0.21	0/4854
24	Q	0.07	0/3527	0.24	0/4748
25	R	0.08	0/3272	0.25	0/4412
26	S	0.08	0/3966	0.25	0/5355
27	T	0.07	0/2279	0.23	0/3077
28	U	0.07	0/2087	0.22	0/2811
29	V	0.10	0/2271	0.32	0/3064
30	W	0.13	0/1557	0.32	0/2111
31	X	0.07	0/931	0.23	0/1262
32	Y	0.12	0/239	0.39	0/322
33	Z	0.12	1/6404 (0.0%)	0.25	0/8686
All	All	0.09	2/107962 (0.0%)	0.24	0/145825

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	75	LEU	C-N	8.19	1.53	1.33
33	Z	468	GLU	C-N	7.64	1.51	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	29	0
1	b	1512	0	1478	33	0
2	2	1719	0	1716	35	0
2	i	1719	0	1716	34	0
3	3	1581	0	1571	48	0
3	h	1581	0	1571	34	0
4	4	1561	0	1569	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	g	1561	0	1569	27	0
5	5	1644	0	1592	23	0
5	f	1644	0	1592	41	0
6	6	1757	0	1708	31	0
6	e	1757	0	1708	35	0
7	7	1790	0	1790	36	0
7	a	1815	0	1818	33	0
8	A	1907	0	1901	28	0
8	c	1921	0	1910	37	0
9	B	1915	0	1929	49	0
9	j	1915	0	1929	35	0
10	C	1904	0	1901	38	0
10	d	1904	0	1901	36	0
11	D	1881	0	1892	39	0
11	n	1890	0	1900	36	0
12	E	1861	0	1836	29	0
12	m	1861	0	1836	33	0
13	F	1795	0	1797	31	0
13	l	1795	0	1797	34	0
14	G	1892	0	1883	31	0
14	k	1896	0	1886	41	0
15	H	2792	0	2879	75	0
16	I	2831	0	2881	78	0
17	J	2928	0	3057	62	0
18	K	3019	0	3084	70	0
19	L	2853	0	2926	54	0
20	M	2866	0	2938	73	0
21	N	6562	0	6625	89	0
22	O	3182	0	3207	45	0
23	P	3545	0	3629	46	0
24	Q	3471	0	3495	53	0
25	R	3218	0	3216	62	0
26	S	3894	0	3938	50	0
27	T	2235	0	2207	26	0
28	U	2061	0	2116	63	0
29	V	2236	0	2242	73	0
30	W	1534	0	1542	31	0
31	X	906	0	888	13	0
32	Y	236	0	203	13	0
33	Z	6290	0	6236	84	0
All	All	106149	0	106483	1721	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 (1721) 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)
20:M:275:PRO:HG3	20:M:320:ARG:HG2	1.19	1.14
20:M:275:PRO:HB3	20:M:320:ARG:HA	1.32	1.08
25:R:348:LEU:HB2	25:R:388:VAL:HB	1.50	0.94
1:1:20:THR:N	1:1:188:SER:HG	1.73	0.86
28:U:210:TYR:HH	28:U:223:HIS:N	1.74	0.85
20:M:274:ALA:HB1	20:M:275:PRO:CD	2.07	0.85
30:W:162:ASN:HA	30:W:168:THR:HG21	1.60	0.82
3:h:124:PHE:HB3	3:h:128:GLY:HA2	1.61	0.82
20:M:274:ALA:HB1	20:M:275:PRO:HD3	1.64	0.80
29:V:62:THR:O	29:V:63:VAL:HG23	1.81	0.80
16:I:186:GLY:H	16:I:357:THR:HG23	1.48	0.78
21:N:221:ASP:HA	21:N:894:ARG:HH22	1.48	0.77
29:V:23:THR:HG21	29:V:171:ARG:HE	1.49	0.77
15:H:313:ALA:HA	16:I:304:ARG:HE	1.50	0.76
20:M:275:PRO:CG	20:M:320:ARG:HG2	2.09	0.75
22:O:15:ARG:HD2	30:W:18:ASN:HD21	1.51	0.75
8:A:112:MET:HE2	8:A:117:LEU:HA	1.69	0.74
10:d:51:LYS:HG3	10:d:52:VAL:HG23	1.67	0.74
5:f:93:SER:HB3	5:f:249:SER:H	1.53	0.74
14:k:36:THR:HA	14:k:166:GLY:HA3	1.70	0.73
2:i:63:LEU:HD11	2:i:71:TRP:HB3	1.70	0.73
29:V:50:MET:HG3	29:V:71:MET:HB2	1.70	0.73
15:H:180:LYS:HE3	15:H:331:ARG:HH11	1.54	0.73
7:7:216:VAL:HG13	2:i:168:GLU:HG3	1.71	0.72
21:N:875:LEU:HD12	21:N:876:PRO:HD2	1.70	0.72
7:a:161:ARG:HE	7:a:169:THR:HB	1.55	0.71
19:L:171:THR:HB	19:L:245:PHE:HB3	1.70	0.71
21:N:781:ALA:O	21:N:873:ARG:NH2	2.23	0.71
7:7:215:ARG:HG2	7:7:247:VAL:HG13	1.71	0.71
16:I:148:LEU:HG	16:I:157:VAL:HG23	1.71	0.71
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.71	0.71
18:K:188:VAL:HG22	18:K:313:LYS:HE2	1.72	0.70
8:A:135:ARG:HB2	14:G:13:SER:HB3	1.71	0.70
15:H:224:VAL:HG11	15:H:373:ARG:HG3	1.73	0.70
21:N:773:MET:HB2	21:N:869:ASP:HB2	1.72	0.70
1:1:131:THR:HG21	7:7:68:ARG:HH21	1.56	0.70
8:c:135:ARG:HB3	14:k:13:SER:HB2	1.73	0.70
17:J:252:SER:HB2	17:J:295:ASN:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:85:LEU:HD11	17:J:93:LYS:HB3	1.75	0.69
29:V:61:TYR:CD1	29:V:172:GLN:NE2	2.60	0.69
12:E:18:GLU:HG2	20:M:426:LYS:HD3	1.75	0.69
3:3:27:LEU:HB3	3:3:39:LYS:HA	1.73	0.69
19:L:149:ASP:HB3	19:L:154:THR:H	1.56	0.69
4:g:53:THR:HG22	4:g:100:VAL:HG22	1.75	0.69
1:b:40:THR:HG22	1:b:45:ILE:HG12	1.75	0.68
28:U:195:LYS:HB3	29:V:226:LYS:HB3	1.75	0.68
16:I:285:ASP:HB2	17:J:270:ARG:HE	1.58	0.68
20:M:275:PRO:HA	20:M:320:ARG:HB3	1.74	0.68
29:V:61:TYR:HD1	29:V:172:GLN:HE21	1.41	0.68
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.74	0.68
15:H:242:PRO:HD2	15:H:346:ARG:HE	1.58	0.68
16:I:290:LYS:HD2	16:I:303:GLN:HG2	1.75	0.68
21:N:528:ARG:HB3	21:N:531:LEU:HB2	1.76	0.68
29:V:62:THR:O	29:V:63:VAL:CG2	2.42	0.68
31:X:38:ASN:HD22	31:X:42:GLU:H	1.42	0.68
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.74	0.68
1:1:80:TYR:HB2	8:A:102:ALA:HB1	1.76	0.68
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.76	0.68
16:I:204:HIS:HB3	16:I:207:LEU:HD13	1.76	0.68
17:J:338:THR:HA	25:R:203:ASP:HB3	1.76	0.68
25:R:359:VAL:HA	32:Y:81:LEU:HD22	1.76	0.67
29:V:188:LEU:HB3	29:V:192:LEU:HA	1.75	0.67
22:O:353:VAL:HG23	22:O:354:GLN:H	1.59	0.67
33:Z:530:LEU:HB3	33:Z:542:ILE:HD11	1.75	0.67
8:A:176:GLN:NE2	18:K:422:ASP:OD2	2.28	0.67
11:D:6:ARG:NH2	12:E:9:ASP:O	2.28	0.67
11:D:37:LYS:HE2	11:D:160:SER:HA	1.77	0.67
8:c:114:CYS:HB2	8:c:145:SER:HB3	1.75	0.67
8:c:59:VAL:HG13	8:c:64:LEU:HD12	1.77	0.67
9:j:71:ILE:HG12	9:j:138:GLY:HA3	1.77	0.67
20:M:289:LYS:HB3	20:M:295:LYS:HE3	1.77	0.67
29:V:232:GLU:HA	29:V:236:SER:HB2	1.77	0.67
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.75	0.66
15:H:98:GLN:HB2	16:I:119:ILE:HG21	1.75	0.66
18:K:90:GLN:HG2	18:K:147:VAL:HG13	1.77	0.66
27:T:92:ASN:HD21	27:T:96:LEU:HD13	1.59	0.66
1:1:40:THR:HG22	1:1:45:ILE:HG12	1.78	0.66
5:5:82:ARG:HH11	5:5:186:THR:HA	1.60	0.66
28:U:210:TYR:OH	28:U:223:HIS:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:71:GLU:OE1	10:d:143:ARG:NH1	2.28	0.66
10:C:124:GLN:NE2	11:D:127:ARG:O	2.28	0.66
20:M:275:PRO:CB	20:M:320:ARG:HA	2.20	0.66
2:2:141:SER:HB3	2:2:154:LEU:HD13	1.78	0.66
17:J:132:PRO:HG2	17:J:137:MET:HE1	1.78	0.65
2:i:70:ILE:HG12	2:i:131:GLY:HA3	1.78	0.65
18:K:289:ASP:OD1	19:L:299:ARG:NH2	2.29	0.65
23:P:432:LEU:HD13	28:U:225:ILE:HG13	1.78	0.65
9:B:42:GLY:HA3	9:B:185:LEU:HD22	1.76	0.65
16:I:132:ILE:HG12	16:I:156:ILE:HD12	1.77	0.65
11:n:66:LYS:HG2	11:n:72:VAL:HG12	1.79	0.65
19:L:393:ASN:ND2	20:M:344:ASP:OD2	2.30	0.65
21:N:421:ASP:HA	21:N:424:LYS:HE2	1.79	0.65
7:7:250:MET:SD	1:b:208:TYR:OH	2.55	0.65
15:H:275:ILE:HA	15:H:309:ASP:HB3	1.79	0.65
11:D:216:LYS:HB2	11:D:220:ASP:HB3	1.79	0.64
29:V:259:LYS:HB2	29:V:279:HIS:HD2	1.63	0.64
33:Z:257:PRO:HB2	33:Z:259:PRO:HD2	1.79	0.64
33:Z:306:MET:HG2	33:Z:973:TYR:HB3	1.79	0.64
17:J:339:ARG:NH2	25:R:205:GLU:OE1	2.30	0.64
12:m:85:ALA:HB2	12:m:140:VAL:HG21	1.80	0.64
23:P:28:ALA:H	23:P:30:ASN:HD22	1.45	0.64
22:O:2:PHE:HB3	22:O:5:HIS:HB3	1.79	0.64
25:R:348:LEU:N	25:R:388:VAL:O	2.31	0.64
26:S:173:LEU:O	26:S:177:ASN:ND2	2.30	0.64
22:O:70:TYR:O	22:O:120:LYS:NZ	2.30	0.64
1:1:194:MET:HB2	1:1:205:LEU:HB2	1.80	0.64
12:m:21:LEU:HD22	12:m:24:VAL:HG23	1.79	0.64
29:V:67:ASP:OD2	29:V:100:ARG:NH1	2.31	0.64
8:A:46:ARG:HH21	8:A:167:LYS:HA	1.63	0.64
25:R:223:ASN:HB3	25:R:226:GLU:HB2	1.79	0.64
33:Z:204:CYS:HA	33:Z:232:LYS:HE2	1.79	0.64
10:d:73:ILE:HG12	10:d:139:GLY:HA3	1.80	0.64
3:3:109:VAL:HB	3:3:122:ALA:HB3	1.80	0.63
21:N:584:ARG:NH1	21:N:614:ASN:OD1	2.31	0.63
25:R:380:VAL:HB	25:R:389:GLU:HB3	1.80	0.63
9:j:33:THR:HA	9:j:165:GLY:HA3	1.78	0.63
21:N:635:GLN:NE2	21:N:667:GLN:OE1	2.31	0.63
1:1:38:ARG:HD2	1:1:45:ILE:HD13	1.80	0.63
2:2:228:LYS:HE2	2:2:231:SER:HA	1.79	0.63
29:V:60:ASP:O	29:V:61:TYR:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:134:SER:O	18:K:259:ARG:NH2	2.31	0.63
10:C:216:ILE:HG12	10:C:227:GLN:HG2	1.79	0.63
7:a:39:VAL:HG13	7:a:62:SER:H	1.64	0.63
17:J:336:ASN:OD1	25:R:207:ARG:NH2	2.31	0.63
23:P:248:ASP:HA	23:P:252:SER:HB3	1.81	0.63
33:Z:773:ARG:NH1	33:Z:802:ASP:OD2	2.31	0.63
8:A:14:ARG:NH2	8:A:30:TYR:OH	2.29	0.62
4:g:62:ALA:HB1	11:n:94:GLN:HB3	1.81	0.62
11:n:118:GLN:NE2	12:m:83:ALA:O	2.31	0.62
3:3:176:ASP:HB3	5:f:104:GLN:HE22	1.62	0.62
21:N:780:ASP:HB2	21:N:874:ILE:HA	1.81	0.62
22:O:98:TYR:HB2	22:O:102:LEU:HD13	1.80	0.62
26:S:421:TYR:HE1	27:T:208:LEU:HG	1.64	0.62
2:2:225:ARG:NH2	3:3:151:GLU:O	2.33	0.62
14:G:68:GLN:OE1	14:G:93:ARG:NH2	2.33	0.62
17:J:336:ASN:ND2	18:K:200:GLN:O	2.32	0.62
25:R:348:LEU:CB	25:R:388:VAL:HB	2.28	0.62
6:6:174:ASN:HB3	6:6:176:LYS:HE2	1.82	0.62
2:i:47:THR:HB	2:i:59:ASN:HA	1.82	0.62
12:m:12:VAL:HG12	12:m:23:GLN:HG3	1.81	0.62
17:J:160:ILE:HG23	17:J:164:ILE:HD12	1.82	0.62
3:h:155:GLU:HB3	3:h:158:LEU:HD21	1.82	0.62
20:M:151:ASP:HB3	29:V:46:PRO:HB2	1.82	0.62
14:k:224:THR:HB	14:k:227:LEU:HB2	1.81	0.61
15:H:203:LYS:HE2	15:H:268:ASP:HB3	1.82	0.61
24:Q:426:LEU:HD21	28:U:292:ILE:HG23	1.82	0.61
31:X:91:PHE:H	31:X:96:ARG:HD3	1.63	0.61
22:O:350:ILE:O	28:U:234:ASN:ND2	2.33	0.61
30:W:132:LEU:HB3	30:W:137:VAL:HB	1.82	0.61
9:B:119:GLN:HE22	10:C:85:GLU:HB2	1.65	0.61
13:l:81:ALA:HB2	13:l:130:VAL:HG21	1.81	0.61
30:W:2:VAL:HG22	30:W:196:SER:HB2	1.82	0.61
30:W:38:GLN:HG3	30:W:42:ASN:HD22	1.65	0.61
4:g:55:GLN:NE2	5:f:160:ASN:OD1	2.31	0.61
17:J:139:VAL:HG22	17:J:211:ILE:HG12	1.82	0.61
26:S:314:ASN:HB3	26:S:332:PHE:HZ	1.66	0.61
29:V:53:MET:HA	29:V:68:VAL:HG12	1.83	0.61
29:V:104:VAL:O	29:V:133:ASN:ND2	2.34	0.61
24:Q:31:LEU:HB3	24:Q:44:ALA:HB1	1.81	0.61
3:3:185:ALA:HB3	3:3:200:LEU:HB2	1.82	0.61
13:l:34:VAL:HA	13:l:162:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:386:MET:HE3	21:N:407:GLY:HA3	1.80	0.61
21:N:494:LYS:HE2	21:N:496:GLU:HB3	1.81	0.61
33:Z:135:LEU:HB3	33:Z:161:ILE:HD13	1.82	0.61
9:B:94:HIS:HA	9:B:98:LYS:HB2	1.83	0.61
19:L:283:VAL:HG21	19:L:325:MET:HB3	1.83	0.61
23:P:286:ASN:HA	23:P:293:LEU:HD11	1.82	0.61
8:A:47:GLY:O	8:A:193:HIS:ND1	2.33	0.60
26:S:227:ASN:HD22	26:S:263:ASP:HB2	1.66	0.60
32:Y:69:VAL:HG12	32:Y:70:ASP:H	1.66	0.60
26:S:283:GLN:HE22	27:T:120:THR:HG23	1.66	0.60
7:a:86:ILE:HG12	7:a:147:ILE:HG12	1.81	0.60
9:j:49:LYS:HE3	9:j:210:GLU:HB2	1.82	0.60
30:W:21:PHE:HB2	30:W:22:PRO:HD3	1.82	0.60
5:5:128:GLN:HB2	6:6:113:GLN:HE22	1.65	0.60
21:N:34:GLN:NE2	26:S:212:SER:OG	2.35	0.60
21:N:273:LEU:HB3	21:N:290:LEU:HD13	1.84	0.60
2:2:153:TYR:HB2	2:2:167:LEU:HD13	1.83	0.60
6:6:212:GLU:OE2	6:6:239:LYS:NZ	2.35	0.60
5:f:172:MET:H	5:f:192:SER:HB3	1.66	0.60
28:U:171:VAL:HB	29:V:217:HIS:HD2	1.66	0.60
7:7:114:ALA:HB1	7:7:117:GLU:HB2	1.84	0.60
10:C:66:LEU:HD23	10:C:76:ALA:HB2	1.84	0.60
16:I:100:ARG:HH11	16:I:133:LEU:HD23	1.67	0.60
29:V:228:TYR:HA	29:V:231:GLU:HB3	1.84	0.60
1:1:64:ARG:HD2	1:1:71:THR:HB	1.83	0.60
14:k:70:VAL:N	14:k:74:ILE:O	2.35	0.60
17:J:75:VAL:HG11	17:J:107:LEU:HB3	1.84	0.60
16:I:294:SER:HB3	16:I:300:ARG:HG3	1.83	0.60
17:J:267:GLU:OE1	18:K:290:ARG:NH2	2.27	0.60
3:3:28:ARG:NH1	3:3:179:ALA:O	2.35	0.59
11:D:201:GLU:O	11:D:204:GLN:NE2	2.33	0.59
16:I:100:ARG:HB3	16:I:157:VAL:HG12	1.84	0.59
17:J:181:GLN:HE22	17:J:287:ASN:H	1.49	0.59
33:Z:754:LYS:NZ	33:Z:787:ASP:OD2	2.32	0.59
10:C:162:ALA:HB3	11:D:54:LEU:HD13	1.84	0.59
20:M:71:ASN:HB3	29:V:74:SER:HA	1.84	0.59
21:N:653:ARG:NH1	21:N:691:GLN:OE1	2.35	0.59
4:4:146:HIS:O	4:4:149:ARG:NH1	2.30	0.59
5:f:273:TRP:HA	5:f:276:LYS:HE2	1.84	0.59
11:n:163:THR:HG21	11:n:171:VAL:HB	1.83	0.59
33:Z:574:TYR:HB2	33:Z:581:VAL:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:813:PHE:HB2	33:Z:850:LEU:HD13	1.83	0.59
6:e:55:ASN:O	7:a:189:ARG:NH2	2.35	0.59
10:d:70:ASN:OD1	10:d:71:ASP:N	2.35	0.59
22:O:4:ASN:ND2	22:O:39:PHE:O	2.36	0.59
22:O:39:PHE:HB2	22:O:52:ALA:HB2	1.83	0.59
25:R:33:LEU:HB3	25:R:74:ASN:HD22	1.66	0.59
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.84	0.59
2:2:239:THR:OG1	3:3:169:GLN:NE2	2.35	0.59
26:S:327:ILE:HG21	32:Y:64:TRP:HE1	1.68	0.59
28:U:125:LYS:HB3	28:U:127:GLN:HE21	1.66	0.59
3:3:28:ARG:HH21	3:3:183:TRP:CD1	2.21	0.59
5:f:251:ASN:ND2	5:f:265:ASN:OD1	2.33	0.59
33:Z:87:LYS:HE2	33:Z:89:LEU:HB2	1.84	0.59
33:Z:327:GLN:HE22	33:Z:463:HIS:HB2	1.66	0.59
8:c:89:ASP:OD1	14:k:121:GLN:NE2	2.34	0.59
9:j:42:GLY:HA3	9:j:185:LEU:HD13	1.85	0.59
16:I:147:VAL:HG12	16:I:159:VAL:HG23	1.83	0.59
18:K:207:ARG:NH2	18:K:302:GLN:O	2.36	0.59
21:N:341:ALA:HA	21:N:374:ILE:HA	1.83	0.59
22:O:30:GLU:OE2	22:O:58:ARG:NH1	2.35	0.59
24:Q:416:VAL:HG23	25:R:410:LEU:HD21	1.85	0.59
6:6:164:LEU:HD11	3:h:148:GLY:H	1.68	0.59
7:a:100:LEU:HD21	7:a:129:LEU:HD11	1.85	0.59
11:D:118:GLN:NE2	12:E:83:ALA:O	2.36	0.59
8:c:144:VAL:HG12	8:c:154:ILE:HG12	1.84	0.59
16:I:147:VAL:HA	16:I:160:LEU:H	1.66	0.59
23:P:48:GLN:O	23:P:88:GLN:NE2	2.31	0.59
9:B:177:LYS:HG3	24:Q:209:TYR:CZ	2.38	0.59
17:J:164:ILE:HG12	17:J:289:LYS:HE2	1.84	0.59
21:N:875:LEU:HG	21:N:877:GLN:H	1.68	0.59
22:O:74:ASN:OD1	22:O:75:GLN:N	2.36	0.59
1:1:117:ILE:HG12	1:1:131:THR:HG23	1.85	0.58
11:D:155:ILE:HG22	12:E:82:THR:HB	1.85	0.58
4:4:149:ARG:HB2	4:4:152:MET:HG3	1.85	0.58
1:b:110:ASP:OD2	7:a:35:GLN:NE2	2.36	0.58
10:C:120:GLN:NE2	10:C:123:THR:OG1	2.35	0.58
10:C:201:THR:HG22	10:C:203:SER:H	1.69	0.58
25:R:154:LEU:HD13	25:R:170:VAL:HA	1.85	0.58
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.83	0.58
1:b:63:CYS:HB2	1:b:117:ILE:HB	1.84	0.58
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:666:GLN:NE2	21:N:711:ARG:O	2.37	0.58
23:P:392:LYS:HB2	23:P:401:ASN:HB2	1.85	0.58
33:Z:358:TYR:HE1	33:Z:962:ARG:HB2	1.67	0.58
3:3:175:ALA:HB1	3:3:182:GLY:HA2	1.83	0.58
13:l:190:ILE:HD13	13:l:213:ILE:HD12	1.85	0.58
2:i:206:VAL:HB	2:i:214:GLU:HB2	1.84	0.58
15:H:223:GLU:HG2	20:M:403:LEU:HD23	1.85	0.58
16:I:319:ARG:HH21	33:Z:828:ALA:HB2	1.68	0.58
16:I:358:LYS:NZ	16:I:380:LEU:O	2.34	0.58
22:O:343:GLN:HB3	23:P:360:ILE:HA	1.85	0.58
2:2:196:LEU:HB3	6:e:215:ILE:HB	1.85	0.58
17:J:335:MET:HA	18:K:202:GLY:HA3	1.85	0.58
4:g:70:ARG:NH2	11:n:87:GLU:OE2	2.36	0.58
9:j:5:TYR:OH	14:k:127:ASN:ND2	2.37	0.58
16:I:195:LYS:HG3	16:I:199:GLU:HB3	1.86	0.58
22:O:218:SER:HA	22:O:251:LEU:HD21	1.86	0.58
7:7:144:TRP:HA	7:7:165:LEU:HD23	1.86	0.58
3:h:30:GLY:HA2	3:h:36:VAL:HG23	1.86	0.58
9:j:222:LEU:HD13	9:j:232:GLY:HA2	1.86	0.58
12:m:165:TYR:HE1	13:l:60:GLN:HB2	1.69	0.58
23:P:52:LEU:HD23	23:P:55:SER:HB3	1.85	0.58
25:R:308:LEU:HD13	25:R:330:VAL:HG13	1.84	0.58
33:Z:116:ALA:HB3	33:Z:141:SER:HB2	1.86	0.58
23:P:23:LYS:HA	23:P:27:LEU:HD11	1.86	0.58
4:4:96:ARG:HH22	5:5:166:LYS:HB3	1.69	0.58
1:b:20:THR:N	1:b:188:SER:HG	2.00	0.58
6:e:214:HIS:HD2	6:e:217:VAL:HG23	1.68	0.58
15:H:145:TYR:CZ	15:H:174:VAL:HA	2.38	0.58
22:O:143:LEU:HD13	22:O:178:TYR:HA	1.86	0.58
10:C:156:ASN:HB2	16:I:437:LEU:HD22	1.86	0.57
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.84	0.57
13:l:153:VAL:HB	14:k:86:ARG:HH12	1.69	0.57
29:V:194:ARG:HG2	29:V:195:HIS:CD2	2.39	0.57
11:D:122:GLN:HA	12:E:136:ARG:HE	1.68	0.57
17:J:183:LYS:NZ	17:J:280:ASP:OD1	2.36	0.57
21:N:330:THR:HG21	21:N:744:PRO:HG2	1.85	0.57
24:Q:51:ARG:HD2	24:Q:88:PHE:HA	1.85	0.57
26:S:136:CYS:HB3	26:S:179:ILE:HG21	1.86	0.57
7:7:226:ARG:HE	7:7:246:GLN:HB3	1.68	0.57
5:f:96:THR:HG22	5:f:101:VAL:HG22	1.86	0.57
21:N:489:MET:HB3	21:N:524:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:218:GLY:HA3	16:I:344:ILE:HG12	1.86	0.57
23:P:269:VAL:HG13	23:P:303:PHE:HZ	1.69	0.57
2:i:254:GLU:OE2	10:d:228:LYS:NZ	2.34	0.57
15:H:144:LYS:HE3	20:M:75:LEU:HG	1.87	0.57
3:3:177:ARG:NH1	6:e:170:ASP:OD2	2.38	0.57
3:h:78:GLU:OE2	9:j:143:ASN:ND2	2.38	0.57
18:K:210:LEU:HD12	18:K:337:LYS:HG2	1.86	0.57
19:L:253:ASP:HB3	20:M:293:SER:HB2	1.86	0.57
21:N:223:LEU:HD11	21:N:897:LYS:HE3	1.86	0.57
33:Z:737:ALA:HA	33:Z:772:ILE:HD13	1.87	0.57
2:2:242:LEU:HB2	3:3:201:LYS:HB2	1.85	0.57
3:3:145:GLN:HE22	3:3:177:ARG:HB2	1.69	0.57
13:l:7:ASP:O	13:l:21:GLN:NE2	2.37	0.57
33:Z:588:ILE:HG12	33:Z:596:THR:HB	1.85	0.57
15:H:337:ILE:HG23	15:H:370:ARG:HH21	1.69	0.57
23:P:392:LYS:HG3	23:P:403:GLU:HB2	1.86	0.57
26:S:485:LYS:HB2	28:U:305:ARG:HH21	1.69	0.57
27:T:104:LYS:NZ	27:T:169:GLN:OE1	2.38	0.57
28:U:279:SER:HB3	29:V:287:THR:HG23	1.87	0.57
29:V:62:THR:C	29:V:63:VAL:HG23	2.30	0.57
14:G:9:ASP:O	14:G:23:GLN:NE2	2.37	0.57
8:c:129:THR:HG22	8:c:136:PRO:HB3	1.87	0.57
10:d:119:LYS:NZ	10:d:151:SER:OG	2.32	0.57
20:M:175:LYS:HE2	20:M:240:ASN:HB3	1.86	0.57
33:Z:321:PHE:HB3	33:Z:326:VAL:HG21	1.86	0.57
2:i:155:SER:OG	2:i:160:SER:OG	2.23	0.56
4:g:8:ARG:HG3	4:g:13:VAL:HG22	1.86	0.56
15:H:243:PRO:HB3	15:H:372:ASP:HB2	1.87	0.56
21:N:562:THR:HA	21:N:597:ARG:HE	1.70	0.56
23:P:377:GLU:OE1	23:P:395:ARG:NH2	2.38	0.56
27:T:170:ASN:HA	27:T:174:PHE:HB2	1.86	0.56
28:U:49:ASN:OD1	28:U:50:SER:N	2.38	0.56
30:W:130:LYS:HA	30:W:133:LYS:HE2	1.87	0.56
3:3:63:LEU:HD22	3:3:105:VAL:HG11	1.85	0.56
9:B:41:ASN:ND2	9:B:184:GLU:OE1	2.37	0.56
10:d:76:ALA:HB3	10:d:136:ILE:HB	1.87	0.56
13:l:129:GLY:HA2	13:l:149:PRO:HB3	1.87	0.56
21:N:762:ARG:NH2	21:N:766:GLN:O	2.38	0.56
24:Q:426:LEU:HD13	28:U:295:LYS:HD2	1.87	0.56
5:5:281:SER:OG	4:g:146:HIS:ND1	2.39	0.56
4:g:4:ILE:HG22	4:g:103:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:19:PHE:HB2	9:B:20:GLN:HE21	1.69	0.56
10:d:207:THR:OG1	10:d:209:ASP:OD1	2.23	0.56
16:I:249:GLY:HA3	16:I:284:ILE:HG12	1.88	0.56
21:N:619:CYS:HB2	21:N:652:VAL:HG22	1.86	0.56
25:R:372:ILE:HB	26:S:398:THR:HG22	1.87	0.56
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.69	0.56
2:2:230:LYS:HB2	6:e:201:LYS:HD3	1.88	0.56
9:B:2:THR:HG22	9:B:3:ASP:H	1.71	0.56
13:F:67:ASP:HB3	13:F:70:MET:HB2	1.87	0.56
12:m:68:VAL:HB	12:m:93:ARG:HH21	1.70	0.56
15:H:225:VAL:HA	15:H:350:LYS:HE2	1.88	0.56
16:I:118:ALA:HB2	16:I:132:ILE:HD11	1.86	0.56
18:K:195:ALA:HA	18:K:198:TYR:HD2	1.70	0.56
27:T:98:GLU:HB2	27:T:101:LYS:HG2	1.87	0.56
8:A:144:VAL:HG12	8:A:154:ILE:HG12	1.87	0.56
12:E:78:MET:HE1	12:E:82:THR:HA	1.87	0.56
26:S:400:LYS:HG3	26:S:445:THR:HB	1.85	0.56
28:U:31:ARG:NH1	28:U:97:LYS:O	2.38	0.56
8:c:35:THR:HG21	8:c:140:ILE:HG13	1.88	0.56
10:d:156:ASN:HB2	11:n:79:ASN:HB2	1.86	0.56
13:l:11:VAL:HA	14:k:130:ARG:HD3	1.87	0.56
17:J:277:ASN:HB2	17:J:309:ARG:HE	1.71	0.56
18:K:224:LYS:NZ	19:L:313:ASP:O	2.38	0.56
22:O:120:LYS:HG2	30:W:81:ILE:HB	1.88	0.56
22:O:283:HIS:HA	22:O:286:PHE:HD2	1.70	0.56
23:P:392:LYS:HE3	23:P:403:GLU:HA	1.87	0.56
29:V:147:VAL:HG12	29:V:149:GLY:H	1.71	0.56
4:g:55:GLN:OE1	5:f:156:LYS:NZ	2.38	0.56
8:c:158:ASP:OD1	8:c:162:TYR:N	2.39	0.56
20:M:143:ASN:HD21	20:M:257:GLY:HA2	1.70	0.56
21:N:330:THR:HG23	21:N:366:THR:HG21	1.88	0.56
7:a:215:ARG:HG2	7:a:247:VAL:HG13	1.88	0.56
8:c:77:ARG:NH2	8:c:111:ASP:OD2	2.37	0.56
12:m:36:THR:HA	12:m:173:GLY:HA3	1.88	0.56
19:L:118:ILE:HG12	19:L:128:ILE:HG12	1.88	0.56
29:V:52:LEU:HD11	29:V:104:VAL:HG13	1.88	0.56
2:2:75:ALA:HB3	2:2:126:TYR:HB2	1.88	0.56
6:e:83:LEU:HD11	6:e:112:ILE:HG23	1.88	0.56
7:a:137:ARG:HA	7:a:142:PRO:HG3	1.88	0.56
19:L:195:GLU:HA	19:L:199:LEU:HD13	1.88	0.56
21:N:22:THR:HG23	21:N:60:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:377:VAL:HG22	28:U:197:LEU:HD22	1.87	0.56
29:V:221:TRP:NE1	29:V:223:SER:OG	2.39	0.56
16:I:330:LYS:HG2	16:I:332:GLU:H	1.71	0.56
19:L:407:ARG:HG2	19:L:409:HIS:H	1.70	0.56
21:N:366:THR:HG22	21:N:747:HIS:HE1	1.70	0.56
29:V:163:ALA:H	29:V:166:ASN:HD21	1.54	0.56
10:d:206:LEU:HD21	10:d:211:LEU:HD11	1.87	0.55
23:P:424:GLU:HB2	28:U:232:VAL:HG11	1.88	0.55
7:a:60:LEU:HB2	7:a:225:SER:HB3	1.88	0.55
14:k:65:VAL:HG12	14:k:67:ILE:H	1.71	0.55
23:P:409:SER:HB3	23:P:412:LEU:HD12	1.88	0.55
24:Q:65:TYR:HD2	24:Q:74:LEU:HD13	1.71	0.55
4:4:29:LYS:HE3	4:4:31:SER:HB2	1.88	0.55
5:f:233:LYS:HB3	5:f:271:LEU:HD21	1.87	0.55
7:a:77:PRO:HA	7:a:83:VAL:HA	1.88	0.55
16:I:174:ASP:HB3	16:I:244:PHE:HB3	1.88	0.55
25:R:373:PRO:HB2	32:Y:64:TRP:HZ3	1.71	0.55
3:3:20:CYS:HA	3:3:112:ILE:HD11	1.88	0.55
6:e:35:ALA:HB2	6:e:141:VAL:HG23	1.89	0.55
8:A:156:LYS:NZ	8:A:170:ALA:O	2.39	0.55
11:D:68:ASP:HB3	11:D:71:VAL:HB	1.88	0.55
13:F:34:VAL:HA	13:F:162:GLY:HA3	1.88	0.55
13:l:120:THR:HG22	13:l:127:PRO:HB3	1.87	0.55
19:L:305:LEU:HD13	19:L:334:ASP:HB2	1.89	0.55
20:M:129:LEU:HD11	20:M:155:ILE:HD12	1.87	0.55
22:O:75:GLN:OE1	22:O:114:GLN:NE2	2.39	0.55
24:Q:104:PHE:HB3	24:Q:114:GLN:HE21	1.71	0.55
29:V:124:ASN:OD1	29:V:194:ARG:NH1	2.36	0.55
33:Z:762:GLY:HA2	33:Z:765:MET:HE2	1.87	0.55
33:Z:812:ILE:HD13	33:Z:848:THR:HA	1.88	0.55
1:b:23:MET:HE2	1:b:174:ILE:HG12	1.89	0.55
9:B:111:VAL:HG21	9:B:148:TYR:HD2	1.72	0.55
12:m:187:TRP:HA	12:m:191:LEU:HD11	1.89	0.55
19:L:357:ARG:NH2	19:L:383:SER:O	2.39	0.55
33:Z:861:THR:OG1	33:Z:962:ARG:NH1	2.39	0.55
1:l:33:LEU:HD21	1:l:119:ALA:HB3	1.88	0.55
3:3:11:ILE:HD12	3:3:146:LEU:HD11	1.88	0.55
25:R:174:ILE:HG21	25:R:190:LYS:HB2	1.88	0.55
3:3:73:LEU:HD23	3:3:76:LEU:HD12	1.89	0.55
10:C:217:ARG:HG2	10:C:219:GLY:H	1.71	0.55
20:M:219:LEU:HD23	20:M:346:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:11:ASP:HA	30:W:55:ALA:HB3	1.89	0.55
33:Z:150:GLY:H	33:Z:210:TYR:HE1	1.53	0.55
33:Z:347:ASN:HB3	33:Z:353:VAL:HG23	1.89	0.55
7:7:48:LYS:HD2	7:7:173:PRO:HA	1.88	0.55
12:m:50:VAL:HG21	12:m:66:LYS:HB2	1.88	0.55
14:k:193:VAL:HG13	14:k:216:ILE:HG21	1.89	0.55
17:J:357:ASP:OD2	18:K:330:ARG:NH1	2.40	0.55
21:N:70:TYR:HE2	26:S:219:LYS:HD2	1.72	0.55
24:Q:127:ARG:HA	24:Q:130:ARG:HB2	1.89	0.55
1:b:209:PRO:HA	1:b:212:TYR:CE2	2.40	0.55
2:i:246:ILE:HG12	3:h:196:VAL:HG22	1.89	0.55
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.89	0.55
15:H:147:ILE:HD11	15:H:157:VAL:HG23	1.89	0.55
20:M:202:LYS:HG2	20:M:203:ARG:HG2	1.87	0.55
21:N:713:VAL:HA	21:N:755:PRO:HA	1.88	0.55
22:O:43:GLU:HA	22:O:82:LEU:HD21	1.89	0.55
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.38	0.55
28:U:283:ARG:HB2	29:V:287:THR:HG21	1.89	0.55
24:Q:188:LEU:HD11	25:R:278:SER:HA	1.87	0.55
27:T:206:LYS:HG3	27:T:211:PHE:HB2	1.89	0.55
10:C:181:LYS:HE2	10:C:183:ASP:HB2	1.89	0.54
13:F:117:GLN:HE21	13:F:121:GLN:HG3	1.72	0.54
33:Z:869:ASP:HB2	33:Z:977:ILE:HG13	1.89	0.54
6:e:170:ASP:HB3	6:e:176:LYS:HD2	1.88	0.54
8:c:162:TYR:HB2	9:j:80:PRO:HD3	1.89	0.54
2:2:32:ILE:HD13	2:2:73:ALA:HB1	1.90	0.54
6:e:76:PHE:HZ	7:a:166:LEU:HB3	1.72	0.54
8:A:18:ILE:HG22	9:B:128:ARG:HB3	1.88	0.54
15:H:275:ILE:HG22	15:H:277:SER:H	1.72	0.54
20:M:295:LYS:HB3	20:M:302:GLN:HB2	1.89	0.54
28:U:66:PHE:HB2	30:W:96:LEU:HD13	1.89	0.54
28:U:273:LEU:HD23	28:U:276:ILE:HD12	1.89	0.54
15:H:96:PRO:HA	15:H:191:ILE:HG13	1.89	0.54
1:1:196:VAL:HB	1:1:203:GLU:HB3	1.90	0.54
4:g:19:LYS:HB3	4:g:31:SER:HA	1.90	0.54
6:e:49:ILE:HG22	6:e:54:ILE:HG12	1.88	0.54
13:F:22:VAL:HG11	13:F:150:SER:HB3	1.88	0.54
21:N:83:LEU:HD11	21:N:136:ILE:HG13	1.89	0.54
21:N:154:LEU:HD22	21:N:189:LEU:HD21	1.88	0.54
26:S:330:LEU:HD12	32:Y:65:ASP:H	1.72	0.54
28:U:47:VAL:HG22	28:U:89:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:81:LYS:HB3	29:V:72:PRO:HB3	1.90	0.54
7:a:136:ARG:HB3	7:a:142:PRO:HA	1.88	0.54
16:I:161:GLN:NE2	16:I:163:ASP:OD2	2.41	0.54
29:V:61:TYR:CD2	29:V:62:THR:N	2.76	0.54
5:f:107:LYS:N	6:e:151:GLU:OE2	2.35	0.54
8:A:141:LEU:HB2	8:A:157:THR:HB	1.90	0.54
9:B:81:ASP:HB3	9:B:130:PHE:HB3	1.89	0.54
11:D:44:LEU:HD11	11:D:136:ALA:HB3	1.89	0.54
16:I:281:ILE:HB	16:I:326:MET:HG2	1.90	0.54
20:M:136:ASP:OD2	20:M:139:LYS:NZ	2.36	0.54
2:2:109:LEU:HD21	2:2:148:THR:HB	1.89	0.54
3:3:103:TYR:OH	4:4:93:ARG:NH1	2.33	0.54
8:c:119:LYS:HG3	9:j:83:ARG:HD2	1.88	0.54
10:d:16:GLU:HB3	11:n:29:ARG:HH12	1.72	0.54
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.90	0.54
21:N:265:ALA:HB1	21:N:269:LEU:HB2	1.89	0.54
21:N:378:ASN:HD21	21:N:381:GLU:HB2	1.73	0.54
5:5:127:CYS:HA	5:5:172:MET:HE3	1.90	0.54
7:a:232:ILE:HB	7:a:240:THR:HB	1.89	0.54
13:l:39:ARG:HH21	14:k:60:VAL:HG21	1.73	0.54
33:Z:99:LEU:HD23	33:Z:102:ILE:HD12	1.90	0.54
2:2:114:GLN:HE22	8:A:107:LYS:HA	1.70	0.54
6:e:110:ARG:NE	6:e:150:TYR:OH	2.36	0.54
28:U:189:ARG:HG3	29:V:296:LEU:HD11	1.90	0.54
3:3:138:VAL:HG11	3:3:146:LEU:HB2	1.89	0.53
10:d:50:ARG:NH1	10:d:209:ASP:O	2.41	0.53
13:l:50:LYS:HB3	13:l:59:TYR:HB3	1.90	0.53
5:f:108:LYS:HB3	5:f:120:MET:HB3	1.89	0.53
9:B:20:GLN:O	9:B:24:ALA:N	2.35	0.53
11:D:37:LYS:HD2	11:D:145:PRO:HB2	1.90	0.53
13:F:31:GLN:NE2	20:M:428:LYS:O	2.40	0.53
15:H:283:TYR:HD2	15:H:286:GLU:HB2	1.73	0.53
16:I:372:SER:HB3	16:I:412:THR:HA	1.91	0.53
17:J:301:ASP:HB3	17:J:304:LEU:HG	1.90	0.53
19:L:147:THR:HG21	19:L:156:MET:HE2	1.91	0.53
24:Q:382:LEU:O	25:R:263:ARG:NH1	2.40	0.53
24:Q:404:ASN:O	25:R:397:ASN:ND2	2.41	0.53
5:5:104:GLN:NE2	3:h:176:ASP:O	2.41	0.53
14:G:73:HIS:ND1	14:G:74:ILE:HG13	2.23	0.53
10:d:70:ASN:HB3	10:d:73:ILE:HB	1.89	0.53
12:m:159:GLU:OE1	12:m:163:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:k:73:HIS:NE2	14:k:107:ILE:O	2.33	0.53
19:L:351:LEU:HD12	19:L:352:PRO:HD2	1.90	0.53
5:f:128:GLN:HB3	6:e:113:GLN:HE22	1.74	0.53
13:l:47:VAL:HG22	13:l:213:ILE:HG22	1.90	0.53
17:J:251:ASP:OD1	17:J:253:ILE:HG12	2.07	0.53
19:L:131:VAL:HB	19:L:135:VAL:HG21	1.89	0.53
21:N:305:ASN:HD22	21:N:871:MET:HE1	1.73	0.53
2:2:48:ARG:NH2	6:e:241:ASP:OD2	2.41	0.53
9:j:119:GLN:OE1	9:j:122:THR:OG1	2.26	0.53
17:J:155:LYS:HD3	17:J:317:PRO:HG3	1.90	0.53
18:K:77:ARG:HH22	21:N:577:SER:HA	1.74	0.53
20:M:290:ARG:H	20:M:332:VAL:HG21	1.73	0.53
25:R:312:TYR:HA	25:R:316:LEU:HD12	1.89	0.53
28:U:265:LEU:HB3	28:U:268:LYS:HE2	1.90	0.53
29:V:116:CYS:HG	29:V:117:TRP:CD1	2.25	0.53
10:d:156:ASN:HA	11:n:83:ARG:HH22	1.74	0.53
15:H:399:GLU:HB3	15:H:402:ILE:HG23	1.89	0.53
16:I:358:LYS:HZ1	16:I:395:MET:HE1	1.73	0.53
28:U:276:ILE:O	28:U:280:ASN:ND2	2.42	0.53
4:4:4:ILE:HG12	4:4:103:LEU:HD12	1.90	0.53
11:n:12:SER:OG	11:n:14:ASP:OD1	2.23	0.53
20:M:219:LEU:HD21	20:M:330:VAL:HG21	1.90	0.53
21:N:510:HIS:HB3	21:N:513:ILE:HB	1.90	0.53
24:Q:431:SER:HA	25:R:422:ARG:HG3	1.91	0.53
29:V:97:GLN:HG3	29:V:98:THR:HG23	1.90	0.53
1:1:89:TYR:HD1	14:G:111:ALA:HB1	1.74	0.53
7:7:161:ARG:HE	7:7:169:THR:HB	1.74	0.53
13:F:2:PHE:N	13:F:24:TYR:HH	2.07	0.53
20:M:357:ARG:NH2	20:M:383:THR:O	2.42	0.53
33:Z:596:THR:HA	33:Z:599:ILE:HD12	1.91	0.53
7:a:48:LYS:HG2	7:a:53:VAL:HG12	1.90	0.53
16:I:93:LYS:H	16:I:96:LEU:HD13	1.73	0.53
18:K:281:ARG:NH2	18:K:285:GLN:H	2.07	0.53
20:M:357:ARG:HD2	20:M:391:LEU:HD21	1.90	0.53
3:h:107:PRO:HD2	3:h:124:PHE:HB2	1.91	0.52
4:g:71:GLU:O	10:d:144:TYR:OH	2.23	0.52
9:B:13:SER:HB2	9:B:18:LEU:HD23	1.91	0.52
18:K:213:GLY:O	18:K:219:LYS:NZ	2.42	0.52
27:T:129:LEU:HD12	27:T:136:LEU:HD12	1.91	0.52
33:Z:512:ILE:HG23	33:Z:521:GLU:HB3	1.91	0.52
3:h:104:PHE:HD1	3:h:126:LEU:HD13	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:77:THR:HG21	5:f:239:ALA:HB1	1.92	0.52
8:A:114:CYS:HA	8:A:117:LEU:HB3	1.90	0.52
12:E:146:GLY:HA2	12:E:222:ILE:HG21	1.90	0.52
15:H:299:ARG:NH2	15:H:339:GLN:OE1	2.42	0.52
18:K:99:PHE:HA	18:K:110:VAL:HG12	1.92	0.52
21:N:424:LYS:NZ	21:N:461:GLU:OE1	2.42	0.52
13:F:76:GLY:HA3	13:F:130:VAL:HA	1.90	0.52
13:F:153:VAL:HB	14:G:86:ARG:HH12	1.74	0.52
12:m:122:ARG:HA	12:m:132:ARG:HD3	1.91	0.52
15:H:279:LEU:HD22	15:H:287:GLY:HA2	1.90	0.52
21:N:259:PHE:HB2	21:N:902:VAL:HG13	1.90	0.52
3:3:28:ARG:HB2	3:3:183:TRP:HB2	1.92	0.52
5:f:82:ARG:NH1	5:f:185:PRO:O	2.41	0.52
10:C:97:ASN:HA	10:C:100:LYS:HD3	1.90	0.52
12:E:166:ARG:HB3	13:F:58:SER:HB2	1.91	0.52
25:R:363:PHE:HD2	32:Y:81:LEU:HD21	1.73	0.52
29:V:29:ILE:HG23	29:V:33:ALA:HB3	1.92	0.52
29:V:221:TRP:NE1	29:V:223:SER:HG	2.07	0.52
8:A:156:LYS:HB3	8:A:166:TYR:HE2	1.75	0.52
9:B:8:SER:HA	9:B:11:THR:O	2.10	0.52
9:B:44:VAL:HG21	9:B:189:ILE:HG12	1.90	0.52
15:H:100:ALA:HB1	15:H:173:ARG:O	2.10	0.52
26:S:311:GLN:NE2	26:S:341:SER:OG	2.42	0.52
1:1:27:PHE:HE2	1:1:32:ILE:HG13	1.73	0.52
4:4:8:ARG:HG3	4:4:13:VAL:HG22	1.91	0.52
6:6:145:ASP:OD1	6:6:156:ARG:NH2	2.43	0.52
14:k:179:LEU:HD11	14:k:187:LEU:HD11	1.92	0.52
15:H:157:VAL:O	15:H:182:ASN:ND2	2.42	0.52
15:H:314:VAL:O	15:H:318:ARG:NH1	2.42	0.52
20:M:221:TYR:HE1	20:M:346:LYS:HB3	1.74	0.52
28:U:46:ARG:NH2	28:U:164:GLU:OE2	2.37	0.52
6:6:107:SER:HB3	12:E:103:TYR:HD1	1.75	0.52
11:n:4:TYR:CZ	11:n:6:ARG:HB3	2.43	0.52
28:U:19:ASP:OD2	28:U:23:ARG:NE	2.42	0.52
9:B:7:PHE:HB2	9:B:9:LEU:HG	1.91	0.52
12:E:99:HIS:ND1	12:E:105:GLU:O	2.38	0.52
10:d:112:VAL:HG22	10:d:137:TYR:HD2	1.75	0.52
20:M:246:LEU:HD22	20:M:262:LEU:HD13	1.92	0.52
21:N:589:ILE:HA	21:N:624:ALA:HB2	1.92	0.52
23:P:55:SER:HA	23:P:59:LEU:HB3	1.90	0.52
7:7:137:ARG:HA	7:7:142:PRO:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:251:PRO:HG2	15:H:254:THR:HB	1.91	0.52
16:I:101:GLY:HA3	16:I:150:HIS:CD2	2.45	0.52
21:N:647:ASP:O	21:N:653:ARG:NE	2.43	0.52
33:Z:446:GLU:HG2	33:Z:484:LYS:HG3	1.91	0.52
16:I:202:LEU:O	33:Z:826:ARG:NH2	2.43	0.52
26:S:393:ARG:NH1	26:S:431:VAL:O	2.43	0.52
26:S:475:TYR:OH	28:U:295:LYS:HG3	2.10	0.52
3:3:123:GLY:HA3	3:3:137:ILE:HG21	1.93	0.51
7:a:40:THR:HG23	7:a:88:GLY:HA2	1.92	0.51
8:c:198:SER:HB3	8:c:201:LYS:HG2	1.92	0.51
17:J:160:ILE:HD11	17:J:198:LEU:HD21	1.91	0.51
22:O:72:LYS:HG2	22:O:73:ILE:HG12	1.92	0.51
22:O:292:CYS:O	22:O:295:THR:OG1	2.26	0.51
25:R:240:SER:HB2	25:R:244:THR:HG22	1.91	0.51
31:X:48:PHE:HB2	31:X:66:LEU:HB3	1.92	0.51
2:2:123:ILE:HG22	2:2:125:ALA:H	1.76	0.51
8:A:14:ARG:O	8:A:27:GLN:NE2	2.43	0.51
13:F:74:LEU:HD13	13:F:81:ALA:HB1	1.92	0.51
19:L:283:VAL:HB	19:L:327:THR:HB	1.91	0.51
24:Q:249:LEU:HB2	24:Q:253:ASN:HB2	1.92	0.51
25:R:347:THR:O	25:R:348:LEU:HD23	2.10	0.51
26:S:425:ARG:NH1	27:T:188:GLU:OE2	2.42	0.51
27:T:190:ALA:HB2	27:T:209:LEU:HD21	1.91	0.51
3:3:30:GLY:HA2	3:3:36:VAL:HG23	1.92	0.51
9:B:21:ILE:O	9:B:25:LEU:N	2.33	0.51
16:I:198:VAL:HG13	16:I:323:LYS:HG3	1.92	0.51
3:3:51:LEU:HD22	3:3:87:PHE:HZ	1.76	0.51
4:4:80:VAL:HG12	4:4:104:ILE:HD13	1.92	0.51
1:b:59:LYS:HD3	1:b:121:TYR:HD2	1.74	0.51
7:a:110:ASP:OD2	13:l:107:ARG:NH1	2.44	0.51
10:C:206:LEU:HD23	10:C:244:ILE:HG21	1.91	0.51
9:j:6:SER:HB2	11:n:4:TYR:HD1	1.75	0.51
18:K:109:ILE:HG12	18:K:119:VAL:HG22	1.92	0.51
18:K:341:PRO:O	18:K:344:ARG:NH1	2.34	0.51
20:M:275:PRO:HB3	20:M:320:ARG:CA	2.22	0.51
27:T:131:LYS:HB3	27:T:134:LYS:HB2	1.92	0.51
28:U:56:GLU:HB2	28:U:66:PHE:HB3	1.92	0.51
28:U:64:VAL:HG22	30:W:92:GLN:HG2	1.92	0.51
29:V:225:LEU:O	29:V:228:TYR:N	2.44	0.51
33:Z:873:LEU:HD13	33:Z:878:LEU:HD21	1.91	0.51
2:2:57:ASP:OD1	2:2:58:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:87:ASP:OD1	9:B:90:ARG:NH2	2.44	0.51
12:E:142:LEU:HB2	12:E:158:ALA:HB3	1.92	0.51
23:P:304:THR:HA	23:P:352:VAL:HG21	1.92	0.51
26:S:82:TYR:CD2	26:S:86:SER:HB3	2.46	0.51
15:H:155:PHE:HZ	20:M:150:LYS:HD2	1.75	0.51
15:H:158:GLY:HA2	20:M:162:GLU:HG3	1.92	0.51
21:N:742:TRP:CE3	21:N:743:PHE:HB3	2.46	0.51
33:Z:352:LYS:HG2	33:Z:462:VAL:HG23	1.91	0.51
14:G:150:MET:HB3	14:G:160:TYR:CE2	2.46	0.51
16:I:148:LEU:HB2	16:I:160:LEU:HG	1.93	0.51
25:R:325:HIS:HB3	25:R:328:PHE:HB2	1.93	0.51
33:Z:217:GLU:HA	33:Z:220:ALA:HB3	1.93	0.51
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.93	0.51
6:6:221:LEU:N	6:6:236:TYR:O	2.41	0.51
7:a:134:TYR:HD1	7:a:137:ARG:HE	1.59	0.51
14:G:54:ILE:HD11	14:G:213:GLU:HG3	1.92	0.51
8:c:54:ILE:HG12	8:c:225:VAL:HG22	1.92	0.51
20:M:116:ALA:HA	20:M:130:PRO:HA	1.93	0.51
28:U:37:LEU:HB2	28:U:49:ASN:HB3	1.92	0.51
33:Z:327:GLN:HG3	33:Z:346:LEU:HD11	1.93	0.51
6:e:76:PHE:CZ	7:a:166:LEU:HB3	2.46	0.51
9:B:16:GLY:O	10:C:28:SER:OG	2.26	0.51
10:C:172:ALA:HB2	10:C:200:THR:HG21	1.93	0.51
12:E:213:ASP:OD1	12:E:214:GLU:N	2.44	0.51
9:j:95:THR:HA	9:j:99:ARG:HD3	1.92	0.51
9:j:179:TRP:HA	9:j:183:LEU:HD11	1.92	0.51
14:k:54:ILE:HB	14:k:211:ASP:HB2	1.92	0.51
20:M:274:ALA:CB	20:M:275:PRO:CD	2.86	0.51
24:Q:426:LEU:HD11	28:U:292:ILE:HG12	1.92	0.51
29:V:28:TYR:CE1	29:V:202:ASP:OD2	2.63	0.51
30:W:109:ARG:HH22	30:W:195:GLY:HA3	1.75	0.51
3:3:27:LEU:HD12	3:3:184:GLY:HA3	1.92	0.51
4:4:73:TYR:HB2	10:C:143:ARG:HH21	1.75	0.51
7:7:58:ASP:HA	7:7:228:PHE:HA	1.93	0.51
5:f:156:LYS:HG2	11:n:101:GLU:HB2	1.92	0.51
12:m:71:ASP:HB3	12:m:74:ILE:HB	1.93	0.51
15:H:227:LEU:HD22	20:M:403:LEU:HD22	1.92	0.51
18:K:120:VAL:HG11	18:K:139:LEU:HD22	1.93	0.51
20:M:62:ILE:HG13	20:M:66:LYS:HG3	1.92	0.51
24:Q:195:LYS:HG2	24:Q:225:LEU:HD13	1.93	0.51
7:7:54:ILE:HD11	7:7:230:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:50:THR:HG22	2:i:55:VAL:HG22	1.93	0.50
2:i:74:GLY:HA3	2:i:81:THR:HG21	1.93	0.50
14:G:150:MET:HB3	14:G:160:TYR:HE2	1.75	0.50
14:G:224:THR:HG22	14:G:229:LYS:HD2	1.93	0.50
16:I:390:ALA:HB1	17:J:307:PRO:HD2	1.93	0.50
17:J:42:ARG:NE	26:S:484:ASP:OD2	2.44	0.50
25:R:58:GLU:HB3	25:R:144:ILE:HA	1.92	0.50
26:S:129:GLU:OE2	26:S:132:ALA:N	2.44	0.50
7:7:107:ASN:HD22	7:7:120:LEU:HG	1.76	0.50
1:b:198:THR:HG23	1:b:200:ALA:H	1.76	0.50
16:I:336:PRO:HA	16:I:339:ILE:HD12	1.92	0.50
19:L:189:GLN:OE1	19:L:345:ARG:NH2	2.43	0.50
19:L:196:VAL:HG23	19:L:197:ILE:HG12	1.92	0.50
24:Q:172:PRO:HA	24:Q:208:ILE:HD13	1.92	0.50
24:Q:419:LEU:HD22	25:R:414:LEU:HD13	1.93	0.50
1:1:102:LYS:HD2	1:1:138:VAL:HG23	1.93	0.50
3:3:173:ASN:ND2	6:e:176:LYS:O	2.41	0.50
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.93	0.50
6:6:78:ALA:HB2	7:7:167:GLY:HA3	1.93	0.50
10:C:44:ILE:HB	10:C:216:ILE:HD12	1.94	0.50
10:d:76:ALA:O	10:d:136:ILE:N	2.42	0.50
16:I:124:THR:HG22	17:J:91:GLU:HB3	1.94	0.50
17:J:304:LEU:HD23	17:J:309:ARG:HD3	1.91	0.50
29:V:61:TYR:CG	29:V:62:THR:N	2.77	0.50
33:Z:537:THR:O	33:Z:577:GLN:NE2	2.44	0.50
33:Z:559:LYS:HG3	33:Z:561:ASP:H	1.76	0.50
33:Z:601:VAL:HG21	33:Z:623:ARG:HD3	1.92	0.50
6:e:71:MET:HE3	6:e:84:VAL:HG22	1.94	0.50
18:K:123:LEU:HG	18:K:125:THR:H	1.76	0.50
18:K:345:ASP:OD1	18:K:346:ARG:N	2.44	0.50
23:P:283:LYS:HD2	23:P:286:ASN:HD21	1.77	0.50
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.93	0.50
17:J:336:ASN:HB3	17:J:376:HIS:ND1	2.27	0.50
20:M:396:VAL:HG12	20:M:400:MET:HE3	1.93	0.50
21:N:533:ASP:OD1	21:N:559:TYR:OH	2.29	0.50
2:i:244:GLU:HG2	3:h:198:ARG:HG2	1.93	0.50
5:f:82:ARG:HD2	5:f:185:PRO:HB2	1.93	0.50
21:N:436:ASP:HB2	21:N:439:VAL:HG23	1.93	0.50
2:2:63:LEU:HD12	2:2:215:TYR:HE1	1.76	0.50
9:B:200:VAL:HG22	9:B:202:GLY:H	1.76	0.50
11:D:79:ASN:HB2	16:I:437:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:124:GLN:HA	11:n:127:ARG:HE	1.77	0.50
15:H:73:ASP:OD1	15:H:173:ARG:NH2	2.39	0.50
17:J:183:LYS:N	17:J:311:ASP:OD2	2.40	0.50
22:O:290:LYS:NZ	22:O:354:GLN:HE21	2.10	0.50
33:Z:138:ARG:HH21	33:Z:157:LEU:HB2	1.76	0.50
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.58	0.50
13:F:67:ASP:OD1	13:F:68:GLU:N	2.44	0.50
13:l:67:ASP:OD1	13:l:68:GLU:N	2.42	0.50
17:J:88:VAL:HB	17:J:92:GLY:H	1.76	0.50
19:L:298:ASP:HB3	19:L:302:GLN:HG2	1.94	0.50
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.76	0.50
2:i:32:ILE:HD13	2:i:73:ALA:HB1	1.92	0.50
10:d:162:ALA:HB3	11:n:54:LEU:HD21	1.94	0.50
15:H:399:GLU:HG2	15:H:401:GLY:H	1.77	0.50
21:N:891:VAL:HB	21:N:908:ARG:HD3	1.94	0.50
25:R:347:THR:HA	25:R:389:GLU:HA	1.94	0.50
3:3:145:GLN:HE21	6:e:167:PRO:HG3	1.77	0.49
1:b:47:ASN:HD21	2:i:151:GLY:HA3	1.76	0.49
3:h:59:ASP:OD2	3:h:103:TYR:HB3	2.11	0.49
19:L:425:VAL:HG21	20:M:345:ARG:HA	1.94	0.49
26:S:418:THR:HG22	26:S:422:MET:HE2	1.93	0.49
29:V:25:GLU:HB3	29:V:63:VAL:HG21	1.94	0.49
29:V:250:GLN:HE22	29:V:253:LYS:HD3	1.77	0.49
30:W:114:VAL:HG21	30:W:141:ILE:HG23	1.94	0.49
2:2:192:ILE:HG23	2:2:199:GLY:HA2	1.94	0.49
7:7:48:LYS:HG2	7:7:53:VAL:HG12	1.93	0.49
2:i:81:THR:HG23	2:i:127:LEU:HD11	1.94	0.49
11:D:181:ARG:NH1	12:E:59:LEU:O	2.45	0.49
12:E:71:ASP:OD1	12:E:72:ARG:N	2.44	0.49
13:F:226:ASP:OD1	13:F:227:GLY:N	2.45	0.49
18:K:241:GLU:O	18:K:243:VAL:HG23	2.12	0.49
19:L:219:LEU:HD11	19:L:327:THR:HG22	1.95	0.49
25:R:236:ALA:HB1	25:R:279:LEU:HD21	1.94	0.49
29:V:95:LEU:HG	29:V:100:ARG:NE	2.27	0.49
29:V:259:LYS:HB2	29:V:279:HIS:CD2	2.45	0.49
31:X:85:ARG:HD2	31:X:101:LEU:HD12	1.94	0.49
2:i:36:LYS:HB2	2:i:152:TYR:HE1	1.77	0.49
14:k:68:GLN:HB3	14:k:93:ARG:HH21	1.76	0.49
15:H:96:PRO:HB3	15:H:191:ILE:HG21	1.94	0.49
15:H:431:ILE:HG21	16:I:200:LEU:HD21	1.95	0.49
24:Q:339:TYR:HE2	24:Q:376:LYS:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:330:LEU:N	32:Y:62:GLU:O	2.44	0.49
30:W:36:ILE:HG12	30:W:191:ILE:HD11	1.94	0.49
7:7:185:ASN:HB3	7:7:186:PRO:HD3	1.93	0.49
8:A:168:ALA:HB3	9:B:55:LEU:HD13	1.94	0.49
11:D:117:GLN:HE22	11:D:129:PHE:HB2	1.78	0.49
12:E:130:GLU:HB3	12:E:132:ARG:HH12	1.77	0.49
13:F:39:ARG:NH2	13:F:155:GLU:OE2	2.46	0.49
11:n:65:SER:HB3	11:n:90:ARG:HH21	1.75	0.49
12:m:201:LEU:HB3	12:m:243:LEU:HD22	1.93	0.49
13:l:72:LEU:HD13	13:l:132:LEU:HD22	1.94	0.49
6:6:84:VAL:HG12	6:6:88:LYS:HE3	1.94	0.49
2:i:36:LYS:HB2	2:i:152:TYR:CE1	2.47	0.49
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.94	0.49
8:c:72:ILE:HG12	8:c:82:VAL:HG22	1.93	0.49
9:j:45:ILE:HD12	9:j:74:VAL:HB	1.93	0.49
16:I:251:GLU:O	16:I:254:GLN:NE2	2.43	0.49
18:K:238:ASN:HB2	18:K:241:GLU:HG3	1.94	0.49
18:K:386:ILE:HG12	18:K:414:GLN:HG3	1.94	0.49
19:L:318:LEU:HB3	19:L:321:THR:HB	1.94	0.49
25:R:40:ILE:HG12	25:R:88:LEU:HD13	1.95	0.49
26:S:30:GLN:OE1	26:S:64:ARG:NH2	2.46	0.49
27:T:29:PRO:HA	27:T:32:ILE:HD12	1.94	0.49
7:7:232:ILE:HB	7:7:240:THR:HB	1.94	0.49
9:B:119:GLN:HB3	10:C:86:ILE:HD11	1.95	0.49
15:H:177:ASP:OD1	15:H:283:TYR:OH	2.22	0.49
17:J:79:VAL:HG12	17:J:81:ASP:H	1.78	0.49
18:K:148:ASP:OD1	18:K:149:ILE:N	2.45	0.49
22:O:366:MET:HE3	28:U:233:PHE:HE2	1.77	0.49
24:Q:81:SER:HA	24:Q:84:TYR:HD2	1.76	0.49
33:Z:518:LEU:HB2	33:Z:562:TRP:HH2	1.77	0.49
5:5:93:SER:OG	5:5:249:SER:N	2.31	0.49
1:b:82:LEU:O	1:b:86:THR:N	2.44	0.49
18:K:283:ASP:OD1	18:K:284:ALA:N	2.44	0.49
19:L:105:ILE:HD11	19:L:145:ARG:HD2	1.94	0.49
21:N:654:GLN:HG3	21:N:698:GLY:HA3	1.95	0.49
27:T:41:ILE:HG23	27:T:87:PRO:HG3	1.95	0.49
7:7:172:SER:OG	7:7:174:THR:O	2.28	0.49
1:b:80:TYR:HB2	8:c:102:ALA:HB1	1.93	0.49
1:b:132:ILE:HG23	1:b:136:GLY:HA2	1.94	0.49
2:i:46:ASP:HA	2:i:202:VAL:HA	1.94	0.49
14:G:204:HIS:CE1	14:G:208:LYS:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:101:GLY:HA3	16:I:150:HIS:HD2	1.78	0.49
16:I:217:LYS:NZ	16:I:318:ASP:OD1	2.40	0.49
18:K:426:PHE:HB3	18:K:428:LYS:NZ	2.28	0.49
21:N:190:LEU:HD13	21:N:207:LEU:HD21	1.93	0.49
24:Q:387:TYR:HB3	24:Q:400:TYR:HD2	1.78	0.49
33:Z:400:ILE:HD13	33:Z:422:ILE:HG23	1.93	0.49
1:b:194:MET:HB2	1:b:205:LEU:HB2	1.95	0.49
4:g:35:THR:HA	4:g:45:SER:HA	1.95	0.49
4:g:60:ILE:HG12	4:g:83:PHE:HE2	1.77	0.49
24:Q:92:LYS:HA	24:Q:129:LYS:HE2	1.95	0.49
26:S:293:ILE:HD13	26:S:316:LEU:HD23	1.95	0.49
26:S:424:SER:HB3	27:T:192:ASN:HB3	1.95	0.49
29:V:55:GLY:HA2	29:V:66:VAL:HG23	1.95	0.49
31:X:66:LEU:HD11	31:X:91:PHE:HE2	1.78	0.49
33:Z:382:ALA:HA	33:Z:846:PHE:HD1	1.76	0.49
3:h:125:ASP:OD1	3:h:128:GLY:N	2.46	0.49
16:I:294:SER:HA	16:I:299:GLU:HA	1.93	0.49
19:L:244:ILE:HB	19:L:278:ILE:HA	1.95	0.49
23:P:177:ILE:HG23	23:P:203:ILE:HD12	1.94	0.49
28:U:226:LEU:HD23	28:U:229:LEU:HD12	1.94	0.49
11:D:17:ILE:HG22	11:D:19:GLN:H	1.77	0.48
15:H:363:PRO:HA	15:H:366:LEU:HB3	1.95	0.48
16:I:408:ARG:NH1	16:I:412:THR:OG1	2.46	0.48
18:K:217:THR:OG1	18:K:380:GLY:N	2.46	0.48
18:K:244:HIS:O	19:L:299:ARG:NH1	2.44	0.48
19:L:108:VAL:HG22	19:L:119:VAL:HG12	1.94	0.48
21:N:521:LEU:HB3	21:N:535:LEU:HD21	1.95	0.48
21:N:664:LEU:HD13	21:N:678:ILE:HG21	1.95	0.48
29:V:228:TYR:HB3	29:V:232:GLU:HB2	1.95	0.48
6:6:76:PHE:CE2	6:6:78:ALA:HB3	2.48	0.48
3:h:65:GLU:OE2	4:g:85:ARG:NH2	2.46	0.48
8:c:192:ASP:OD1	8:c:193:HIS:ND1	2.43	0.48
15:H:368:PRO:HD2	20:M:389:ALA:HB1	1.95	0.48
18:K:91:SER:OG	18:K:92:VAL:N	2.45	0.48
18:K:271:ILE:N	18:K:315:ILE:O	2.41	0.48
20:M:135:VAL:HG12	20:M:158:THR:HG23	1.94	0.48
20:M:220:MET:HB3	20:M:349:PHE:HE2	1.77	0.48
21:N:239:LEU:HG	21:N:243:LYS:HE3	1.95	0.48
23:P:361:THR:HG22	23:P:363:LEU:H	1.78	0.48
23:P:411:LEU:HD13	29:V:297:THR:HG21	1.95	0.48
24:Q:97:LEU:HB3	24:Q:130:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:486:LYS:HE2	28:U:301:ILE:HG22	1.95	0.48
5:5:162:VAL:HG11	5:5:192:SER:HA	1.95	0.48
2:i:32:ILE:HB	2:i:156:LEU:HB3	1.95	0.48
9:j:157:PHE:HE1	10:d:64:GLU:HB3	1.77	0.48
11:n:56:ASP:HB3	11:n:59:ILE:HG12	1.96	0.48
18:K:271:ILE:HB	18:K:316:MET:HA	1.95	0.48
18:K:418:ASP:OD1	18:K:419:ASN:N	2.45	0.48
19:L:104:LEU:HD23	20:M:127:VAL:HG12	1.95	0.48
21:N:96:GLN:HG3	26:S:220:ILE:HG12	1.94	0.48
21:N:756:THR:HG21	21:N:876:PRO:HD3	1.95	0.48
24:Q:129:LYS:HG3	24:Q:133:LEU:HD12	1.95	0.48
1:b:208:TYR:CD1	1:b:209:PRO:HD2	2.48	0.48
5:f:126:ASP:HB3	5:f:172:MET:HE2	1.95	0.48
6:e:48:ASN:O	6:e:55:ASN:N	2.45	0.48
11:D:161:ALA:HB1	11:D:175:LEU:HD22	1.95	0.48
13:F:9:ASP:OD1	13:F:10:THR:N	2.47	0.48
15:H:328:GLU:CD	15:H:329:VAL:HG23	2.39	0.48
16:I:184:ILE:HB	16:I:187:LEU:HD12	1.94	0.48
17:J:162:GLU:HA	17:J:166:LEU:HD13	1.95	0.48
18:K:102:PRO:HA	18:K:108:GLY:HA2	1.94	0.48
23:P:89:LEU:HG	23:P:91:LEU:H	1.78	0.48
29:V:225:LEU:O	29:V:229:ASP:N	2.47	0.48
1:b:103:GLU:HG2	14:k:102:LEU:HD23	1.95	0.48
9:B:35:LEU:HD22	9:B:175:LEU:HD21	1.95	0.48
13:F:176:LEU:HD13	14:G:58:LEU:HD23	1.95	0.48
14:G:80:GLY:HA3	14:G:134:VAL:HG12	1.94	0.48
9:j:49:LYS:HD3	9:j:58:SER:HB2	1.95	0.48
11:n:181:ARG:HH22	12:m:60:GLU:HA	1.78	0.48
15:H:217:GLN:NE2	15:H:378:SER:H	2.11	0.48
16:I:282:ASP:OD1	16:I:283:GLU:N	2.46	0.48
17:J:61:GLU:OE2	18:K:121:ARG:NH2	2.45	0.48
18:K:60:LEU:HD21	21:N:601:THR:HB	1.95	0.48
18:K:399:ARG:HD3	23:P:198:VAL:HG11	1.95	0.48
20:M:324:LEU:HA	20:M:343:LEU:HD21	1.94	0.48
23:P:94:GLN:HA	23:P:97:ILE:HD12	1.96	0.48
33:Z:475:GLN:HE22	33:Z:502:ASN:HD22	1.61	0.48
4:4:33:ASP:OD1	4:4:34:LYS:N	2.46	0.48
6:6:50:THR:OG1	6:6:55:ASN:ND2	2.36	0.48
1:b:57:HIS:HB3	1:b:60:ILE:HB	1.95	0.48
13:F:81:ALA:HB2	13:F:130:VAL:HG21	1.96	0.48
8:c:44:ALA:HB2	8:c:53:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:72:LYS:HG2	10:d:225:VAL:HB	1.94	0.48
14:k:168:GLY:HA3	14:k:203:ALA:HB1	1.95	0.48
15:H:240:ILE:HD13	20:M:399:GLY:HA3	1.95	0.48
29:V:38:LEU:O	29:V:42:ARG:HG3	2.13	0.48
3:3:113:ASN:ND2	3:3:116:SER:OG	2.47	0.48
14:G:68:GLN:O	14:G:76:CYS:N	2.46	0.48
15:H:357:ARG:HH21	15:H:359:ASN:HD22	1.62	0.48
21:N:25:LEU:HD23	21:N:28:ILE:HD12	1.96	0.48
21:N:301:THR:HG21	21:N:921:ARG:HB3	1.96	0.48
21:N:303:LEU:HD21	21:N:755:PRO:HB3	1.96	0.48
29:V:51:GLY:HA3	29:V:108:TYR:CZ	2.48	0.48
33:Z:598:ALA:HB3	33:Z:738:TYR:HB3	1.96	0.48
5:5:91:VAL:HG21	5:5:108:LYS:HB2	1.94	0.48
10:C:144:TYR:HB3	11:D:59:ILE:HG22	1.94	0.48
17:J:156:GLN:HE21	17:J:198:LEU:HD22	1.78	0.48
11:n:41:CYS:HA	11:n:138:PHE:HZ	1.78	0.48
11:n:118:GLN:HE22	12:m:86:ARG:HB2	1.79	0.48
31:X:17:TYR:HH	31:X:97:TYR:HH	1.60	0.48
3:3:205:ASP:OD2	5:f:94:ARG:NH2	2.45	0.48
7:a:131:THR:HG21	13:l:98:VAL:HG22	1.95	0.48
21:N:728:LYS:HB3	21:N:751:LEU:HB3	1.95	0.48
25:R:240:SER:HB3	25:R:243:LEU:HB2	1.96	0.48
29:V:59:ASP:O	29:V:60:ASP:CB	2.62	0.48
4:4:29:LYS:HE3	4:4:32:ASP:H	1.78	0.47
4:4:36:ARG:HG2	4:4:46:PHE:HE1	1.79	0.47
3:h:10:GLY:HA3	3:h:42:LYS:HE2	1.96	0.47
5:f:191:ASP:OD1	5:f:192:SER:N	2.46	0.47
8:A:200:GLU:HB3	8:A:244:ARG:HH12	1.79	0.47
13:F:121:GLN:NE2	14:G:84:ASP:OD1	2.46	0.47
10:d:120:GLN:NE2	11:n:81:ASP:OD1	2.46	0.47
11:n:92:GLU:HA	11:n:95:SER:HB3	1.96	0.47
15:H:107:LYS:HB2	15:H:144:LYS:HG3	1.95	0.47
16:I:105:SER:O	16:I:149:LEU:HB2	2.14	0.47
20:M:165:SER:HB3	20:M:258:GLU:HG2	1.96	0.47
21:N:416:GLY:HA3	21:N:453:ALA:HB1	1.96	0.47
21:N:600:THR:HA	21:N:634:LEU:HD22	1.96	0.47
9:B:44:VAL:HG23	9:B:213:ILE:HG22	1.95	0.47
9:j:5:TYR:HE1	10:d:3:SER:HA	1.78	0.47
17:J:64:LEU:HB3	18:K:121:ARG:HD2	1.95	0.47
20:M:78:LEU:HD22	20:M:150:LYS:HA	1.96	0.47
21:N:104:LYS:HG3	21:N:108:MET:HE2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:630:ALA:HB2	21:N:662:MET:HE2	1.96	0.47
4:4:146:HIS:HA	5:f:281:SER:HB2	1.96	0.47
9:j:95:THR:HA	9:j:99:ARG:HB2	1.96	0.47
14:k:95:GLU:HB3	14:k:115:ARG:HD3	1.96	0.47
18:K:212:TYR:HB2	18:K:339:GLU:HA	1.96	0.47
26:S:119:TYR:CE2	26:S:121:VAL:HB	2.50	0.47
29:V:197:TYR:CE2	29:V:199:LEU:HB2	2.49	0.47
12:E:161:SER:HB2	20:M:433:TYR:HD2	1.79	0.47
11:n:162:GLN:HE22	11:n:172:ARG:HD3	1.79	0.47
25:R:331:ARG:NH2	32:Y:72:ASP:O	2.47	0.47
26:S:428:ARG:NH1	27:T:191:LYS:O	2.48	0.47
30:W:186:ALA:HA	30:W:191:ILE:HD12	1.97	0.47
33:Z:342:LEU:HB2	33:Z:345:GLU:HG2	1.96	0.47
1:1:23:MET:HE2	1:1:174:ILE:HG12	1.95	0.47
3:h:56:LEU:HD23	3:h:59:ASP:HB2	1.95	0.47
10:C:44:ILE:H	10:C:216:ILE:HB	1.78	0.47
10:C:50:ARG:NH1	10:C:59:GLN:O	2.29	0.47
18:K:325:ASP:OD2	18:K:329:LEU:HB2	2.14	0.47
26:S:26:ALA:HB2	26:S:68:LEU:HD12	1.96	0.47
28:U:175:LEU:HD23	29:V:205:LYS:HE3	1.97	0.47
33:Z:415:MET:HE2	33:Z:447:VAL:HG22	1.97	0.47
5:5:113:ASN:OD1	5:5:116:LEU:N	2.47	0.47
4:g:58:GLU:CD	5:f:156:LYS:HZ1	2.23	0.47
9:B:94:HIS:O	9:B:99:ARG:N	2.43	0.47
11:D:139:ASP:HB2	11:D:142:ASP:HB3	1.96	0.47
10:d:208:TYR:HB2	10:d:235:ILE:HG22	1.95	0.47
18:K:268:ILE:HG12	18:K:313:LYS:HB3	1.97	0.47
24:Q:419:LEU:HD12	25:R:410:LEU:HD13	1.97	0.47
26:S:480:ARG:HD2	26:S:483:GLU:HB2	1.95	0.47
33:Z:358:TYR:HA	33:Z:361:HIS:HD2	1.80	0.47
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.97	0.47
8:A:78:THR:H	8:A:233:PHE:HB2	1.79	0.47
13:F:39:ARG:NH1	13:F:142:ALA:O	2.48	0.47
8:c:73:PHE:O	8:c:81:MET:N	2.47	0.47
10:d:112:VAL:HG22	10:d:137:TYR:CD2	2.49	0.47
12:m:184:LEU:HA	13:l:56:LEU:HD11	1.97	0.47
13:l:156:LEU:HG	14:k:59:LEU:HA	1.95	0.47
13:l:226:ASP:OD1	13:l:227:GLY:N	2.47	0.47
15:H:98:GLN:HG3	16:I:110:GLU:HB3	1.96	0.47
16:I:100:ARG:HD3	16:I:133:LEU:HD23	1.97	0.47
16:I:135:PHE:CD2	16:I:136:VAL:HG13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:281:ARG:HH22	18:K:285:GLN:H	1.62	0.47
20:M:144:ASP:OD1	20:M:145:LEU:N	2.47	0.47
20:M:149:ASN:OD1	20:M:150:LYS:N	2.47	0.47
20:M:187:ASP:HA	20:M:190:ILE:HB	1.96	0.47
21:N:360:GLN:HG3	29:V:168:LEU:HD12	1.97	0.47
23:P:119:ILE:HG23	23:P:125:VAL:HG11	1.96	0.47
3:3:80:ARG:HE	9:B:142:PHE:HB3	1.79	0.47
7:a:148:ILE:HD11	7:a:177:THR:HG23	1.95	0.47
8:c:14:ARG:O	8:c:27:GLN:NE2	2.32	0.47
11:n:65:SER:O	11:n:73:LEU:N	2.43	0.47
12:m:51:GLU:HG2	12:m:53:ARG:HG3	1.96	0.47
18:K:123:LEU:H	18:K:146:LEU:HD23	1.79	0.47
18:K:357:ALA:HB1	18:K:362:LEU:HD11	1.97	0.47
19:L:371:THR:HG22	19:L:407:ARG:HH21	1.80	0.47
21:N:286:LEU:HD23	21:N:289:ILE:HD12	1.97	0.47
22:O:76:LEU:HA	22:O:79:VAL:HG12	1.97	0.47
25:R:213:TYR:HD1	25:R:216:ILE:HD12	1.80	0.47
28:U:262:GLN:HG2	28:U:265:LEU:HD12	1.95	0.47
29:V:159:ILE:HB	29:V:195:HIS:HB3	1.97	0.47
33:Z:331:GLY:HA3	33:Z:346:LEU:HD22	1.96	0.47
6:6:81:ASP:OD2	7:7:169:THR:OG1	2.33	0.47
3:h:35:GLY:HA3	3:h:183:TRP:HH2	1.80	0.47
6:e:32:LEU:HD21	6:e:169:LEU:HD11	1.96	0.47
10:C:156:ASN:ND2	16:I:436:TYR:O	2.48	0.47
11:n:93:ALA:HA	11:n:104:VAL:HG11	1.96	0.47
33:Z:249:MET:HG3	33:Z:253:VAL:HG21	1.96	0.47
33:Z:577:GLN:HB3	33:Z:580:GLN:HB2	1.96	0.47
1:1:214:GLN:HE21	7:a:226:ARG:HH12	1.63	0.47
3:3:107:PRO:HG2	3:3:124:PHE:HB2	1.97	0.47
7:a:92:ASP:HB3	7:a:145:ASN:HD21	1.80	0.47
8:c:60:PRO:HD2	8:c:64:LEU:HD11	1.97	0.47
11:n:159:TRP:HZ3	12:m:56:SER:HB3	1.80	0.47
12:m:108:ASN:HB3	12:m:111:SER:HB3	1.97	0.47
14:k:73:HIS:CD2	14:k:74:ILE:HG13	2.50	0.47
24:Q:47:ASP:OD1	24:Q:48:ASP:N	2.47	0.47
2:2:189:GLN:HB2	2:2:220:LEU:HD21	1.97	0.46
8:c:77:ARG:NH1	8:c:231:ASP:O	2.48	0.46
9:j:31:GLY:HA3	9:j:77:GLY:HA2	1.97	0.46
9:j:189:ILE:HD11	9:j:213:ILE:HD13	1.96	0.46
29:V:59:ASP:O	29:V:60:ASP:HB3	2.16	0.46
6:6:29:GLY:H	6:6:216:GLN:HG3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:11:ILE:HG21	3:h:142:ALA:HB3	1.97	0.46
5:f:138:CYS:HB3	5:f:149:ILE:HG13	1.96	0.46
14:G:218:TRP:HH2	14:G:223:GLU:HB2	1.80	0.46
8:c:81:MET:HE1	8:c:94:ALA:HB2	1.98	0.46
16:I:358:LYS:HD3	16:I:381:VAL:HA	1.98	0.46
18:K:326:PRO:HD2	18:K:328:LEU:HG	1.98	0.46
23:P:123:ARG:HA	23:P:126:THR:HB	1.97	0.46
24:Q:426:LEU:HD22	28:U:295:LYS:HB2	1.96	0.46
25:R:381:ILE:HB	26:S:399:TYR:HD1	1.80	0.46
28:U:82:ILE:HG23	29:V:70:ALA:HB3	1.95	0.46
30:W:163:ASN:HB3	30:W:164:PRO:HD3	1.96	0.46
33:Z:613:ASP:OD1	33:Z:614:VAL:N	2.48	0.46
3:3:65:GLU:HG2	10:C:100:LYS:HA	1.97	0.46
4:4:89:ALA:O	4:4:93:ARG:NE	2.48	0.46
4:4:165:VAL:HG13	4:4:176:PHE:HZ	1.80	0.46
1:b:210:ASP:HA	1:b:213:GLU:HB2	1.97	0.46
7:a:44:VAL:HG12	7:a:148:ILE:HD12	1.97	0.46
9:B:38:LYS:HA	9:B:43:VAL:HG22	1.98	0.46
10:C:50:ARG:HH21	10:C:212:GLU:HG2	1.80	0.46
11:n:65:SER:N	11:n:73:LEU:O	2.45	0.46
22:O:114:GLN:HG2	22:O:118:GLY:HA3	1.95	0.46
23:P:47:ARG:HG2	23:P:52:LEU:HG	1.97	0.46
23:P:393:VAL:H	24:Q:354:PHE:HB3	1.80	0.46
24:Q:135:HIS:ND1	24:Q:169:ASP:OD2	2.49	0.46
24:Q:374:GLU:O	25:R:345:TYR:OH	2.33	0.46
28:U:15:LEU:HD22	29:V:213:LEU:HD21	1.96	0.46
33:Z:87:LYS:HD3	33:Z:90:LYS:HG3	1.98	0.46
9:B:77:GLY:HA3	9:B:132:VAL:HG12	1.98	0.46
11:D:149:GLN:NE2	11:D:157:SER:OG	2.48	0.46
10:d:120:GLN:HE22	11:n:81:ASP:HA	1.80	0.46
15:H:106:ILE:HG12	20:M:76:PRO:HD3	1.97	0.46
15:H:226:GLU:HA	15:H:267:THR:HG22	1.97	0.46
22:O:306:ARG:NH2	28:U:234:ASN:OD1	2.49	0.46
25:R:117:ILE:HD12	25:R:137:LEU:HD22	1.98	0.46
1:1:103:GLU:HG3	14:G:102:LEU:HA	1.97	0.46
3:3:53:ILE:HG22	3:3:60:VAL:HG22	1.97	0.46
6:e:50:THR:OG1	6:e:55:ASN:ND2	2.39	0.46
10:C:226:TYR:CE2	10:C:228:LYS:HB2	2.51	0.46
13:F:54:ASP:H	13:F:57:SER:HB3	1.81	0.46
15:H:248:LEU:HB2	15:H:354:ALA:HA	1.97	0.46
15:H:396:MET:HA	16:I:212:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:341:ILE:HG22	22:O:348:VAL:HG13	1.98	0.46
23:P:388:ILE:HG22	23:P:389:ILE:HG23	1.97	0.46
29:V:67:ASP:OD1	29:V:68:VAL:N	2.48	0.46
2:2:126:TYR:HB3	2:2:156:LEU:HD21	1.97	0.46
6:6:220:GLY:H	6:6:238:LEU:HB2	1.80	0.46
19:L:182:GLY:HA2	19:L:363:ILE:HD13	1.97	0.46
21:N:602:VAL:HB	21:N:603:PRO:HD3	1.98	0.46
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.48	0.46
33:Z:911:LYS:HE3	33:Z:964:GLU:HB3	1.97	0.46
2:2:36:LYS:HD2	2:2:152:TYR:HD1	1.81	0.46
15:H:311:ILE:HD12	15:H:314:VAL:HB	1.97	0.46
19:L:298:ASP:O	19:L:301:ILE:N	2.48	0.46
23:P:144:VAL:HG12	23:P:148:LYS:HE3	1.98	0.46
24:Q:98:LYS:HD2	24:Q:136:SER:HB3	1.98	0.46
24:Q:249:LEU:HB3	24:Q:252:HIS:HB2	1.96	0.46
26:S:357:LEU:HB3	26:S:384:ARG:HH22	1.80	0.46
28:U:273:LEU:HA	28:U:276:ILE:HD12	1.98	0.46
33:Z:256:LEU:HB3	33:Z:257:PRO:HD3	1.97	0.46
33:Z:841:GLU:H	33:Z:844:ALA:HB3	1.81	0.46
5:f:130:TRP:CZ3	5:f:161:LEU:HD13	2.51	0.46
7:a:234:ASP:OD1	7:a:235:LYS:N	2.49	0.46
11:n:189:GLU:HG3	11:n:232:TYR:HE1	1.81	0.46
22:O:2:PHE:HE1	22:O:35:GLU:HA	1.81	0.46
9:B:68:THR:HG21	9:B:105:PRO:HD2	1.98	0.46
9:B:90:ARG:O	9:B:94:HIS:ND1	2.29	0.46
15:H:105:ILE:HB	15:H:146:VAL:HG22	1.97	0.46
18:K:211:LEU:HD23	18:K:338:ILE:HB	1.97	0.46
19:L:374:PHE:HA	19:L:412:PRO:HG3	1.98	0.46
3:3:138:VAL:HG12	3:3:143:SER:HB2	1.98	0.46
4:4:142:SER:HB3	5:f:210:PHE:HA	1.98	0.46
5:5:283:ASN:HD22	4:g:149:ARG:HA	1.81	0.46
6:e:76:PHE:HE2	6:e:78:ALA:HB3	1.81	0.46
10:C:70:ASN:OD1	10:C:73:ILE:N	2.49	0.46
9:j:10:THR:HG22	9:j:18:LEU:HD22	1.97	0.46
23:P:59:LEU:HD21	23:P:82:LEU:HD13	1.97	0.46
30:W:143:ASN:ND2	30:W:149:GLN:O	2.49	0.46
1:1:143:TYR:OH	1:1:158:ASP:OD1	2.33	0.45
3:h:13:VAL:HG13	3:h:167:ILE:HD11	1.97	0.45
10:C:119:LYS:NZ	10:C:151:SER:OG	2.45	0.45
11:D:79:ASN:HD22	16:I:437:LEU:HG	1.81	0.45
12:E:19:GLY:HA2	13:F:24:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:68:GLN:HB2	14:G:76:CYS:HB3	1.98	0.45
10:d:222:ASP:OD1	10:d:223:GLY:N	2.49	0.45
25:R:331:ARG:HH12	32:Y:69:VAL:HG12	1.80	0.45
26:S:445:THR:HG22	26:S:447:GLU:H	1.81	0.45
28:U:289:ASP:O	28:U:293:GLU:N	2.45	0.45
33:Z:301:THR:O	33:Z:307:HIS:NE2	2.48	0.45
1:1:122:ASP:OD1	1:1:123:ASP:N	2.49	0.45
5:f:234:ARG:HA	5:f:237:LEU:HB3	1.98	0.45
5:f:237:LEU:HD11	5:f:272:PHE:HD1	1.81	0.45
6:e:106:ASN:HA	6:e:142:TYR:HE2	1.80	0.45
9:B:35:LEU:HB2	9:B:175:LEU:HD11	1.97	0.45
9:B:45:ILE:HD12	9:B:74:VAL:HB	1.98	0.45
18:K:212:TYR:N	18:K:338:ILE:O	2.49	0.45
19:L:145:ARG:HH21	19:L:159:LEU:HB3	1.81	0.45
23:P:164:GLN:HG3	23:P:168:TYR:HE2	1.82	0.45
24:Q:423:VAL:HA	24:Q:426:LEU:HD12	1.99	0.45
1:1:64:ARG:HG2	1:1:116:ILE:HG12	1.98	0.45
5:5:134:LEU:HD22	5:5:158:LEU:HB2	1.97	0.45
3:h:188:TYR:HE1	3:h:197:LYS:HG3	1.81	0.45
6:e:89:ASN:ND2	13:l:93:ASN:OD1	2.50	0.45
9:B:214:ILE:HG13	9:B:235:PHE:HD1	1.81	0.45
12:E:41:ALA:HA	12:E:46:VAL:HG22	1.98	0.45
13:F:39:ARG:HD3	13:F:144:LEU:HB2	1.99	0.45
12:m:18:GLU:OE1	12:m:20:ARG:NH2	2.47	0.45
14:k:48:PHE:HE1	14:k:137:ILE:HG22	1.81	0.45
21:N:653:ARG:NH1	21:N:692:GLU:OE1	2.50	0.45
21:N:885:ILE:HG12	21:N:887:ASP:H	1.81	0.45
22:O:270:ILE:HD12	22:O:274:ILE:HG13	1.98	0.45
24:Q:93:THR:O	24:Q:130:ARG:NH2	2.50	0.45
26:S:164:ILE:HB	26:S:165:PRO:HD3	1.98	0.45
1:1:145:ILE:HD12	1:1:150:SER:HB2	1.97	0.45
5:f:206:SER:OG	5:f:243:ASP:OD2	2.34	0.45
11:D:56:ASP:HB3	11:D:59:ILE:HG12	1.98	0.45
8:c:123:ASN:OD1	9:j:83:ARG:NE	2.36	0.45
8:c:147:ASP:OD2	8:c:150:LEU:N	2.44	0.45
8:c:167:LYS:HB2	9:j:55:LEU:HB3	1.98	0.45
14:k:126:TYR:HB2	14:k:129:VAL:HG22	1.97	0.45
17:J:188:TYR:HB2	17:J:315:GLU:HA	1.98	0.45
17:J:335:MET:SD	17:J:362:CYS:HB3	2.56	0.45
18:K:175:GLY:HA3	18:K:351:LEU:HB3	1.98	0.45
21:N:376:LYS:HA	21:N:411:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:90:LYS:HG3	23:P:129:LYS:HB3	1.98	0.45
25:R:220:ALA:HA	25:R:324:ARG:HE	1.82	0.45
30:W:30:ILE:HG23	30:W:73:LEU:HD22	1.98	0.45
7:7:183:MET:HE1	7:7:220:ARG:HB2	1.97	0.45
5:f:113:ASN:OD1	5:f:116:LEU:N	2.49	0.45
12:E:175:GLY:O	15:H:409:ARG:NH2	2.50	0.45
16:I:261:PRO:HB2	16:I:265:ARG:HH12	1.82	0.45
19:L:222:GLY:HA3	19:L:349:ILE:HB	1.97	0.45
19:L:360:ILE:HG22	19:L:391:ILE:HD13	1.98	0.45
21:N:277:LEU:HG	21:N:282:TYR:HB3	1.99	0.45
25:R:348:LEU:HD13	25:R:353:MET:SD	2.57	0.45
3:3:25:CYS:HB2	3:3:42:LYS:NZ	2.32	0.45
5:5:285:VAL:HA	3:h:38:ASN:HD21	1.82	0.45
7:7:187:LEU:HD11	7:7:216:VAL:HG11	1.98	0.45
3:h:12:VAL:HG13	3:h:43:ILE:HD11	1.99	0.45
19:L:156:MET:HG2	19:L:157:ARG:HG2	1.99	0.45
20:M:124:ARG:HH22	20:M:255:TYR:HE1	1.64	0.45
22:O:137:TYR:HB2	22:O:146:ALA:HB2	1.97	0.45
24:Q:97:LEU:HB3	24:Q:130:ARG:NH2	2.32	0.45
28:U:93:HIS:HE1	28:U:121:ILE:HG12	1.81	0.45
33:Z:865:ASP:HB3	33:Z:909:ARG:HD3	1.98	0.45
4:4:135:TYR:HA	4:4:138:PHE:HE2	1.81	0.45
5:f:220:LYS:HB2	5:f:223:LEU:HB2	1.99	0.45
8:A:35:THR:HG21	8:A:140:ILE:HG13	1.99	0.45
10:C:76:ALA:HB3	10:C:136:ILE:HD12	1.98	0.45
8:c:105:ARG:HA	8:c:109:GLY:H	1.82	0.45
11:n:62:SER:OG	11:n:211:GLU:OE2	2.33	0.45
12:m:165:TYR:CE1	13:l:60:GLN:HB2	2.51	0.45
14:k:18:ASP:OD2	14:k:20:ARG:NH2	2.45	0.45
14:k:37:SER:O	14:k:165:THR:OG1	2.28	0.45
15:H:57:LYS:NZ	16:I:95:GLN:O	2.50	0.45
21:N:161:TYR:HE1	21:N:197:VAL:HG22	1.82	0.45
7:7:44:VAL:HG13	7:7:57:ALA:HB2	1.97	0.45
1:b:47:ASN:OD1	1:b:49:VAL:HG22	2.16	0.45
17:J:167:PRO:HG3	17:J:182:PRO:HG2	1.99	0.45
25:R:394:ASP:O	25:R:397:ASN:ND2	2.49	0.45
28:U:293:GLU:HA	28:U:296:ILE:HD12	1.99	0.45
30:W:4:GLU:CD	30:W:109:ARG:HE	2.25	0.45
1:1:63:CYS:HB2	1:1:117:ILE:HB	1.99	0.45
2:2:129:VAL:HB	2:2:140:PHE:HB2	1.98	0.45
2:2:153:TYR:OH	2:2:168:GLU:OE1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:163:SER:O	3:h:145:GLN:HG2	2.17	0.45
3:h:113:ASN:HB3	3:h:117:GLY:H	1.82	0.45
5:f:105:THR:OG1	6:e:153:GLU:OE1	2.35	0.45
9:j:185:LEU:HD11	9:j:213:ILE:HB	1.98	0.45
16:I:287:ILE:HG13	16:I:302:ILE:HG23	1.98	0.45
16:I:427:LYS:HG3	16:I:428:VAL:H	1.82	0.45
17:J:87:LYS:HA	17:J:93:LYS:HA	1.98	0.45
18:K:237:VAL:O	18:K:271:ILE:HA	2.17	0.45
21:N:578:ASP:O	21:N:584:ARG:NE	2.42	0.45
27:T:164:LEU:HB3	27:T:178:THR:HG23	1.98	0.45
27:T:235:PHE:CZ	27:T:237:ASN:HB2	2.51	0.45
28:U:140:GLU:OE2	28:U:152:LYS:NZ	2.39	0.45
3:3:189:ILE:HB	3:3:196:VAL:HB	1.99	0.45
1:b:27:PHE:CE1	1:b:32:ILE:HG13	2.52	0.45
3:h:113:ASN:OD1	3:h:114:SER:N	2.49	0.45
6:e:50:THR:HG1	6:e:55:ASN:HD21	1.60	0.45
6:e:214:HIS:NE2	6:e:216:GLN:HB2	2.32	0.45
9:B:8:SER:OG	9:B:18:LEU:HD21	2.17	0.45
12:m:65:GLU:HB2	12:m:86:ARG:HH22	1.82	0.45
21:N:491:GLY:H	21:N:526:TYR:HB3	1.81	0.45
25:R:204:TRP:CG	25:R:235:LEU:HD12	2.52	0.45
27:T:110:LEU:HD21	27:T:125:GLU:HB2	1.99	0.45
33:Z:571:GLY:HA2	33:Z:574:TYR:HE2	1.82	0.45
4:4:192:VAL:HG12	4:4:194:ASP:H	1.82	0.44
5:5:82:ARG:HH21	5:5:200:ASP:HA	1.80	0.44
5:5:244:ALA:HB1	3:h:179:ALA:HB1	1.99	0.44
9:B:193:LEU:HD21	9:B:211:LEU:HD22	1.99	0.44
13:F:11:VAL:HA	14:G:130:ARG:HD3	1.99	0.44
16:I:116:ASP:HA	16:I:132:ILE:HB	2.00	0.44
16:I:387:LEU:HD22	16:I:391:ASP:HB2	1.99	0.44
18:K:106:ASN:HA	18:K:122:ILE:HB	1.98	0.44
19:L:187:THR:HA	19:L:190:ILE:HB	1.99	0.44
20:M:82:VAL:HG21	20:M:140:LEU:HB3	1.99	0.44
22:O:376:GLN:O	22:O:381:GLY:N	2.43	0.44
32:Y:69:VAL:HG12	32:Y:70:ASP:N	2.30	0.44
33:Z:347:ASN:HA	33:Z:352:LYS:HD2	1.99	0.44
3:3:108:VAL:HA	3:3:123:GLY:HA2	1.98	0.44
6:6:134:ASP:OD1	6:6:138:LYS:N	2.50	0.44
7:7:256:LYS:HG2	1:b:206:ILE:HG21	1.99	0.44
12:m:39:GLY:HA3	12:m:48:LEU:HD23	1.98	0.44
12:m:70:ILE:HG21	12:m:112:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:149:LEU:HD23	15:H:177:ASP:HB2	1.99	0.44
18:K:210:LEU:HD23	18:K:316:MET:HB2	1.99	0.44
21:N:207:LEU:HB3	21:N:228:VAL:HG13	1.98	0.44
21:N:302:PHE:HB3	21:N:757:THR:HG21	2.00	0.44
28:U:93:HIS:CE1	28:U:121:ILE:HG12	2.52	0.44
30:W:30:ILE:HG12	30:W:76:LEU:HD13	2.00	0.44
5:f:93:SER:OG	5:f:104:GLN:O	2.26	0.44
9:B:9:LEU:HB3	9:B:125:GLY:HA2	1.98	0.44
10:C:34:THR:OG1	10:C:167:ALA:O	2.32	0.44
11:D:56:ASP:O	11:D:60:THR:OG1	2.34	0.44
11:D:81:ASP:CG	11:D:127:ARG:HH22	2.24	0.44
11:D:163:THR:HG21	11:D:171:VAL:HB	1.99	0.44
17:J:61:GLU:O	17:J:65:LEU:HG	2.17	0.44
17:J:252:SER:H	17:J:294:THR:HA	1.82	0.44
18:K:349:ARG:NH2	18:K:375:ASN:O	2.50	0.44
20:M:62:ILE:HD12	20:M:65:ASN:HB2	1.98	0.44
20:M:248:ALA:HB2	20:M:282:GLU:HB2	2.00	0.44
23:P:438:ILE:HD11	28:U:98:LEU:HD12	2.00	0.44
33:Z:224:LEU:HD21	33:Z:232:LYS:HB2	1.98	0.44
1:b:77:ILE:HA	1:b:80:TYR:CE2	2.52	0.44
2:i:95:HIS:HD2	2:i:103:PRO:HB3	1.82	0.44
10:C:22:VAL:HG13	10:C:153:PRO:HG2	1.97	0.44
17:J:68:PRO:HB2	17:J:118:ASP:HB2	2.00	0.44
17:J:297:LEU:HD21	17:J:302:PRO:HA	2.00	0.44
18:K:164:ASN:HB3	18:K:234:PHE:HD2	1.82	0.44
19:L:281:ASP:OD1	19:L:282:GLU:N	2.50	0.44
21:N:416:GLY:O	21:N:420:THR:N	2.51	0.44
33:Z:819:GLY:HA2	33:Z:827:LEU:HD13	2.00	0.44
1:l:85:TYR:CZ	1:l:96:THR:HG21	2.53	0.44
2:i:47:THR:O	2:i:60:CYS:N	2.48	0.44
10:C:107:PRO:HD2	10:C:110:ILE:HD12	2.00	0.44
8:c:135:ARG:HB2	14:k:15:PHE:HE2	1.83	0.44
12:m:34:GLY:HA3	12:m:80:GLY:HA2	1.98	0.44
14:k:11:SER:HB2	14:k:14:VAL:HG23	1.98	0.44
17:J:184:GLY:HA3	17:J:309:ARG:O	2.17	0.44
19:L:220:LEU:HD23	19:L:347:VAL:HB	1.99	0.44
23:P:364:ARG:NH1	23:P:367:GLU:OE1	2.50	0.44
26:S:93:LEU:O	26:S:98:SER:OG	2.27	0.44
30:W:166:GLU:HB3	30:W:195:GLY:HA2	1.99	0.44
31:X:37:PRO:HB3	31:X:46:TRP:HD1	1.82	0.44
31:X:48:PHE:HD2	31:X:66:LEU:HD23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:159:LEU:HD21	33:Z:223:LEU:HD22	1.99	0.44
6:6:170:ASP:O	6:6:176:LYS:N	2.36	0.44
3:h:50:PHE:HE2	3:h:190:ILE:HG12	1.83	0.44
15:H:57:LYS:NZ	16:I:99:ILE:HB	2.33	0.44
15:H:311:ILE:O	15:H:315:GLY:N	2.51	0.44
17:J:329:ARG:HG2	17:J:343:LEU:HD13	1.99	0.44
21:N:662:MET:HE3	21:N:715:ILE:HD13	2.00	0.44
22:O:222:LEU:HB3	22:O:280:LEU:HD13	1.99	0.44
30:W:9:VAL:HB	30:W:112:ALA:HA	2.00	0.44
33:Z:740:VAL:HA	33:Z:743:ILE:HD12	1.99	0.44
3:3:28:ARG:HG3	3:3:183:TRP:CE3	2.51	0.44
3:3:109:VAL:N	3:3:122:ALA:O	2.41	0.44
2:i:94:LEU:HB3	2:i:98:TYR:CE2	2.52	0.44
8:A:20:SER:HB2	8:A:21:PRO:HD2	1.99	0.44
8:A:165:GLY:H	9:B:60:THR:HG21	1.83	0.44
11:D:5:ASP:HB3	11:D:22:TYR:HE2	1.82	0.44
11:n:12:SER:OG	11:n:16:HIS:O	2.36	0.44
17:J:267:GLU:HG3	17:J:270:ARG:HH12	1.83	0.44
18:K:232:ALA:HA	18:K:266:PRO:HB2	1.99	0.44
19:L:252:VAL:HG13	19:L:300:GLU:HB2	2.00	0.44
29:V:28:TYR:CE1	29:V:202:ASP:CG	2.96	0.44
30:W:52:ILE:HG22	30:W:61:VAL:HG13	2.00	0.44
30:W:110:ILE:HD12	30:W:139:VAL:HG22	1.98	0.44
1:b:85:TYR:CZ	1:b:96:THR:HG21	2.53	0.44
5:f:130:TRP:CD1	5:f:172:MET:HE1	2.53	0.44
15:H:146:VAL:HG11	20:M:76:PRO:HB3	1.98	0.44
16:I:104:LEU:HD23	17:J:95:ILE:HG21	1.98	0.44
16:I:184:ILE:HG22	16:I:231:LEU:HB3	1.99	0.44
24:Q:426:LEU:HB3	28:U:295:LYS:HD3	1.99	0.44
25:R:138:GLY:HA2	25:R:141:TYR:HD2	1.83	0.44
33:Z:228:GLU:HA	33:Z:264:PHE:HZ	1.82	0.44
33:Z:400:ILE:HG12	33:Z:422:ILE:HG12	1.99	0.44
1:b:122:ASP:OD1	1:b:123:ASP:N	2.50	0.44
9:B:2:THR:HG22	9:B:3:ASP:N	2.33	0.44
12:E:120:ALA:HB1	12:E:160:PRO:HA	1.99	0.44
13:F:187:ASP:OD1	13:F:233:TYR:OH	2.32	0.44
12:m:79:SER:HB3	12:m:141:ALA:HB3	1.99	0.44
19:L:387:ASN:OD1	19:L:390:ASP:N	2.46	0.44
21:N:117:TYR:HD1	21:N:123:PHE:HE2	1.66	0.44
21:N:475:ALA:O	21:N:512:ASN:ND2	2.46	0.44
22:O:189:TYR:HB2	22:O:220:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:51:ARG:NH1	24:Q:89:ALA:H	2.16	0.44
24:Q:389:VAL:CG2	25:R:346:LYS:HB2	2.47	0.44
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.31	0.44
28:U:166:ALA:HB3	29:V:42:ARG:HE	1.81	0.44
33:Z:375:ASP:H	33:Z:379:GLN:HE21	1.64	0.44
33:Z:427:GLN:HG2	33:Z:428:TRP:CD1	2.53	0.44
1:1:64:ARG:HD3	1:1:75:ALA:HB2	1.99	0.43
2:2:244:GLU:HG3	3:3:198:ARG:HG2	1.99	0.43
7:7:198:ILE:HB	7:7:199:PRO:HD3	1.99	0.43
9:B:217:GLU:OE1	9:B:232:GLY:N	2.36	0.43
18:K:53:LYS:HA	18:K:56:LYS:HD3	1.99	0.43
20:M:149:ASN:ND2	20:M:152:SER:OG	2.51	0.43
20:M:216:LYS:NZ	20:M:316:SER:O	2.47	0.43
23:P:94:GLN:HB3	23:P:135:GLU:HG2	1.99	0.43
25:R:347:THR:O	25:R:348:LEU:HG	2.18	0.43
26:S:475:TYR:OH	28:U:294:ASN:HB2	2.18	0.43
28:U:280:ASN:HA	28:U:283:ARG:HB3	2.00	0.43
7:a:58:ASP:O	7:a:74:ARG:NH2	2.51	0.43
9:B:82:TYR:CZ	9:B:86:VAL:HG21	2.53	0.43
9:j:185:LEU:HD21	9:j:213:ILE:HD12	2.00	0.43
10:d:44:ILE:HG21	10:d:138:ALA:HB1	2.00	0.43
21:N:352:ASN:HB3	21:N:355:TRP:CE3	2.53	0.43
23:P:392:LYS:HD2	23:P:401:ASN:HB2	1.99	0.43
4:g:182:LYS:HE2	4:g:191:GLN:HE21	1.83	0.43
11:D:95:SER:HA	11:D:98:LEU:HB3	2.00	0.43
9:j:122:THR:HA	9:j:129:PRO:HG3	1.99	0.43
15:H:221:LEU:O	15:H:225:VAL:HB	2.19	0.43
18:K:391:GLY:HA3	19:L:212:ILE:HG21	1.99	0.43
33:Z:905:ASN:HA	33:Z:908:ILE:HD12	2.00	0.43
1:1:61:TRP:HD1	1:1:197:LEU:HD11	1.83	0.43
5:5:120:MET:HE2	5:5:128:GLN:HE21	1.84	0.43
2:i:141:SER:HB3	2:i:154:LEU:HD13	2.01	0.43
4:g:86:GLN:HE21	4:g:90:LYS:HE3	1.83	0.43
6:e:76:PHE:CE2	6:e:78:ALA:HB3	2.53	0.43
15:H:105:ILE:HG22	15:H:107:LYS:HG2	2.00	0.43
16:I:188:GLU:HA	16:I:191:ILE:HB	2.01	0.43
22:O:40:GLN:O	22:O:58:ARG:NH2	2.38	0.43
22:O:127:LEU:HD22	22:O:167:ILE:HG12	2.00	0.43
25:R:225:LYS:O	25:R:229:LYS:HG3	2.18	0.43
3:h:78:GLU:HG3	3:h:80:ARG:HG2	1.99	0.43
4:g:17:SER:HB3	4:g:34:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:179:TRP:HB2	9:B:191:ILE:HG21	2.00	0.43
8:c:135:ARG:HB2	14:k:15:PHE:CE2	2.54	0.43
11:n:96:HIS:CD2	11:n:100:LEU:HD12	2.54	0.43
19:L:102:GLY:H	20:M:154:LEU:HD21	1.84	0.43
23:P:125:VAL:O	23:P:136:ARG:NE	2.51	0.43
23:P:350:LEU:HD11	23:P:369:LEU:HD21	2.01	0.43
33:Z:796:LEU:HA	33:Z:799:PHE:HB3	1.99	0.43
33:Z:911:LYS:HG3	33:Z:964:GLU:HB2	2.00	0.43
3:h:138:VAL:HG21	3:h:146:LEU:HB2	1.99	0.43
5:f:110:ILE:HD11	5:f:120:MET:HE3	2.01	0.43
13:l:6:TYR:HB2	13:l:20:PHE:CE2	2.54	0.43
15:H:57:LYS:HE3	16:I:96:LEU:HA	2.00	0.43
17:J:116:ARG:HG2	17:J:118:ASP:H	1.84	0.43
28:U:52:ALA:O	29:V:97:GLN:NE2	2.52	0.43
7:7:90:ILE:HG23	7:7:93:MET:HE2	2.00	0.43
4:g:37:GLN:O	4:g:61:GLN:NE2	2.52	0.43
10:C:11:THR:HG22	11:D:127:ARG:HB2	2.00	0.43
14:G:65:VAL:HG12	14:G:67:ILE:H	1.82	0.43
8:c:146:VAL:HG13	8:c:152:PRO:HG3	2.00	0.43
9:j:213:ILE:HD11	9:j:236:ARG:HH21	1.84	0.43
16:I:433:GLU:CG	16:I:435:LEU:HD13	2.48	0.43
21:N:340:HIS:HB2	21:N:374:ILE:HG12	1.99	0.43
21:N:344:THR:HG22	21:N:375:HIS:HA	2.01	0.43
23:P:19:GLU:HB3	23:P:58:VAL:HG11	2.01	0.43
24:Q:359:ILE:HA	24:Q:362:ILE:HD12	2.00	0.43
26:S:427:ILE:HD12	27:T:196:SER:HB3	2.01	0.43
28:U:126:GLN:HE22	29:V:212:MET:HA	1.83	0.43
33:Z:255:LEU:HD13	33:Z:260:GLU:HB2	2.00	0.43
1:1:47:ASN:HA	7:a:220:ARG:HH12	1.84	0.43
2:2:46:ASP:OD1	2:2:62:LYS:NZ	2.45	0.43
4:4:34:LYS:HB3	4:4:46:PHE:CE2	2.54	0.43
5:5:229:LEU:HD22	5:5:252:LEU:HD13	2.00	0.43
5:f:133:TRP:HE3	12:m:101:LEU:HD22	1.84	0.43
9:j:157:PHE:CE1	10:d:64:GLU:HB3	2.54	0.43
14:k:38:ILE:HG22	14:k:164:ALA:HA	2.01	0.43
15:H:162:ARG:HB2	15:H:183:ILE:HD12	2.01	0.43
17:J:96:VAL:HB	17:J:121:MET:HA	2.00	0.43
17:J:181:GLN:HE21	17:J:183:LYS:HE2	1.82	0.43
18:K:233:ALA:O	18:K:268:ILE:N	2.39	0.43
25:R:208:ASN:O	25:R:212:THR:N	2.50	0.43
28:U:34:GLY:HA3	28:U:92:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:168:GLU:O	29:V:217:HIS:NE2	2.51	0.43
30:W:87:MET:HE3	30:W:91:LEU:HD11	2.00	0.43
3:3:52:GLY:O	3:3:107:PRO:HA	2.18	0.43
8:A:236:LEU:HD22	8:A:240:ASN:HB3	2.01	0.43
15:H:298:ALA:HB1	15:H:349:ILE:HG12	2.01	0.43
19:L:109:MET:N	19:L:118:ILE:O	2.51	0.43
19:L:308:LEU:HB3	19:L:342:ARG:HH21	1.83	0.43
20:M:142:PRO:HG2	20:M:264:ARG:HH22	1.83	0.43
9:j:35:LEU:HA	9:j:163:ALA:HA	1.99	0.43
14:k:120:VAL:HG21	14:k:151:LEU:HD21	2.00	0.43
22:O:357:ILE:HB	28:U:223:HIS:HB2	1.99	0.43
25:R:59:MET:O	25:R:63:TYR:N	2.39	0.43
26:S:428:ARG:HD3	27:T:192:ASN:HA	2.01	0.43
33:Z:327:GLN:HE21	33:Z:464:ASP:CG	2.27	0.43
2:2:58:LYS:NZ	3:3:135:ASP:OD2	2.37	0.42
3:3:35:GLY:HA3	3:3:183:TRP:HH2	1.83	0.42
4:4:23:ARG:HG3	4:4:28:LEU:HD12	2.00	0.42
7:a:126:PHE:CZ	7:a:163:VAL:HB	2.54	0.42
11:D:122:GLN:HA	12:E:136:ARG:NE	2.33	0.42
9:j:111:VAL:HG21	9:j:148:TYR:HD2	1.84	0.42
9:j:224:TYR:OH	9:j:230:ASP:OD2	2.28	0.42
14:k:37:SER:OG	14:k:165:THR:OG1	2.35	0.42
15:H:150:LYS:HG2	15:H:152:ILE:H	1.84	0.42
20:M:379:LEU:HD21	20:M:416:VAL:HG22	2.00	0.42
25:R:238:PHE:HD2	25:R:249:ILE:HG13	1.84	0.42
25:R:316:LEU:HD13	25:R:329:PHE:CD2	2.54	0.42
28:U:163:ALA:HB3	28:U:168:GLU:HG3	2.00	0.42
29:V:42:ARG:CZ	29:V:145:GLN:HE21	2.32	0.42
31:X:91:PHE:HB3	31:X:94:ASN:ND2	2.34	0.42
33:Z:263:ALA:HA	33:Z:288:LEU:HD11	2.01	0.42
2:2:166:VAL:O	2:2:170:HIS:ND1	2.45	0.42
4:4:38:LEU:HD23	4:4:61:GLN:HG3	2.00	0.42
2:i:139:LEU:HG	2:i:154:LEU:HD12	2.01	0.42
12:E:99:HIS:HE1	12:E:105:GLU:HB3	1.83	0.42
14:G:91:ARG:HG2	14:G:119:TYR:CE1	2.54	0.42
12:m:71:ASP:OD1	12:m:72:ARG:N	2.48	0.42
15:H:197:MET:SD	15:H:278:GLU:HB2	2.59	0.42
18:K:64:GLN:HA	18:K:67:TYR:HB3	2.01	0.42
21:N:283:ASP:HB3	21:N:286:LEU:HB2	2.00	0.42
23:P:126:THR:O	23:P:136:ARG:NH2	2.52	0.42
23:P:319:GLU:OE1	23:P:323:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:234:ILE:HD11	26:S:258:GLU:HG2	2.01	0.42
33:Z:498:ALA:HA	33:Z:533:VAL:HA	2.00	0.42
5:5:233:LYS:HD2	5:5:271:LEU:HD11	2.01	0.42
3:h:56:LEU:O	3:h:60:VAL:HG23	2.19	0.42
8:A:69:VAL:HG22	14:G:158:TRP:CD1	2.53	0.42
10:d:67:TYR:HD2	10:d:88:ILE:HD13	1.84	0.42
11:n:68:ASP:OD1	11:n:69:SER:N	2.48	0.42
14:k:28:VAL:HA	14:k:153:PRO:HG2	2.00	0.42
14:k:54:ILE:HG12	14:k:59:LEU:HD23	2.02	0.42
14:k:231:VAL:HG12	14:k:236:LEU:HB2	2.01	0.42
15:H:164:SER:OG	15:H:167:ASP:O	2.35	0.42
21:N:518:ALA:HB1	21:N:550:GLY:HA3	2.00	0.42
28:U:36:ILE:HG23	28:U:92:TYR:HD2	1.84	0.42
30:W:115:CYS:HA	30:W:144:PHE:HB2	2.01	0.42
30:W:143:ASN:HD21	30:W:149:GLN:H	1.65	0.42
33:Z:225:LEU:HD21	33:Z:253:VAL:HA	2.02	0.42
2:2:239:THR:HG21	3:3:168:SER:HB3	2.01	0.42
3:3:105:VAL:HG23	3:3:107:PRO:HD3	2.01	0.42
7:7:48:LYS:HE3	7:7:160:LEU:HB3	2.00	0.42
10:C:232:PRO:HA	10:C:235:ILE:HD12	2.01	0.42
13:F:168:ALA:N	13:F:200:SER:OG	2.53	0.42
9:j:161:ALA:HB1	9:j:175:LEU:HD13	2.01	0.42
13:l:213:ILE:HG12	13:l:230:VAL:HG12	1.99	0.42
15:H:106:ILE:HD12	29:V:76:THR:HG22	2.01	0.42
15:H:253:GLY:HA2	15:H:256:LYS:HE2	2.01	0.42
24:Q:94:VAL:HB	24:Q:133:LEU:HD13	2.01	0.42
25:R:241:ILE:N	25:R:244:THR:O	2.53	0.42
4:4:71:GLU:OE2	10:C:113:ARG:NH2	2.41	0.42
4:4:135:TYR:HA	4:4:138:PHE:CE2	2.54	0.42
6:6:221:LEU:HB2	6:6:238:LEU:HD11	2.01	0.42
1:b:85:TYR:HE2	1:b:92:PRO:HA	1.85	0.42
4:g:140:THR:HG23	4:g:168:LEU:HD21	2.00	0.42
6:e:43:ALA:HB1	6:e:221:LEU:HD11	2.01	0.42
8:A:35:THR:HA	8:A:85:GLY:HA2	2.00	0.42
14:G:179:LEU:HA	14:G:182:HIS:HD2	1.84	0.42
10:d:9:ARG:O	10:d:12:ILE:HG12	2.19	0.42
10:d:12:ILE:HA	11:n:19:GLN:HE22	1.84	0.42
13:l:157:TYR:CE2	14:k:60:VAL:HG22	2.55	0.42
14:k:71:ASP:CG	14:k:72:ARG:H	2.27	0.42
15:H:312:ASP:OD1	15:H:360:THR:OG1	2.34	0.42
17:J:230:VAL:HG11	17:J:272:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:267:GLU:O	17:J:270:ARG:HG2	2.19	0.42
18:K:209:VAL:HG23	18:K:336:ARG:HB2	2.00	0.42
19:L:290:ARG:HG2	19:L:291:PHE:H	1.84	0.42
22:O:130:ASP:HA	22:O:133:ILE:HD12	2.00	0.42
24:Q:239:PHE:HB3	24:Q:265:MET:HG2	2.00	0.42
24:Q:343:LEU:O	24:Q:347:LEU:N	2.48	0.42
28:U:36:ILE:HD11	28:U:118:LEU:HB3	2.01	0.42
29:V:173:THR:HG22	29:V:174:THR:HG23	2.00	0.42
31:X:85:ARG:HH22	31:X:104:LYS:HG3	1.85	0.42
4:4:41:HIS:NE2	4:4:186:LYS:O	2.52	0.42
1:b:151:THR:HA	1:b:154:TYR:HE2	1.85	0.42
2:i:252:ILE:HD12	10:d:226:TYR:HB2	2.01	0.42
10:C:13:PHE:CD2	11:D:19:GLN:HB3	2.54	0.42
11:D:70:HIS:ND1	11:D:71:VAL:HG23	2.35	0.42
13:l:171:TYR:OH	13:l:195:GLU:OE1	2.34	0.42
19:L:421:LYS:HB3	20:M:345:ARG:HH22	1.84	0.42
29:V:126:GLN:NE2	29:V:130:GLU:OE2	2.53	0.42
3:3:203:ARG:HB3	5:f:269:GLY:HA3	2.01	0.42
6:e:110:ARG:HG2	12:m:104:ASP:HB2	2.01	0.42
9:B:4:ARG:HH21	9:B:11:THR:HG21	1.84	0.42
16:I:104:LEU:HD13	16:I:148:LEU:HD12	2.02	0.42
16:I:196:GLU:O	16:I:208:TYR:OH	2.33	0.42
18:K:351:LEU:HD22	24:Q:234:THR:HA	2.01	0.42
24:Q:210:CYS:HB3	24:Q:214:THR:HB	2.00	0.42
33:Z:211:PHE:CG	33:Z:220:ALA:HB2	2.54	0.42
4:4:8:ARG:N	4:4:129:PRO:O	2.44	0.42
6:6:35:ALA:HB3	6:6:154:GLN:HA	2.02	0.42
7:7:107:ASN:ND2	7:7:120:LEU:HG	2.35	0.42
3:h:8:ASN:HA	3:h:30:GLY:O	2.20	0.42
9:B:119:GLN:HE21	10:C:82:ALA:HA	1.85	0.42
8:c:14:ARG:HG2	8:c:26:TYR:CG	2.55	0.42
8:c:194:ILE:HG22	8:c:196:GLU:HG2	2.01	0.42
13:l:110:HIS:CE1	14:k:86:ARG:HB3	2.55	0.42
13:l:225:TYR:HD1	13:l:229:ALA:HB1	1.84	0.42
15:H:51:GLN:HA	15:H:54:ASN:HD22	1.85	0.42
16:I:253:ILE:HG13	16:I:302:ILE:HG12	2.01	0.42
16:I:405:ARG:NH2	17:J:162:GLU:OE2	2.50	0.42
17:J:70:SER:O	18:K:119:VAL:HG23	2.20	0.42
17:J:102:ILE:HG21	17:J:122:LEU:HD21	2.02	0.42
18:K:239:GLY:HA2	18:K:277:ILE:HG13	2.02	0.42
19:L:114:GLU:OE1	19:L:137:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:54:SER:HA	23:P:58:VAL:HB	2.00	0.42
25:R:401:HIS:CD2	25:R:402:LEU:HG	2.55	0.42
29:V:114:PHE:H	29:V:118:LEU:HG	1.85	0.42
1:1:38:ARG:NH2	1:1:186:GLY:O	2.53	0.42
4:4:25:ILE:HD11	5:5:209:THR:HG21	2.02	0.42
1:b:56:VAL:HB	1:b:82:LEU:HD12	2.02	0.42
2:i:137:SER:HB2	2:i:209:ILE:HD11	2.01	0.42
12:E:123:PHE:CD1	12:E:137:PRO:HA	2.54	0.42
12:E:125:GLU:OE2	12:E:135:SER:OG	2.33	0.42
11:n:31:THR:O	11:n:76:SER:OG	2.37	0.42
11:n:202:VAL:HG13	11:n:203:VAL:N	2.35	0.42
16:I:293:ASP:CG	16:I:294:SER:H	2.28	0.42
18:K:55:GLU:HA	18:K:58:TYR:HD2	1.85	0.42
20:M:432:PHE:CG	20:M:433:TYR:N	2.87	0.42
21:N:83:LEU:HD13	21:N:135:SER:HB3	2.02	0.42
22:O:22:LEU:HD22	22:O:26:PHE:CG	2.55	0.42
24:Q:78:ILE:HG12	24:Q:100:LEU:HD13	2.02	0.42
25:R:262:GLU:O	25:R:266:LEU:HG	2.20	0.42
33:Z:925:VAL:HG12	33:Z:927:VAL:HG13	2.00	0.42
2:2:171:TRP:HA	2:2:175:LEU:HD11	2.02	0.42
7:7:183:MET:O	7:7:186:PRO:HD2	2.20	0.42
7:7:184:ALA:HA	7:7:187:LEU:HD12	2.01	0.42
3:h:91:VAL:HG11	3:h:107:PRO:HG3	2.02	0.42
4:g:126:VAL:HG12	4:g:128:LEU:HG	2.01	0.42
5:f:78:THR:HB	5:f:91:VAL:HG23	2.01	0.42
14:G:68:GLN:HG3	14:G:89:VAL:HG21	2.01	0.42
8:c:12:TYR:HA	8:c:15:HIS:HD1	1.85	0.42
13:l:50:LYS:HG2	13:l:62:LYS:HG2	2.01	0.42
16:I:306:MET:HE1	16:I:335:ASP:H	1.85	0.42
17:J:279:LEU:O	17:J:284:THR:N	2.53	0.42
18:K:159:SER:HA	18:K:242:PHE:HA	2.01	0.42
19:L:307:GLU:OE2	19:L:311:GLN:NE2	2.52	0.42
22:O:51:ASP:OD1	22:O:52:ALA:N	2.53	0.42
27:T:264:MET:HE1	29:V:295:VAL:HG21	2.02	0.42
2:2:95:HIS:HE1	8:A:104:PHE:CZ	2.38	0.41
2:i:192:ILE:HG12	2:i:199:GLY:HA2	2.02	0.41
7:a:133:MET:SD	7:a:165:LEU:HA	2.60	0.41
8:A:87:ILE:N	8:A:88:PRO:HD2	2.35	0.41
9:B:18:LEU:HB2	9:B:21:ILE:HD12	2.02	0.41
11:D:159:TRP:CZ3	12:E:56:SER:HB3	2.55	0.41
13:F:50:LYS:HG2	13:F:61:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:202:VAL:HG13	11:n:203:VAL:H	1.85	0.41
13:l:52:ASN:HB2	13:l:57:SER:OG	2.20	0.41
19:L:274:GLU:HB3	19:L:320:GLN:HG3	2.00	0.41
25:R:370:LYS:NZ	32:Y:70:ASP:OD1	2.36	0.41
4:4:130:TYR:OH	5:f:242:ARG:NH2	2.48	0.41
2:i:66:ILE:HG23	2:i:88:ILE:HG12	2.02	0.41
2:i:84:VAL:HA	2:i:87:LEU:HD12	2.02	0.41
2:i:125:ALA:H	2:i:144:ALA:HA	1.85	0.41
4:g:52:ASP:HA	5:f:163:TYR:HE1	1.84	0.41
8:A:218:PHE:HB3	8:A:222:ASP:HB2	2.02	0.41
12:E:21:LEU:HD12	20:M:433:TYR:CE1	2.56	0.41
13:l:157:TYR:CD2	14:k:60:VAL:HG22	2.56	0.41
17:J:196:THR:HG21	18:K:305:GLY:HA2	2.02	0.41
20:M:284:ASP:O	20:M:288:THR:OG1	2.29	0.41
21:N:759:ILE:HD11	21:N:769:PRO:HD2	2.00	0.41
22:O:308:LEU:HD23	22:O:348:VAL:HB	2.02	0.41
24:Q:151:TYR:HB2	24:Q:184:VAL:HG13	2.02	0.41
29:V:57:PHE:O	29:V:135:ARG:NH1	2.53	0.41
5:5:243:ASP:OD1	3:h:33:SER:OG	2.38	0.41
6:6:183:THR:HG21	6:6:187:VAL:HB	2.02	0.41
6:6:194:LEU:HB3	6:6:198:GLU:HB2	2.01	0.41
7:a:96:ILE:HD13	7:a:147:ILE:HD11	2.02	0.41
8:c:50:CYS:HB3	8:c:229:THR:HG22	2.03	0.41
13:l:132:LEU:HB2	13:l:147:PHE:HB3	2.02	0.41
14:k:16:SER:OG	14:k:18:ASP:OD1	2.28	0.41
15:H:157:VAL:HB	15:H:182:ASN:HD22	1.85	0.41
15:H:161:GLU:HG3	15:H:183:ILE:HG22	2.02	0.41
16:I:117:HIS:HA	16:I:131:SER:HA	2.01	0.41
17:J:261:SER:HA	18:K:293:GLN:HG3	2.02	0.41
20:M:157:ASP:OD1	20:M:158:THR:N	2.53	0.41
28:U:296:ILE:HG12	29:V:266:LEU:HD22	2.02	0.41
31:X:7:VAL:HG12	31:X:8:ILE:HG13	2.02	0.41
2:2:64:HIS:CE1	2:2:82:GLU:HG2	2.55	0.41
3:3:51:LEU:HD22	3:3:87:PHE:CZ	2.56	0.41
5:5:255:VAL:HA	5:5:260:TRP:HA	2.03	0.41
4:g:81:SER:HB3	4:g:119:ILE:HD11	2.01	0.41
6:e:194:LEU:HB3	6:e:198:GLU:HB2	2.01	0.41
9:B:216:ASP:OD1	9:B:217:GLU:N	2.53	0.41
15:H:249:TYR:HD2	15:H:376:GLU:HG2	1.84	0.41
17:J:339:ARG:HD3	25:R:206:ARG:HE	1.85	0.41
25:R:76:GLN:HB2	25:R:86:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:40:GLU:HA	26:S:46:LEU:HD12	2.02	0.41
26:S:205:ASN:HA	26:S:208:ILE:HD12	2.01	0.41
29:V:235:GLU:HG2	29:V:297:THR:HA	2.02	0.41
4:4:130:TYR:HB2	4:4:144:LEU:HD13	2.02	0.41
6:e:77:ALA:HB3	7:a:168:VAL:HA	2.02	0.41
11:D:133:THR:OG1	11:D:150:THR:OG1	2.38	0.41
14:G:119:TYR:CZ	14:G:123:HIS:HE1	2.38	0.41
15:H:147:ILE:HA	15:H:155:PHE:HB2	2.02	0.41
15:H:251:PRO:HA	15:H:252:PRO:HD3	1.97	0.41
21:N:58:ARG:HA	21:N:61:ALA:HB3	2.03	0.41
22:O:44:SER:O	22:O:47:LYS:N	2.54	0.41
22:O:290:LYS:HZ2	22:O:354:GLN:HE21	1.69	0.41
23:P:265:VAL:HG21	23:P:296:GLN:HB3	2.02	0.41
25:R:316:LEU:HD13	25:R:329:PHE:HD2	1.85	0.41
25:R:368:LEU:HD23	25:R:371:PHE:HD2	1.86	0.41
2:2:48:ARG:HE	2:2:199:GLY:HA3	1.85	0.41
2:2:109:LEU:HD22	2:2:140:PHE:HB3	2.02	0.41
3:3:184:GLY:N	3:3:204:GLN:HE21	2.18	0.41
1:b:60:ILE:HG12	1:b:120:GLY:HA3	2.03	0.41
1:b:209:PRO:O	1:b:213:GLU:HG3	2.20	0.41
2:i:97:LEU:HD21	9:j:66:LEU:HD23	2.02	0.41
2:i:170:HIS:HB3	2:i:183:LEU:HD13	2.02	0.41
3:h:190:ILE:HG12	3:h:195:VAL:HG22	2.02	0.41
7:a:185:ASN:HB2	7:a:186:PRO:HD3	2.03	0.41
9:B:72:GLY:N	9:B:137:ALA:O	2.47	0.41
10:d:119:LYS:HG2	10:d:131:PHE:CD2	2.56	0.41
12:m:208:MET:SD	12:m:216:ASN:ND2	2.94	0.41
15:H:227:LEU:HD11	15:H:234:ARG:HD2	2.01	0.41
15:H:235:PHE:CZ	15:H:242:PRO:HG3	2.55	0.41
16:I:218:GLY:HA2	16:I:324:VAL:O	2.21	0.41
20:M:336:ALA:O	20:M:342:ARG:NH1	2.48	0.41
30:W:9:VAL:HG22	30:W:52:ILE:HD11	2.01	0.41
33:Z:495:ILE:HA	33:Z:532:HIS:CE1	2.56	0.41
5:5:125:ALA:HB2	6:6:149:SER:N	2.35	0.41
13:F:37:GLY:HA3	13:F:46:LEU:HD23	2.02	0.41
13:l:13:PHE:HE2	14:k:131:PRO:HD2	1.86	0.41
17:J:57:PHE:O	17:J:61:GLU:HG2	2.21	0.41
21:N:23:TYR:HB3	27:T:35:ILE:HG21	2.01	0.41
21:N:79:VAL:HG22	21:N:101:ILE:HG23	2.01	0.41
23:P:122:ILE:HG22	23:P:124:VAL:H	1.86	0.41
24:Q:282:LEU:HD23	24:Q:300:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:359:ILE:HD12	24:Q:395:GLY:HA2	2.02	0.41
26:S:469:ASN:HA	26:S:472:HIS:ND1	2.36	0.41
33:Z:777:PRO:HB3	33:Z:796:LEU:HD21	2.02	0.41
6:6:114:HIS:CD2	12:E:102:TYR:HA	2.55	0.41
6:6:226:VAL:HG22	6:6:231:VAL:HG22	2.01	0.41
2:i:33:VAL:HG22	2:i:188:ILE:HD11	2.03	0.41
6:e:41:VAL:HG12	6:e:225:ILE:HA	2.03	0.41
7:a:184:ALA:HB2	7:a:217:LEU:HD21	2.03	0.41
11:D:79:ASN:N	16:I:437:LEU:O	2.40	0.41
8:c:88:PRO:HB3	14:k:156:SER:HB3	2.03	0.41
10:d:166:GLY:O	10:d:169:THR:OG1	2.32	0.41
12:m:169:ALA:HB1	12:m:183:LEU:HD13	2.01	0.41
17:J:211:ILE:HB	17:J:245:ILE:HA	2.02	0.41
19:L:336:ALA:HA	19:L:339:ARG:NH1	2.36	0.41
21:N:758:VAL:HG12	21:N:773:MET:HE1	2.02	0.41
28:U:31:ARG:HH21	28:U:57:GLU:CD	2.28	0.41
33:Z:166:ASN:HB2	33:Z:227:ILE:HG22	2.03	0.41
2:2:119:TYR:OH	3:3:99:ARG:NH1	2.53	0.41
2:2:172:LYS:H	2:2:175:LEU:HD11	1.85	0.41
4:4:66:LEU:HD11	11:D:90:ARG:HB3	2.03	0.41
6:6:55:ASN:HB3	7:7:170:TYR:CZ	2.55	0.41
6:6:96:PHE:HB3	13:F:89:ARG:NH1	2.36	0.41
7:7:115:ASP:OD1	7:7:116:ALA:N	2.54	0.41
7:7:124:TYR:HD1	13:F:100:ASN:HB3	1.86	0.41
1:b:38:ARG:HA	1:b:48:ARG:HA	2.02	0.41
2:i:189:GLN:HA	2:i:192:ILE:HD12	2.02	0.41
4:g:56:PHE:CD2	4:g:100:VAL:HG11	2.56	0.41
10:C:191:GLU:HG2	10:C:242:THR:HG22	2.03	0.41
10:C:231:LYS:HE3	10:C:233:GLN:HB2	2.03	0.41
11:D:31:THR:O	11:D:76:SER:OG	2.33	0.41
14:G:28:VAL:HG22	14:G:153:PRO:HG2	2.03	0.41
8:c:79:ILE:HG12	8:c:145:SER:HB2	2.02	0.41
9:j:42:GLY:HA2	9:j:145:PHE:CE1	2.56	0.41
12:m:167:TYR:HB3	12:m:170:LYS:HB2	2.03	0.41
15:H:280:VAL:HG22	15:H:313:ALA:HB1	2.03	0.41
16:I:113:ILE:HD12	16:I:115:ASP:HB2	2.02	0.41
17:J:388:LYS:O	17:J:392:LYS:N	2.49	0.41
18:K:104:ASP:OD1	18:K:105:GLN:N	2.46	0.41
18:K:351:LEU:HD21	24:Q:237:SER:HB3	2.03	0.41
20:M:353:SER:N	20:M:356:SER:OG	2.54	0.41
21:N:339:MET:HE2	21:N:707:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:378:ASN:HA	21:N:924:LYS:HG3	2.02	0.41
22:O:294:MET:SD	22:O:356:ARG:NE	2.94	0.41
24:Q:204:ALA:O	24:Q:208:ILE:HG13	2.21	0.41
25:R:67:CYS:HA	25:R:75:GLY:HA2	2.03	0.41
25:R:163:SER:O	25:R:167:LYS:HG2	2.20	0.41
26:S:208:ILE:HD13	27:T:44:LEU:HB3	2.03	0.41
28:U:35:VAL:HA	28:U:91:TRP:HA	2.03	0.41
29:V:37:MET:HG3	29:V:68:VAL:HG21	2.03	0.41
29:V:50:MET:HE1	29:V:83:VAL:HG22	2.02	0.41
31:X:73:THR:HG23	31:X:90:VAL:H	1.85	0.41
32:Y:67:VAL:O	32:Y:69:VAL:HG23	2.21	0.41
33:Z:434:GLN:HA	33:Z:437:ASP:OD2	2.21	0.41
33:Z:493:LEU:HB3	33:Z:497:PHE:CE2	2.55	0.41
6:6:46:THR:OG1	6:6:219:ASP:O	2.38	0.41
7:7:117:GLU:HG2	13:F:140:SER:HA	2.03	0.41
3:h:89:GLN:HG2	9:j:102:GLY:HA3	2.03	0.41
4:g:23:ARG:NH2	5:f:191:ASP:OD2	2.55	0.41
6:e:106:ASN:HA	6:e:142:TYR:CE2	2.56	0.41
11:D:11:PHE:HZ	12:E:138:PHE:HA	1.85	0.41
13:F:157:TYR:CZ	14:G:60:VAL:HG22	2.56	0.41
12:m:21:LEU:HD23	12:m:23:GLN:N	2.36	0.41
19:L:149:ASP:OD2	19:L:152:THR:OG1	2.37	0.41
20:M:50:ARG:HH21	30:W:30:ILE:HD13	1.85	0.41
26:S:330:LEU:HB3	26:S:334:HIS:CE1	2.56	0.41
27:T:92:ASN:ND2	27:T:96:LEU:HD13	2.32	0.41
33:Z:212:LEU:HD11	33:Z:238:ASP:HB3	2.03	0.41
1:1:61:TRP:CD1	1:1:197:LEU:HD21	2.55	0.40
1:1:82:LEU:HA	1:1:85:TYR:HB3	2.02	0.40
3:3:155:GLU:O	3:3:158:LEU:HG	2.21	0.40
6:6:220:GLY:HA2	6:6:237:GLU:HA	2.04	0.40
7:7:220:ARG:HH12	1:b:47:ASN:HA	1.84	0.40
5:f:210:PHE:CE2	5:f:242:ARG:HB2	2.55	0.40
10:C:11:THR:HA	11:D:127:ARG:HB2	2.02	0.40
8:c:87:ILE:N	8:c:88:PRO:HD2	2.37	0.40
14:k:103:TYR:C	14:k:105:THR:H	2.29	0.40
16:I:109:LEU:HD23	16:I:120:VAL:HG12	2.03	0.40
16:I:427:LYS:HG3	16:I:428:VAL:N	2.36	0.40
18:K:186:GLU:HA	18:K:190:LEU:HD13	2.03	0.40
19:L:120:LYS:HA	19:L:126:ARG:HA	2.02	0.40
21:N:515:ARG:HB2	21:N:546:LEU:HD22	2.03	0.40
23:P:254:GLU:HA	23:P:257:TRP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:40:THR:HG21	1:b:187:SER:HA	2.03	0.40
14:G:193:VAL:HG13	14:G:216:ILE:HG21	2.04	0.40
15:H:404:TRP:O	15:H:408:SER:OG	2.30	0.40
17:J:327:ILE:HG22	17:J:358:VAL:HG11	2.03	0.40
20:M:194:VAL:HA	20:M:198:VAL:HB	2.03	0.40
20:M:275:PRO:O	20:M:276:THR:HB	2.21	0.40
26:S:290:ASN:OD1	26:S:321:GLN:NE2	2.54	0.40
33:Z:145:ASP:HB3	33:Z:210:TYR:HD1	1.86	0.40
33:Z:327:GLN:C	33:Z:329:ILE:H	2.30	0.40
2:2:50:THR:HG22	2:2:55:VAL:HG13	2.03	0.40
6:6:224:LEU:HG	6:6:233:LYS:HG2	2.04	0.40
1:b:82:LEU:HA	1:b:85:TYR:HB3	2.03	0.40
4:g:19:LYS:HG2	4:g:180:ILE:HG13	2.04	0.40
9:B:95:THR:HA	9:B:99:ARG:HD2	2.03	0.40
11:D:65:SER:HB3	11:D:90:ARG:HH21	1.86	0.40
8:c:156:LYS:HE2	8:c:166:TYR:CE2	2.57	0.40
13:l:60:GLN:HE22	13:l:78:ALA:HB1	1.86	0.40
15:H:145:TYR:CD1	15:H:174:VAL:HG13	2.56	0.40
19:L:223:PRO:HA	19:L:224:PRO:HD3	2.00	0.40
25:R:309:LEU:HD21	32:Y:78:LYS:HD3	2.03	0.40
28:U:121:ILE:HD12	28:U:136:TYR:HE2	1.84	0.40
14:G:41:LYS:HA	14:G:46:VAL:HG12	2.04	0.40
14:G:65:VAL:HG22	14:G:215:GLU:OE2	2.21	0.40
20:M:379:LEU:HD13	20:M:419:ILE:HD12	2.04	0.40
22:O:74:ASN:ND2	30:W:82:GLU:OE1	2.55	0.40
24:Q:378:SER:HA	24:Q:381:ILE:HD12	2.03	0.40
26:S:282:ILE:HA	26:S:382:ARG:HH12	1.85	0.40
2:i:32:ILE:O	2:i:156:LEU:N	2.54	0.40
5:f:94:ARG:NH1	5:f:244:ALA:O	2.55	0.40
6:e:221:LEU:HB3	6:e:236:TYR:HB3	2.03	0.40
7:a:227:ASN:OD1	7:a:228:PHE:N	2.55	0.40
9:B:240:SER:HA	9:B:243:ILE:HD12	2.03	0.40
10:d:94:HIS:CD2	10:d:114:ARG:HG2	2.57	0.40
13:l:157:TYR:CD2	13:l:176:LEU:HD11	2.57	0.40
15:H:281:GLN:HE22	16:I:258:GLY:HA3	1.87	0.40
16:I:193:GLU:HB3	16:I:346:ARG:HD2	2.04	0.40
19:L:251:ILE:N	20:M:293:SER:OG	2.54	0.40
22:O:20:PRO:HD2	22:O:22:LEU:HG	2.03	0.40
22:O:157:LEU:HD12	22:O:171:PHE:HD2	1.87	0.40
27:T:105:LEU:HD12	27:T:108:LEU:HD12	2.03	0.40
27:T:229:VAL:HG21	27:T:234:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:12:LEU:HD13	29:V:35:LEU:HB2	2.02	0.40
33:Z:155:ARG:HA	33:Z:158:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	194/215 (90%)	189 (97%)	5 (3%)	0	100	100
1	b	194/215 (90%)	189 (97%)	5 (3%)	0	100	100
2	2	224/261 (86%)	218 (97%)	6 (3%)	0	100	100
2	i	224/261 (86%)	220 (98%)	4 (2%)	0	100	100
3	3	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
3	h	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	24	63
4	4	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
4	g	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
5	5	210/287 (73%)	208 (99%)	2 (1%)	0	100	100
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
6	6	220/241 (91%)	215 (98%)	5 (2%)	0	100	100
6	e	220/241 (91%)	213 (97%)	7 (3%)	0	100	100
7	7	227/266 (85%)	218 (96%)	9 (4%)	0	100	100
7	a	230/266 (86%)	223 (97%)	7 (3%)	0	100	100
8	A	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
9	j	248/250 (99%)	238 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	C	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
10	d	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
11	D	238/254 (94%)	228 (96%)	10 (4%)	0	100	100
11	n	239/254 (94%)	231 (97%)	8 (3%)	0	100	100
12	E	240/260 (92%)	229 (95%)	11 (5%)	0	100	100
12	m	240/260 (92%)	233 (97%)	7 (3%)	0	100	100
13	F	231/234 (99%)	220 (95%)	11 (5%)	0	100	100
13	l	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
14	G	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
14	k	242/288 (84%)	237 (98%)	5 (2%)	0	100	100
15	H	353/467 (76%)	311 (88%)	41 (12%)	1 (0%)	36	72
16	I	361/437 (83%)	334 (92%)	27 (8%)	0	100	100
17	J	371/405 (92%)	350 (94%)	21 (6%)	0	100	100
18	K	379/428 (89%)	343 (90%)	35 (9%)	1 (0%)	36	72
19	L	359/437 (82%)	335 (93%)	24 (7%)	0	100	100
20	M	363/434 (84%)	336 (93%)	24 (7%)	3 (1%)	16	54
21	N	843/945 (89%)	793 (94%)	47 (6%)	3 (0%)	30	67
22	O	385/393 (98%)	348 (90%)	36 (9%)	1 (0%)	36	72
23	P	430/445 (97%)	390 (91%)	40 (9%)	0	100	100
24	Q	429/434 (99%)	398 (93%)	31 (7%)	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%)	239 (88%)	31 (12%)	0	100	100
28	U	245/338 (72%)	240 (98%)	4 (2%)	1 (0%)	30	67
29	V	282/306 (92%)	243 (86%)	33 (12%)	6 (2%)	5	30
30	W	195/268 (73%)	174 (89%)	18 (9%)	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%)	743 (92%)	64 (8%)	0	100	100
All	All	13382/15139 (88%)	12602 (94%)	755 (6%)	25 (0%)	44	78

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	H	329	VAL
29	V	61	TYR
3	h	105	VAL
20	M	274	ALA
29	V	62	THR
21	N	874	ILE
21	N	903	VAL
28	U	129	VAL
29	V	60	ASP
32	Y	69	VAL
20	M	276	THR
21	N	761	ILE
25	R	241	ILE
25	R	421	VAL
29	V	189	ILE
29	V	305	ILE
30	W	147	ILE
30	W	22	PRO
18	K	326	PRO
25	R	72	VAL
20	M	167	VAL
26	S	83	PRO
29	V	271	VAL
22	O	227	ILE
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	207/210 (99%)	207 (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%)	203 (100%)	0	100	100
11	D	212/226 (94%)	212 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	254 (100%)	0	100	100
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	11628/13054 (89%)	11628 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	214	GLN
2	2	64	HIS
2	2	95	HIS
2	2	115	HIS
3	3	145	GLN
3	3	169	GLN
3	3	204	GLN
4	4	55	GLN
4	4	86	GLN
5	5	104	GLN
5	5	128	GLN
5	5	160	ASN
5	5	251	ASN
5	5	283	ASN
6	6	55	ASN
6	6	113	GLN
6	6	172	GLN
6	6	216	GLN
7	7	95	HIS
7	7	107	ASN

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Mol	Chain	Res	Type
1	b	81	HIS
1	b	180	GLN
2	i	51	GLN
3	h	145	GLN
4	g	65	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	55	ASN
6	e	89	ASN
6	e	113	GLN
6	e	172	GLN
7	a	70	ASN
7	a	95	HIS
7	a	145	ASN
8	A	84	ASN
8	A	209	HIS
9	B	20	GLN
9	B	30	GLN
9	B	119	GLN
10	C	59	GLN
10	C	120	GLN
11	D	79	ASN
11	D	94	GLN
11	D	122	GLN
11	D	149	GLN
12	E	218	GLN
13	F	4	ASN
13	F	43	HIS
13	F	90	GLN
13	F	117	GLN
13	F	143	HIS
13	F	152	ASN
13	F	166	GLN
14	G	23	GLN
14	G	64	ASN
14	G	182	HIS
14	G	183	HIS
8	c	126	GLN

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Mol	Chain	Res	Type
9	j	190	HIS
10	d	94	HIS
10	d	120	GLN
10	d	227	GLN
11	n	19	GLN
11	n	162	GLN
11	n	178	ASN
12	m	154	GLN
12	m	180	GLN
13	l	60	GLN
13	l	117	GLN
13	l	119	ASN
14	k	12	ASN
14	k	127	ASN
14	k	147	HIS
14	k	183	HIS
15	H	54	ASN
15	H	182	ASN
15	H	281	GLN
15	H	327	ASN
15	H	330	GLN
15	H	359	ASN
15	H	413	ASN
16	I	190	GLN
16	I	204	HIS
17	J	170	HIS
17	J	181	GLN
17	J	240	HIS
17	J	376	HIS
18	K	72	GLN
19	L	67	HIS
19	L	311	GLN
19	L	409	HIS
20	M	81	ASN
20	M	238	GLN
20	M	407	GLN
21	N	34	GLN
21	N	116	GLN
21	N	176	GLN
21	N	305	ASN
21	N	340	HIS
21	N	375	HIS

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Mol	Chain	Res	Type
21	N	747	HIS
22	O	4	ASN
22	O	107	GLN
22	O	235	HIS
22	O	247	ASN
22	O	354	GLN
22	O	376	GLN
23	P	30	ASN
23	P	183	GLN
23	P	263	HIS
23	P	286	ASN
23	P	401	ASN
24	Q	19	GLN
24	Q	114	GLN
24	Q	178	HIS
24	Q	226	HIS
24	Q	346	ASN
24	Q	418	GLN
25	R	399	GLN
26	S	19	HIS
26	S	32	GLN
26	S	135	ASN
26	S	139	HIS
26	S	159	ASN
26	S	191	HIS
26	S	227	ASN
26	S	261	HIS
26	S	283	GLN
26	S	311	GLN
26	S	321	GLN
26	S	334	HIS
26	S	369	GLN
26	S	386	ASN
26	S	450	ASN
26	S	458	GLN
26	S	470	GLN
27	T	123	HIS
28	U	127	GLN
28	U	173	HIS
28	U	201	GLN
28	U	270	ASN
29	V	111	HIS

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Mol	Chain	Res	Type
29	V	126	GLN
29	V	145	GLN
29	V	195	HIS
29	V	204	HIS
29	V	222	GLN
29	V	237	ASN
29	V	250	GLN
29	V	279	HIS
30	W	18	ASN
30	W	42	ASN
30	W	92	GLN
30	W	170	HIS
31	X	38	ASN
31	X	94	ASN
33	Z	215	ASN
33	Z	276	ASN
33	Z	309	GLN
33	Z	327	GLN
33	Z	361	HIS
33	Z	379	GLN
33	Z	427	GLN
33	Z	475	GLN
33	Z	618	GLN
33	Z	760	HIS
33	Z	766	HIS
33	Z	801	HIS
33	Z	829	GLN
33	Z	833	GLN
33	Z	959	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

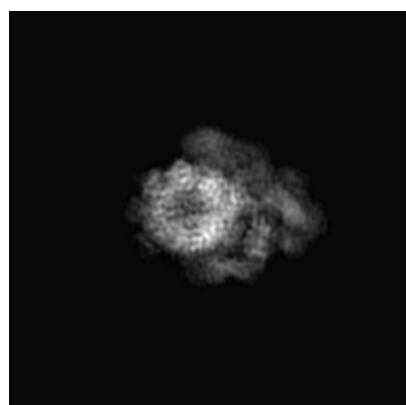
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9769. These allow visual inspection of the internal detail of the map and identification of artifacts.

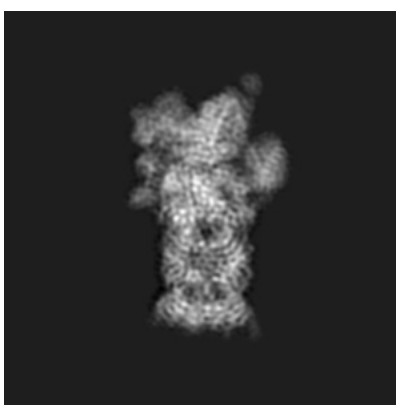
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

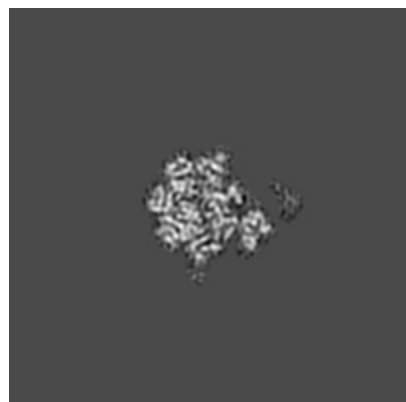


Z

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

6.2 Central slices [i](#)

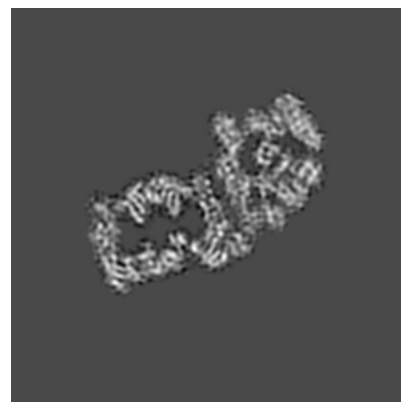
6.2.1 Primary map



X Index: 180



Y Index: 180

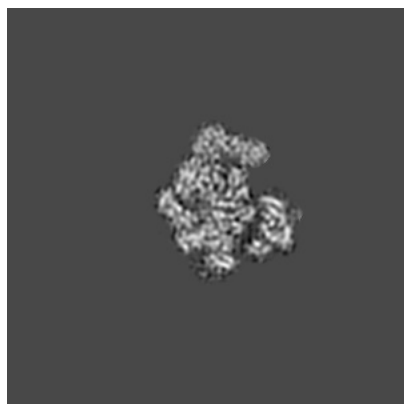


Z Index: 180

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

6.3 Largest variance slices [i](#)

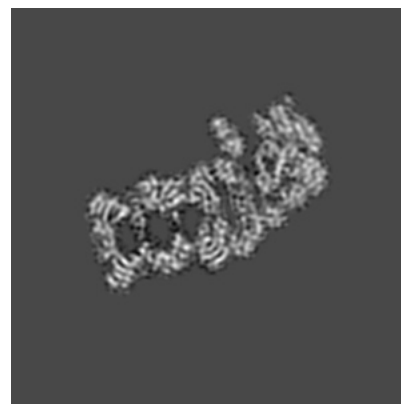
6.3.1 Primary map



X Index: 204



Y Index: 183

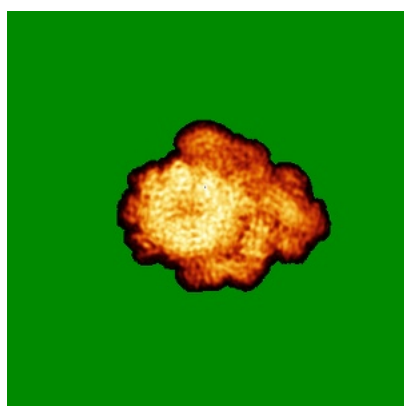


Z Index: 187

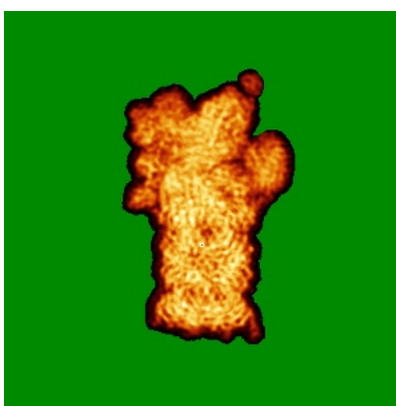
The images above show the largest variance slices of the map in three orthogonal directions.

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

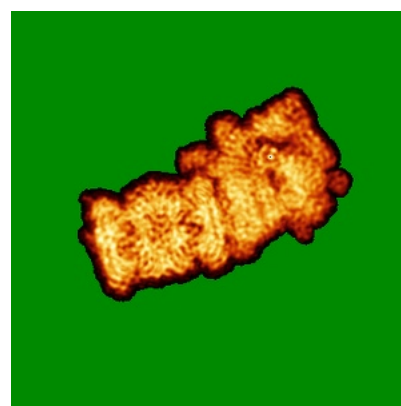
6.4.1 Primary map



X



Y

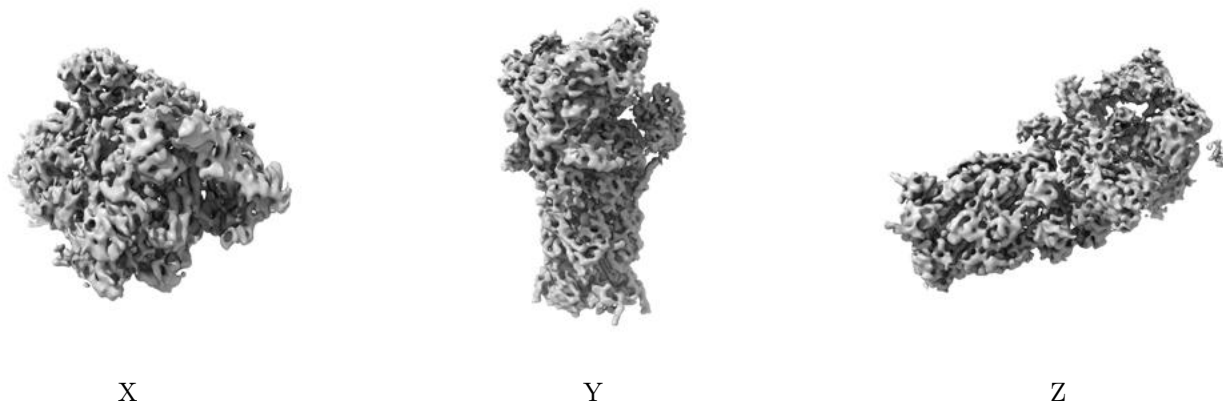


Z

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 0.657. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

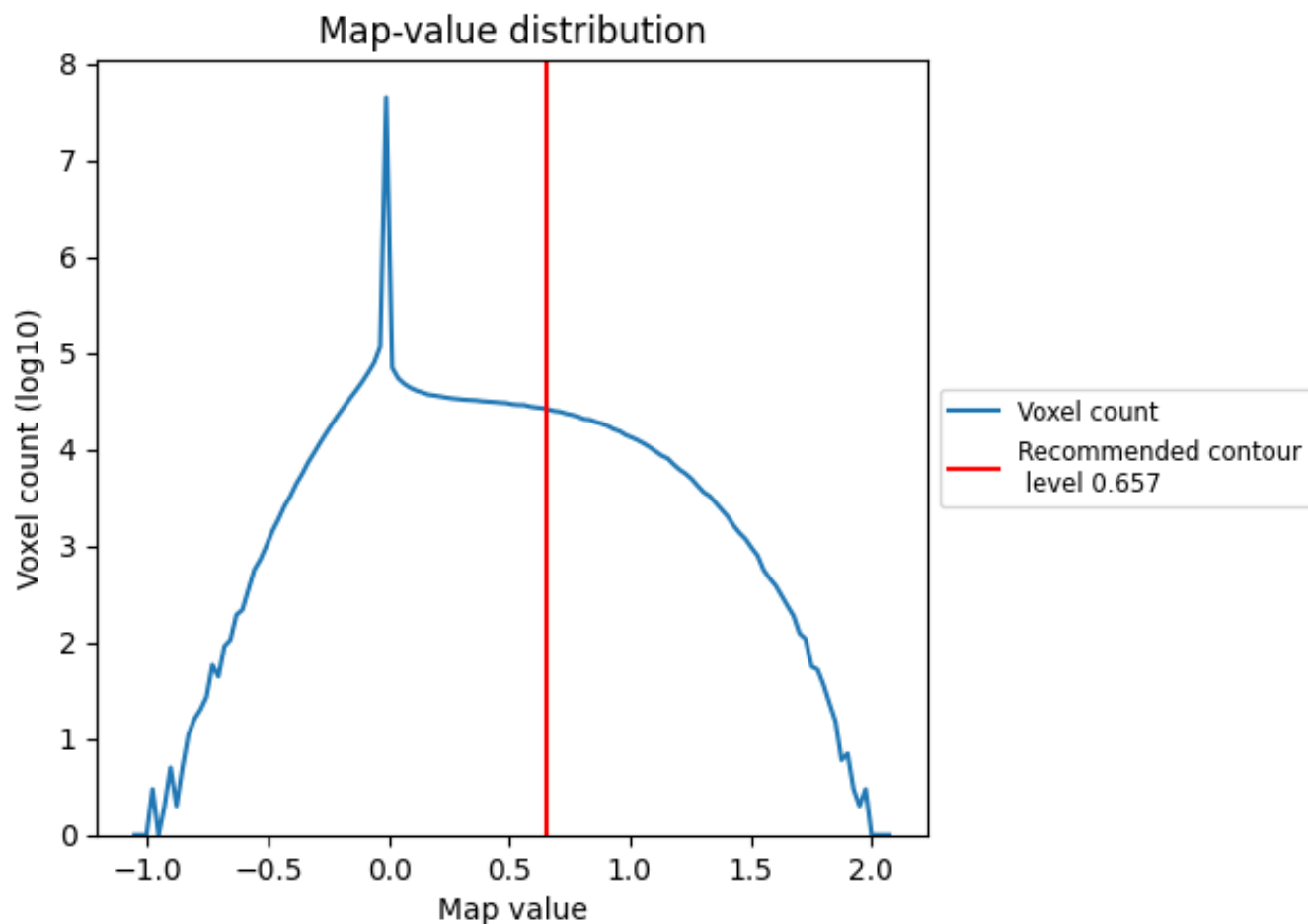
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

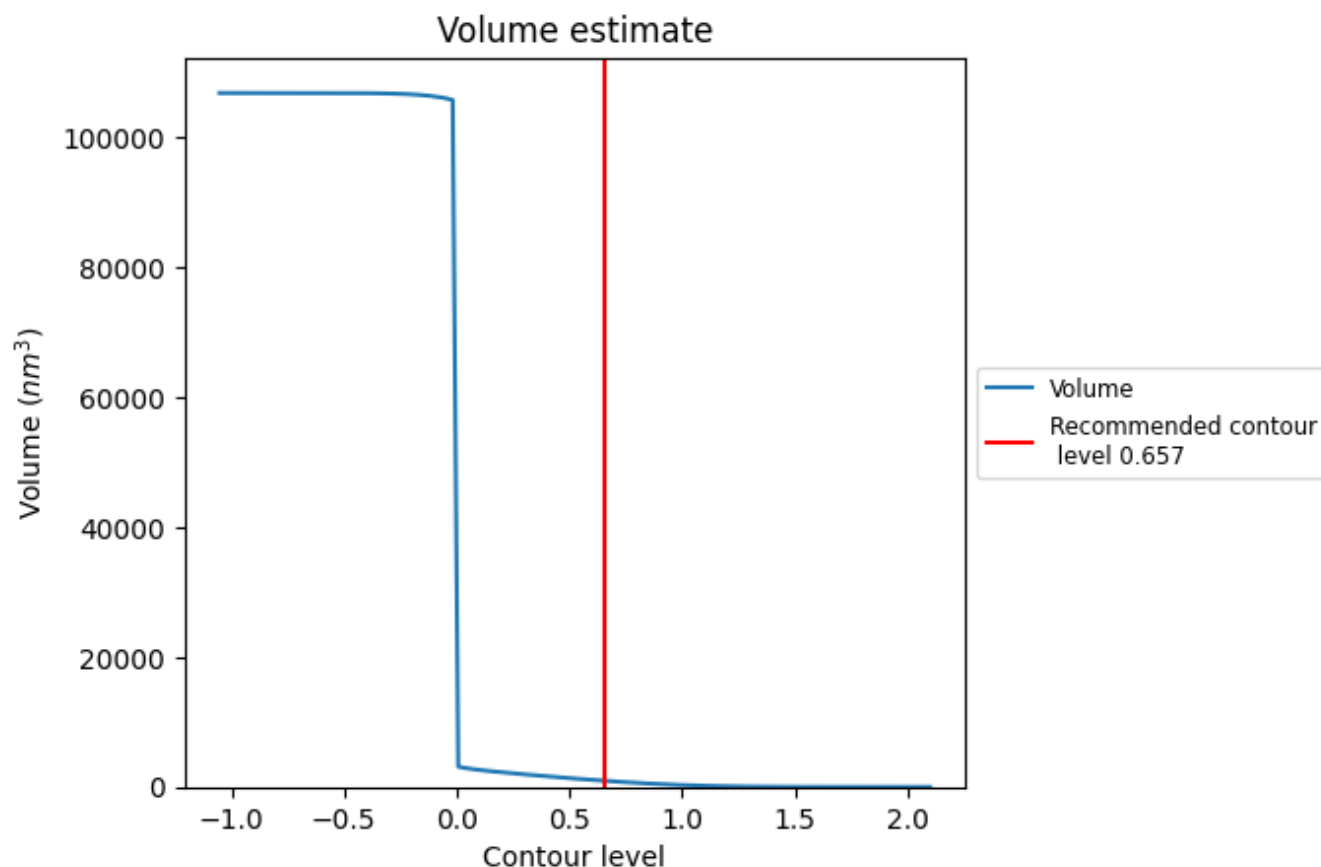
This section contains the results of statistical analysis of the map.

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.

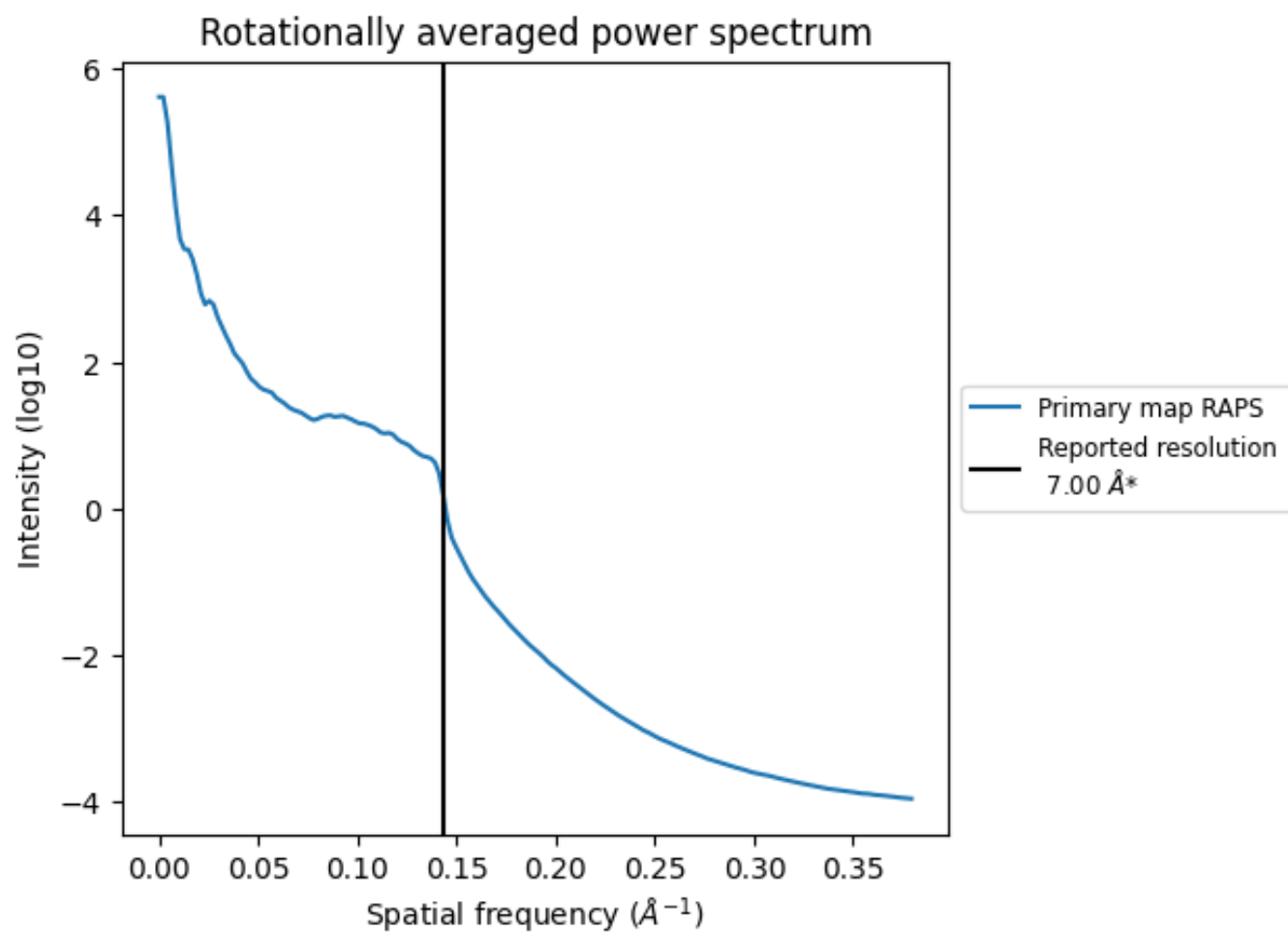
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 945 nm^3 ; this corresponds to an approximate mass of 854 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 0.143 Å⁻¹

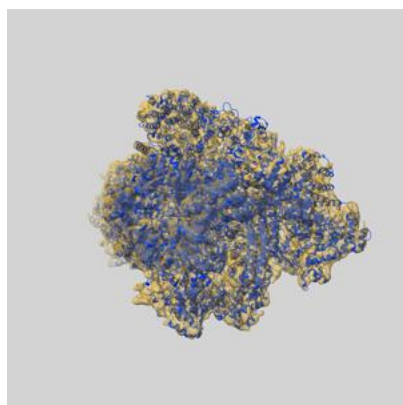
8 Fourier-Shell correlation

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

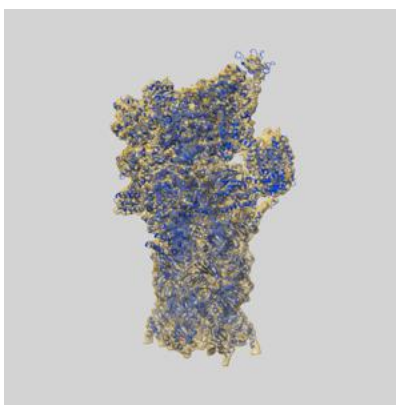
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9769 and PDB model 6J2C. Per-residue inclusion information can be found in section [3](#) on page [11](#).

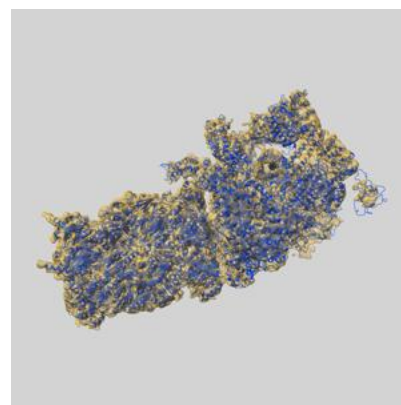
9.1 Map-model overlay [i](#)



X



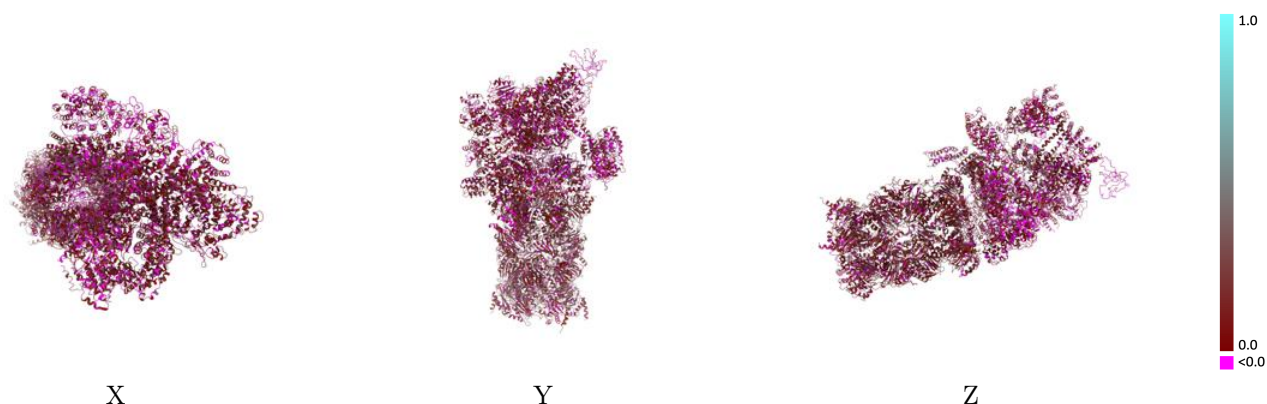
Y



Z

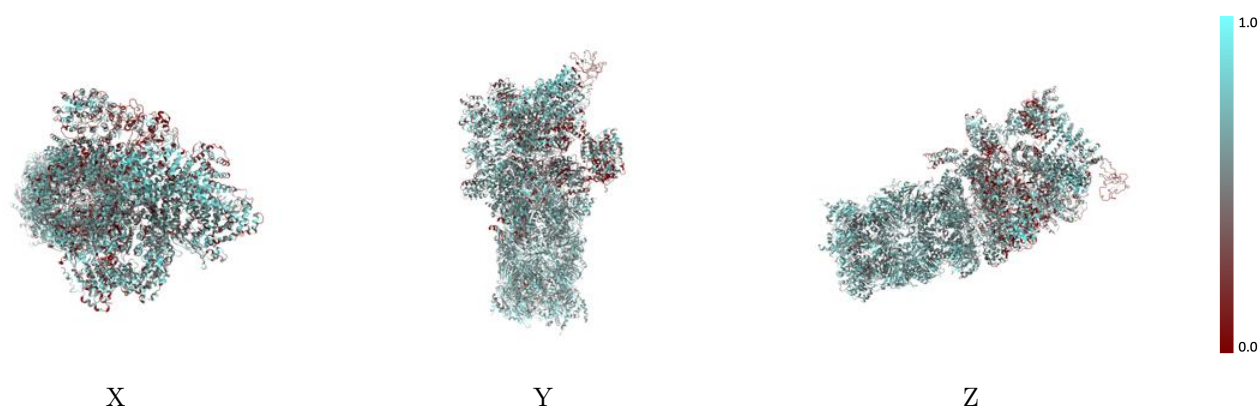
The images above show the 3D surface view of the map at the recommended contour level 0.657 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



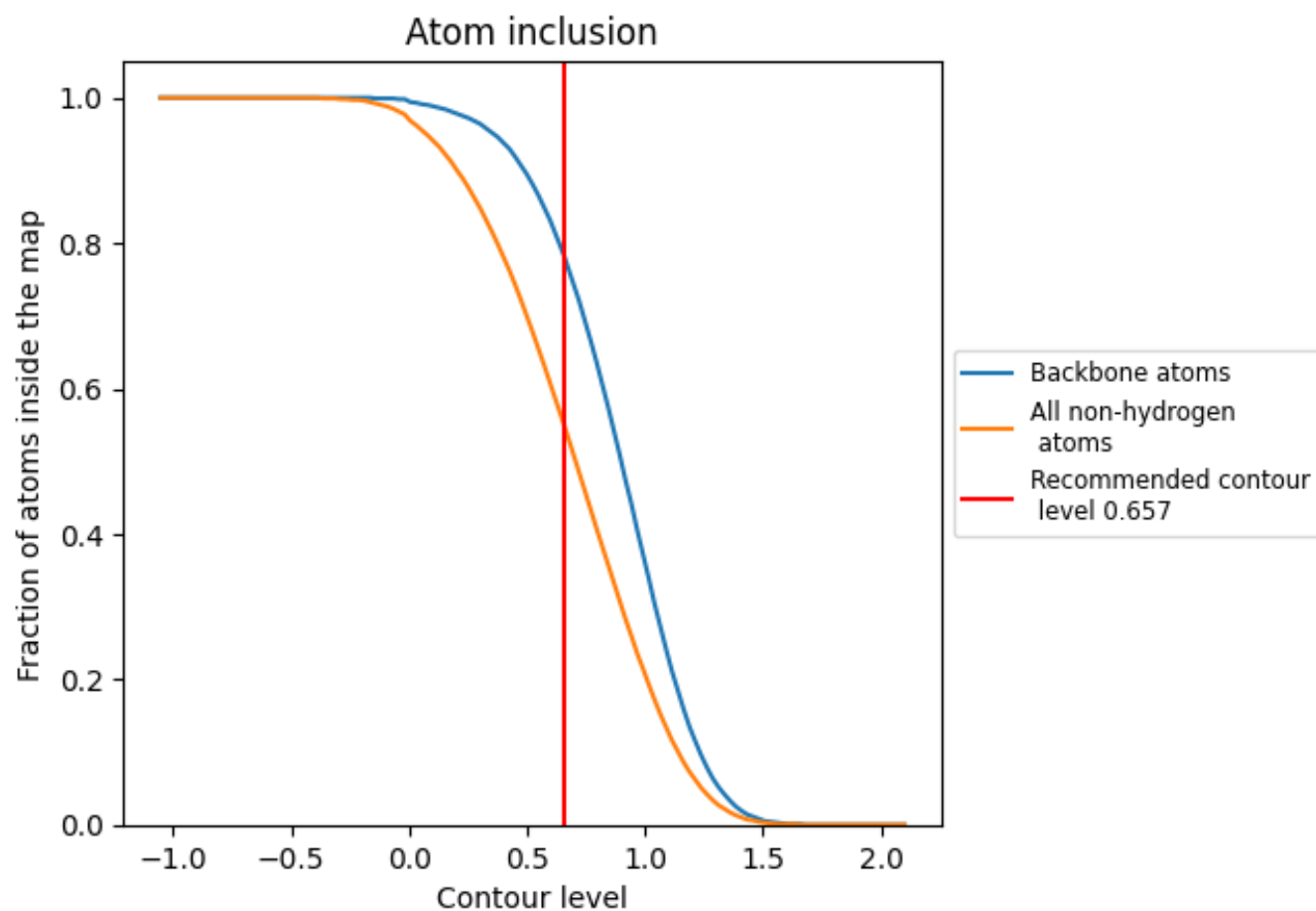
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.657).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 55% 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 (0.657) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5500	 0.1170
1	 0.6150	 0.1440
2	 0.6270	 0.1540
3	 0.6060	 0.1300
4	 0.5990	 0.1350
5	 0.6350	 0.1470
6	 0.6360	 0.1430
7	 0.6370	 0.1480
A	 0.5770	 0.1440
B	 0.5670	 0.1330
C	 0.5880	 0.1410
D	 0.6060	 0.1390
E	 0.5910	 0.1500
F	 0.6130	 0.1320
G	 0.6190	 0.1440
H	 0.4720	 0.0780
I	 0.4640	 0.0960
J	 0.4290	 0.0980
K	 0.4830	 0.1140
L	 0.4620	 0.0930
M	 0.4680	 0.0860
N	 0.6170	 0.1120
O	 0.5060	 0.0970
P	 0.5600	 0.1200
Q	 0.5280	 0.1140
R	 0.5700	 0.1160
S	 0.4880	 0.1050
T	 0.4600	 0.0960
U	 0.5300	 0.1090
V	 0.4920	 0.0890
W	 0.4660	 0.0720
X	 0.1230	 -0.0200
Y	 0.4960	 0.0870
Z	 0.4280	 0.0620
a	 0.6030	 0.1490



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Chain	Atom inclusion	Q-score
b	 0.6210	 0.1380
c	 0.6240	 0.1380
d	 0.5990	 0.1270
e	 0.6270	 0.1470
f	 0.6400	 0.1500
g	 0.6240	 0.1490
h	 0.6200	 0.1400
i	 0.6100	 0.1430
j	 0.5920	 0.1300
k	 0.6400	 0.1400
l	 0.6410	 0.1380
m	 0.6130	 0.1370
n	 0.6180	 0.1390