



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:39 PM UTC

PDB ID : 6J2Q / pdb_00006j2q
EMDB ID : EMD-9771
Title : Yeast proteasome in Ub-accepted state (C1-b)
Authors : Cong, Y.
Deposited on : 2019-01-02
Resolution : 3.80 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

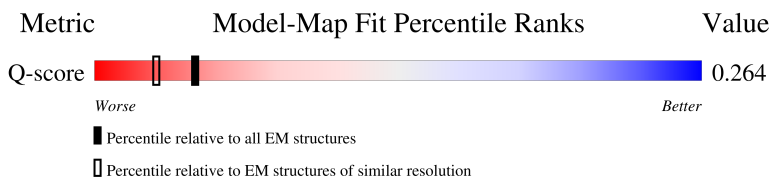
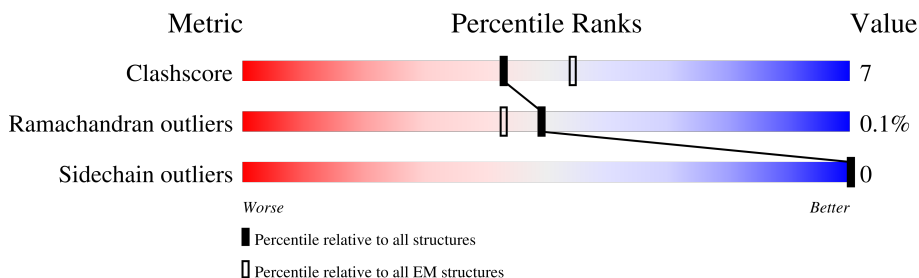
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



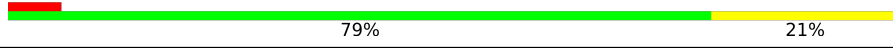
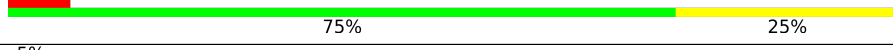
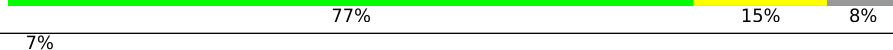
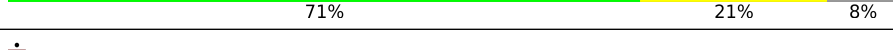
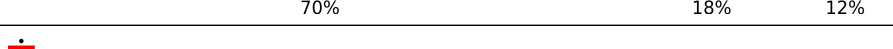
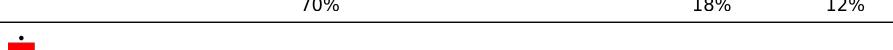
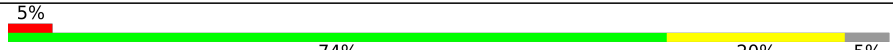
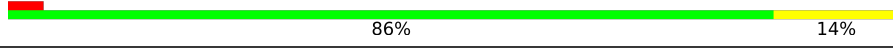
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	 7% 73% 22% 5%
1	b	215	 7% 80% 15% 5%
2	2	261	 70% 15% 15%
2	i	261	 67% 18% 15%

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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 106311 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	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
1	b	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
2	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	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	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
4	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	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	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
7	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	243	Total	C	N	O	S	0	0
			1921	1221	322	370	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	241	Total	C	N	O	S	0	0
			1890	1181	331	374	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
			1888	1201	328	355	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	355	Total	C	N	O	S	0	0
			2787	1755	500	515	17		

- 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	371	Total	C	N	O	S	0	0
			2937	1852	519	554	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	258	Total	C	N	O	S	0	0
			2025	1273	344	395	13		

- 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	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- 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		

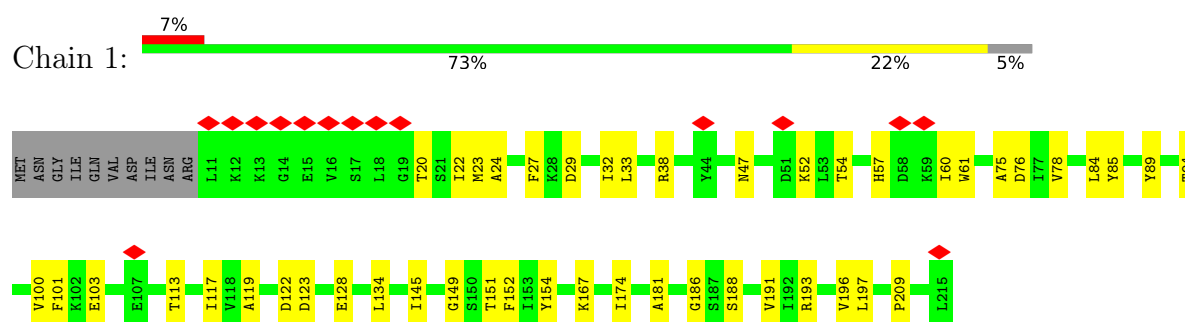
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

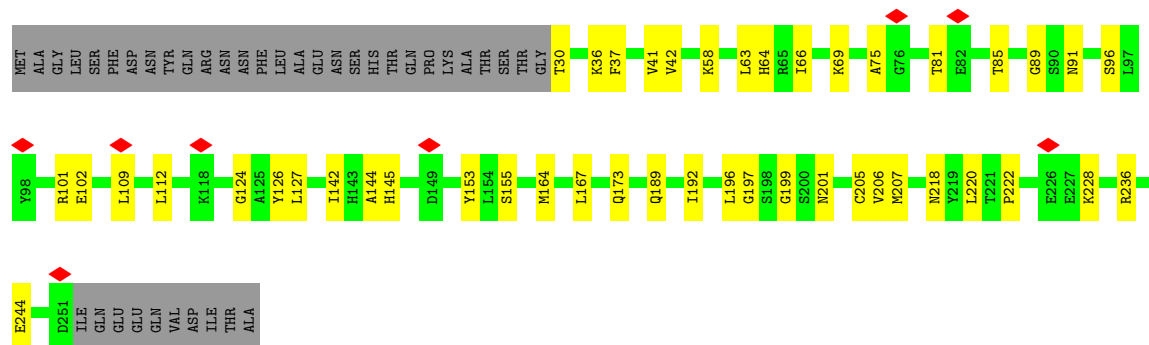
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

3 Residue-property plots

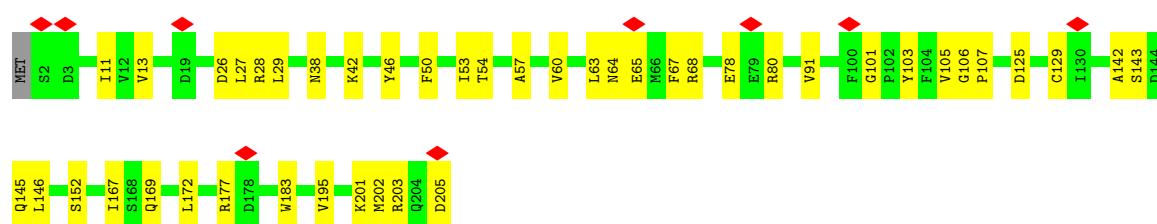
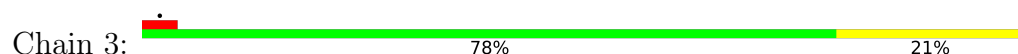
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

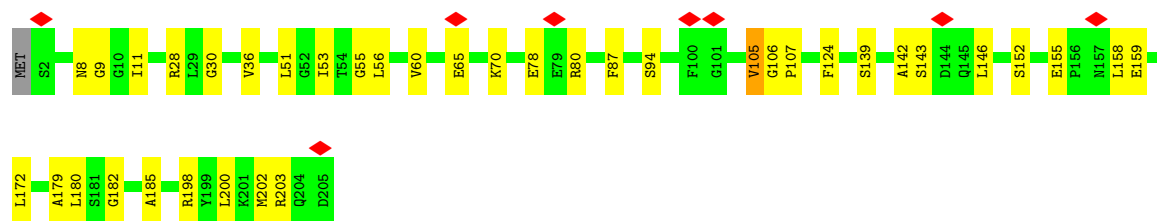
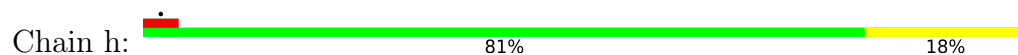




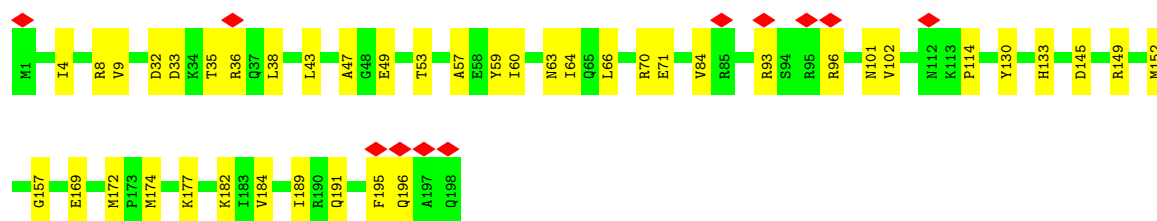
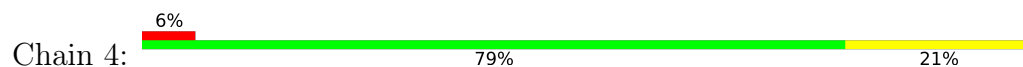
• Molecule 3: Proteasome subunit beta type-3



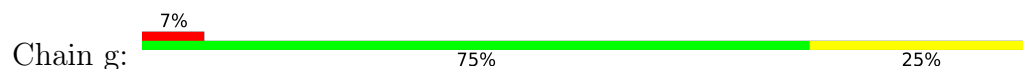
• Molecule 3: Proteasome subunit beta type-3

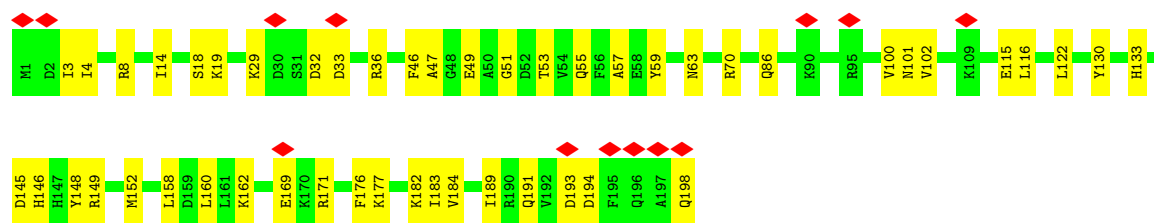


• Molecule 4: Proteasome subunit beta type-4

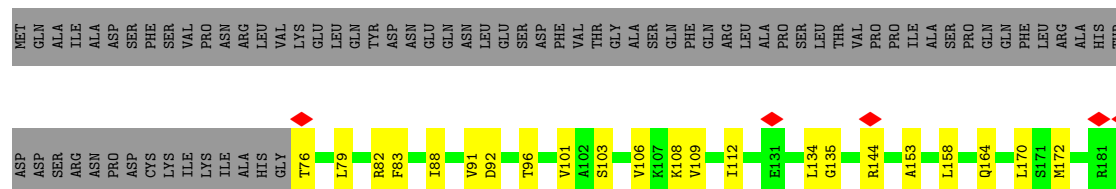


• Molecule 4: Proteasome subunit beta type-4

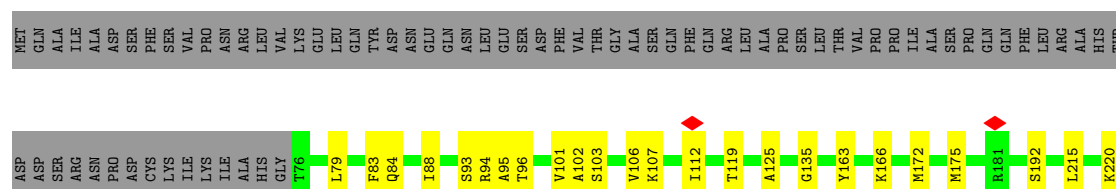




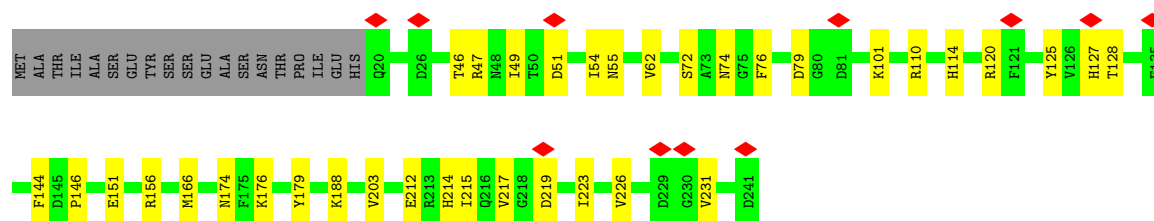
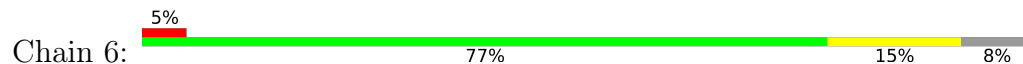
• Molecule 5: Proteasome subunit beta type-5



• Molecule 5: Proteasome subunit beta type-5

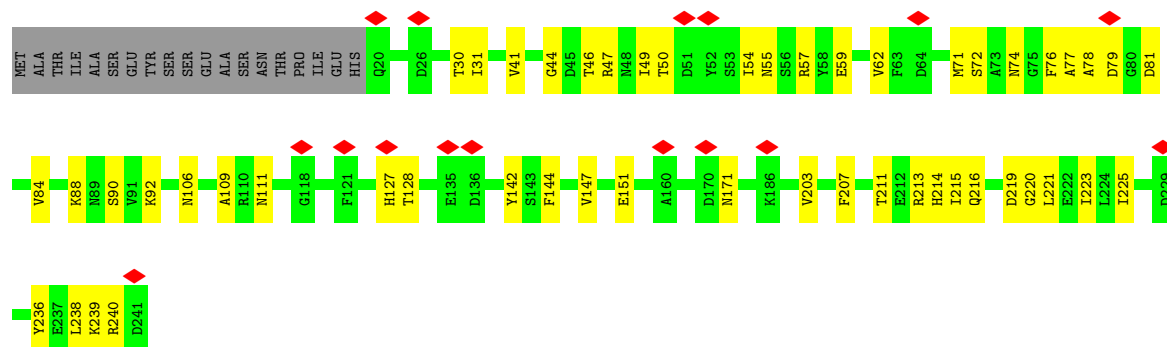


• Molecule 6: Proteasome subunit beta type-6



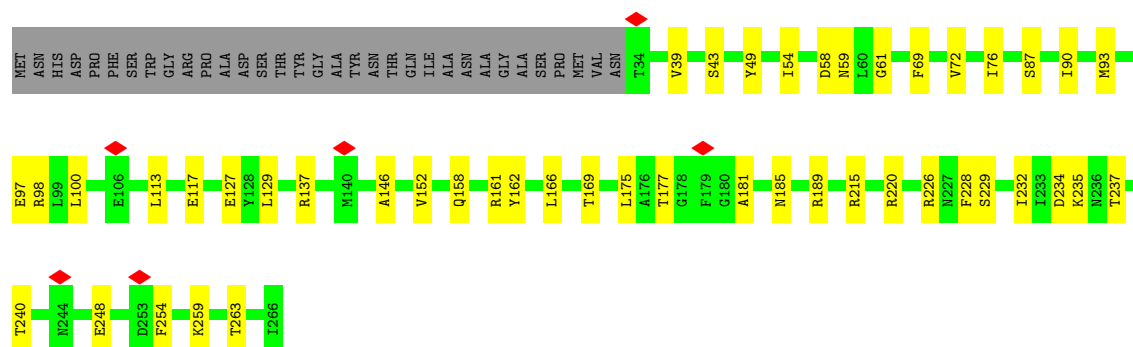
• Molecule 6: Proteasome subunit beta type-6





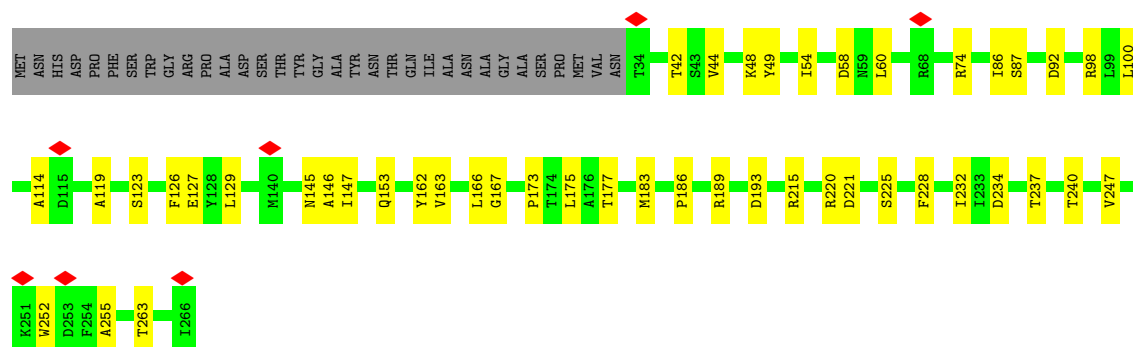
• Molecule 7: Proteasome subunit beta type-7

Chain 7: 70% 18% 12%



• Molecule 7: Proteasome subunit beta type-7

Chain a: 70% 18% 12%



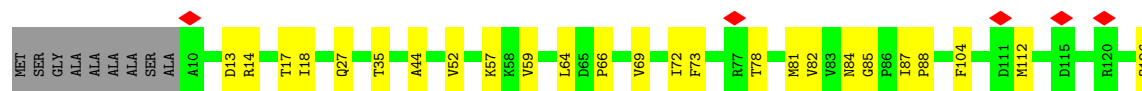
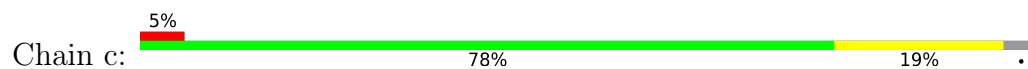
• Molecule 8: Proteasome subunit alpha type-1

Chain A: 77% 19% 4%

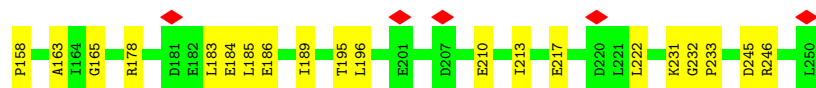
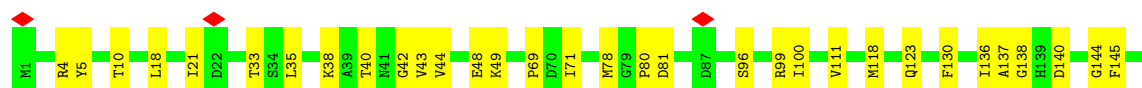
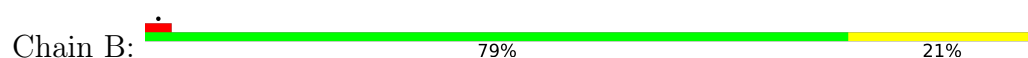




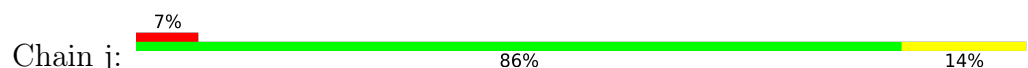
- Molecule 8: Proteasome subunit alpha type-1



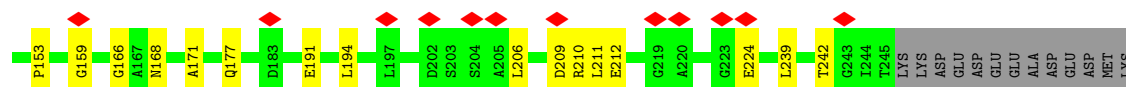
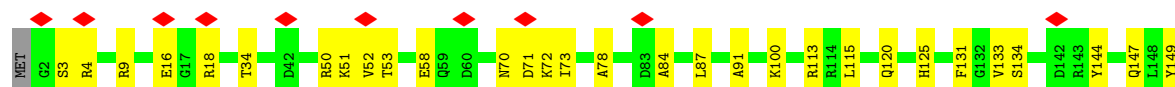
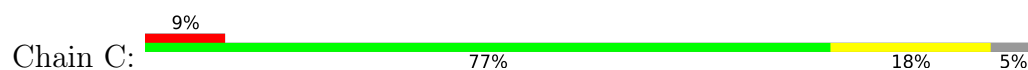
- Molecule 9: Proteasome subunit alpha type-2



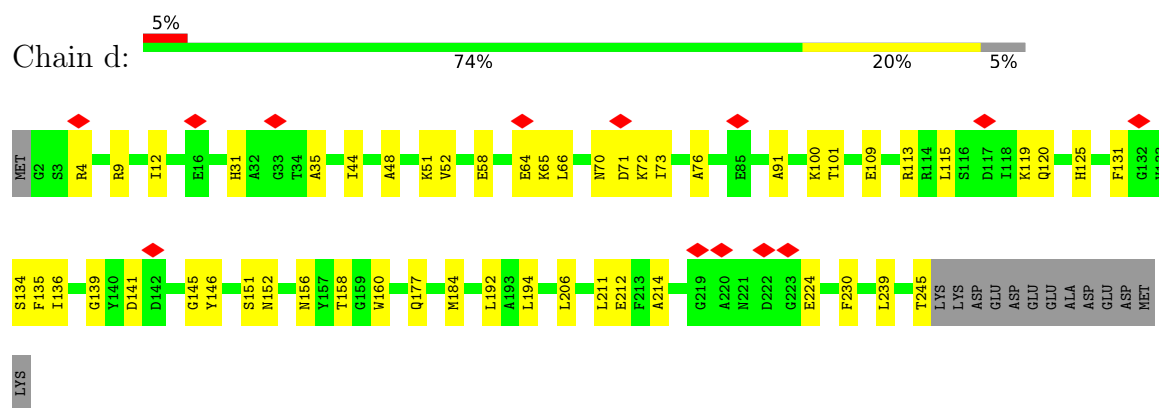
- Molecule 9: Proteasome subunit alpha type-2



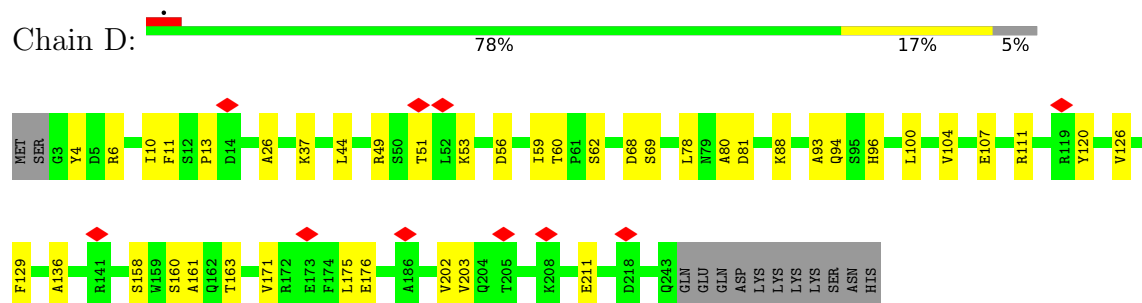
- Molecule 10: Proteasome subunit alpha type-3



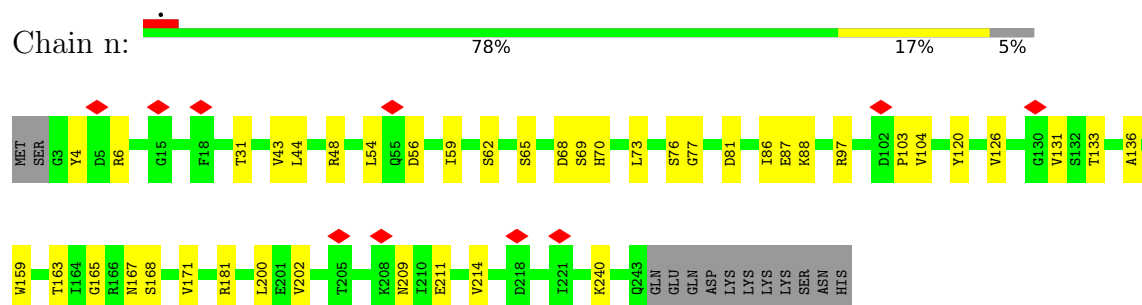
- Molecule 10: Proteasome subunit alpha type-3



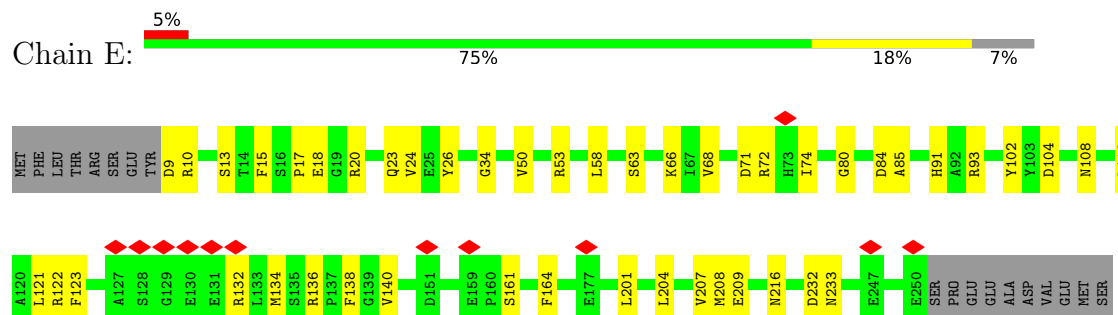
- Molecule 11: Proteasome subunit alpha type-4



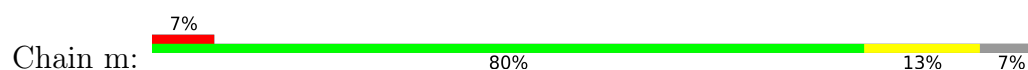
- Molecule 11: Proteasome subunit alpha type-4

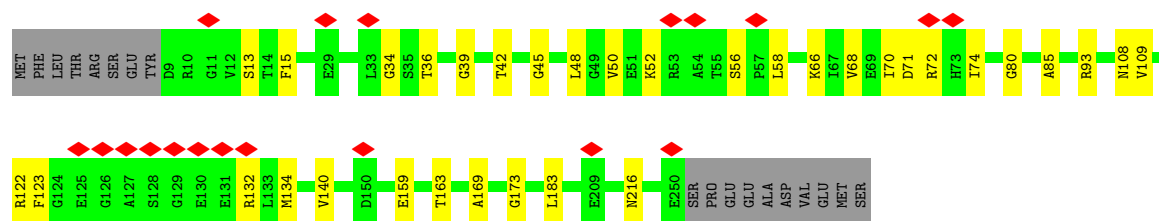


- Molecule 12: Proteasome subunit alpha type-5

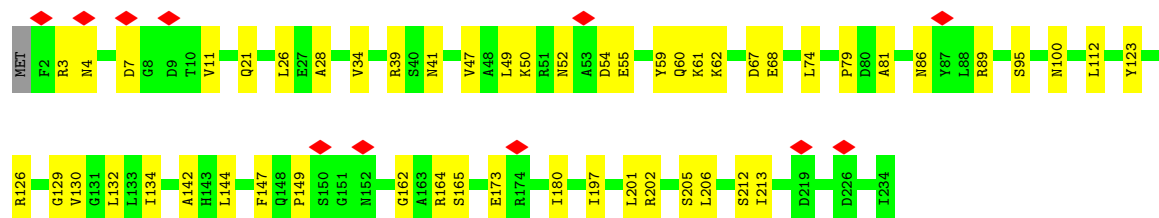
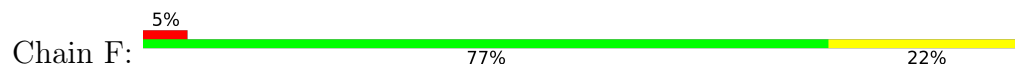


- Molecule 12: Proteasome subunit alpha type-5

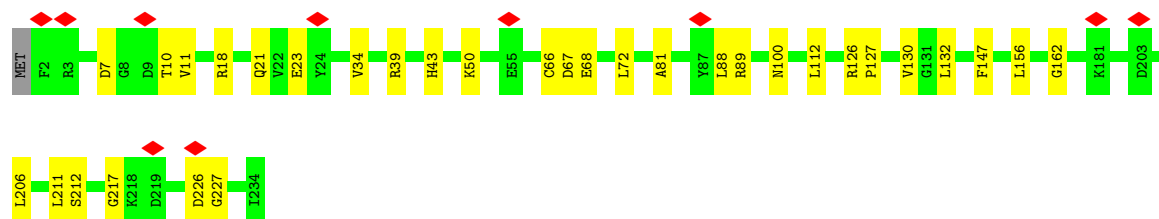
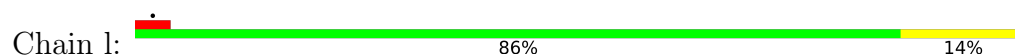




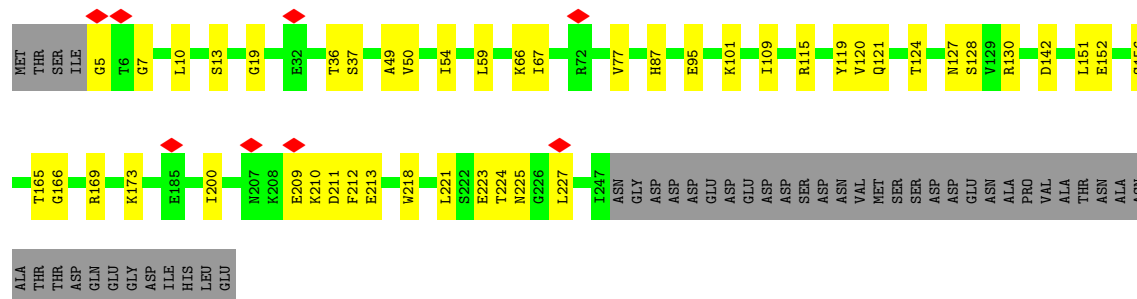
- Molecule 13: Proteasome subunit alpha type-6



- Molecule 13: Proteasome subunit alpha type-6



- Molecule 14: Probable proteasome subunit alpha type-7

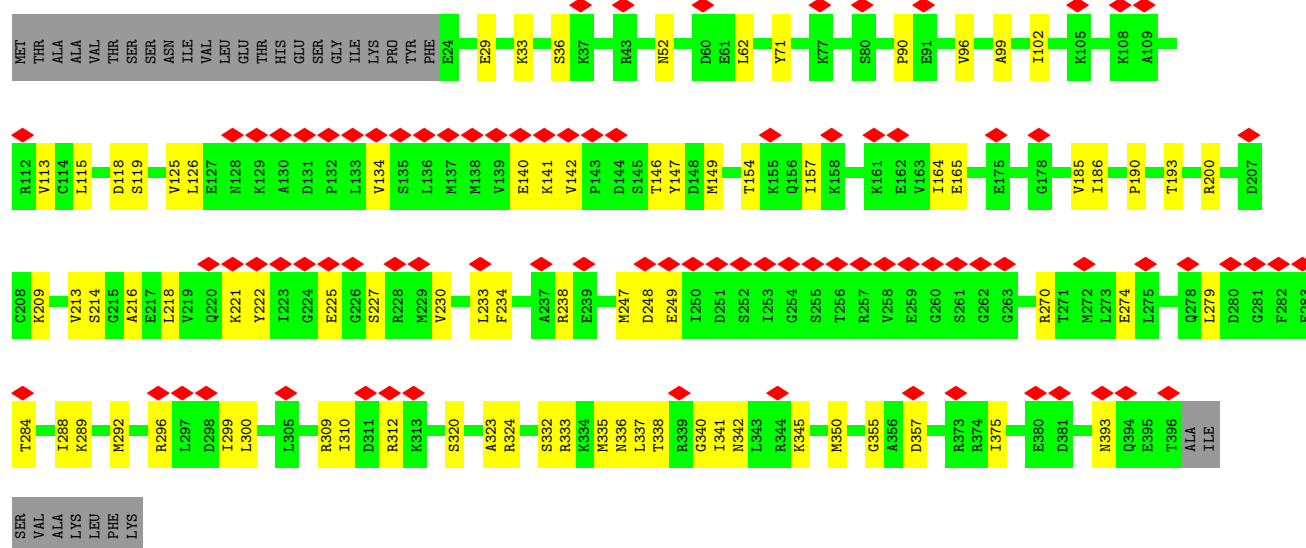


- Molecule 14: Probable proteasome subunit alpha type-7

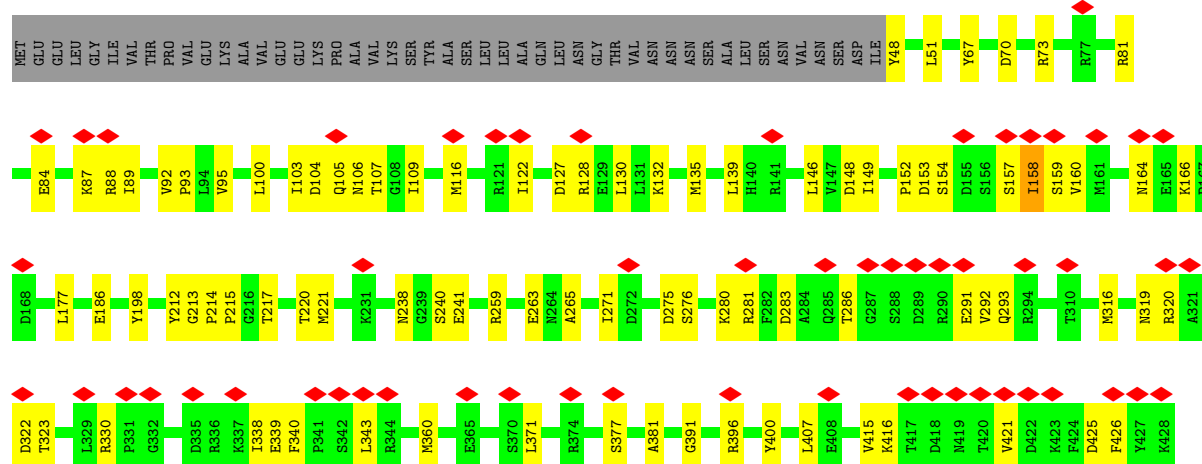




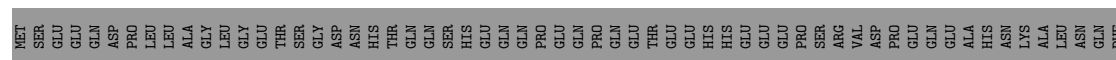
- Molecule 17: 26S protease regulatory subunit 8 homolog



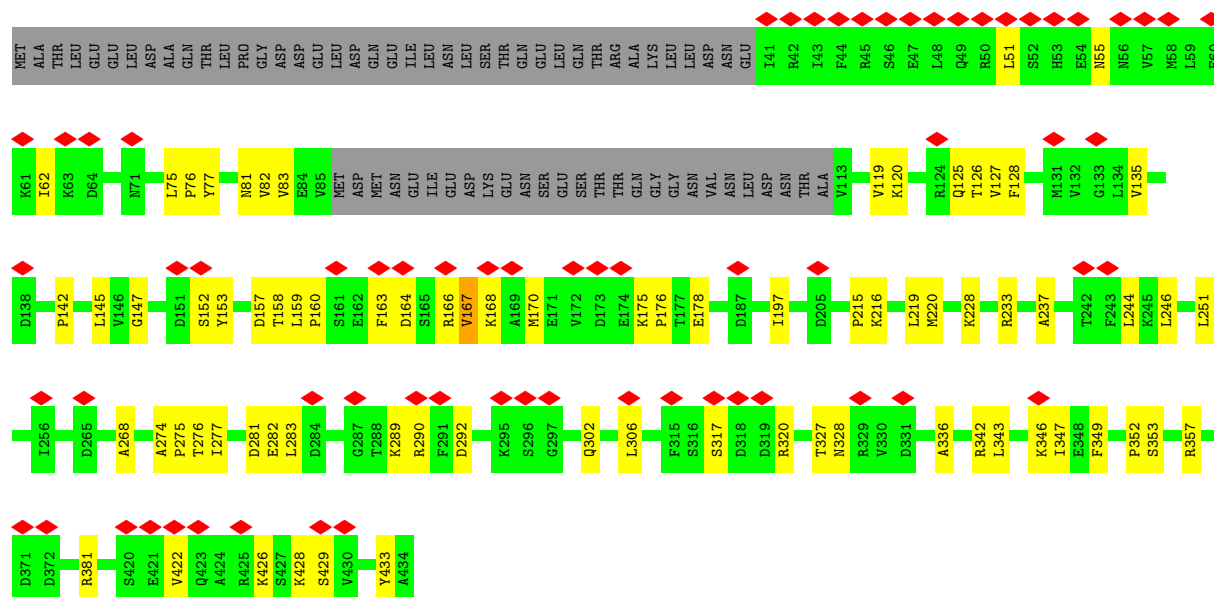
- Molecule 18: 26S protease regulatory subunit 6B homolog



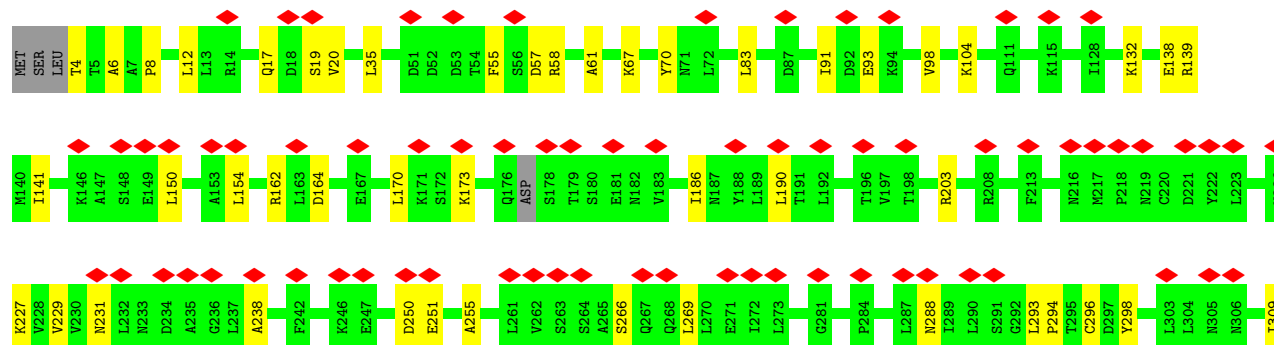
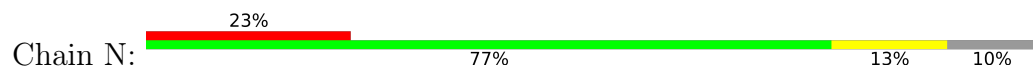
- Molecule 19: 26S protease subunit RPT4

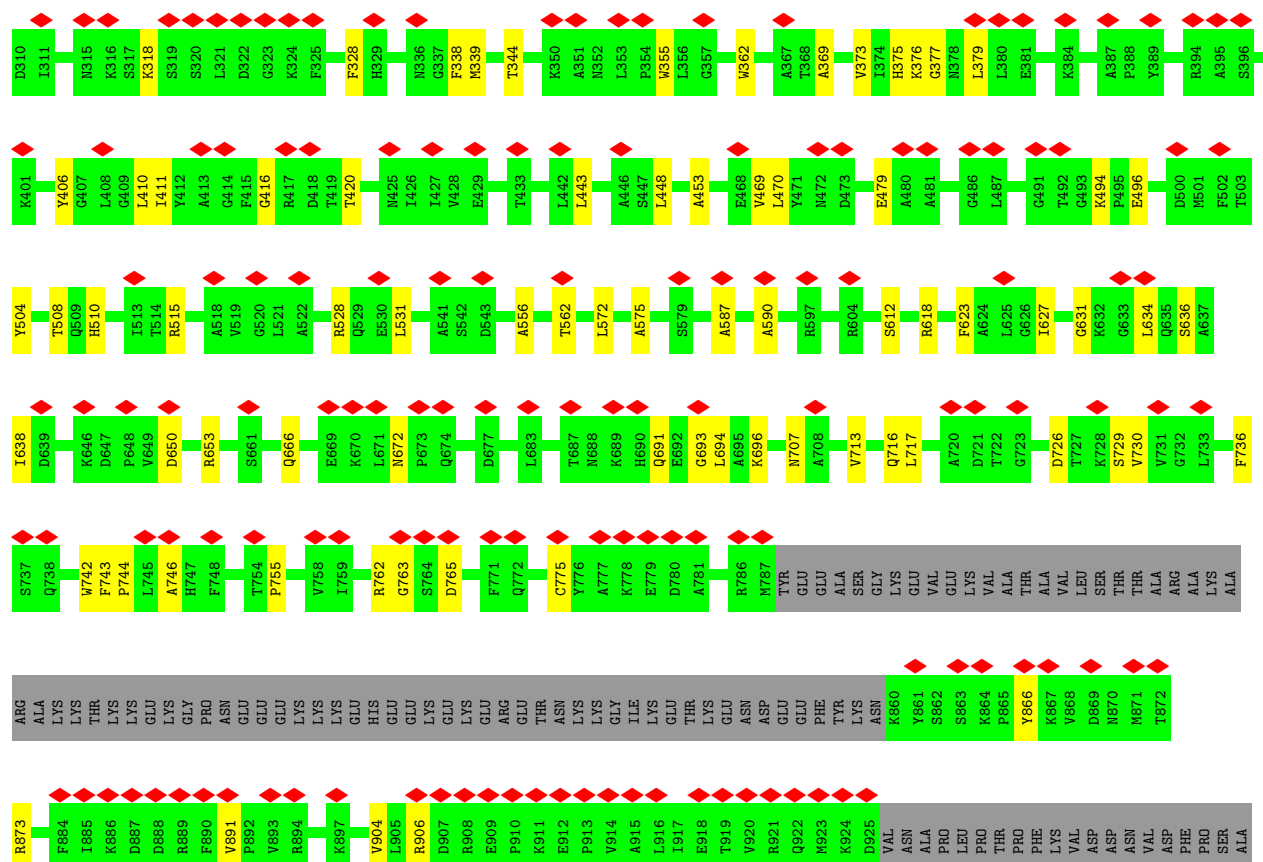


- Molecule 20: 26S protease regulatory subunit 6A

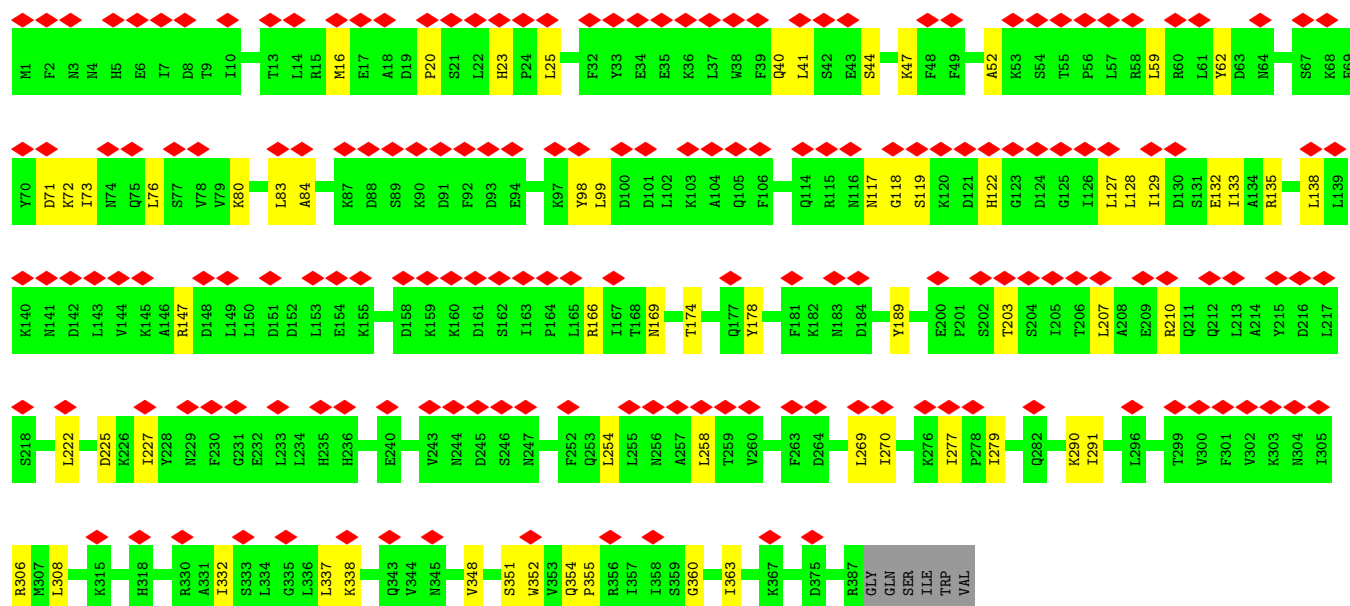
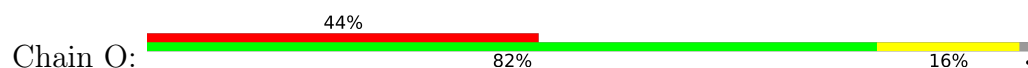


- Molecule 21: 26S proteasome regulatory subunit RPN2



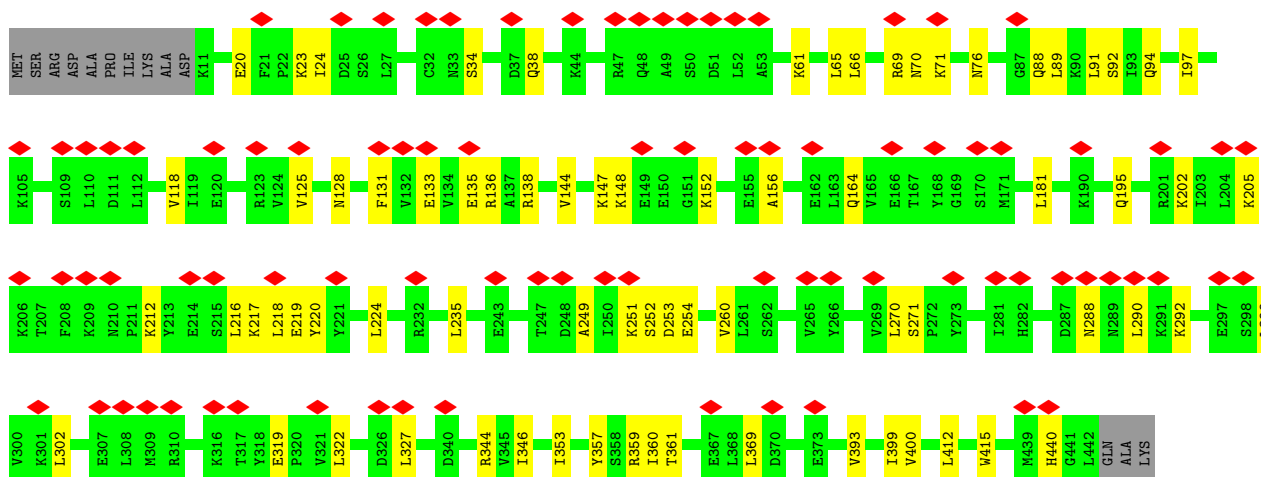


• Molecule 22: 26S proteasome regulatory subunit RPN9



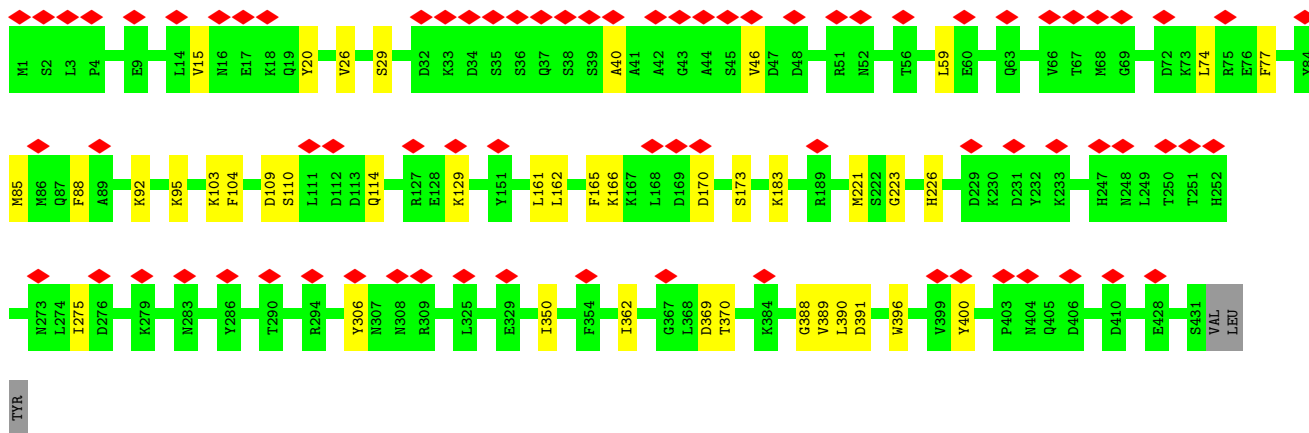
• Molecule 23: 26S proteasome regulatory subunit RPN5

Chain P: 19% 80% 17% .



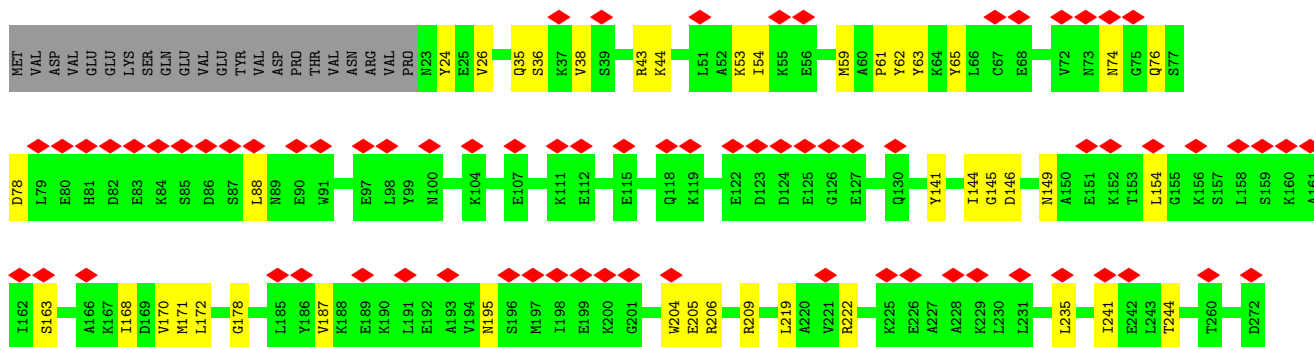
• Molecule 24: 26S proteasome regulatory subunit RPN6

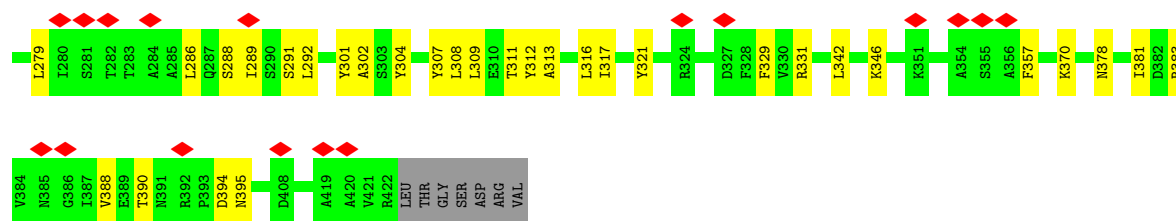
Chain Q: 18% 90% 9% .



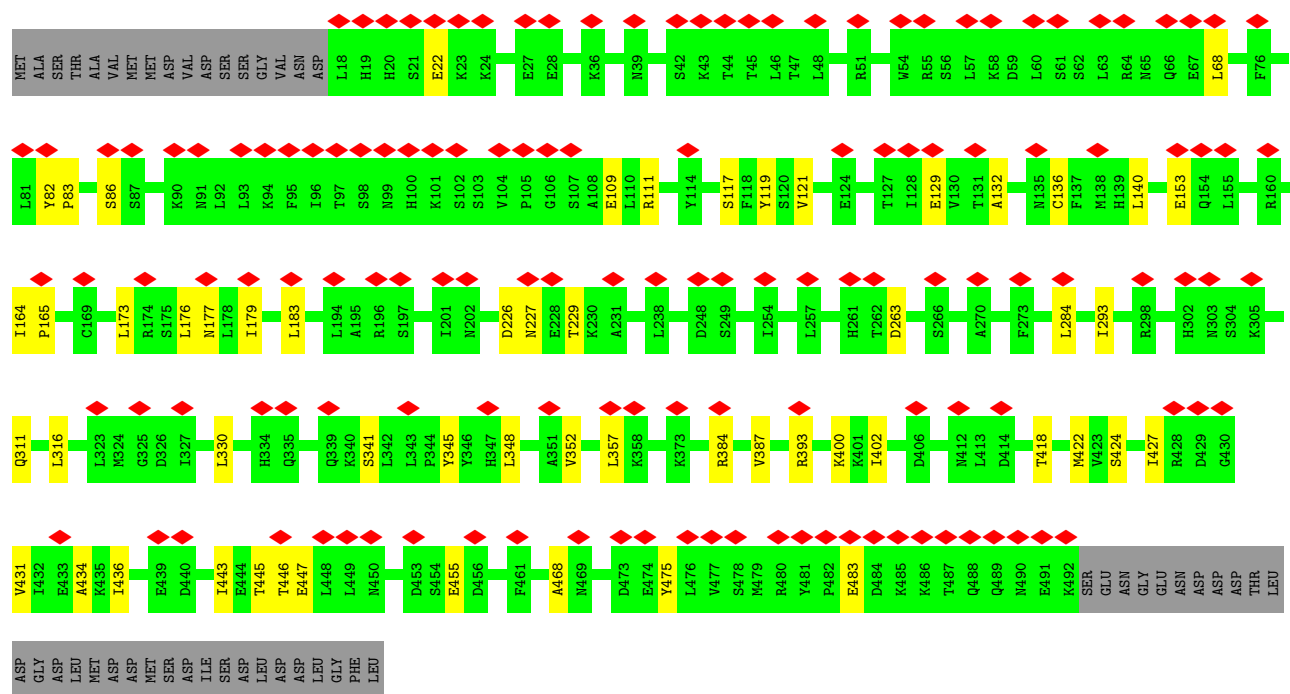
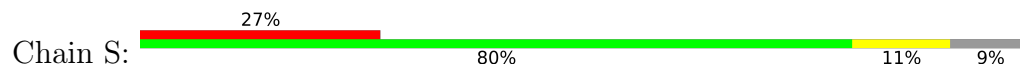
• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R: 21% 76% 17% 7% .

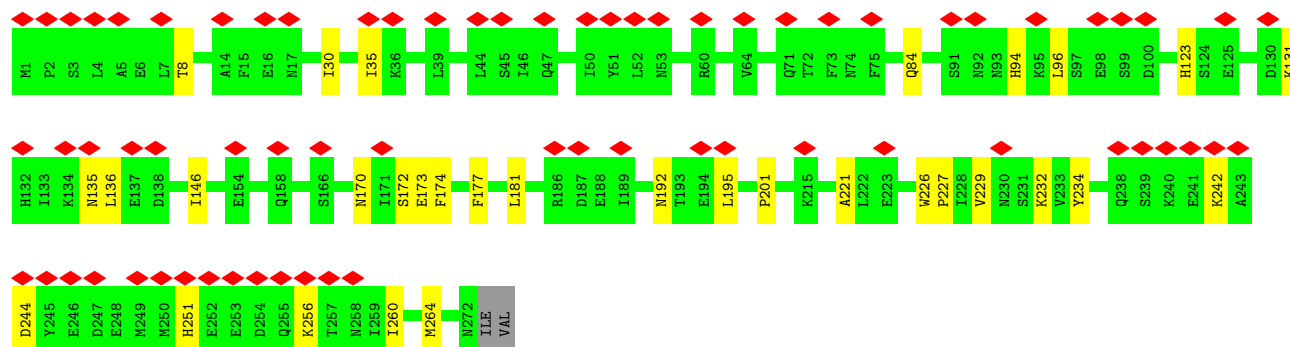
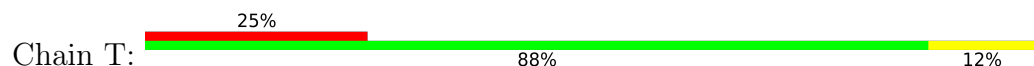




• Molecule 26: 26S proteasome regulatory subunit RPN3

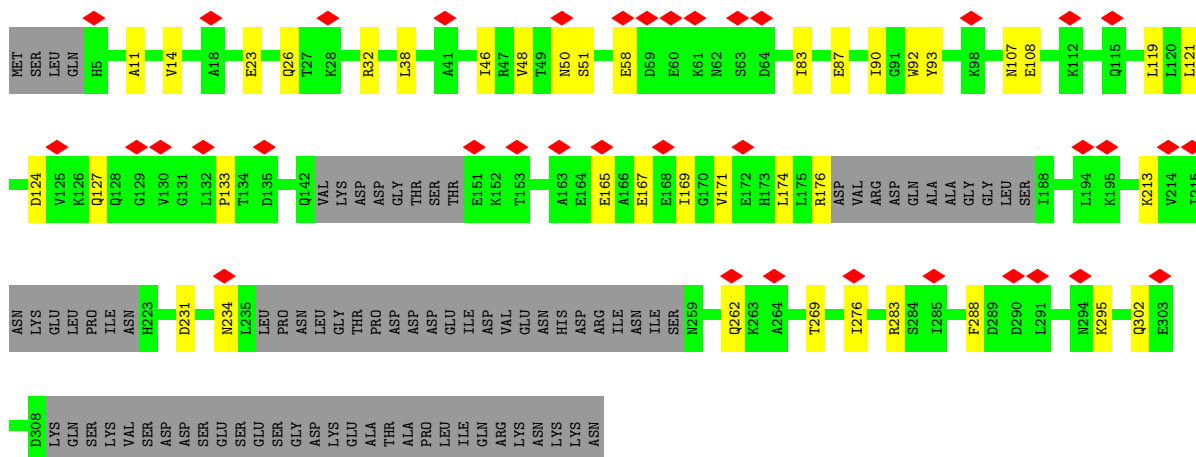


• Molecule 27: 26S proteasome regulatory subunit RPN12

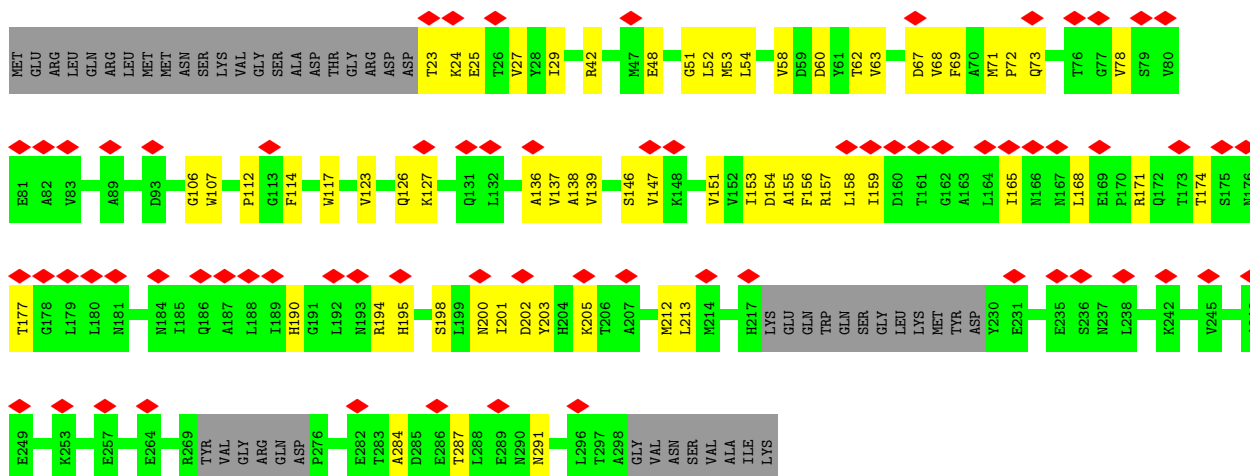


• Molecule 28: 26S proteasome regulatory subunit RPN8

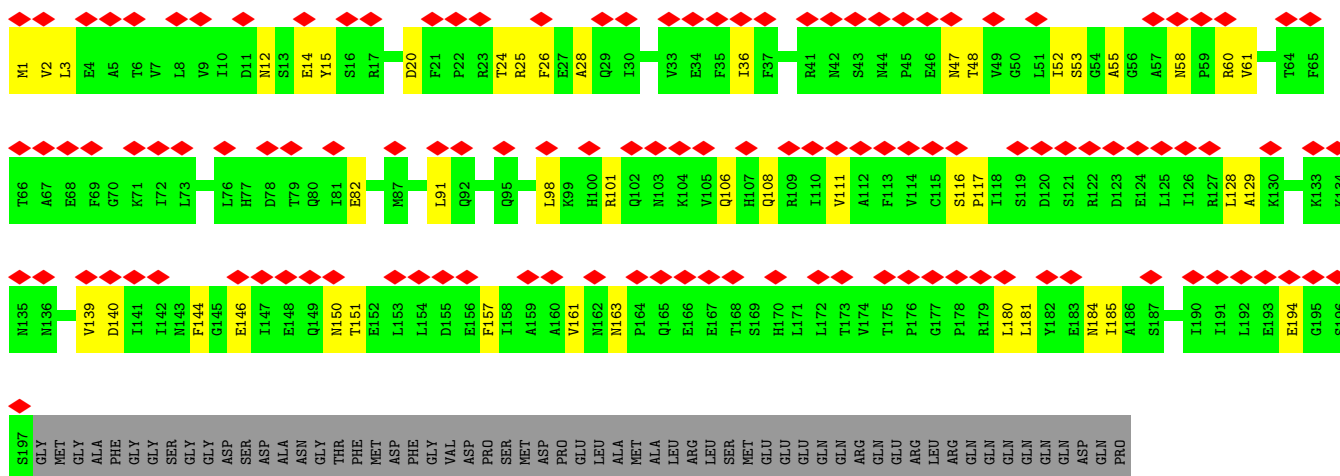




• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11



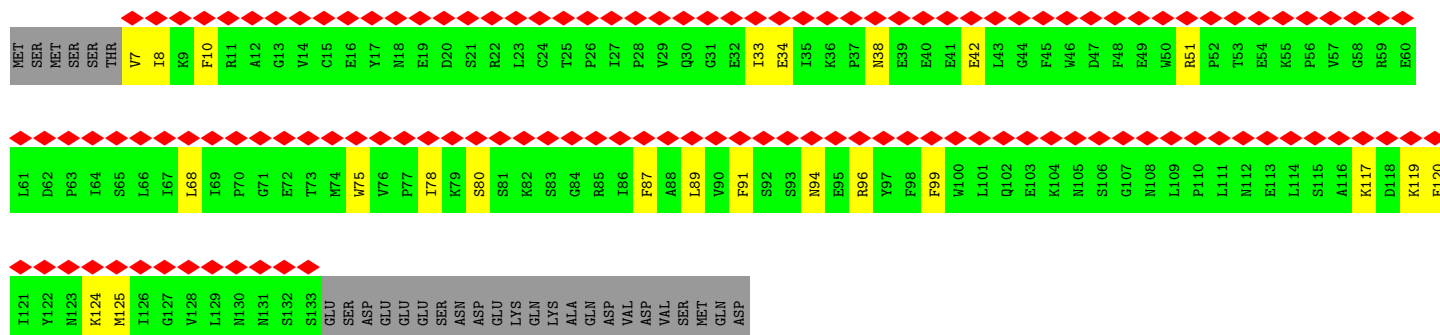
• Molecule 30: 26S proteasome regulatory subunit RPN10



GLU
GLN
SER
GLU
GLN
PRO
GLU
GLN
HIS
GLN
ASP
LYS

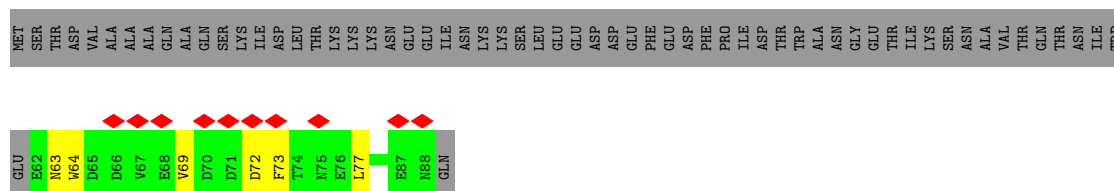
• Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X:



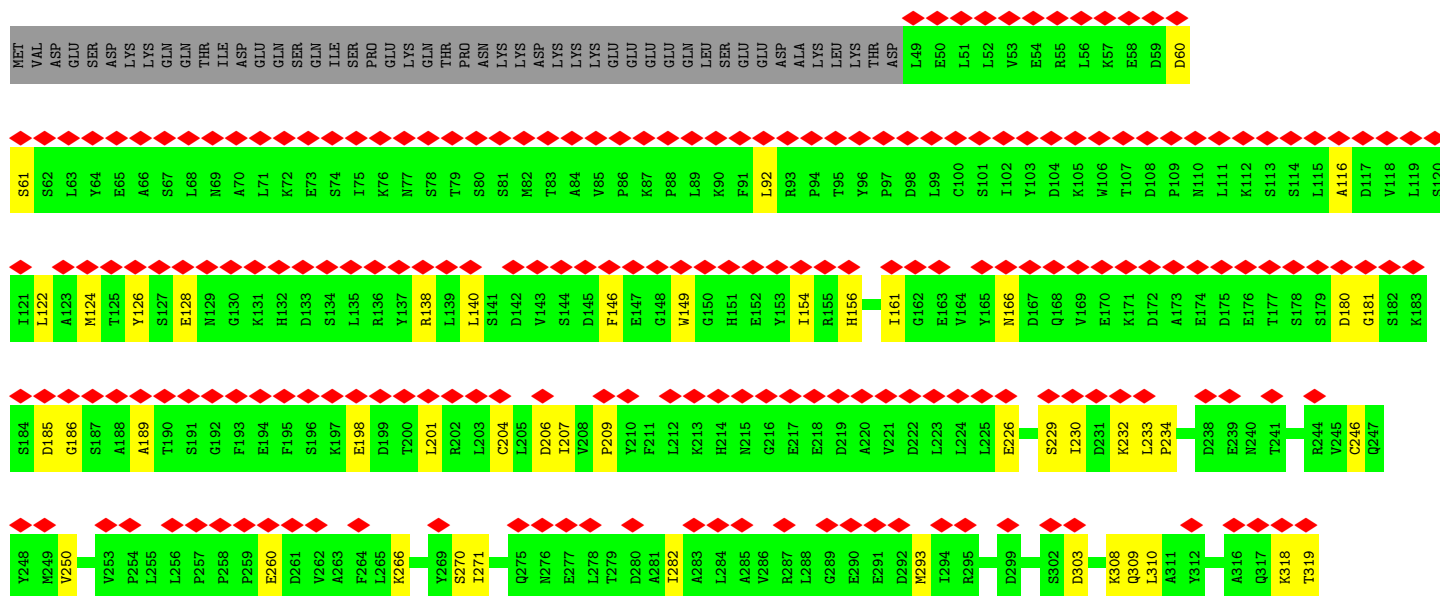
• Molecule 32: 26S proteasome complex subunit SEM1

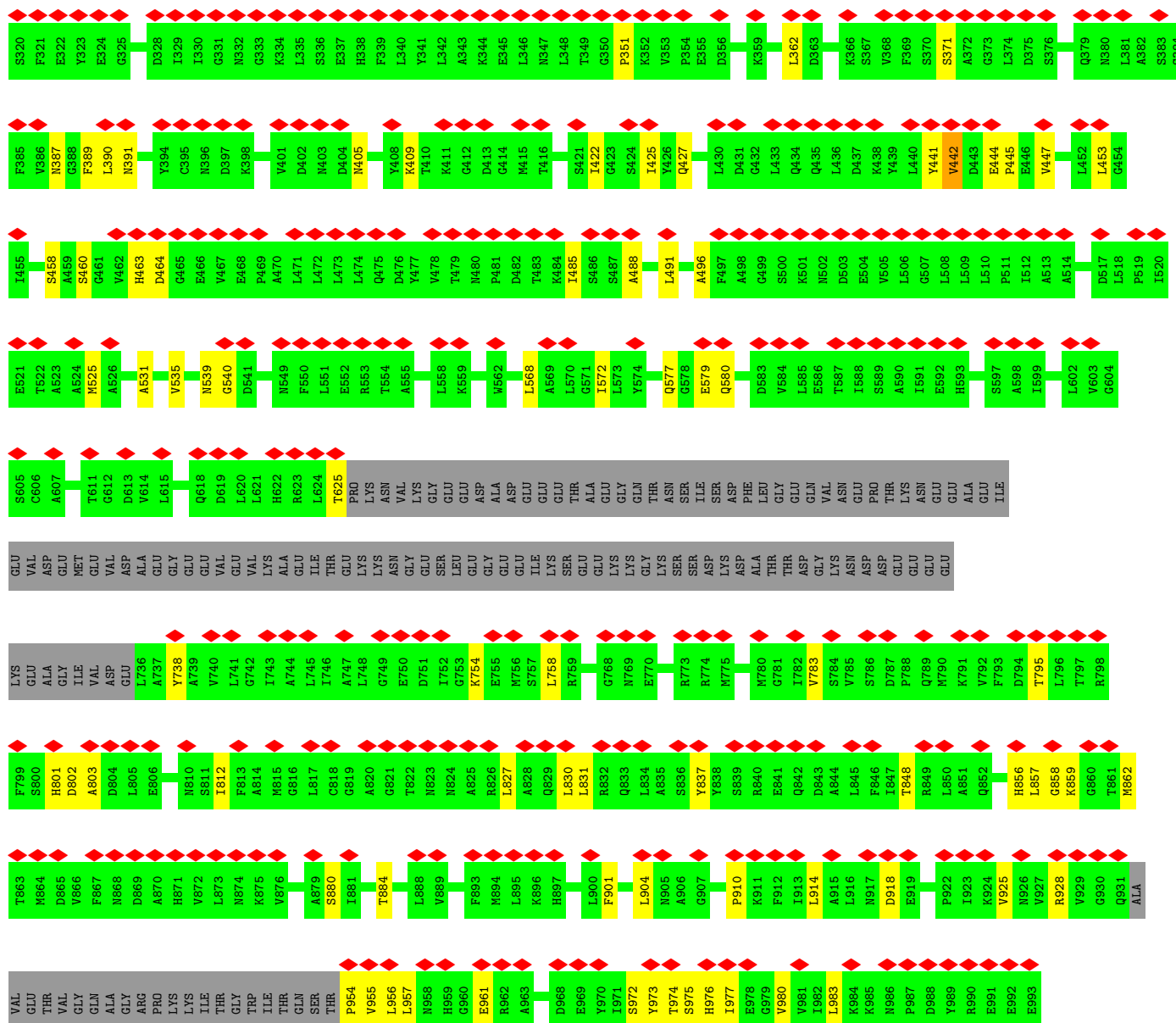
Chain Y:



• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77729	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	2.361	Depositor
Minimum map value	-1.289	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.477	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	0/1605	0.22	0/2171
1	b	0.07	0/1605	0.23	0/2171
2	2	0.06	0/1715	0.21	0/2326
2	i	0.06	0/1715	0.21	0/2326
3	3	0.08	0/1611	0.25	0/2174
3	h	0.08	0/1611	0.26	0/2174
4	4	0.07	0/1613	0.24	0/2173
4	g	0.07	0/1613	0.22	0/2173
5	5	0.07	0/1681	0.22	0/2274
5	f	0.07	0/1681	0.25	0/2274
6	6	0.08	0/1795	0.26	1/2420 (0.0%)
6	e	0.07	0/1795	0.23	0/2420
7	7	0.08	0/1855	0.25	0/2514
7	a	0.07	0/1855	0.25	0/2514
8	A	0.07	0/1959	0.24	0/2652
8	c	0.07	0/1959	0.22	0/2652
9	B	0.07	0/1952	0.22	0/2642
9	j	0.06	0/1952	0.20	0/2642
10	C	0.07	0/1934	0.23	0/2618
10	d	0.07	0/1934	0.22	0/2618
11	D	0.07	0/1919	0.23	0/2598
11	n	0.07	0/1919	0.22	0/2598
12	E	0.07	0/1886	0.24	0/2541
12	m	0.06	0/1886	0.19	0/2541
13	F	0.07	0/1823	0.23	0/2463
13	l	0.07	0/1823	0.22	0/2463
14	G	0.08	0/1928	0.24	0/2603
14	k	0.07	0/1936	0.22	0/2614
15	H	0.10	0/2834	0.32	0/3816
16	I	0.09	0/2869	0.30	0/3867
17	J	0.09	0/2964	0.26	0/3981
18	K	0.19	1/3062 (0.0%)	0.31	0/4132
19	L	0.21	1/2981 (0.0%)	0.28	0/4008
20	M	0.09	0/2903	0.29	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	N	0.09	0/6670	0.22	0/9023
22	O	0.11	0/3243	0.27	0/4374
23	P	0.07	0/3599	0.23	0/4854
24	Q	0.07	0/3527	0.22	0/4748
25	R	0.07	0/3272	0.25	0/4412
26	S	0.08	0/3966	0.26	1/5355 (0.0%)
27	T	0.07	0/2279	0.27	1/3077 (0.0%)
28	U	0.06	0/2087	0.19	0/2811
29	V	0.07	0/2054	0.25	0/2770
30	W	0.07	0/1557	0.24	0/2111
31	X	0.07	0/1058	0.23	0/1432
32	Y	0.12	0/239	0.30	0/322
33	Z	0.08	0/6404	0.24	1/8686 (0.0%)
All	All	0.09	2/108128 (0.0%)	0.24	4/146037 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	274	GLU	C-N	10.28	1.57	1.33
18	K	265	ALA	C-N	9.32	1.55	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	244	ASP	CB-CA-C	-6.26	109.34	116.54
26	S	153	GLU	CB-CA-C	-5.33	109.99	117.23
33	Z	318	LYS	CB-CA-C	-5.28	110.05	117.23
6	6	51	ASP	CB-CA-C	-5.27	110.48	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1576	0	1552	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1576	0	1552	20	0
2	2	1684	0	1685	26	0
2	i	1684	0	1685	32	0
3	3	1581	0	1571	30	0
3	h	1581	0	1571	26	0
4	4	1585	0	1590	30	0
4	g	1585	0	1590	34	0
5	5	1644	0	1592	31	0
5	f	1644	0	1592	25	0
6	6	1757	0	1708	26	0
6	e	1757	0	1708	41	0
7	7	1824	0	1829	34	0
7	a	1824	0	1829	31	0
8	A	1921	0	1910	34	0
8	c	1921	0	1910	29	0
9	B	1915	0	1929	34	0
9	j	1915	0	1929	21	0
10	C	1904	0	1901	32	0
10	d	1904	0	1901	36	0
11	D	1890	0	1900	30	0
11	n	1890	0	1900	27	0
12	E	1861	0	1836	36	0
12	m	1861	0	1836	20	0
13	F	1795	0	1797	36	0
13	l	1795	0	1797	22	0
14	G	1888	0	1880	33	0
14	k	1896	0	1886	24	0
15	H	2787	0	2851	58	0
16	I	2831	0	2881	52	0
17	J	2928	0	3057	52	0
18	K	3019	0	3084	59	0
19	L	2937	0	3011	55	0
20	M	2866	0	2938	52	0
21	N	6562	0	6625	73	0
22	O	3182	0	3207	36	0
23	P	3545	0	3629	46	0
24	Q	3471	0	3495	23	0
25	R	3218	0	3216	45	0
26	S	3894	0	3938	34	0
27	T	2235	0	2207	20	0
28	U	2061	0	2116	31	0
29	V	2025	0	2035	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	W	1534	0	1542	27	0
31	X	1032	0	1015	13	0
32	Y	236	0	203	6	0
33	Z	6290	0	6236	69	0
All	All	106311	0	106652	1405	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 7.

All (1405) 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)
3:h:107:PRO:HD2	3:h:124:PHE:HB2	1.58	0.84
5:f:93:SER:HB2	5:f:106:VAL:H	1.46	0.79
22:O:147:ARG:HD3	23:P:288:ASN:HD21	1.47	0.78
29:V:24:LYS:H	29:V:174:THR:HG22	1.50	0.77
19:L:165:PRO:HD2	20:M:83:VAL:HB	1.67	0.75
9:B:78:MET:HG2	9:B:80:PRO:HD2	1.69	0.73
30:W:12:ASN:ND2	30:W:53:SER:OG	2.23	0.72
8:A:135:ARG:HB3	14:G:13:SER:HB2	1.71	0.71
5:f:172:MET:H	5:f:192:SER:HB3	1.54	0.71
6:e:128:THR:HB	6:e:144:PHE:HB2	1.73	0.71
13:F:34:VAL:HA	13:F:162:GLY:HA3	1.72	0.71
23:P:66:LEU:HD13	23:P:70:ASN:HD22	1.56	0.71
1:b:20:THR:HG21	1:b:52:LYS:HE3	1.72	0.71
10:C:51:LYS:HG2	10:C:52:VAL:HG23	1.73	0.71
20:M:178:GLU:HG3	20:M:233:ARG:HE	1.57	0.70
29:V:52:LEU:HB2	29:V:69:PHE:HB3	1.74	0.70
10:d:51:LYS:HG2	10:d:52:VAL:HG23	1.74	0.69
6:6:101:LYS:HD2	12:E:108:ASN:HD21	1.57	0.69
7:a:87:SER:HB3	7:a:146:ALA:HB3	1.75	0.69
15:H:243:PRO:HB3	15:H:372:ASP:HB2	1.74	0.69
18:K:275:ASP:OD2	18:K:319:ASN:ND2	2.24	0.69
19:L:118:ILE:HG12	19:L:128:ILE:HG12	1.75	0.68
19:L:280:MET:HB2	19:L:325:MET:HA	1.75	0.68
15:H:247:LEU:HB3	15:H:374:LYS:HA	1.75	0.68
5:f:94:ARG:HH21	5:f:247:GLY:HA3	1.58	0.68
28:U:32:ARG:NH2	28:U:58:GLU:OE1	2.27	0.68
10:C:34:THR:HA	10:C:166:GLY:HA3	1.76	0.68
2:i:101:ARG:NH2	8:c:149:GLU:OE1	2.26	0.67
11:D:10:ILE:HG23	12:E:23:GLN:HE22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:72:ILE:HG12	8:c:82:VAL:HG22	1.77	0.67
25:R:346:LYS:NZ	25:R:390:THR:O	2.27	0.67
5:f:220:LYS:HE2	5:f:222:ASP:HB2	1.76	0.67
12:E:53:ARG:HH12	12:E:209:GLU:H	1.40	0.67
17:J:193:THR:HA	17:J:355:GLY:H	1.59	0.67
15:H:185:LEU:HD12	15:H:186:PRO:HD2	1.77	0.67
12:E:121:LEU:HD11	13:F:79:PRO:HB2	1.77	0.67
13:l:34:VAL:HA	13:l:162:GLY:HA3	1.77	0.67
26:S:330:LEU:O	32:Y:63:ASN:ND2	2.27	0.67
5:5:220:LYS:HE2	5:5:222:ASP:HB2	1.77	0.67
22:O:41:LEU:HD22	22:O:62:TYR:HB2	1.77	0.67
3:3:28:ARG:NH2	3:3:205:ASP:OXT	2.27	0.66
28:U:169:ILE:HG21	29:V:147:VAL:HA	1.78	0.66
33:Z:928:ARG:HG3	33:Z:955:VAL:HG13	1.77	0.66
4:g:158:LEU:HD21	4:g:183:ILE:HD11	1.77	0.66
16:I:246:ARG:NH2	17:J:274:GLU:OE2	2.27	0.66
28:U:38:LEU:HB2	28:U:50:ASN:HB3	1.78	0.66
13:l:11:VAL:HA	14:k:130:ARG:HD3	1.77	0.66
23:P:89:LEU:HG	23:P:91:LEU:H	1.61	0.66
24:Q:183:LYS:HG2	24:Q:221:MET:HE2	1.78	0.66
1:1:47:ASN:HD22	2:2:149:ASP:HB3	1.61	0.66
18:K:276:SER:HB2	19:L:303:ARG:HG2	1.78	0.66
18:K:416:LYS:HE3	18:K:421:VAL:HG12	1.78	0.66
13:l:66:CYS:O	13:l:89:ARG:NH1	2.29	0.65
15:H:321:ASP:OD1	20:M:290:ARG:NH2	2.29	0.65
33:Z:362:LEU:HD13	33:Z:859:LYS:HD2	1.78	0.65
18:K:281:ARG:NH2	19:L:293:GLU:OE1	2.27	0.65
23:P:135:GLU:OE1	23:P:138:ARG:NH2	2.29	0.65
15:H:364:ALA:O	15:H:370:ARG:NH1	2.29	0.65
20:M:274:ALA:HA	20:M:320:ARG:HH21	1.59	0.65
22:O:225:ASP:O	22:O:290:LYS:NZ	2.29	0.65
10:C:84:ALA:HB2	10:C:133:VAL:HG21	1.79	0.65
19:L:248:ALA:HB2	19:L:283:VAL:HG22	1.78	0.65
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.79	0.64
13:F:52:ASN:ND2	13:F:54:ASP:O	2.30	0.64
19:L:329:ARG:NH2	19:L:435:GLN:OE1	2.29	0.64
25:R:383:ARG:HG3	26:S:402:ILE:HG13	1.78	0.64
16:I:104:LEU:HB3	16:I:148:LEU:HD11	1.79	0.64
22:O:118:GLY:HA3	22:O:128:LEU:HD22	1.80	0.64
28:U:48:VAL:HG22	28:U:90:ILE:HD11	1.80	0.64
8:A:14:ARG:O	8:A:27:GLN:NE2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:91:ALA:HB2	10:C:115:LEU:HD11	1.79	0.64
15:H:103:THR:O	20:M:166:ARG:NH1	2.30	0.64
19:L:219:LEU:HB2	19:L:343:LEU:HD13	1.80	0.64
14:G:87:HIS:HE2	14:G:119:TYR:HH	1.42	0.64
13:l:7:ASP:O	13:l:21:GLN:NE2	2.31	0.64
25:R:219:LEU:O	25:R:222:ARG:NH1	2.30	0.64
8:c:135:ARG:HB3	14:k:13:SER:HB2	1.80	0.64
21:N:190:LEU:HD22	21:N:227:LYS:HE2	1.79	0.64
29:V:23:THR:HG23	29:V:190:HIS:HE1	1.63	0.64
15:H:318:ARG:HB3	16:I:300:ARG:HH21	1.62	0.64
21:N:494:LYS:HE2	21:N:496:GLU:HB2	1.80	0.64
16:I:285:ASP:OD2	17:J:270:ARG:NH1	2.30	0.64
25:R:172:LEU:HD21	25:R:209:ARG:HD3	1.79	0.64
33:Z:387:ASN:O	33:Z:391:ASN:ND2	2.31	0.64
9:B:49:LYS:HE3	9:B:210:GLU:HB2	1.78	0.64
16:I:172:LYS:HG3	16:I:246:ARG:HB2	1.80	0.64
24:Q:40:ALA:HA	24:Q:46:VAL:HA	1.80	0.63
26:S:173:LEU:O	26:S:177:ASN:ND2	2.32	0.63
7:7:263:THR:HG23	2:i:109:LEU:HD22	1.79	0.63
10:C:9:ARG:NH1	12:E:9:ASP:OD2	2.32	0.63
17:J:29:GLU:OE2	21:N:104:LYS:NZ	2.31	0.63
1:l:23:MET:HE2	1:l:174:ILE:HG12	1.79	0.63
9:j:49:LYS:HE3	9:j:210:GLU:HB2	1.81	0.63
21:N:203:ARG:HH22	21:N:562:THR:HG21	1.63	0.63
7:a:60:LEU:HD22	7:a:225:SER:HB3	1.80	0.63
4:g:86:GLN:HG3	10:d:101:THR:HA	1.81	0.63
33:Z:138:ARG:HE	33:Z:161:ILE:HD11	1.63	0.63
1:b:57:HIS:HB3	1:b:60:ILE:HB	1.80	0.63
12:E:85:ALA:HB2	12:E:140:VAL:HG21	1.80	0.62
17:J:320:SER:H	17:J:323:ALA:HB3	1.64	0.62
26:S:227:ASN:HD22	26:S:263:ASP:HB2	1.63	0.62
28:U:127:GLN:HE22	29:V:212:MET:HA	1.64	0.62
20:M:336:ALA:O	20:M:342:ARG:NH2	2.31	0.62
14:k:224:THR:HB	14:k:227:LEU:HB2	1.81	0.62
22:O:269:LEU:HD23	22:O:270:ILE:HG13	1.82	0.62
30:W:20:ASP:HB2	30:W:25:ARG:HD2	1.80	0.62
20:M:246:LEU:HD11	20:M:251:LEU:HD21	1.81	0.62
10:C:50:ARG:NH2	10:C:209:ASP:O	2.33	0.62
10:d:70:ASN:OD1	10:d:71:ASP:N	2.33	0.62
20:M:82:VAL:HG22	20:M:119:VAL:HG12	1.82	0.62
29:V:287:THR:O	29:V:291:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:163:THR:HG21	11:D:171:VAL:HB	1.82	0.61
18:K:371:LEU:HD11	18:K:407:LEU:HB3	1.80	0.61
17:J:332:SER:HB2	17:J:337:LEU:HD21	1.82	0.61
7:a:58:ASP:OD1	7:a:74:ARG:NH2	2.31	0.61
12:m:36:THR:HA	12:m:173:GLY:HA3	1.82	0.61
24:Q:170:ASP:HB3	24:Q:173:SER:HB2	1.80	0.61
26:S:136:CYS:HB3	26:S:179:ILE:HG21	1.82	0.61
8:A:40:ILE:HG23	8:A:56:GLN:HB2	1.80	0.61
8:A:78:THR:HG22	8:A:231:ASP:HA	1.83	0.61
17:J:338:THR:HG22	17:J:340:GLY:H	1.65	0.61
7:a:127:GLU:HG2	13:l:100:ASN:HB2	1.81	0.61
26:S:475:TYR:HE1	28:U:295:LYS:HB2	1.66	0.61
33:Z:229:SER:HB2	33:Z:232:LYS:HB2	1.83	0.61
1:1:193:ARG:NH2	7:a:255:ALA:O	2.33	0.61
4:4:177:LYS:NZ	4:g:169:GLU:O	2.34	0.61
20:M:77:TYR:HB3	20:M:147:GLY:HA3	1.83	0.61
25:R:154:LEU:HB3	25:R:170:VAL:HG13	1.81	0.61
22:O:258:LEU:HD13	22:O:291:ILE:HG13	1.83	0.61
9:B:33:THR:HA	9:B:165:GLY:HA3	1.83	0.60
18:K:84:GLU:HA	18:K:87:LYS:HE2	1.82	0.60
22:O:207:LEU:HD23	22:O:210:ARG:HD2	1.83	0.60
23:P:147:LYS:HB3	23:P:152:LYS:HB2	1.83	0.60
31:X:87:PHE:HB2	31:X:99:PHE:HB2	1.83	0.60
4:g:51:GLY:HA3	5:f:166:LYS:HE3	1.83	0.60
13:F:173:GLU:OE2	20:M:381:ARG:NH1	2.33	0.60
25:R:76:GLN:HG3	25:R:78:ASP:H	1.65	0.60
25:R:178:GLY:HA3	25:R:187:VAL:HG21	1.83	0.60
28:U:14:VAL:HG21	28:U:48:VAL:HG12	1.83	0.60
4:4:169:GLU:O	4:g:177:LYS:NZ	2.35	0.60
1:b:23:MET:HE2	1:b:174:ILE:HG12	1.84	0.60
4:g:182:LYS:HE2	4:g:191:GLN:HE21	1.67	0.60
10:C:144:TYR:HB2	10:C:147:GLN:HE21	1.67	0.60
17:J:149:MET:SD	17:J:333:ARG:NH2	2.74	0.60
26:S:311:GLN:NE2	26:S:341:SER:OG	2.34	0.60
31:X:34:GLU:HB3	31:X:51:ARG:HE	1.65	0.60
2:2:47:THR:HB	2:2:59:ASN:HA	1.83	0.60
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.82	0.60
8:A:114:CYS:HB2	8:A:145:SER:HB3	1.83	0.60
10:C:70:ASN:OD1	10:C:71:ASP:N	2.34	0.60
9:j:71:ILE:HG12	9:j:138:GLY:HA3	1.82	0.60
25:R:331:ARG:NH2	25:R:370:LYS:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:128:THR:HB	6:6:144:PHE:HB2	1.83	0.60
10:d:76:ALA:HB3	10:d:136:ILE:HB	1.83	0.60
11:D:88:LYS:NZ	11:D:120:TYR:OH	2.34	0.60
6:e:49:ILE:HG22	6:e:54:ILE:HA	1.84	0.60
23:P:38:GLN:O	23:P:88:GLN:NE2	2.35	0.60
33:Z:389:PHE:HB3	33:Z:857:LEU:HA	1.83	0.60
6:6:212:GLU:OE1	2:i:58:LYS:NZ	2.35	0.59
13:F:11:VAL:HA	14:G:130:ARG:HD3	1.84	0.59
13:F:50:LYS:HE2	13:F:61:LYS:HA	1.84	0.59
13:l:81:ALA:HB2	13:l:130:VAL:HG21	1.84	0.59
22:O:117:ASN:HB3	22:O:127:LEU:HB2	1.84	0.59
29:V:114:PHE:HB3	29:V:117:TRP:HE1	1.67	0.59
10:C:191:GLU:HG2	10:C:242:THR:HG22	1.83	0.59
16:I:247:ILE:HB	16:I:281:ILE:HG12	1.83	0.59
3:3:203:ARG:HG2	5:f:269:GLY:HA3	1.84	0.59
12:m:13:SER:HB2	13:l:126:ARG:HB3	1.84	0.59
19:L:228:LYS:NZ	19:L:327:THR:O	2.35	0.59
20:M:51:LEU:O	20:M:55:ASN:ND2	2.36	0.59
6:e:55:ASN:O	7:a:189:ARG:NH2	2.35	0.59
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.84	0.59
29:V:24:LYS:HB2	29:V:174:THR:HA	1.85	0.59
11:D:37:LYS:HE2	11:D:160:SER:HA	1.85	0.59
3:3:101:GLY:O	4:4:93:ARG:NH1	2.35	0.59
5:5:144:ARG:O	11:D:111:ARG:NH1	2.35	0.59
8:c:14:ARG:O	8:c:27:GLN:NE2	2.36	0.59
15:H:98:GLN:N	15:H:176:VAL:O	2.33	0.59
21:N:891:VAL:HB	21:N:906:ARG:HB2	1.85	0.59
7:7:232:ILE:HB	7:7:240:THR:HB	1.85	0.59
15:H:224:VAL:HG23	15:H:225:VAL:HG23	1.85	0.59
3:h:51:LEU:HD11	3:h:107:PRO:HB3	1.85	0.59
23:P:353:ILE:HG23	23:P:357:TYR:HB2	1.85	0.59
3:3:103:TYR:HA	4:4:93:ARG:HH22	1.68	0.59
12:E:34:GLY:HA3	12:E:80:GLY:HA2	1.85	0.59
7:7:58:ASP:HA	7:7:228:PHE:HA	1.84	0.58
8:c:141:LEU:HB2	8:c:157:THR:HB	1.84	0.58
9:j:33:THR:HA	9:j:165:GLY:HA3	1.84	0.58
30:W:150:ASN:OD1	30:W:151:THR:N	2.36	0.58
33:Z:351:PRO:HG2	33:Z:464:ASP:HB3	1.84	0.58
18:K:415:VAL:HG13	18:K:416:LYS:HG2	1.85	0.58
19:L:172:SER:OG	19:L:174:GLU:OE2	2.20	0.58
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T:170:ASN:HA	27:T:174:PHE:HB2	1.85	0.58
8:A:37:GLN:NE2	14:G:19:GLY:O	2.36	0.58
11:D:13:PRO:HB2	15:H:462:ARG:HB3	1.85	0.58
16:I:173:MET:HG3	16:I:243:THR:HG23	1.84	0.58
2:i:201:ASN:ND2	2:i:218:ASN:OD1	2.35	0.58
14:G:224:THR:HB	14:G:227:LEU:HB2	1.86	0.58
15:H:456:LYS:O	16:I:347:LYS:NZ	2.30	0.58
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.85	0.58
30:W:161:VAL:O	30:W:163:ASN:ND2	2.36	0.58
5:5:283:ASN:ND2	4:g:148:TYR:O	2.36	0.58
4:g:149:ARG:HB2	4:g:152:MET:HG3	1.85	0.58
4:4:130:TYR:OH	5:f:242:ARG:NH2	2.36	0.58
7:7:54:ILE:HG12	7:7:232:ILE:HG12	1.83	0.58
5:f:83:PHE:HE2	5:f:88:ILE:HG12	1.68	0.58
8:c:78:THR:HG22	8:c:231:ASP:HA	1.86	0.58
29:V:146:SER:HB2	29:V:151:VAL:HA	1.85	0.58
29:V:153:ILE:HG23	29:V:201:ILE:HG13	1.85	0.58
1:1:103:GLU:OE2	7:7:98:ARG:NH1	2.36	0.58
5:5:112:ILE:HG23	5:5:135:GLY:HA2	1.85	0.58
33:Z:975:SER:HB3	33:Z:977:ILE:HG12	1.86	0.58
6:6:55:ASN:O	7:7:189:ARG:NH2	2.37	0.58
11:n:163:THR:HG21	11:n:171:VAL:HB	1.85	0.58
25:R:54:ILE:HG21	25:R:63:TYR:HB2	1.85	0.58
5:5:170:LEU:HD23	6:6:120:ARG:HH21	1.68	0.58
19:L:402:ALA:HB1	19:L:407:ARG:HB2	1.86	0.58
22:O:83:LEU:HD21	22:O:98:TYR:HB2	1.85	0.58
33:Z:972:SER:OG	33:Z:976:HIS:ND1	2.37	0.58
6:6:74:ASN:HB3	6:6:127:HIS:HB2	1.85	0.57
17:J:62:LEU:HD13	18:K:89:ILE:HD13	1.84	0.57
31:X:89:LEU:O	31:X:96:ARG:NE	2.37	0.57
6:e:211:THR:HG21	6:e:239:LYS:HB2	1.86	0.57
12:E:207:VAL:HG12	15:H:409:ARG:HH12	1.69	0.57
1:b:16:VAL:HG13	1:b:41:THR:HG22	1.85	0.57
3:3:65:GLU:OE1	3:3:68:ARG:NH2	2.37	0.57
10:d:152:ASN:ND2	10:d:156:ASN:OD1	2.32	0.57
22:O:338:LYS:HB3	22:O:351:SER:HB3	1.87	0.57
4:4:4:ILE:HG13	4:4:47:ALA:HB2	1.85	0.57
4:g:146:HIS:O	4:g:149:ARG:NH1	2.32	0.57
17:J:146:THR:HG21	25:R:163:SER:HB3	1.86	0.57
23:P:212:LYS:HA	23:P:216:LEU:HD22	1.87	0.57
7:a:42:THR:OG1	7:a:221:ASP:OD2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.84	0.57
17:J:52:ASN:HD21	21:N:612:SER:HA	1.70	0.57
33:Z:233:LEU:HB3	33:Z:271:ILE:HD11	1.86	0.57
4:g:14:ILE:HG12	4:g:183:ILE:HG12	1.86	0.57
12:E:84:ASP:OD2	12:E:136:ARG:NH1	2.38	0.57
18:K:70:ASP:OD1	18:K:73:ARG:NH2	2.38	0.57
5:f:253:TYR:HE1	5:f:262:TYR:HD1	1.53	0.57
11:n:88:LYS:NZ	11:n:120:TYR:OH	2.37	0.57
12:m:85:ALA:HB2	12:m:140:VAL:HG21	1.87	0.57
15:H:311:ILE:HG22	15:H:355:THR:HB	1.86	0.57
2:i:91:ASN:OD1	9:j:99:ARG:NH2	2.38	0.57
9:B:38:LYS:HG3	9:B:43:VAL:HG22	1.87	0.57
20:M:166:ARG:HD2	20:M:170:MET:HB3	1.87	0.57
29:V:126:GLN:HG2	29:V:158:LEU:HD21	1.85	0.57
7:7:226:ARG:NH1	1:b:213:GLU:OE1	2.38	0.57
8:A:53:VAL:HG21	8:A:82:VAL:HG21	1.87	0.57
10:C:168:ASN:HB3	10:C:171:ALA:HB3	1.86	0.57
10:d:158:THR:OG1	10:d:160:TRP:NE1	2.38	0.57
21:N:344:THR:HG22	21:N:375:HIS:HA	1.87	0.57
31:X:120:GLU:HG2	31:X:124:LYS:HE3	1.86	0.57
33:Z:371:SER:HA	33:Z:387:ASN:HB3	1.87	0.57
5:f:266:HIS:HB3	5:f:271:LEU:HD11	1.87	0.56
14:G:120:VAL:HG21	14:G:151:LEU:HD21	1.87	0.56
5:5:76:THR:N	5:5:206:SER:HG	2.03	0.56
14:G:210:LYS:HE3	20:M:353:SER:HB2	1.87	0.56
21:N:162:ARG:HE	21:N:164:ASP:HB3	1.69	0.56
25:R:292:LEU:HD11	25:R:311:THR:HG21	1.85	0.56
29:V:24:LYS:HD2	29:V:200:ASN:HD21	1.69	0.56
4:4:130:TYR:OH	4:4:145:ASP:OD1	2.22	0.56
2:i:69:LYS:NZ	2:i:102:GLU:OE1	2.37	0.56
3:h:185:ALA:HB3	3:h:200:LEU:HD12	1.88	0.56
6:e:46:THR:OG1	6:e:219:ASP:O	2.24	0.56
6:e:71:MET:HE3	6:e:84:VAL:HG22	1.86	0.56
21:N:650:ASP:HB3	21:N:694:LEU:HB2	1.87	0.56
30:W:180:LEU:O	30:W:184:ASN:ND2	2.37	0.56
8:A:126:GLN:HE22	9:B:81:ASP:HA	1.69	0.56
19:L:300:GLU:OE1	19:L:303:ARG:NH2	2.38	0.56
22:O:44:SER:O	22:O:47:LYS:NZ	2.37	0.56
1:1:54:THR:HG21	1:1:75:ALA:HB1	1.87	0.56
2:2:126:TYR:HB3	2:2:156:LEU:HD13	1.87	0.56
8:A:61:ASP:OD2	14:G:173:LYS:NZ	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:435:LEU:HG	16:I:437:LEU:H	1.70	0.56
21:N:362:TRP:HZ3	29:V:168:LEU:HB3	1.70	0.56
23:P:70:ASN:OD1	23:P:71:LYS:N	2.38	0.56
28:U:50:ASN:OD1	28:U:51:SER:N	2.39	0.56
3:3:105:VAL:HG23	3:3:107:PRO:HD3	1.86	0.56
29:V:58:VAL:HB	29:V:62:THR:HB	1.87	0.56
33:Z:309:GLN:NE2	33:Z:980:VAL:O	2.34	0.56
2:i:220:LEU:HG	2:i:222:PRO:HD3	1.87	0.56
8:A:178:ILE:HD11	8:A:214:LEU:HD21	1.88	0.56
12:m:159:GLU:OE1	12:m:163:THR:OG1	2.24	0.56
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.88	0.56
2:2:48:ARG:O	2:2:62:LYS:NZ	2.33	0.56
5:f:220:LYS:HB3	5:f:223:LEU:HG	1.87	0.56
13:F:50:LYS:HE3	13:F:212:SER:HB2	1.88	0.56
14:G:152:GLU:OE1	14:G:156:SER:OG	2.24	0.56
10:d:4:ARG:O	11:n:6:ARG:NH1	2.39	0.56
10:d:120:GLN:NE2	11:n:81:ASP:OD1	2.39	0.56
30:W:1:MET:HG2	30:W:2:VAL:HG13	1.86	0.56
30:W:28:ALA:HB1	30:W:181:LEU:HD22	1.87	0.56
33:Z:282:ILE:HD11	33:Z:310:LEU:HD22	1.88	0.56
33:Z:925:VAL:HG12	33:Z:983:LEU:HD11	1.87	0.56
6:6:174:ASN:HB3	6:6:176:LYS:HE2	1.86	0.56
2:i:236:ARG:NH2	3:h:159:GLU:OE1	2.39	0.56
4:g:3:ILE:HD12	4:g:176:PHE:HB3	1.87	0.56
14:k:54:ILE:HD11	14:k:213:GLU:HB2	1.88	0.56
14:k:120:VAL:HG21	14:k:151:LEU:HD21	1.88	0.56
19:L:102:GLY:N	20:M:152:SER:O	2.39	0.56
5:f:119:THR:HG21	5:f:175:MET:HE3	1.87	0.55
13:l:132:LEU:HB2	13:l:147:PHE:HB3	1.88	0.55
3:3:54:THR:O	3:3:106:GLY:N	2.39	0.55
24:Q:389:VAL:HG12	24:Q:400:TYR:HB2	1.88	0.55
26:S:173:LEU:H	26:S:176:LEU:HD12	1.70	0.55
28:U:14:VAL:HG13	28:U:51:SER:HB3	1.88	0.55
6:6:214:HIS:HD2	6:6:217:VAL:HG23	1.71	0.55
6:6:215:ILE:HB	2:i:196:LEU:HB3	1.87	0.55
12:m:50:VAL:HG21	12:m:66:LYS:HB2	1.89	0.55
15:H:294:LEU:HD13	15:H:306:ILE:HD11	1.87	0.55
5:5:242:ARG:NH2	4:g:130:TYR:OH	2.39	0.55
14:G:7:GLY:HA2	14:G:10:LEU:HG	1.89	0.55
15:H:90:ARG:HE	16:I:133:LEU:HD22	1.71	0.55
16:I:287:ILE:HG12	16:I:302:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:100:LEU:HB2	18:K:109:ILE:HG23	1.89	0.55
26:S:418:THR:HG22	26:S:422:MET:HE2	1.88	0.55
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.89	0.55
7:a:86:ILE:HG12	7:a:147:ILE:HG12	1.88	0.55
13:F:201:LEU:HD11	13:F:206:LEU:HG	1.89	0.55
11:n:31:THR:O	11:n:76:SER:OG	2.24	0.55
23:P:440:HIS:HB3	28:U:213:LYS:HE3	1.89	0.55
3:3:46:TYR:OH	3:3:64:ASN:OD1	2.24	0.55
2:i:153:TYR:HB2	2:i:167:LEU:HD13	1.89	0.55
8:c:13:ASP:HA	8:c:18:ILE:HD11	1.88	0.55
17:J:96:VAL:HG11	17:J:115:LEU:HD11	1.89	0.55
21:N:634:LEU:HG	21:N:636:SER:H	1.72	0.55
25:R:146:ASP:HB3	25:R:149:ASN:HB2	1.88	0.55
4:g:184:VAL:HG22	4:g:189:ILE:HG12	1.88	0.55
21:N:742:TRP:CD2	21:N:744:PRO:HD2	2.42	0.55
23:P:249:ALA:HB1	23:P:252:SER:HB3	1.88	0.55
18:K:217:THR:HA	18:K:381:ALA:HB2	1.88	0.55
18:K:240:SER:OG	19:L:307:GLU:OE2	2.24	0.55
19:L:150:ILE:HG13	19:L:151:THR:HG23	1.88	0.55
20:M:220:MET:HB3	20:M:349:PHE:HE2	1.72	0.55
23:P:319:GLU:HB3	23:P:322:LEU:HB2	1.88	0.55
28:U:11:ALA:HB1	28:U:167:GLU:HG2	1.89	0.55
29:V:52:LEU:HD23	29:V:107:TRP:HB3	1.89	0.55
30:W:129:ALA:HB1	30:W:161:VAL:HB	1.87	0.55
32:Y:63:ASN:OD1	32:Y:64:TRP:N	2.36	0.55
4:4:149:ARG:HB2	4:4:152:MET:HG2	1.89	0.55
6:6:125:TYR:HA	6:6:146:PRO:HB3	1.89	0.55
4:4:71:GLU:OE2	10:C:113:ARG:NH1	2.37	0.55
5:5:256:THR:HG23	5:5:258:ASP:H	1.71	0.55
2:i:96:SER:OG	2:i:101:ARG:O	2.24	0.55
7:a:100:LEU:HD21	7:a:129:LEU:HD11	1.89	0.55
13:l:72:LEU:HD13	13:l:132:LEU:HD22	1.88	0.55
17:J:186:ILE:HD13	17:J:300:LEU:HD11	1.89	0.55
29:V:53:MET:HG2	29:V:68:VAL:HG12	1.89	0.54
2:i:37:PHE:HE2	2:i:42:VAL:HG23	1.71	0.54
15:H:318:ARG:NH1	15:H:360:THR:O	2.40	0.54
19:L:107:GLU:OE2	19:L:145:ARG:NH2	2.40	0.54
11:D:4:TYR:CZ	11:D:6:ARG:HB3	2.43	0.54
9:j:222:LEU:HD13	9:j:232:GLY:HA2	1.90	0.54
19:L:348:GLU:OE2	19:L:436:LYS:NZ	2.40	0.54
29:V:53:MET:HA	29:V:68:VAL:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:200:LEU:HD11	16:I:207:LEU:HD22	1.89	0.54
20:M:244:LEU:HD12	20:M:276:THR:HG21	1.88	0.54
22:O:119:SER:HB2	22:O:166:ARG:HH11	1.73	0.54
29:V:106:GLY:HA3	29:V:137:VAL:H	1.73	0.54
6:e:214:HIS:HE1	6:e:216:GLN:HB2	1.73	0.54
8:A:52:VAL:HG21	8:A:203:VAL:HG22	1.90	0.54
8:A:72:ILE:HG12	8:A:82:VAL:HG22	1.90	0.54
8:c:144:VAL:HG12	8:c:154:ILE:HG12	1.88	0.54
16:I:229:LYS:NZ	16:I:328:THR:O	2.41	0.54
21:N:150:LEU:HD21	21:N:173:LYS:HG3	1.89	0.54
26:S:445:THR:HG22	26:S:447:GLU:H	1.72	0.54
28:U:23:GLU:O	28:U:26:GLN:NE2	2.40	0.54
28:U:276:ILE:HG23	29:V:291:ASN:HB3	1.89	0.54
30:W:1:MET:N	30:W:194:GLU:OE1	2.40	0.54
30:W:14:GLU:HG2	30:W:82:GLU:HB2	1.90	0.54
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.55	0.54
10:d:76:ALA:O	10:d:136:ILE:N	2.41	0.54
11:n:4:TYR:CZ	11:n:6:ARG:HB3	2.43	0.54
12:m:123:PHE:HA	12:m:134:MET:HB3	1.88	0.54
17:J:147:TYR:OH	17:J:165:GLU:OE1	2.26	0.54
17:J:332:SER:HA	17:J:335:MET:HE3	1.89	0.54
27:T:136:LEU:HD22	27:T:146:ILE:HD11	1.90	0.54
4:g:47:ALA:HB3	4:g:101:ASN:HB2	1.90	0.54
6:e:74:ASN:O	6:e:127:HIS:N	2.33	0.54
12:m:122:ARG:HA	12:m:132:ARG:HD3	1.88	0.54
13:l:39:ARG:HH21	14:k:60:VAL:HG21	1.73	0.54
15:H:448:ASP:HA	15:H:452:SER:HB2	1.90	0.54
17:J:279:LEU:HD11	17:J:288:ILE:HD12	1.90	0.54
27:T:177:PHE:HB3	27:T:181:LEU:HD13	1.90	0.54
1:1:85:TYR:HA	1:1:89:TYR:HD2	1.73	0.54
6:6:74:ASN:O	6:6:127:HIS:N	2.39	0.54
4:g:36:ARG:HG3	4:g:57:ALA:HB1	1.90	0.54
8:A:194:ILE:HG22	8:A:196:GLU:H	1.72	0.54
17:J:185:VAL:HG22	17:J:312:ARG:HB3	1.88	0.54
17:J:248:ASP:OD2	18:K:330:ARG:NH2	2.33	0.54
17:J:296:ARG:H	17:J:299:ILE:HD12	1.73	0.54
25:R:309:LEU:HD11	32:Y:77:LEU:HB2	1.90	0.54
33:Z:405:ASN:HB3	33:Z:409:LYS:HE3	1.90	0.54
3:h:9:GLY:HA3	3:h:180:LEU:HB3	1.89	0.54
15:H:428:MET:HG3	16:I:346:ARG:HH22	1.72	0.54
23:P:89:LEU:HB3	23:P:92:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:149:ARG:HD3	5:f:283:ASN:HD21	1.73	0.54
3:h:11:ILE:HG21	3:h:142:ALA:HB3	1.89	0.54
6:e:74:ASN:HB3	6:e:127:HIS:HB2	1.88	0.54
12:E:68:VAL:HB	12:E:93:ARG:HH21	1.71	0.54
15:H:275:ILE:HG23	16:I:311:ASN:HD22	1.73	0.54
16:I:80:GLU:HG3	33:Z:625:THR:HG21	1.90	0.54
18:K:95:VAL:O	18:K:139:LEU:N	2.40	0.54
25:R:36:SER:HB3	25:R:43:ARG:HE	1.73	0.54
6:6:46:THR:OG1	6:6:219:ASP:O	2.27	0.53
3:h:8:ASN:ND2	3:h:30:GLY:O	2.36	0.53
17:J:141:LYS:HG2	17:J:142:VAL:HG23	1.88	0.53
19:L:104:LEU:O	19:L:148:LEU:N	2.39	0.53
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.90	0.53
7:a:98:ARG:HD2	14:k:101:LYS:HA	1.90	0.53
9:j:157:PHE:HE1	10:d:64:GLU:HB3	1.73	0.53
17:J:221:LYS:HE2	18:K:286:THR:HG21	1.90	0.53
17:J:324:ARG:NH2	17:J:350:MET:O	2.41	0.53
21:N:4:THR:HG22	21:N:35:LEU:HD21	1.89	0.53
26:S:393:ARG:NH1	26:S:431:VAL:O	2.42	0.53
1:1:181:ALA:O	1:1:188:SER:OG	2.27	0.53
14:G:121:GLN:OE1	14:G:124:THR:OG1	2.26	0.53
11:n:73:LEU:HD11	11:n:133:THR:HB	1.91	0.53
30:W:20:ASP:HB3	30:W:144:PHE:HE2	1.72	0.53
5:5:83:PHE:HE2	5:5:88:ILE:HG12	1.73	0.53
7:7:181:ALA:O	7:7:185:ASN:ND2	2.40	0.53
2:i:66:ILE:HG23	2:i:89:GLY:HA2	1.91	0.53
5:f:260:TRP:HZ3	5:f:262:TYR:HB2	1.74	0.53
6:e:46:THR:HB	6:e:59:GLU:H	1.74	0.53
11:n:56:ASP:HB3	11:n:59:ILE:HG12	1.91	0.53
26:S:424:SER:HB3	27:T:192:ASN:HB3	1.89	0.53
6:e:47:ARG:NH1	6:e:215:ILE:O	2.42	0.53
16:I:216:PRO:O	16:I:323:LYS:NZ	2.37	0.53
15:H:402:ILE:HD12	15:H:440:GLU:HB2	1.91	0.53
19:L:105:ILE:HD11	20:M:128:PHE:HB2	1.90	0.53
29:V:138:ALA:N	29:V:156:PHE:O	2.37	0.53
4:4:38:LEU:HB3	4:4:64:ILE:HG21	1.91	0.53
12:m:68:VAL:HB	12:m:93:ARG:HH21	1.74	0.53
18:K:400:TYR:HB3	23:P:128:ASN:HB3	1.90	0.53
4:4:8:ARG:NH2	4:4:114:PRO:O	2.40	0.53
5:5:106:VAL:HA	6:6:151:GLU:HG2	1.91	0.53
8:A:126:GLN:NE2	9:B:81:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:56:LEU:HD11	4:g:122:LEU:HD13	1.90	0.53
20:M:422:VAL:HA	20:M:426:LYS:HB2	1.91	0.53
4:g:19:LYS:HG2	4:g:33:ASP:HB3	1.90	0.52
25:R:38:VAL:HG11	25:R:313:ALA:HB1	1.89	0.52
28:U:171:VAL:HG13	29:V:213:LEU:HD13	1.89	0.52
30:W:3:LEU:HB3	30:W:106:GLN:HG2	1.91	0.52
6:e:50:THR:OG1	6:e:55:ASN:ND2	2.30	0.52
6:e:106:ASN:OD1	6:e:142:TYR:OH	2.23	0.52
14:G:36:THR:HA	14:G:166:GLY:HA3	1.91	0.52
9:j:216:ASP:OD1	9:j:217:GLU:N	2.42	0.52
17:J:190:PRO:HG2	17:J:193:THR:HG21	1.91	0.52
21:N:508:THR:HG22	21:N:510:HIS:H	1.73	0.52
22:O:16:MET:HG2	22:O:20:PRO:HD3	1.91	0.52
2:i:192:ILE:HD13	2:i:222:PRO:HG3	1.90	0.52
15:H:160:GLY:H	15:H:163:VAL:HB	1.74	0.52
21:N:250:ASP:OD1	21:N:251:GLU:N	2.41	0.52
33:Z:862:MET:HG2	33:Z:910:PRO:HB3	1.92	0.52
1:b:54:THR:HG21	1:b:75:ALA:HB1	1.91	0.52
6:e:76:PHE:HZ	7:a:166:LEU:HB3	1.75	0.52
6:e:219:ASP:HA	6:e:240:ARG:HG2	1.92	0.52
8:A:44:ALA:HB2	8:A:53:VAL:HG23	1.91	0.52
14:k:36:THR:HA	14:k:166:GLY:HA3	1.90	0.52
23:P:181:LEU:HD13	23:P:219:GLU:HB2	1.91	0.52
31:X:10:PHE:HD2	31:X:33:ILE:HD11	1.74	0.52
33:Z:166:ASN:ND2	33:Z:226:GLU:O	2.42	0.52
33:Z:186:GLY:HA2	33:Z:201:LEU:HD13	1.91	0.52
3:3:172:LEU:HD22	3:3:202:MET:HB3	1.91	0.52
12:E:71:ASP:OD1	12:E:72:ARG:N	2.42	0.52
23:P:20:GLU:OE2	23:P:34:SER:OG	2.27	0.52
2:2:107:SER:HB3	8:A:110:TYR:HE2	1.73	0.52
2:2:201:ASN:ND2	2:2:218:ASN:OD1	2.43	0.52
3:3:50:PHE:HE2	3:3:195:VAL:HG11	1.75	0.52
26:S:82:TYR:CD1	26:S:86:SER:HB3	2.44	0.52
4:4:47:ALA:HB3	4:4:101:ASN:HB2	1.91	0.52
1:b:40:THR:HG22	1:b:45:ILE:HG12	1.91	0.52
1:b:47:ASN:OD1	1:b:49:VAL:HG22	2.10	0.52
3:h:53:ILE:HG22	3:h:60:VAL:HG22	1.92	0.52
4:g:8:ARG:HH11	4:g:116:LEU:H	1.58	0.52
13:F:54:ASP:OD1	13:F:55:GLU:N	2.43	0.52
8:c:158:ASP:OD1	8:c:162:TYR:N	2.41	0.52
10:d:66:LEU:HD12	10:d:212:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:355:THR:HG21	15:H:361:LEU:HD21	1.91	0.52
13:F:81:ALA:HB2	13:F:130:VAL:HG21	1.91	0.52
9:j:65:SER:OG	9:j:82:TYR:OH	2.20	0.52
33:Z:460:SER:HA	33:Z:496:ALA:HA	1.91	0.52
3:3:125:ASP:OD1	3:3:129:CYS:N	2.36	0.52
4:4:32:ASP:OD1	4:4:33:ASP:N	2.43	0.52
10:d:125:HIS:HB3	11:n:126:VAL:HG12	1.91	0.52
22:O:76:LEU:HB3	22:O:122:HIS:HB3	1.92	0.52
5:5:134:LEU:HD21	5:5:158:LEU:HB2	1.91	0.52
12:E:232:ASP:OD1	12:E:233:ASN:N	2.42	0.52
16:I:279:VAL:HB	16:I:324:VAL:HA	1.91	0.52
20:M:159:LEU:HD12	20:M:160:PRO:HD2	1.91	0.52
20:M:228:LYS:NZ	20:M:327:THR:O	2.33	0.52
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.91	0.52
6:e:90:SER:HB2	6:e:111:ASN:HD21	1.75	0.51
17:J:248:ASP:OD1	17:J:249:GLU:N	2.41	0.51
22:O:135:ARG:NH1	22:O:174:THR:OG1	2.39	0.51
25:R:195:ASN:O	25:R:206:ARG:NH2	2.42	0.51
33:Z:827:LEU:HD23	33:Z:830:LEU:HD12	1.91	0.51
3:3:67:PHE:HE1	3:3:91:VAL:HA	1.74	0.51
7:7:113:LEU:HB3	7:7:117:GLU:HB2	1.91	0.51
6:e:47:ARG:HB2	6:e:219:ASP:HB2	1.91	0.51
6:e:220:GLY:HA2	6:e:238:LEU:H	1.74	0.51
8:A:54:ILE:HG12	8:A:225:VAL:HG22	1.93	0.51
10:C:194:LEU:HD11	10:C:239:LEU:HD23	1.92	0.51
33:Z:390:LEU:HD21	33:Z:856:HIS:HB3	1.91	0.51
1:1:38:ARG:O	1:1:52:LYS:NZ	2.44	0.51
1:1:167:LYS:HE3	1:1:196:VAL:HG11	1.92	0.51
2:2:168:GLU:OE2	7:a:220:ARG:NE	2.41	0.51
25:R:342:LEU:HD21	25:R:378:ASN:HB2	1.92	0.51
27:T:8:THR:HG23	27:T:30:ILE:HG23	1.91	0.51
29:V:177:THR:OG1	29:V:200:ASN:OD1	2.29	0.51
33:Z:802:ASP:OD1	33:Z:803:ALA:N	2.43	0.51
33:Z:954:PRO:HG2	33:Z:961:GLU:HG2	1.91	0.51
6:6:47:ARG:NH1	6:6:215:ILE:O	2.44	0.51
7:7:137:ARG:HD3	7:7:166:LEU:HA	1.91	0.51
9:B:69:PRO:HB3	9:B:233:PRO:HB3	1.92	0.51
14:G:54:ILE:HG23	14:G:59:LEU:HD22	1.92	0.51
11:n:43:VAL:HG22	11:n:214:VAL:HG22	1.91	0.51
18:K:213:GLY:HA3	18:K:340:PHE:HB3	1.92	0.51
20:M:75:LEU:HB2	20:M:76:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:219:LEU:HB2	20:M:343:LEU:HD13	1.93	0.51
25:R:222:ARG:NH2	25:R:321:TYR:O	2.36	0.51
29:V:60:ASP:O	29:V:157:ARG:NH1	2.42	0.51
18:K:276:SER:HB3	19:L:306:MET:HG3	1.91	0.51
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.42	0.51
30:W:24:THR:HG22	30:W:26:PHE:H	1.74	0.51
2:2:50:THR:HG21	2:2:197:GLY:HA2	1.92	0.51
1:b:78:VAL:HG22	1:b:100:VAL:HG12	1.91	0.51
4:g:162:LYS:HD3	4:g:198:GLN:HB3	1.93	0.51
7:a:58:ASP:HA	7:a:228:PHE:HA	1.92	0.51
10:C:125:HIS:HB3	11:D:126:VAL:HG12	1.92	0.51
26:S:427:ILE:HD12	27:T:195:LEU:HD23	1.92	0.51
9:B:245:ASP:OD2	24:Q:92:LYS:NZ	2.38	0.51
10:C:50:ARG:NH1	10:C:212:GLU:OE2	2.41	0.51
10:C:72:LYS:HE2	10:C:224:GLU:HA	1.92	0.51
22:O:277:ILE:HG22	22:O:279:ILE:H	1.74	0.51
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.38	0.51
29:V:67:ASP:OD1	29:V:68:VAL:N	2.43	0.51
33:Z:391:ASN:HB2	33:Z:425:ILE:HG12	1.92	0.51
11:D:44:LEU:HD11	11:D:136:ALA:HB3	1.93	0.51
24:Q:369:ASP:OD1	24:Q:370:THR:N	2.43	0.51
30:W:52:ILE:HG12	30:W:61:VAL:HG22	1.92	0.51
1:1:33:LEU:HD11	1:1:119:ALA:HB3	1.93	0.51
2:2:239:THR:OG1	3:3:169:GLN:NE2	2.44	0.51
2:i:42:VAL:HG22	2:i:206:VAL:HA	1.92	0.51
6:e:41:VAL:HG12	6:e:225:ILE:HG12	1.93	0.51
13:F:164:ARG:HH11	13:F:202:ARG:HG3	1.74	0.51
19:L:284:ASP:HB2	20:M:306:LEU:HD21	1.91	0.51
21:N:170:LEU:HD11	21:N:186:ILE:HG12	1.92	0.51
29:V:25:GLU:OE2	29:V:157:ARG:NH1	2.43	0.51
2:2:91:ASN:OD1	9:B:99:ARG:NH2	2.43	0.51
6:6:76:PHE:HZ	7:7:166:LEU:HB3	1.76	0.51
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.91	0.51
5:f:84:GLN:OE1	5:f:221:TRP:NE1	2.43	0.51
16:I:406:GLU:O	16:I:408:ARG:NH1	2.44	0.51
4:4:182:LYS:HE2	4:4:191:GLN:HE21	1.76	0.50
20:M:157:ASP:OD1	20:M:158:THR:N	2.43	0.50
24:Q:104:PHE:HE2	24:Q:114:GLN:HA	1.76	0.50
28:U:174:LEU:O	29:V:205:LYS:NZ	2.31	0.50
33:Z:189:ALA:HB2	33:Z:198:GLU:HB2	1.93	0.50
7:7:59:ASN:ND2	7:7:229:SER:OG	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:30:THR:N	2:i:197:GLY:O	2.44	0.50
4:g:101:ASN:HB3	4:g:133:HIS:CG	2.46	0.50
14:k:193:VAL:HG13	14:k:216:ILE:HG21	1.93	0.50
18:K:104:ASP:OD1	18:K:105:GLN:N	2.42	0.50
31:X:38:ASN:HD22	31:X:42:GLU:H	1.59	0.50
33:Z:914:LEU:HB3	33:Z:980:VAL:HG22	1.94	0.50
3:3:78:GLU:HG2	3:3:80:ARG:HG2	1.94	0.50
5:5:79:LEU:HD13	5:5:215:LEU:HD11	1.93	0.50
6:6:76:PHE:CZ	7:7:166:LEU:HB3	2.47	0.50
10:C:159:GLY:HA3	11:D:59:ILE:HG13	1.93	0.50
11:D:93:ALA:HA	11:D:104:VAL:HG11	1.92	0.50
17:J:336:ASN:ND2	17:J:375:ILE:O	2.44	0.50
19:L:104:LEU:HD21	20:M:125:GLN:HE21	1.76	0.50
23:P:253:ASP:OD1	23:P:254:GLU:N	2.44	0.50
3:3:29:LEU:HD11	3:3:57:ALA:HB2	1.92	0.50
13:F:86:ASN:OD1	13:F:89:ARG:NH2	2.44	0.50
15:H:146:VAL:HG22	15:H:156:VAL:HG22	1.94	0.50
15:H:207:THR:HA	15:H:265:ASN:HD22	1.76	0.50
3:h:28:ARG:HH21	3:h:182:GLY:HA3	1.75	0.50
5:f:112:ILE:HG23	5:f:135:GLY:HA2	1.93	0.50
14:G:54:ILE:HD11	14:G:213:GLU:HB2	1.93	0.50
16:I:423:VAL:HG22	16:I:427:LYS:HD2	1.92	0.50
18:K:104:ASP:HB3	18:K:107:THR:HB	1.92	0.50
23:P:415:TRP:HE1	28:U:262:GLN:HG2	1.77	0.50
6:6:62:VAL:HG22	6:6:72:SER:HB2	1.92	0.50
14:G:49:ALA:HB1	14:G:200:ILE:HD11	1.94	0.50
16:I:286:ALA:HB1	16:I:287:ILE:HD12	1.94	0.50
17:J:90:PRO:HG3	18:K:116:MET:HA	1.94	0.50
22:O:169:ASN:HD22	22:O:203:THR:HB	1.77	0.50
25:R:279:LEU:HD23	25:R:289:ILE:HD13	1.93	0.50
5:f:233:LYS:HB2	5:f:252:LEU:HD11	1.93	0.50
6:e:214:HIS:CE1	6:e:216:GLN:HB2	2.47	0.50
10:C:16:GLU:OE1	10:C:18:ARG:NH2	2.36	0.50
15:H:177:ASP:OD1	15:H:178:ARG:N	2.45	0.50
18:K:135:MET:HE1	18:K:152:PRO:HB3	1.94	0.50
18:K:343:LEU:HD22	18:K:377:SER:HB3	1.93	0.50
19:L:149:ASP:OD2	19:L:152:THR:N	2.43	0.50
20:M:289:LYS:HA	20:M:302:GLN:HE21	1.77	0.50
21:N:556:ALA:HB2	21:N:590:ALA:HB1	1.93	0.50
21:N:631:GLY:HA2	21:N:716:GLN:HG2	1.93	0.50
23:P:346:ILE:HG23	23:P:369:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:455:GLU:HB3	27:T:256:LYS:HE2	1.94	0.50
28:U:83:ILE:HA	29:V:73:GLN:HG2	1.93	0.50
33:Z:812:ILE:HG21	33:Z:848:THR:HA	1.94	0.50
33:Z:858:GLY:HA3	33:Z:862:MET:HB2	1.92	0.50
33:Z:884:THR:HG21	33:Z:904:LEU:HG	1.94	0.50
1:1:22:ILE:HG13	1:1:117:ILE:HD12	1.93	0.50
5:5:153:ALA:HB1	11:D:100:LEU:HD22	1.94	0.50
9:B:4:ARG:HE	14:G:128:SER:HB2	1.76	0.50
9:B:158:PRO:HB2	10:C:58:GLU:HB3	1.94	0.50
14:k:211:ASP:OD1	14:k:212:PHE:N	2.45	0.50
15:H:425:GLU:OE1	16:I:346:ARG:NH1	2.45	0.50
18:K:132:LYS:NZ	18:K:263:GLU:OE2	2.44	0.50
21:N:190:LEU:HD11	21:N:231:ASN:HD22	1.77	0.50
21:N:266:SER:H	21:N:269:LEU:HD12	1.76	0.50
7:7:100:LEU:HD21	7:7:129:LEU:HD11	1.93	0.50
9:B:245:ASP:OD1	24:Q:95:LYS:NZ	2.45	0.50
20:M:352:PRO:O	20:M:357:ARG:NH1	2.45	0.50
3:3:177:ARG:HH12	5:f:103:SER:HA	1.77	0.49
7:a:232:ILE:HB	7:a:240:THR:HB	1.94	0.49
9:B:4:ARG:NH2	13:F:123:TYR:O	2.45	0.49
14:G:54:ILE:HB	14:G:211:ASP:HB3	1.93	0.49
8:c:57:LYS:NZ	8:c:66:PRO:O	2.33	0.49
11:n:62:SER:OG	11:n:211:GLU:OE2	2.29	0.49
14:k:167:LYS:HE2	14:k:206:ASP:HB3	1.94	0.49
21:N:575:ALA:HB2	21:N:587:ALA:HB3	1.94	0.49
22:O:20:PRO:HG3	22:O:71:ASP:HB2	1.93	0.49
25:R:168:ILE:HD13	25:R:205:GLU:HB3	1.94	0.49
26:S:284:LEU:HD11	27:T:123:HIS:HE1	1.77	0.49
27:T:260:ILE:HG22	27:T:264:MET:HE2	1.94	0.49
5:5:268:VAL:HG23	3:h:203:ARG:HD3	1.94	0.49
24:Q:388:GLY:HA2	24:Q:400:TYR:HB3	1.95	0.49
33:Z:880:SER:HB3	33:Z:904:LEU:HD23	1.95	0.49
6:6:203:VAL:HG11	6:6:223:ILE:HD12	1.94	0.49
7:7:162:TYR:HB2	7:7:175:LEU:HD13	1.95	0.49
9:B:96:SER:HA	9:B:100:ILE:HD12	1.94	0.49
19:L:329:ARG:HG2	19:L:331:ASP:H	1.78	0.49
23:P:125:VAL:HG12	23:P:136:ARG:HB2	1.94	0.49
26:S:129:GLU:OE2	26:S:132:ALA:N	2.44	0.49
5:5:82:ARG:HE	5:5:185:PRO:HB2	1.76	0.49
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.94	0.49
7:a:92:ASP:HB3	7:a:145:ASN:HD21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:17:PRO:HG2	13:F:3:ARG:HG2	1.94	0.49
12:m:70:ILE:HA	12:m:93:ARG:HG2	1.94	0.49
14:k:132:PHE:HB3	14:k:134:VAL:HG22	1.93	0.49
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.28	0.49
2:2:106:VAL:HB	7:a:263:THR:HG22	1.93	0.49
11:D:68:ASP:OD1	11:D:69:SER:N	2.42	0.49
9:j:118:MET:HE3	9:j:130:PHE:HB2	1.95	0.49
10:d:73:ILE:HG12	10:d:139:GLY:HA3	1.93	0.49
33:Z:444:GLU:HB2	33:Z:447:VAL:HG23	1.95	0.49
7:7:161:ARG:HE	7:7:169:THR:HB	1.78	0.49
12:E:123:PHE:HA	12:E:134:MET:HB3	1.95	0.49
14:G:109:ILE:H	14:G:142:ASP:HB3	1.77	0.49
22:O:99:LEU:HD22	22:O:129:ILE:HG23	1.95	0.49
9:B:178:ARG:NH1	9:B:195:THR:OG1	2.45	0.49
10:C:70:ASN:HB3	10:C:73:ILE:HB	1.94	0.49
13:F:28:ALA:O	20:M:433:TYR:OH	2.30	0.49
31:X:91:PHE:H	31:X:96:ARG:HH21	1.61	0.49
4:4:195:PHE:CE1	4:4:196:GLN:HG3	2.48	0.49
5:5:220:LYS:HB3	5:5:223:LEU:HG	1.93	0.49
7:a:48:LYS:HD3	7:a:173:PRO:HA	1.94	0.49
15:H:380:PRO:O	15:H:385:ARG:NH1	2.45	0.49
17:J:213:VAL:HG22	17:J:233:LEU:HD13	1.94	0.49
21:N:255:ALA:HB3	21:N:904:VAL:HG11	1.94	0.49
25:R:141:TYR:HA	25:R:144:ILE:HG12	1.94	0.49
5:5:82:ARG:NH1	5:5:200:ASP:OD1	2.41	0.49
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.93	0.49
7:7:220:ARG:HH12	1:b:47:ASN:HA	1.78	0.49
1:b:122:ASP:OD1	1:b:123:ASP:N	2.46	0.49
2:i:30:THR:HG21	2:i:75:ALA:HA	1.95	0.49
5:f:95:ALA:HB3	5:f:102:ALA:HB3	1.95	0.49
8:c:84:ASN:OD1	8:c:85:GLY:N	2.46	0.49
21:N:339:MET:HE2	21:N:707:ASN:HB2	1.95	0.49
33:Z:319:THR:HG21	33:Z:535:VAL:HB	1.95	0.49
6:6:156:ARG:HG3	6:6:166:MET:HE3	1.94	0.49
10:C:120:GLN:NE2	11:D:80:ALA:O	2.46	0.49
22:O:360:GLY:HA2	22:O:363:ILE:HD12	1.93	0.49
2:2:75:ALA:HB3	2:2:126:TYR:HB2	1.95	0.48
7:7:259:LYS:HG2	1:b:193:ARG:HH22	1.77	0.48
5:f:79:LEU:HD13	5:f:215:LEU:HD11	1.95	0.48
10:d:120:GLN:HE22	11:n:81:ASP:HA	1.78	0.48
12:m:39:GLY:HA3	12:m:48:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:71:ASP:OD1	12:m:72:ARG:N	2.42	0.48
13:l:226:ASP:OD1	13:l:227:GLY:N	2.45	0.48
18:K:135:MET:HA	18:K:259:ARG:HH21	1.78	0.48
18:K:280:LYS:N	18:K:323:THR:O	2.46	0.48
23:P:299:LEU:HD23	23:P:302:LEU:HD12	1.95	0.48
29:V:136:ALA:HB3	29:V:158:LEU:HD12	1.94	0.48
1:1:122:ASP:OD1	1:1:123:ASP:N	2.46	0.48
3:h:172:LEU:HD22	3:h:202:MET:HB3	1.94	0.48
11:D:176:GLU:HG2	12:E:58:LEU:HD13	1.94	0.48
12:E:84:ASP:HB3	12:E:138:PHE:HD1	1.78	0.48
15:H:282:LYS:HD2	17:J:221:LYS:HD2	1.95	0.48
26:S:119:TYR:CE2	26:S:121:VAL:HB	2.48	0.48
2:2:55:VAL:HB	6:e:213:ARG:HA	1.95	0.48
7:7:152:VAL:HG22	7:7:158:GLN:HG3	1.95	0.48
6:e:62:VAL:HG22	6:e:72:SER:HB2	1.95	0.48
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.94	0.48
10:d:214:ALA:HA	10:d:230:PHE:HD2	1.79	0.48
22:O:354:GLN:NE2	22:O:355:PRO:HD2	2.27	0.48
4:4:66:LEU:HB2	11:D:94:GLN:HG3	1.94	0.48
2:i:192:ILE:HG23	2:i:199:GLY:HA2	1.94	0.48
23:P:20:GLU:HB3	23:P:23:LYS:HB2	1.95	0.48
27:T:229:VAL:HG23	27:T:232:LYS:HB2	1.95	0.48
3:h:55:GLY:HA3	3:h:105:VAL:HG12	1.95	0.48
8:A:128:TYR:HB3	8:A:136:PRO:HA	1.96	0.48
11:D:81:ASP:HB3	11:D:129:PHE:HD1	1.78	0.48
20:M:145:LEU:HD12	20:M:164:ASP:H	1.77	0.48
22:O:306:ARG:NH2	28:U:234:ASN:OD1	2.35	0.48
24:Q:74:LEU:HD23	24:Q:77:PHE:HD2	1.79	0.48
33:Z:758:LEU:HD11	33:Z:795:THR:HG21	1.95	0.48
3:3:28:ARG:HH21	3:3:183:TRP:CD1	2.32	0.48
6:e:76:PHE:CZ	7:a:166:LEU:HB3	2.49	0.48
11:D:6:ARG:NH2	12:E:9:ASP:OD1	2.47	0.48
8:c:104:PHE:HB2	8:c:112:MET:HE3	1.96	0.48
17:J:141:LYS:HD2	17:J:209:LYS:HE2	1.94	0.48
18:K:157:SER:C	18:K:159:SER:H	2.20	0.48
18:K:396:ARG:NH2	19:L:192:GLU:OE2	2.36	0.48
22:O:352:TRP:NE1	28:U:231:ASP:OD1	2.41	0.48
25:R:36:SER:O	25:R:43:ARG:NH2	2.46	0.48
10:d:66:LEU:HD13	10:d:214:ALA:HB3	1.96	0.48
15:H:190:ARG:HG3	15:H:296:GLU:HG2	1.94	0.48
15:H:278:GLU:O	15:H:281:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:33:LYS:HA	17:J:36:SER:HB3	1.95	0.48
23:P:76:ASN:HD21	23:P:118:VAL:HG22	1.78	0.48
24:Q:59:LEU:HD22	24:Q:103:LYS:HG3	1.96	0.48
8:A:12:TYR:HA	8:A:15:HIS:HD1	1.77	0.48
10:C:206:LEU:HD11	10:C:211:LEU:HD21	1.96	0.48
8:c:44:ALA:N	8:c:169:THR:O	2.40	0.48
17:J:216:ALA:HB1	18:K:281:ARG:HD3	1.95	0.48
23:P:94:GLN:HG3	23:P:133:GLU:HG2	1.96	0.48
30:W:111:VAL:HA	30:W:140:ASP:HB3	1.95	0.48
4:4:96:ARG:NH1	5:5:164:GLN:O	2.47	0.48
5:f:96:THR:HG22	5:f:101:VAL:HG22	1.94	0.48
33:Z:60:ASP:OD1	33:Z:61:SER:N	2.47	0.48
11:n:44:LEU:HD11	11:n:136:ALA:HB3	1.96	0.48
13:l:156:LEU:HG	14:k:59:LEU:HA	1.94	0.48
17:J:222:TYR:HB2	17:J:225:GLU:HB2	1.94	0.48
23:P:220:TYR:HD1	23:P:224:LEU:HD11	1.79	0.48
8:A:158:ASP:OD1	8:A:162:TYR:N	2.46	0.47
10:d:135:PHE:N	10:d:151:SER:OG	2.44	0.47
15:H:454:TYR:CD1	16:I:347:LYS:HD3	2.49	0.47
21:N:91:ILE:HD11	21:N:139:ARG:HH11	1.80	0.47
21:N:775:CYS:O	21:N:866:TYR:N	2.43	0.47
29:V:123:VAL:HG12	29:V:127:LYS:HE3	1.96	0.47
33:Z:204:CYS:HA	33:Z:207:ILE:HD12	1.96	0.47
9:B:185:LEU:HD11	9:B:213:ILE:HB	1.95	0.47
12:E:208:MET:HE2	12:E:216:ASN:HB3	1.95	0.47
13:F:62:LYS:O	13:F:74:LEU:N	2.45	0.47
13:F:95:SER:O	13:F:100:ASN:N	2.46	0.47
17:J:164:ILE:HG12	17:J:289:LYS:HE2	1.95	0.47
26:S:22:GLU:HB3	26:S:68:LEU:HD22	1.97	0.47
26:S:140:LEU:HA	26:S:183:LEU:HD21	1.96	0.47
27:T:172:SER:OG	27:T:173:GLU:OE1	2.22	0.47
1:1:38:ARG:NH1	1:1:186:GLY:O	2.47	0.47
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.95	0.47
7:a:123:SER:HB3	7:a:153:GLN:HE21	1.79	0.47
8:c:52:VAL:HG11	8:c:203:VAL:HA	1.96	0.47
8:c:168:ALA:HB3	9:j:55:LEU:HD13	1.97	0.47
17:J:218:LEU:HB3	17:J:230:VAL:HA	1.95	0.47
21:N:376:LYS:HA	21:N:411:ILE:HG12	1.95	0.47
30:W:58:ASN:O	30:W:60:ARG:N	2.48	0.47
33:Z:260:GLU:HB2	33:Z:579:GLU:HB3	1.96	0.47
3:h:51:LEU:HD22	3:h:87:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:156:LYS:HD3	8:A:166:TYR:HE2	1.80	0.47
11:n:165:GLY:O	11:n:168:SER:OG	2.30	0.47
29:V:154:ASP:OD1	29:V:155:ALA:N	2.47	0.47
30:W:139:VAL:HG11	30:W:157:PHE:HE2	1.79	0.47
33:Z:234:PRO:HG3	33:Z:270:SER:HB2	1.96	0.47
3:3:63:LEU:HD12	3:3:105:VAL:HG11	1.96	0.47
5:f:107:LYS:N	6:e:151:GLU:OE2	2.42	0.47
11:D:56:ASP:O	11:D:60:THR:OG1	2.26	0.47
11:n:65:SER:N	11:n:73:LEU:O	2.46	0.47
16:I:116:ASP:HA	16:I:132:ILE:HD12	1.97	0.47
22:O:117:ASN:HB2	22:O:128:LEU:HB2	1.95	0.47
25:R:44:LYS:HB2	25:R:88:LEU:HD12	1.96	0.47
1:1:78:VAL:HG22	1:1:100:VAL:HG12	1.95	0.47
7:7:215:ARG:NH2	7:7:248:GLU:O	2.46	0.47
10:C:87:LEU:HD22	10:C:115:LEU:HD22	1.96	0.47
20:M:274:ALA:HB1	20:M:275:PRO:HD2	1.96	0.47
22:O:72:LYS:HG2	22:O:73:ILE:HG13	1.96	0.47
25:R:36:SER:H	25:R:43:ARG:HH21	1.63	0.47
26:S:483:GLU:HG3	28:U:302:GLN:HE21	1.79	0.47
33:Z:308:LYS:NZ	33:Z:918:ASP:O	2.37	0.47
1:1:113:THR:HG22	1:1:134:LEU:HD22	1.95	0.47
3:3:53:ILE:HG22	3:3:60:VAL:HG22	1.95	0.47
7:7:234:ASP:OD2	7:7:237:THR:N	2.42	0.47
2:i:41:VAL:HG23	2:i:207:MET:HE3	1.96	0.47
9:B:10:THR:HG22	9:B:18:LEU:HD22	1.96	0.47
14:G:209:GLU:HG2	14:G:210:LYS:HG3	1.96	0.47
15:H:105:ILE:HG23	15:H:145:TYR:CE1	2.50	0.47
19:L:290:ARG:NH1	20:M:292:ASP:OD2	2.47	0.47
21:N:470:LEU:O	21:N:504:TYR:OH	2.22	0.47
23:P:144:VAL:HG13	23:P:156:ALA:HB1	1.96	0.47
25:R:59:MET:HB3	25:R:62:TYR:HD2	1.79	0.47
27:T:221:ALA:HB1	27:T:226:TRP:HB2	1.97	0.47
31:X:78:ILE:HG12	31:X:80:SER:H	1.79	0.47
32:Y:72:ASP:OD1	32:Y:73:PHE:N	2.47	0.47
1:1:151:THR:HA	1:1:154:TYR:HE2	1.79	0.47
10:C:4:ARG:HD2	12:E:10:ARG:HA	1.97	0.47
30:W:15:TYR:HB2	30:W:116:SER:HB3	1.97	0.47
3:3:11:ILE:HG22	3:3:142:ALA:HB3	1.96	0.47
4:4:60:ILE:HD13	4:4:84:VAL:HG22	1.96	0.47
13:F:4:ASN:ND2	15:H:359:ASN:O	2.48	0.47
10:d:184:MET:HE1	10:d:192:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:432:ILE:HG12	19:L:436:LYS:HB2	1.96	0.47
23:P:24:ILE:O	23:P:69:ARG:NH1	2.48	0.47
29:V:138:ALA:O	29:V:156:PHE:N	2.48	0.47
1:1:76:ASP:OD2	2:2:113:LYS:NZ	2.42	0.47
4:g:29:LYS:HD3	4:g:32:ASP:HB2	1.97	0.47
4:g:59:TYR:O	4:g:63:ASN:ND2	2.47	0.47
11:D:161:ALA:HB1	11:D:175:LEU:HD13	1.98	0.47
10:d:31:HIS:O	10:d:51:LYS:NZ	2.43	0.47
18:K:320:ARG:NH2	18:K:322:ASP:OD2	2.47	0.47
23:P:217:LYS:HA	23:P:220:TYR:HD2	1.80	0.47
25:R:302:ALA:HB2	25:R:357:PHE:HA	1.96	0.47
33:Z:266:LYS:HA	33:Z:293:MET:HE1	1.97	0.47
33:Z:827:LEU:HB3	33:Z:831:LEU:HD13	1.96	0.47
8:A:104:PHE:HB2	8:A:112:MET:HE3	1.97	0.46
11:D:107:GLU:OE2	11:D:111:ARG:NH2	2.48	0.46
21:N:138:GLU:HA	21:N:141:ILE:HD12	1.97	0.46
21:N:736:PHE:HD1	21:N:746:ALA:HA	1.80	0.46
22:O:23:HIS:CE1	22:O:25:LEU:HB2	2.50	0.46
1:1:209:PRO:HG2	7:a:252:TRP:CE2	2.50	0.46
9:j:161:ALA:HB1	9:j:175:LEU:HD13	1.98	0.46
14:k:12:ASN:O	14:k:21:ASN:ND2	2.47	0.46
17:J:279:LEU:O	17:J:284:THR:N	2.48	0.46
19:L:277:ILE:HG23	19:L:322:LYS:HB2	1.97	0.46
21:N:17:GLN:HB3	21:N:20:VAL:HB	1.98	0.46
29:V:54:LEU:N	29:V:67:ASP:O	2.48	0.46
33:Z:92:LEU:HD12	33:Z:122:LEU:HD21	1.97	0.46
33:Z:138:ARG:HH22	33:Z:146:PHE:HZ	1.62	0.46
33:Z:531:ALA:HB1	33:Z:572:ILE:HB	1.97	0.46
9:B:5:TYR:HE1	10:C:3:SER:HA	1.80	0.46
9:B:18:LEU:HD12	9:B:21:ILE:HD12	1.97	0.46
10:d:35:ALA:HA	10:d:48:ALA:HA	1.98	0.46
12:m:71:ASP:HB3	12:m:74:ILE:HB	1.97	0.46
17:J:71:TYR:N	17:J:115:LEU:O	2.40	0.46
19:L:137:ARG:HA	19:L:140:LEU:HD12	1.95	0.46
21:N:416:GLY:HA3	21:N:453:ALA:HB1	1.96	0.46
5:5:92:ASP:HB2	5:5:247:GLY:O	2.15	0.46
12:E:122:ARG:HG2	12:E:132:ARG:HH21	1.79	0.46
17:J:99:ALA:HB3	17:J:102:ILE:HG12	1.96	0.46
20:M:281:ASP:OD1	20:M:282:GLU:N	2.49	0.46
22:O:308:LEU:O	22:O:348:VAL:N	2.42	0.46
7:a:215:ARG:HG2	7:a:247:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:26:TYR:OH	15:H:465:GLN:OE1	2.32	0.46
14:G:165:THR:HA	14:G:169:ARG:HD3	1.97	0.46
17:J:247:MET:HG3	17:J:292:MET:HG2	1.96	0.46
20:M:175:LYS:HG3	20:M:237:ALA:HA	1.97	0.46
22:O:132:GLU:OE2	22:O:135:ARG:NH2	2.48	0.46
22:O:189:TYR:HE2	22:O:227:ILE:HB	1.81	0.46
30:W:12:ASN:H	30:W:55:ALA:HB3	1.81	0.46
33:Z:126:TYR:HD2	33:Z:128:GLU:HB2	1.81	0.46
2:2:242:LEU:HA	3:3:201:LYS:HE3	1.98	0.46
5:5:109:VAL:HG21	5:5:253:TYR:HE2	1.80	0.46
7:a:234:ASP:OD2	7:a:237:THR:N	2.44	0.46
9:B:140:ASP:OD1	9:B:144:GLY:N	2.44	0.46
12:E:50:VAL:HG21	12:E:66:LYS:HB2	1.98	0.46
13:F:7:ASP:O	13:F:21:GLN:NE2	2.49	0.46
14:G:5:GLY:HA2	15:H:322:GLY:HA3	1.96	0.46
10:d:91:ALA:HB2	10:d:115:LEU:HD21	1.97	0.46
15:H:414:SER:OG	15:H:418:GLU:OE1	2.29	0.46
19:L:105:ILE:HD12	20:M:126:THR:HG22	1.98	0.46
20:M:220:MET:HG2	20:M:347:ILE:HB	1.98	0.46
5:5:103:SER:HB3	5:5:106:VAL:HG23	1.97	0.46
4:g:100:VAL:HG12	4:g:102:VAL:HG13	1.98	0.46
6:e:207:PHE:O	6:e:211:THR:OG1	2.33	0.46
15:H:277:SER:OG	16:I:308:GLU:OE1	2.33	0.46
27:T:94:HIS:NE2	27:T:96:LEU:HB2	2.31	0.46
2:i:81:THR:HB	2:i:127:LEU:HD21	1.97	0.46
10:d:44:ILE:HD11	10:d:146:TYR:HB3	1.98	0.46
16:I:299:GLU:HA	16:I:302:ILE:HD12	1.96	0.46
21:N:713:VAL:HG12	21:N:755:PRO:HB3	1.97	0.46
27:T:201:PRO:HA	27:T:232:LYS:HA	1.98	0.46
33:Z:246:CYS:HB2	33:Z:250:VAL:HG23	1.98	0.46
33:Z:491:LEU:HD21	33:Z:525:MET:HE2	1.98	0.46
2:2:196:LEU:HB3	6:e:215:ILE:HB	1.98	0.46
7:7:49:TYR:HE2	7:7:54:ILE:HG13	1.80	0.46
9:B:123:GLN:HE22	10:C:131:PHE:HE1	1.64	0.46
13:F:201:LEU:HD13	13:F:205:SER:HA	1.97	0.46
8:c:35:THR:HG21	8:c:140:ILE:HG13	1.98	0.46
14:k:48:PHE:HE1	14:k:137:ILE:HG22	1.81	0.46
16:I:254:GLN:NE2	17:J:227:SER:OG	2.49	0.46
19:L:167:VAL:HB	20:M:142:PRO:HG2	1.97	0.46
30:W:181:LEU:HA	30:W:184:ASN:HD22	1.81	0.46
8:A:219:SER:H	8:A:222:ASP:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:11:PHE:CE2	12:E:136:ARG:HB2	2.51	0.46
16:I:248:VAL:HG12	16:I:250:SER:H	1.81	0.46
20:M:274:ALA:O	20:M:276:THR:N	2.48	0.46
20:M:282:GLU:OE1	20:M:328:ASN:ND2	2.49	0.46
29:V:48:GLU:HG2	29:V:112:PRO:HD2	1.98	0.46
33:Z:441:TYR:CD2	33:Z:442:VAL:HG22	2.51	0.46
3:3:11:ILE:HD11	3:3:26:ASP:HB3	1.96	0.45
11:D:26:ALA:HB1	11:D:78:LEU:HG	1.96	0.45
19:L:263:ILE:HD11	19:L:304:THR:HG23	1.98	0.45
19:L:400:PHE:HZ	20:M:215:PRO:HD3	1.81	0.45
21:N:373:VAL:HG23	21:N:410:LEU:HD13	1.98	0.45
27:T:242:LYS:HB3	27:T:251:HIS:HD2	1.80	0.45
1:b:151:THR:HA	1:b:154:TYR:HE2	1.81	0.45
12:m:108:ASN:OD1	12:m:109:VAL:N	2.49	0.45
18:K:153:ASP:OD1	19:L:110:LYS:NZ	2.50	0.45
4:4:70:ARG:HE	10:C:113:ARG:CZ	2.28	0.45
12:E:201:LEU:HD23	12:E:204:LEU:HD12	1.99	0.45
21:N:67:LYS:HA	21:N:70:TYR:HB3	1.98	0.45
3:h:30:GLY:HA2	3:h:36:VAL:HG23	1.97	0.45
6:e:31:ILE:HA	6:e:44:GLY:HA2	1.98	0.45
9:B:111:VAL:HG23	9:B:136:ILE:HD12	1.98	0.45
15:H:312:ASP:O	15:H:318:ARG:NH2	2.49	0.45
18:K:127:ASP:OD1	18:K:128:ARG:N	2.49	0.45
18:K:164:ASN:H	18:K:166:LYS:HG2	1.81	0.45
19:L:364:HIS:CE1	19:L:392:ARG:HE	2.34	0.45
33:Z:149:TRP:HA	33:Z:154:ILE:HD12	1.98	0.45
2:i:112:LEU:HD23	2:i:142:ILE:HD12	1.98	0.45
12:E:204:LEU:HA	12:E:207:VAL:HG22	1.99	0.45
10:d:70:ASN:HB3	10:d:73:ILE:HB	1.98	0.45
15:H:101:ARG:HE	15:H:171:GLY:HA2	1.82	0.45
9:B:118:MET:HE3	9:B:130:PHE:HB2	1.99	0.45
15:H:98:GLN:NE2	16:I:127:ASP:O	2.49	0.45
5:5:244:ALA:HB1	3:h:179:ALA:HB1	1.98	0.45
8:A:20:SER:HG	8:A:24:ARG:H	1.63	0.45
8:c:73:PHE:HB2	8:c:81:MET:HE2	1.99	0.45
10:d:177:GLN:HA	11:n:54:LEU:HD11	1.98	0.45
25:R:312:TYR:HD1	25:R:316:LEU:HD22	1.82	0.45
25:R:346:LYS:HD2	25:R:390:THR:HB	1.99	0.45
28:U:46:ILE:HG21	28:U:119:LEU:HD22	1.97	0.45
7:7:254:PHE:HB3	2:i:173:GLN:HE21	1.81	0.45
3:h:11:ILE:HD12	3:h:146:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:183:MET:O	7:a:186:PRO:HD2	2.17	0.45
11:n:97:ARG:HH21	11:n:103:PRO:HB3	1.81	0.45
16:I:253:ILE:HG22	16:I:254:GLN:H	1.82	0.45
21:N:296:CYS:HB3	21:N:377:GLY:HA2	1.98	0.45
23:P:270:LEU:O	23:P:344:ARG:NE	2.50	0.45
26:S:293:ILE:HD13	26:S:316:LEU:HD23	1.99	0.45
2:2:141:SER:HB2	2:2:154:LEU:HD13	1.99	0.45
4:g:49:GLU:O	4:g:53:THR:HG23	2.17	0.45
15:H:291:VAL:HG11	15:H:336:LEU:HA	1.99	0.45
15:H:385:ARG:NH1	15:H:413:ASN:OD1	2.41	0.45
19:L:113:SER:HB3	19:L:116:LYS:HB2	1.97	0.45
23:P:97:ILE:HG21	23:P:136:ARG:HB3	1.97	0.45
28:U:165:GLU:OE2	29:V:42:ARG:NH2	2.35	0.45
29:V:29:ILE:HD12	29:V:201:ILE:HG23	1.98	0.45
9:B:217:GLU:OE1	9:B:231:LYS:HB2	2.17	0.45
12:m:42:THR:OG1	12:m:45:GLY:O	2.33	0.45
25:R:62:TYR:HE2	25:R:145:GLY:HA2	1.81	0.45
1:1:23:MET:HB3	1:1:145:ILE:HG22	1.98	0.44
6:e:30:THR:HA	6:e:74:ASN:HD21	1.82	0.44
8:A:14:ARG:HG2	8:A:26:TYR:CG	2.52	0.44
9:B:43:VAL:HG11	9:B:137:ALA:HB1	1.99	0.44
13:F:26:LEU:HD23	13:F:149:PRO:HD2	1.98	0.44
14:G:109:ILE:HG12	14:G:142:ASP:HB3	1.99	0.44
1:1:94:THR:OG1	1:1:128:GLU:OE1	2.30	0.44
2:i:189:GLN:HA	2:i:192:ILE:HD12	1.99	0.44
14:G:95:GLU:HB3	14:G:115:ARG:HH11	1.83	0.44
17:J:154:THR:HA	17:J:157:ILE:HD12	1.99	0.44
19:L:88:TYR:HD1	20:M:62:ILE:HG13	1.83	0.44
21:N:742:TRP:CH2	21:N:744:PRO:HG2	2.51	0.44
31:X:117:LYS:HE2	31:X:119:LYS:HB2	1.98	0.44
33:Z:445:PRO:HB2	33:Z:485:ILE:HD11	2.00	0.44
33:Z:577:GLN:NE2	33:Z:580:GLN:OE1	2.51	0.44
1:b:70:ASP:OD2	1:b:113:THR:N	2.46	0.44
9:B:186:GLU:OE1	9:B:246:ARG:NE	2.50	0.44
10:d:239:LEU:HB3	10:d:245:THR:H	1.82	0.44
16:I:222:TYR:HE1	16:I:330:LYS:HA	1.82	0.44
22:O:138:LEU:HD11	22:O:178:TYR:HA	1.99	0.44
23:P:361:THR:HG22	23:P:399:ILE:HG22	1.98	0.44
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.99	0.44
31:X:75:TRP:HB2	31:X:125:MET:HE2	1.99	0.44
5:5:220:LYS:HG2	5:5:222:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:61:GLY:N	7:7:69:PHE:O	2.37	0.44
1:b:61:TRP:CD1	1:b:197:LEU:HD21	2.52	0.44
5:f:83:PHE:CE2	5:f:88:ILE:HG12	2.49	0.44
11:n:68:ASP:OD1	11:n:69:SER:N	2.47	0.44
13:l:43:HIS:CD2	13:l:217:GLY:HA3	2.53	0.44
14:k:108:PRO:HB2	14:k:110:PRO:HD2	1.99	0.44
15:H:422:VAL:HA	15:H:450:VAL:HG21	1.98	0.44
19:L:143:GLY:O	19:L:161:ARG:NH2	2.50	0.44
21:N:294:PRO:HB2	21:N:298:TYR:CZ	2.53	0.44
21:N:717:LEU:HD22	21:N:730:VAL:HA	1.99	0.44
24:Q:223:GLY:HA2	24:Q:226:HIS:HD2	1.82	0.44
25:R:61:PRO:HB2	25:R:65:TYR:CZ	2.53	0.44
7:a:44:VAL:N	7:a:177:THR:OG1	2.48	0.44
16:I:196:GLU:O	16:I:208:TYR:OH	2.28	0.44
21:N:8:PRO:HB3	27:T:84:GLN:HA	1.99	0.44
26:S:111:ARG:HA	26:S:117:SER:HB3	2.00	0.44
29:V:202:ASP:OD1	29:V:203:TYR:N	2.50	0.44
30:W:47:ASN:OD1	30:W:48:THR:N	2.50	0.44
16:I:300:ARG:HB3	16:I:304:ARG:HH12	1.83	0.44
16:I:340:ARG:NH1	16:I:341:PRO:O	2.51	0.44
18:K:67:TYR:HB2	21:N:572:LEU:HD13	2.00	0.44
19:L:427:LYS:HD2	20:M:346:LYS:HE2	1.99	0.44
20:M:127:VAL:HG11	20:M:153:TYR:HB3	2.00	0.44
24:Q:15:VAL:HG13	24:Q:20:TYR:HB3	1.98	0.44
26:S:357:LEU:HB3	26:S:384:ARG:HH22	1.83	0.44
28:U:108:GLU:OE1	30:W:60:ARG:NH2	2.50	0.44
8:c:178:ILE:HD11	8:c:214:LEU:HD21	2.00	0.44
11:n:77:GLY:HA3	11:n:131:VAL:HG22	2.00	0.44
12:m:52:LYS:HB2	12:m:216:ASN:HA	2.00	0.44
15:H:261:ARG:NH2	16:I:315:GLY:O	2.33	0.44
18:K:271:ILE:HD12	18:K:316:MET:HE2	1.99	0.44
2:2:104:ARG:HG2	2:2:133:ASP:HB2	2.00	0.44
5:5:96:THR:HG22	5:5:101:VAL:HG22	2.00	0.44
5:5:172:MET:H	5:5:192:SER:HB3	1.82	0.44
13:F:41:ASN:ND2	13:F:180:ILE:O	2.51	0.44
9:j:95:THR:HA	9:j:99:ARG:HD2	1.99	0.44
11:n:159:TRP:HZ3	12:m:56:SER:HB3	1.82	0.44
14:k:103:TYR:C	14:k:105:THR:H	2.26	0.44
21:N:406:TYR:HD1	21:N:448:LEU:HB3	1.82	0.44
23:P:144:VAL:HG12	23:P:148:LYS:HE3	1.99	0.44
2:2:123:ILE:HG22	2:2:125:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:53:THR:OG1	10:C:210:ARG:NE	2.51	0.44
14:G:37:SER:HB3	14:G:50:VAL:HG23	2.00	0.44
10:d:194:LEU:HD13	10:d:239:LEU:HD23	1.99	0.44
13:l:206:LEU:HD11	13:l:211:LEU:HB2	2.00	0.44
14:k:114:ASP:OD1	14:k:157:TYR:OH	2.36	0.44
14:k:217:SER:OG	14:k:229:LYS:O	2.31	0.44
15:H:247:LEU:HD13	15:H:374:LYS:HG2	2.00	0.44
15:H:304:CYS:SG	15:H:349:ILE:HG21	2.58	0.44
16:I:104:LEU:HD22	16:I:148:LEU:HD21	2.00	0.44
18:K:177:LEU:HD11	18:K:221:MET:HE3	2.00	0.44
18:K:360:MET:HE1	19:L:212:ILE:HA	1.99	0.44
30:W:36:ILE:HD11	30:W:185:ILE:HD12	1.98	0.44
33:Z:206:ASP:C	33:Z:209:PRO:HD2	2.43	0.44
2:i:228:LYS:HE2	3:h:152:SER:HA	1.99	0.43
3:h:78:GLU:HG3	3:h:80:ARG:HG2	2.00	0.43
7:a:49:TYR:HE2	7:a:54:ILE:HG13	1.82	0.43
11:n:200:LEU:HD21	11:n:240:LYS:HD2	1.99	0.43
15:H:102:CYS:HA	15:H:147:ILE:HA	2.01	0.43
16:I:253:ILE:HG22	16:I:254:GLN:N	2.33	0.43
18:K:158:ILE:C	18:K:160:VAL:H	2.26	0.43
19:L:107:GLU:HA	19:L:145:ARG:HA	2.00	0.43
27:T:227:PRO:HG2	27:T:234:TYR:HB3	2.00	0.43
30:W:91:LEU:HB2	30:W:128:LEU:HD21	1.99	0.43
5:5:92:ASP:OD1	5:5:108:LYS:NZ	2.51	0.43
14:G:13:SER:OG	14:G:127:ASN:ND2	2.45	0.43
11:n:48:ARG:HB2	11:n:209:ASN:HA	1.99	0.43
15:H:273:ARG:HG3	15:H:307:PHE:HD2	1.83	0.43
19:L:129:VAL:HG11	19:L:148:LEU:HD22	1.99	0.43
19:L:257:GLY:HA2	19:L:303:ARG:HH22	1.82	0.43
7:7:39:VAL:HB	7:7:90:ILE:HG22	2.00	0.43
4:g:130:TYR:OH	4:g:145:ASP:OD1	2.31	0.43
9:j:97:TYR:O	9:j:101:TYR:N	2.52	0.43
10:d:134:SER:OG	10:d:151:SER:O	2.28	0.43
19:L:293:GLU:O	19:L:295:THR:HG23	2.19	0.43
21:N:6:ALA:HB2	21:N:35:LEU:HB3	1.99	0.43
23:P:131:PHE:HA	23:P:136:ARG:HH21	1.83	0.43
23:P:218:LEU:HD23	23:P:251:LYS:HE2	2.01	0.43
28:U:93:TYR:HB3	28:U:121:LEU:HD23	2.00	0.43
2:2:85:THR:HA	2:2:88:ILE:HG22	1.99	0.43
8:A:88:PRO:HD3	14:G:156:SER:HB3	2.01	0.43
9:j:10:THR:HG22	9:j:18:LEU:HD22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:45:ILE:HD12	9:j:74:VAL:HB	2.00	0.43
21:N:666:GLN:HG2	21:N:873:ARG:HH21	1.83	0.43
22:O:332:ILE:HG12	22:O:337:LEU:HB2	2.00	0.43
25:R:394:ASP:OD1	25:R:395:ASN:N	2.52	0.43
26:S:434:ALA:HA	26:S:446:THR:H	1.83	0.43
28:U:124:ASP:HB3	28:U:133:PRO:HB2	2.00	0.43
33:Z:116:ALA:HB2	33:Z:140:LEU:HD23	2.01	0.43
1:l:152:PHE:HB3	1:b:154:TYR:HB2	2.01	0.43
6:e:76:PHE:HD2	6:e:79:ASP:H	1.64	0.43
10:C:177:GLN:HE22	11:D:53:LYS:HD2	1.83	0.43
16:I:313:LEU:HD21	16:I:324:VAL:HG21	2.00	0.43
18:K:48:TYR:HA	18:K:51:LEU:HD12	2.00	0.43
18:K:212:TYR:HB2	18:K:339:GLU:HA	2.00	0.43
20:M:283:LEU:HB2	20:M:327:THR:HB	2.00	0.43
24:Q:162:LEU:HD22	24:Q:166:LYS:HE3	2.00	0.43
25:R:286:LEU:HG	25:R:288:SER:H	1.82	0.43
30:W:117:PRO:HD3	30:W:146:GLU:HB2	2.01	0.43
7:7:152:VAL:HG11	7:7:235:LYS:HB3	2.00	0.43
4:g:4:ILE:HG13	4:g:47:ALA:HB2	2.00	0.43
9:j:140:ASP:OD1	9:j:144:GLY:N	2.51	0.43
11:n:70:HIS:NE2	11:n:104:VAL:O	2.38	0.43
12:m:34:GLY:HA3	12:m:80:GLY:HA2	2.01	0.43
13:l:88:LEU:HD21	13:l:112:LEU:HB2	2.01	0.43
17:J:118:ASP:OD1	17:J:119:SER:N	2.49	0.43
17:J:126:LEU:HD22	18:K:103:ILE:HD13	2.01	0.43
19:L:193:LEU:HD11	19:L:231:LEU:HD13	2.00	0.43
31:X:7:VAL:HG12	31:X:8:ILE:HG13	2.00	0.43
33:Z:957:LEU:HD22	33:Z:961:GLU:HB2	2.00	0.43
12:E:15:PHE:CE2	13:F:126:ARG:HB2	2.53	0.43
14:G:50:VAL:HG11	14:G:66:LYS:HB2	2.00	0.43
8:c:203:VAL:HG13	8:c:225:VAL:HG11	2.01	0.43
16:I:280:PHE:CE2	16:I:282:ASP:HB2	2.53	0.43
18:K:148:ASP:OD1	18:K:149:ILE:N	2.51	0.43
21:N:19:SER:HB3	27:T:35:ILE:HG21	2.01	0.43
4:4:59:TYR:O	4:4:63:ASN:ND2	2.52	0.43
1:b:15:GLU:HA	2:i:145:HIS:NE2	2.33	0.43
2:i:124:GLY:HA2	2:i:144:ALA:HB1	2.01	0.43
6:e:109:ALA:HA	6:e:144:PHE:HZ	1.84	0.43
8:A:181:ASN:HD22	8:A:213:ALA:HB2	1.84	0.43
13:F:39:ARG:NH1	13:F:142:ALA:O	2.52	0.43
8:c:59:VAL:HG13	8:c:64:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:286:ALA:C	16:I:288:GLY:H	2.25	0.43
25:R:309:LEU:HD21	32:Y:77:LEU:HD12	2.01	0.43
25:R:381:ILE:HA	25:R:388:VAL:HA	2.00	0.43
2:2:228:LYS:HE2	3:3:152:SER:HA	1.99	0.43
8:A:135:ARG:HD3	14:G:13:SER:HA	2.01	0.43
12:E:119:LEU:HB3	12:E:138:PHE:CE2	2.54	0.43
17:J:342:ASN:HB3	17:J:345:LYS:HB3	2.01	0.43
18:K:92:VAL:HB	18:K:93:PRO:HD2	2.01	0.43
18:K:281:ARG:C	18:K:283:ASP:H	2.26	0.43
26:S:468:ALA:HA	28:U:288:PHE:HZ	1.84	0.43
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.84	0.43
3:h:65:GLU:HB3	10:d:100:LYS:HG3	2.00	0.43
13:l:18:ARG:HH21	13:l:23:GLU:HG2	1.83	0.43
16:I:387:LEU:HD21	16:I:424:MET:HG2	2.00	0.43
17:J:113:VAL:HG12	17:J:125:VAL:HA	2.01	0.43
21:N:338:PHE:HZ	21:N:746:ALA:HB1	1.84	0.43
22:O:222:LEU:HD23	22:O:254:LEU:HD22	2.01	0.43
25:R:304:TYR:CZ	25:R:308:LEU:HD21	2.54	0.43
29:V:139:VAL:HA	29:V:155:ALA:HA	2.00	0.43
7:7:90:ILE:HG13	7:7:93:MET:HE2	2.01	0.42
1:b:196:VAL:HB	1:b:203:GLU:HB3	2.01	0.42
13:F:67:ASP:OD1	13:F:68:GLU:N	2.45	0.42
9:j:38:LYS:NZ	10:d:58:GLU:OE1	2.52	0.42
10:d:9:ARG:O	10:d:12:ILE:HG12	2.19	0.42
10:d:206:LEU:HD21	10:d:211:LEU:HD11	2.01	0.42
29:V:137:VAL:HG22	29:V:157:ARG:HG3	2.01	0.42
33:Z:422:ILE:HA	33:Z:425:ILE:HD12	1.99	0.42
3:3:27:LEU:HB3	3:3:38:ASN:O	2.18	0.42
3:3:65:GLU:HB3	10:C:100:LYS:HG3	2.01	0.42
4:4:84:VAL:HG11	4:4:102:VAL:HG21	2.01	0.42
9:B:35:LEU:HA	9:B:163:ALA:HA	1.99	0.42
13:F:39:ARG:HD3	13:F:144:LEU:HB2	2.00	0.42
13:F:112:LEU:HD12	13:F:134:ILE:HD11	2.01	0.42
18:K:122:ILE:HA	18:K:146:LEU:HD23	2.01	0.42
18:K:238:ASN:HB3	18:K:241:GLU:HB2	2.00	0.42
20:M:81:ASN:O	20:M:120:LYS:N	2.47	0.42
20:M:216:LYS:HG2	20:M:317:SER:HB3	2.01	0.42
21:N:653:ARG:NH1	21:N:691:GLN:OE1	2.52	0.42
23:P:393:VAL:HG13	23:P:400:VAL:HG22	1.99	0.42
3:h:70:LYS:NZ	3:h:94:SER:OG	2.50	0.42
9:B:48:GLU:HB2	9:B:196:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:131:PHE:O	10:C:153:PRO:HB3	2.19	0.42
12:E:13:SER:HB2	13:F:126:ARG:HD3	2.01	0.42
13:F:50:LYS:HB3	13:F:59:TYR:HB3	2.02	0.42
8:c:78:THR:O	8:c:145:SER:OG	2.35	0.42
8:c:156:LYS:HE2	8:c:166:TYR:HE2	1.85	0.42
9:j:44:VAL:HG22	9:j:213:ILE:HG22	2.01	0.42
17:J:214:SER:O	17:J:218:LEU:HG	2.19	0.42
17:J:234:PHE:O	17:J:238:ARG:HG3	2.19	0.42
21:N:309:ILE:HD13	21:N:707:ASN:HB3	2.01	0.42
23:P:290:LEU:HD21	23:P:292:LYS:HE3	2.01	0.42
33:Z:974:THR:HG23	33:Z:975:SER:N	2.34	0.42
8:A:215:GLY:O	19:L:353:ASN:ND2	2.52	0.42
12:E:24:VAL:HG11	12:E:161:SER:HA	2.00	0.42
13:F:49:LEU:HB2	13:F:197:ILE:HD11	2.01	0.42
14:G:67:ILE:HG12	14:G:77:VAL:HB	2.01	0.42
8:c:87:ILE:N	8:c:88:PRO:HD2	2.34	0.42
14:k:95:GLU:HB3	14:k:115:ARG:HD3	2.01	0.42
15:H:99:VAL:HB	16:I:127:ASP:CG	2.44	0.42
17:J:357:ASP:OD2	17:J:393:ASN:ND2	2.48	0.42
18:K:220:THR:HG21	19:L:313:ASP:OD1	2.18	0.42
19:L:187:THR:HA	19:L:190:ILE:HD12	2.01	0.42
19:L:327:THR:HG21	19:L:333:LEU:HD11	2.02	0.42
19:L:400:PHE:HA	19:L:403:ILE:HD12	2.01	0.42
20:M:428:LYS:HG3	20:M:429:SER:H	1.84	0.42
24:Q:26:VAL:O	24:Q:29:SER:OG	2.33	0.42
24:Q:390:LEU:O	25:R:346:LYS:N	2.52	0.42
26:S:345:TYR:HD1	26:S:348:LEU:HD12	1.85	0.42
26:S:400:LYS:HG3	26:S:445:THR:HB	2.00	0.42
28:U:92:TRP:CH2	28:U:107:ASN:HA	2.55	0.42
29:V:171:ARG:NH1	29:V:198:SER:O	2.53	0.42
33:Z:928:ARG:HA	33:Z:956:LEU:H	1.84	0.42
2:2:95:HIS:HE1	8:A:104:PHE:HE1	1.67	0.42
11:D:202:VAL:HG13	11:D:203:VAL:H	1.84	0.42
8:c:133:TYR:CD1	8:c:134:MET:HG3	2.54	0.42
16:I:219:VAL:HG12	16:I:346:ARG:HB2	2.00	0.42
16:I:279:VAL:O	16:I:325:ILE:N	2.45	0.42
17:J:186:ILE:HG22	17:J:310:ILE:HG21	2.02	0.42
20:M:135:VAL:HG12	20:M:158:THR:HG22	2.00	0.42
21:N:288:ASN:HB3	21:N:293:LEU:HB2	2.01	0.42
23:P:412:LEU:HD21	28:U:269:THR:HA	2.00	0.42
33:Z:180:ASP:OD1	33:Z:181:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:539:ASN:OD1	33:Z:540:GLY:N	2.52	0.42
33:Z:884:THR:HG22	33:Z:901:PHE:HA	2.02	0.42
4:4:172:MET:HG2	4:4:174:MET:H	1.85	0.42
3:h:155:GLU:HB3	3:h:158:LEU:HD11	2.00	0.42
6:e:203:VAL:HG11	6:e:223:ILE:HD12	2.02	0.42
6:e:221:LEU:N	6:e:236:TYR:O	2.45	0.42
10:C:78:ALA:O	10:C:134:SER:OG	2.35	0.42
12:E:164:PHE:O	13:F:60:GLN:NE2	2.51	0.42
10:d:64:GLU:HG3	10:d:65:LYS:HG2	2.01	0.42
12:m:15:PHE:HE1	13:l:126:ARG:HD2	1.85	0.42
14:k:27:ALA:HB1	14:k:133:GLY:HA2	2.01	0.42
28:U:38:LEU:HD23	28:U:87:GLU:HB3	2.02	0.42
29:V:127:LYS:HE2	29:V:195:HIS:CE1	2.55	0.42
30:W:98:LEU:O	30:W:101:ARG:NH1	2.49	0.42
4:g:152:MET:HE1	4:g:160:LEU:HB2	2.02	0.42
11:n:181:ARG:HD3	12:m:58:LEU:HA	2.00	0.42
15:H:95:HIS:O	15:H:97:LEU:N	2.53	0.42
15:H:100:ALA:HB2	15:H:149:LEU:HD23	2.00	0.42
21:N:328:PHE:HE1	21:N:696:LYS:HB2	1.84	0.42
21:N:379:LEU:HD23	21:N:411:ILE:HG22	2.02	0.42
21:N:623:PHE:O	21:N:627:ILE:HG12	2.20	0.42
1:1:191:VAL:HG12	1:1:209:PRO:HD3	2.02	0.42
1:b:182:ILE:HG23	1:b:189:GLY:HA2	2.01	0.42
4:g:8:ARG:HH11	4:g:115:GLU:HA	1.85	0.42
15:H:252:PRO:HB2	15:H:460:THR:HG21	2.01	0.42
18:K:212:TYR:N	18:K:338:ILE:O	2.52	0.42
19:L:217:GLY:HA3	19:L:343:LEU:HD23	2.02	0.42
28:U:283:ARG:NE	29:V:284:ALA:O	2.53	0.42
4:g:46:PHE:HE1	4:g:53:THR:HB	1.85	0.42
11:D:96:HIS:NE2	11:D:100:LEU:HD12	2.35	0.42
11:D:158:SER:HB3	12:E:63:SER:HB2	2.02	0.42
13:F:129:GLY:HA2	13:F:149:PRO:HG3	2.01	0.42
13:F:132:LEU:HB2	13:F:147:PHE:HB3	2.01	0.42
8:c:44:ALA:HB3	8:c:169:THR:HB	2.02	0.42
9:j:217:GLU:OE1	9:j:231:LYS:HB2	2.19	0.42
16:I:219:VAL:HG22	16:I:325:ILE:HG12	2.00	0.42
16:I:287:ILE:HG12	16:I:302:ILE:HG12	2.02	0.42
17:J:274:GLU:OE1	17:J:309:ARG:NH2	2.45	0.42
18:K:106:ASN:O	18:K:122:ILE:N	2.49	0.42
21:N:251:GLU:HB3	21:N:763:GLY:HA3	2.02	0.42
23:P:357:TYR:CG	23:P:360:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:204:TRP:CZ3	25:R:235:LEU:HD13	2.55	0.42
33:Z:303:ASP:OD2	33:Z:973:TYR:OH	2.27	0.42
4:4:96:ARG:HH22	5:5:164:GLN:HE22	1.67	0.42
11:D:49:ARG:HG2	11:D:51:THR:H	1.84	0.42
13:F:34:VAL:HG23	13:F:165:SER:HB3	2.02	0.42
10:d:141:ASP:OD1	10:d:145:GLY:N	2.52	0.42
18:K:127:ASP:HB3	18:K:130:LEU:HG	2.02	0.42
18:K:154:SER:HB3	18:K:259:ARG:NH1	2.35	0.42
21:N:612:SER:O	21:N:618:ARG:NH1	2.48	0.42
1:1:84:LEU:HD21	8:A:99:ALA:HA	2.02	0.41
5:5:91:VAL:HG21	5:5:109:VAL:HG23	2.02	0.41
7:a:126:PHE:CZ	7:a:163:VAL:HB	2.55	0.41
7:a:162:TYR:HB2	7:a:175:LEU:HD13	2.00	0.41
14:G:221:LEU:HA	14:G:225:ASN:HA	2.02	0.41
8:c:148:GLU:HG2	8:c:149:GLU:HG3	2.02	0.41
16:I:168:VAL:HG13	16:I:171:MET:HB2	2.01	0.41
18:K:81:ARG:NH2	28:U:176:ARG:O	2.53	0.41
18:K:93:PRO:HG2	19:L:153:LEU:HB2	2.02	0.41
21:N:369:ALA:HB1	21:N:406:TYR:HD2	1.85	0.41
23:P:235:LEU:HD23	23:P:271:SER:HB2	2.00	0.41
31:X:68:LEU:HD21	31:X:89:LEU:HD13	2.01	0.41
2:2:192:ILE:HG12	2:2:199:GLY:HA2	2.01	0.41
6:6:110:ARG:HG2	12:E:104:ASP:HB2	2.01	0.41
6:e:92:LYS:HB3	13:l:89:ARG:HH22	1.85	0.41
9:B:42:GLY:HA2	9:B:145:PHE:CE1	2.55	0.41
12:E:18:GLU:OE1	12:E:20:ARG:NH2	2.38	0.41
12:m:169:ALA:HB1	12:m:183:LEU:HD13	2.03	0.41
13:l:50:LYS:HD2	13:l:212:SER:HB2	2.01	0.41
15:H:201:GLU:HG3	15:H:273:ARG:HH12	1.85	0.41
18:K:425:ASP:CG	18:K:426:PHE:H	2.28	0.41
21:N:229:VAL:HG11	21:N:238:ALA:HB2	2.01	0.41
21:N:416:GLY:O	21:N:420:THR:N	2.52	0.41
21:N:528:ARG:HB3	21:N:531:LEU:HB2	2.02	0.41
25:R:291:SER:HB3	25:R:307:TYR:CD2	2.55	0.41
29:V:159:ILE:HG13	29:V:194:ARG:HA	2.02	0.41
32:Y:63:ASN:CG	32:Y:64:TRP:H	2.27	0.41
1:1:27:PHE:HE1	1:1:29:ASP:HB2	1.85	0.41
2:i:244:GLU:HG3	3:h:198:ARG:HG2	2.02	0.41
7:a:54:ILE:HG12	7:a:232:ILE:HG12	2.03	0.41
17:J:52:ASN:ND2	21:N:612:SER:HA	2.34	0.41
18:K:186:GLU:O	18:K:198:TYR:OH	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.85	0.41
25:R:35:GLN:HG3	25:R:74:ASN:HB2	2.00	0.41
29:V:27:VAL:HG13	29:V:63:VAL:HB	2.02	0.41
3:3:42:LYS:HD3	3:3:54:THR:HG22	2.02	0.41
6:6:114:HIS:CD2	12:E:102:TYR:HA	2.55	0.41
7:7:49:TYR:CE2	7:7:54:ILE:HG13	2.55	0.41
2:i:75:ALA:HB3	2:i:126:TYR:HB2	2.03	0.41
14:G:211:ASP:OD1	14:G:212:PHE:N	2.53	0.41
13:l:10:THR:HG21	13:l:127:PRO:HD3	2.02	0.41
21:N:743:PHE:HB2	21:N:744:PRO:HD3	2.01	0.41
22:O:40:GLN:HA	22:O:52:ALA:HA	2.02	0.41
22:O:99:LEU:HD13	22:O:133:ILE:HG12	2.01	0.41
23:P:202:LYS:HA	23:P:205:LYS:HE2	2.03	0.41
24:Q:85:MET:HA	24:Q:88:PHE:CE2	2.56	0.41
2:i:36:LYS:HA	2:i:41:VAL:HG12	2.02	0.41
7:a:114:ALA:O	7:a:119:ALA:HB2	2.21	0.41
10:d:72:LYS:HE2	10:d:224:GLU:HA	2.01	0.41
14:k:54:ILE:HB	14:k:211:ASP:HB3	2.03	0.41
14:k:221:LEU:HA	14:k:225:ASN:HA	2.01	0.41
20:M:163:PHE:HZ	20:M:268:ALA:HB1	1.85	0.41
21:N:55:PHE:CZ	21:N:57:ASP:HB2	2.55	0.41
21:N:58:ARG:HA	21:N:61:ALA:HB3	2.03	0.41
21:N:762:ARG:HH21	21:N:765:ASP:HB2	1.85	0.41
22:O:80:LYS:O	22:O:84:ALA:HB3	2.21	0.41
23:P:353:ILE:HA	23:P:357:TYR:HD2	1.86	0.41
25:R:301:TYR:HD2	25:R:357:PHE:HB3	1.85	0.41
2:2:177:LYS:HE3	2:2:206:VAL:HG11	2.03	0.41
3:3:143:SER:HA	3:3:146:LEU:HD12	2.03	0.41
4:4:101:ASN:HB3	4:4:133:HIS:CG	2.56	0.41
7:7:43:SER:HA	7:7:177:THR:HB	2.02	0.41
4:g:3:ILE:HB	4:g:18:SER:HB3	2.01	0.41
8:A:17:THR:HG22	8:A:27:GLN:HB2	2.01	0.41
19:L:108:VAL:HG22	19:L:119:VAL:HG22	2.01	0.41
21:N:443:LEU:HD21	21:N:469:VAL:HG13	2.01	0.41
21:N:638:ILE:HD11	21:N:672:ASN:HD21	1.86	0.41
26:S:357:LEU:HA	26:S:384:ARG:HH12	1.85	0.41
1:1:61:TRP:CD1	1:1:197:LEU:HD21	2.55	0.41
4:4:9:VAL:HG11	4:4:157:GLY:HA3	2.03	0.41
7:7:72:VAL:HG13	7:7:93:MET:HE1	2.02	0.41
3:h:139:SER:C	3:h:143:SER:HB3	2.45	0.41
8:A:87:ILE:N	8:A:88:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:109:GLU:HG2	10:d:113:ARG:HH12	1.85	0.41
15:H:177:ASP:HB3	15:H:180:LYS:O	2.21	0.41
15:H:253:GLY:O	15:H:417:ALA:N	2.51	0.41
21:N:93:GLU:HB3	21:N:98:VAL:HG21	2.03	0.41
23:P:359:ARG:HD3	23:P:399:ILE:HD12	2.02	0.41
25:R:24:TYR:CD1	25:R:244:THR:HA	2.56	0.41
29:V:71:MET:HE3	29:V:72:PRO:HD2	2.01	0.41
1:1:78:VAL:HG21	1:1:101:PHE:CE1	2.56	0.41
6:6:179:TYR:HD1	6:6:188:LYS:HA	1.85	0.41
6:6:226:VAL:HG22	6:6:231:VAL:HG22	2.03	0.41
7:7:127:GLU:HG2	13:F:100:ASN:HB2	2.02	0.41
8:A:128:TYR:HA	8:A:134:MET:HG3	2.03	0.41
9:B:184:GLU:HG3	24:Q:129:LYS:HB2	2.02	0.41
16:I:219:VAL:HA	16:I:344:ILE:HG23	2.02	0.41
16:I:298:GLY:C	16:I:300:ARG:H	2.29	0.41
23:P:260:VAL:HG22	23:P:327:LEU:HB3	2.02	0.41
25:R:222:ARG:HE	25:R:329:PHE:HZ	1.68	0.41
27:T:131:LYS:HB2	27:T:135:ASN:ND2	2.36	0.41
33:Z:801:HIS:ND1	33:Z:837:TYR:OH	2.39	0.41
1:1:24:ALA:HB2	1:1:33:LEU:HG	2.02	0.41
1:1:61:TRP:HD1	1:1:197:LEU:HD11	1.86	0.41
4:4:49:GLU:O	4:4:53:THR:HG23	2.21	0.41
2:i:155:SER:HB3	2:i:164:MET:HE2	2.02	0.41
3:h:107:PRO:HB2	3:h:124:PHE:HD2	1.86	0.41
4:g:193:ASP:OD1	4:g:194:ASP:N	2.54	0.41
6:e:57:ARG:NH1	7:a:193:ASP:OD1	2.48	0.41
6:e:78:ALA:HB2	7:a:167:GLY:HA3	2.02	0.41
9:B:44:VAL:HG11	9:B:189:ILE:HA	2.03	0.41
11:D:62:SER:OG	11:D:211:GLU:OE2	2.36	0.41
12:E:91:HIS:CD2	12:E:119:LEU:HD11	2.56	0.41
8:c:17:THR:HG22	8:c:27:GLN:HB2	2.02	0.41
9:j:69:PRO:HB3	9:j:233:PRO:HB3	2.03	0.41
18:K:214:PRO:HA	18:K:215:PRO:HD3	1.90	0.41
20:M:167:VAL:HG12	20:M:168:LYS:HG3	2.02	0.41
20:M:176:PRO:HG2	20:M:237:ALA:HB2	2.03	0.41
21:N:12:LEU:HD21	27:T:84:GLN:HE22	1.86	0.41
21:N:154:LEU:HD21	21:N:170:LEU:HD12	2.03	0.41
21:N:479:GLU:OE2	21:N:515:ARG:NH2	2.54	0.41
24:Q:350:ILE:HD13	24:Q:362:ILE:HG23	2.02	0.41
3:3:145:GLN:HG2	3:3:177:ARG:HB2	2.02	0.41
4:g:55:GLN:HG3	5:f:163:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:77:ALA:O	6:e:81:ASP:N	2.54	0.41
10:C:147:GLN:HB3	10:C:149:TYR:CE2	2.56	0.41
11:n:167:ASN:HD22	11:n:202:VAL:HG12	1.86	0.41
16:I:282:ASP:OD1	16:I:283:GLU:N	2.54	0.41
17:J:338:THR:O	17:J:341:ILE:HG12	2.21	0.41
18:K:84:GLU:O	18:K:88:ARG:NE	2.48	0.41
21:N:726:ASP:HB3	21:N:729:SER:HB3	2.03	0.41
23:P:164:GLN:HE22	23:P:195:GLN:NE2	2.19	0.41
24:Q:275:ILE:HD11	24:Q:306:TYR:HD2	1.85	0.41
33:Z:124:MET:O	33:Z:156:HIS:ND1	2.53	0.41
33:Z:463:HIS:HB2	33:Z:496:ALA:HB1	2.03	0.41
33:Z:568:LEU:HD21	33:Z:738:TYR:CZ	2.55	0.41
1:1:20:THR:O	1:1:149:GLY:N	2.52	0.40
2:2:191:GLY:O	2:2:195:ASP:HB3	2.22	0.40
5:f:125:ALA:HB3	6:e:147:VAL:HG12	2.02	0.40
6:e:84:VAL:HG12	6:e:88:LYS:HE3	2.03	0.40
8:c:126:GLN:NE2	9:j:81:ASP:HA	2.36	0.40
13:l:67:ASP:OD1	13:l:68:GLU:N	2.44	0.40
16:I:423:VAL:HA	16:I:427:LYS:HB2	2.03	0.40
18:K:291:GLU:C	18:K:293:GLN:H	2.29	0.40
19:L:88:TYR:CD1	20:M:62:ILE:HG13	2.56	0.40
21:N:83:LEU:HD13	21:N:132:LYS:HB3	2.03	0.40
26:S:352:VAL:HG22	26:S:387:VAL:HG22	2.03	0.40
3:3:13:VAL:HG13	3:3:167:ILE:HD11	2.03	0.40
5:5:212:TYR:HB3	4:g:171:ARG:HG3	2.03	0.40
9:B:40:THR:OG1	9:B:183:LEU:O	2.30	0.40
14:G:218:TRP:HH2	14:G:223:GLU:HB3	1.86	0.40
15:H:104:LYS:HB3	15:H:146:VAL:HB	2.03	0.40
18:K:391:GLY:HA3	19:L:212:ILE:HG21	2.02	0.40
21:N:318:LYS:HD2	21:N:355:TRP:CD1	2.57	0.40
23:P:61:LYS:O	23:P:65:LEU:HG	2.21	0.40
26:S:164:ILE:HB	26:S:165:PRO:HD3	2.03	0.40
33:Z:185:ASP:HB3	33:Z:230:ILE:HD12	2.02	0.40
33:Z:427:GLN:HA	33:Z:458:SER:HA	2.02	0.40
4:4:35:THR:HB	4:4:43:LEU:HD11	2.03	0.40
5:5:96:THR:HG21	5:5:245:TYR:HA	2.03	0.40
3:h:106:GLY:HA2	3:h:107:PRO:HD3	1.92	0.40
6:e:92:LYS:HB3	13:l:89:ARG:NH2	2.36	0.40
10:d:119:LYS:HG2	10:d:131:PHE:CD2	2.57	0.40
15:H:215:LYS:HB3	15:H:217:GLN:OE1	2.20	0.40
15:H:289:ARG:O	15:H:293:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:197:ILE:HB	20:M:277:ILE:HD13	2.03	0.40
21:N:328:PHE:HZ	21:N:693:GLY:HA2	1.87	0.40
23:P:147:LYS:HB2	23:P:156:ALA:HB2	2.03	0.40
3:3:63:LEU:HB3	3:3:67:PHE:CE2	2.56	0.40
6:6:76:PHE:HD2	6:6:79:ASP:H	1.69	0.40
1:b:172:ASP:O	1:b:176:HIS:ND1	2.31	0.40
4:g:70:ARG:HH12	11:n:87:GLU:HG2	1.86	0.40
6:e:46:THR:O	6:e:59:GLU:N	2.54	0.40
11:D:202:VAL:HG13	11:D:203:VAL:N	2.36	0.40
8:c:69:VAL:HG22	14:k:158:TRP:CD1	2.56	0.40
11:n:73:LEU:HD23	11:n:86:ILE:HG12	2.03	0.40
17:J:140:GLU:OE2	17:J:200:ARG:NH2	2.52	0.40
24:Q:161:LEU:HD22	24:Q:165:PHE:CZ	2.56	0.40
25:R:168:ILE:HG13	25:R:171:MET:HE2	2.01	0.40
33:Z:754:LYS:HG3	33:Z:783:VAL:HB	2.03	0.40
1:1:32:ILE:HG12	1:1:196:VAL:HA	2.03	0.40
2:2:234:PHE:HZ	6:e:171:ASN:HD21	1.69	0.40
7:7:76:ILE:HG21	7:7:97:GLU:HG3	2.03	0.40
2:i:63:LEU:HD13	2:i:205:CYS:HB2	2.03	0.40
2:i:64:HIS:HB3	2:i:85:THR:HG21	2.04	0.40
22:O:41:LEU:HD23	22:O:59:LEU:HD23	2.03	0.40
25:R:26:VAL:HG22	25:R:53:LYS:HG2	2.03	0.40
29:V:51:GLY:HA2	29:V:71:MET:HG2	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	203/215 (94%)	191 (94%)	12 (6%)	0	100	100
1	b	203/215 (94%)	193 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	220/261 (84%)	213 (97%)	7 (3%)	0	100	100
2	i	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
3	3	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
3	h	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	24	57
4	4	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
4	g	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
5	5	210/287 (73%)	204 (97%)	6 (3%)	0	100	100
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
6	6	220/241 (91%)	212 (96%)	8 (4%)	0	100	100
6	e	220/241 (91%)	211 (96%)	9 (4%)	0	100	100
7	7	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
7	a	231/266 (87%)	221 (96%)	10 (4%)	0	100	100
8	A	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
9	j	248/250 (99%)	238 (96%)	10 (4%)	0	100	100
10	C	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
10	d	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
11	D	239/254 (94%)	229 (96%)	10 (4%)	0	100	100
11	n	239/254 (94%)	230 (96%)	9 (4%)	0	100	100
12	E	240/260 (92%)	227 (95%)	13 (5%)	0	100	100
12	m	240/260 (92%)	234 (98%)	6 (2%)	0	100	100
13	F	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
13	l	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
14	G	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
14	k	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
15	H	351/467 (75%)	319 (91%)	32 (9%)	0	100	100
16	I	361/437 (83%)	331 (92%)	29 (8%)	1 (0%)	36	67
17	J	371/405 (92%)	338 (91%)	32 (9%)	1 (0%)	36	67
18	K	379/428 (89%)	340 (90%)	37 (10%)	2 (0%)	24	57
19	L	369/437 (84%)	336 (91%)	33 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	M	363/434 (84%)	326 (90%)	36 (10%)	1 (0%)	36	67
21	N	843/945 (89%)	814 (97%)	29 (3%)	0	100	100
22	O	385/393 (98%)	352 (91%)	33 (9%)	0	100	100
23	P	430/445 (97%)	398 (93%)	32 (7%)	0	100	100
24	Q	429/434 (99%)	407 (95%)	22 (5%)	0	100	100
25	R	398/429 (93%)	360 (90%)	37 (9%)	1 (0%)	36	67
26	S	473/523 (90%)	453 (96%)	19 (4%)	1 (0%)	43	73
27	T	270/274 (98%)	246 (91%)	24 (9%)	0	100	100
28	U	245/338 (72%)	241 (98%)	4 (2%)	0	100	100
29	V	252/306 (82%)	227 (90%)	23 (9%)	2 (1%)	16	48
30	W	195/268 (73%)	181 (93%)	14 (7%)	0	100	100
31	X	125/156 (80%)	113 (90%)	12 (10%)	0	100	100
32	Y	25/89 (28%)	19 (76%)	5 (20%)	1 (4%)	2	20
33	Z	807/993 (81%)	757 (94%)	49 (6%)	1 (0%)	48	79
All	All	13400/15139 (88%)	12648 (94%)	740 (6%)	12 (0%)	49	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	I	287	ILE
18	K	158	ILE
18	K	292	VAL
25	R	241	ILE
3	h	105	VAL
17	J	134	VAL
20	M	167	VAL
29	V	165	ILE
32	Y	69	VAL
33	Z	442	VAL
26	S	83	PRO
29	V	78	VAL

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	169/178 (95%)	169 (100%)	0	100	100
1	b	169/178 (95%)	169 (100%)	0	100	100
2	2	181/214 (85%)	181 (100%)	0	100	100
2	i	181/214 (85%)	181 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
4	g	175/175 (100%)	175 (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	199/224 (89%)	199 (100%)	0	100	100
7	a	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (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	213/226 (94%)	213 (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	200/239 (84%)	200 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	317/377 (84%)	317 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	447/489 (91%)	447 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	227/268 (85%)	227 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	116/144 (81%)	116 (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	11646/13054 (89%)	11646 (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 (159) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	115	HIS
2	2	145	HIS
2	2	189	GLN
3	3	169	GLN
4	4	10	GLN
4	4	65	GLN
4	4	191	GLN
5	5	128	GLN
5	5	164	GLN
5	5	251	ASN
5	5	254	HIS
5	5	263	HIS

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Mol	Chain	Res	Type
6	6	55	ASN
6	6	214	HIS
7	7	36	GLN
7	7	59	ASN
1	b	139	HIS
2	i	114	GLN
2	i	122	HIS
2	i	173	GLN
3	h	89	GLN
3	h	204	GLN
4	g	191	GLN
5	f	251	ASN
5	f	283	ASN
6	e	55	ASN
6	e	111	ASN
7	a	59	ASN
7	a	145	ASN
7	a	153	GLN
7	a	185	ASN
8	A	36	ASN
8	A	84	ASN
8	A	126	GLN
8	A	181	ASN
10	C	31	HIS
10	C	120	GLN
10	C	177	GLN
11	D	16	HIS
11	D	209	ASN
12	E	23	GLN
12	E	73	HIS
12	E	91	HIS
12	E	108	ASN
12	E	168	ASN
13	F	4	ASN
13	F	41	ASN
14	G	33	ASN
14	G	43	ASN
14	G	118	GLN
8	c	37	GLN
8	c	181	ASN
9	j	139	HIS
10	d	94	HIS

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Mol	Chain	Res	Type
11	n	117	GLN
11	n	167	ASN
11	n	209	ASN
12	m	100	ASN
12	m	147	HIS
12	m	180	GLN
12	m	188	HIS
13	l	43	HIS
14	k	12	ASN
14	k	121	GLN
15	H	80	HIS
15	H	98	GLN
15	H	265	ASN
15	H	281	GLN
15	H	359	ASN
16	I	254	GLN
16	I	303	GLN
16	I	311	ASN
16	I	312	GLN
17	J	52	ASN
17	J	204	HIS
17	J	205	HIS
17	J	376	HIS
18	K	74	HIS
18	K	98	GLN
18	K	293	GLN
19	L	189	GLN
19	L	328	ASN
19	L	364	HIS
19	L	409	HIS
20	M	125	GLN
20	M	149	ASN
20	M	302	GLN
20	M	328	ASN
21	N	231	ASN
21	N	315	ASN
21	N	375	HIS
21	N	565	ASN
21	N	747	HIS
21	N	900	ASN
22	O	169	ASN
22	O	186	ASN

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Mol	Chain	Res	Type
22	O	229	ASN
22	O	282	GLN
22	O	283	HIS
22	O	343	GLN
22	O	354	GLN
23	P	78	GLN
23	P	86	HIS
23	P	88	GLN
23	P	195	GLN
23	P	263	HIS
23	P	288	ASN
23	P	296	GLN
23	P	348	HIS
23	P	349	ASN
24	Q	150	GLN
24	Q	178	HIS
24	Q	226	HIS
24	Q	247	HIS
24	Q	379	GLN
24	Q	392	GLN
24	Q	418	GLN
24	Q	420	ASN
25	R	73	ASN
25	R	378	ASN
26	S	20	HIS
26	S	32	GLN
26	S	135	ASN
26	S	159	ASN
26	S	172	ASN
26	S	207	ASN
26	S	227	ASN
26	S	311	GLN
26	S	321	GLN
26	S	347	HIS
26	S	369	GLN
26	S	437	ASN
26	S	450	ASN
26	S	470	GLN
26	S	488	GLN
27	T	37	ASN
27	T	84	GLN
27	T	112	ASN

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Mol	Chain	Res	Type
27	T	123	HIS
28	U	26	GLN
28	U	84	ASN
28	U	94	HIS
28	U	127	GLN
28	U	302	GLN
29	V	133	ASN
29	V	190	HIS
29	V	204	HIS
29	V	217	HIS
29	V	291	ASN
30	W	12	ASN
30	W	95	GLN
31	X	94	ASN
33	Z	247	GLN
33	Z	435	GLN
33	Z	577	GLN
33	Z	622	HIS
33	Z	824	ASN
33	Z	931	GLN
33	Z	958	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

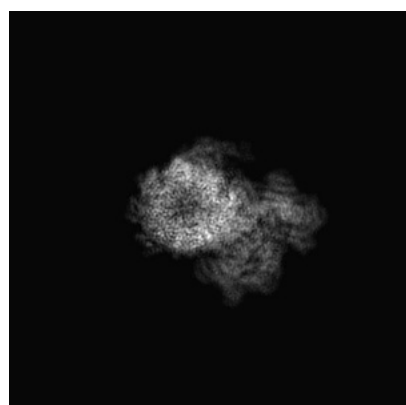
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9771. These allow visual inspection of the internal detail of the map and identification of artifacts.

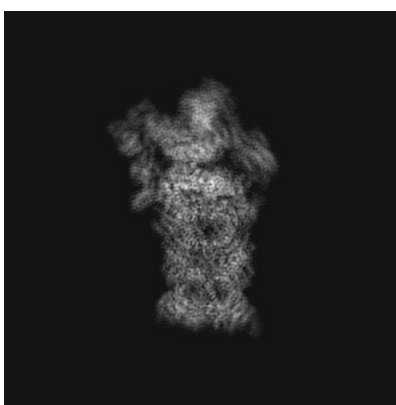
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

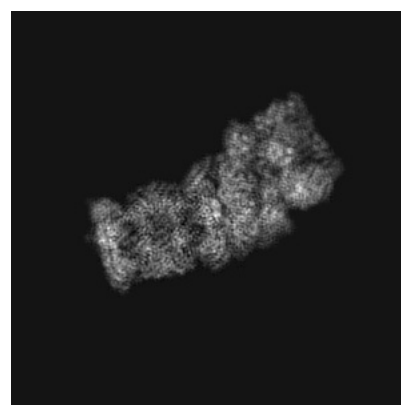
6.1.1 Primary map



X



Y

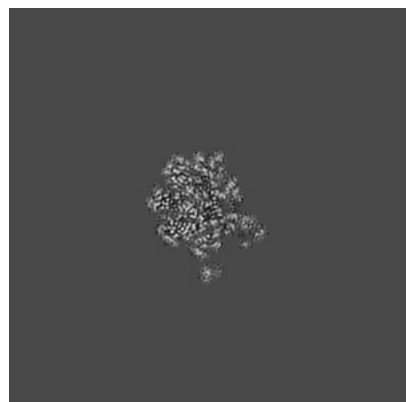


Z

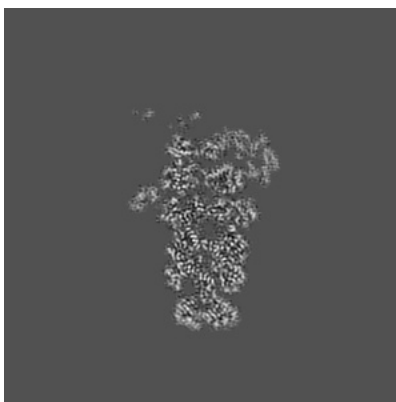
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

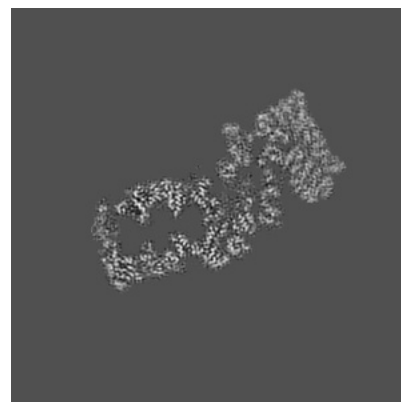
6.2.1 Primary map



X Index: 180



Y Index: 180

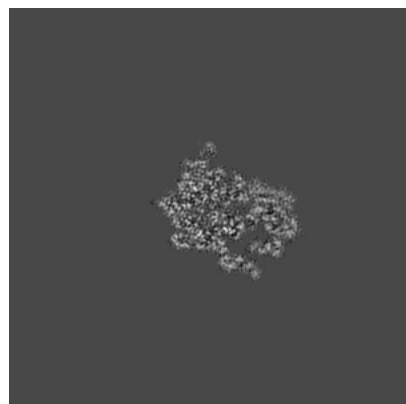


Z Index: 180

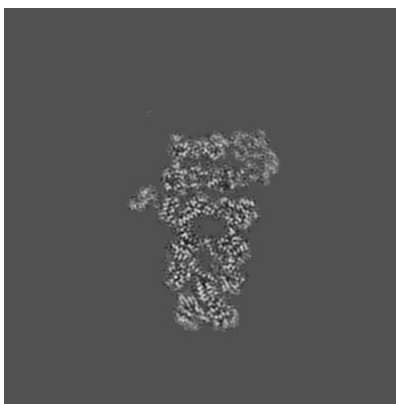
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

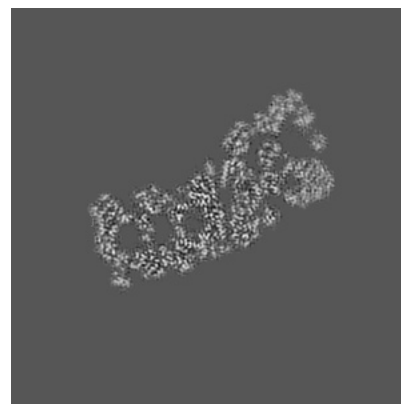
6.3.1 Primary map



X Index: 204



Y Index: 177

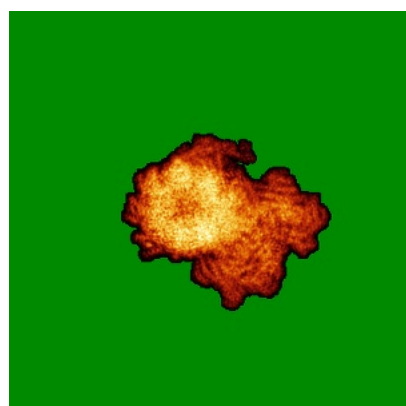


Z Index: 170

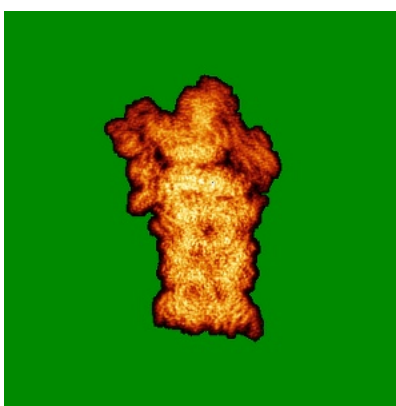
The images above show the largest variance slices of the map in three orthogonal directions.

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

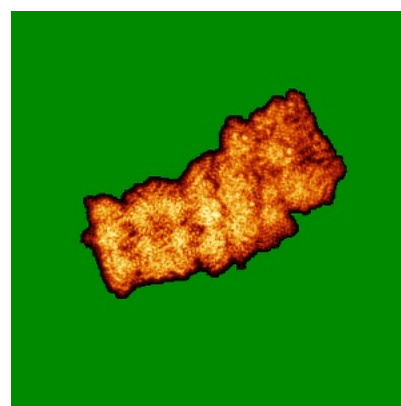
6.4.1 Primary map



X



Y

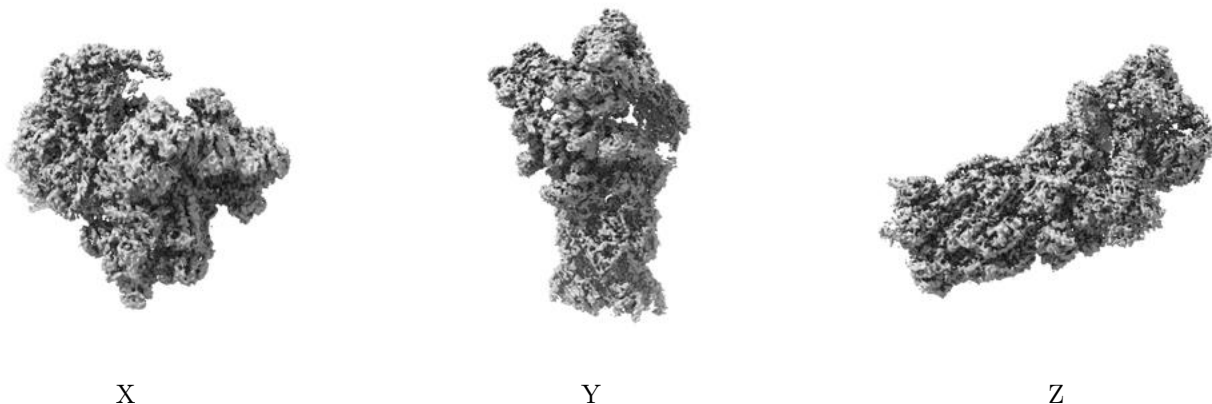


Z

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

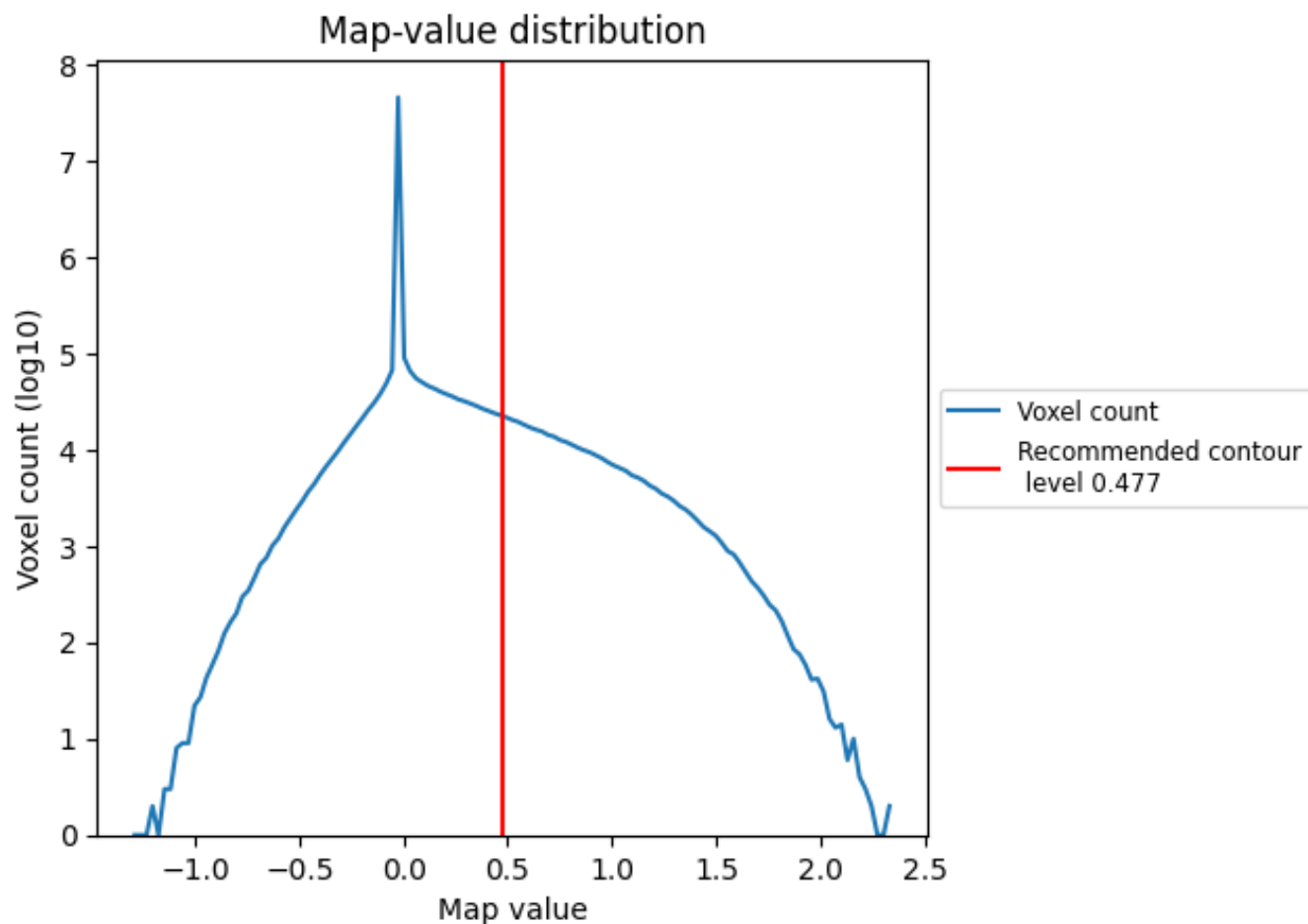
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

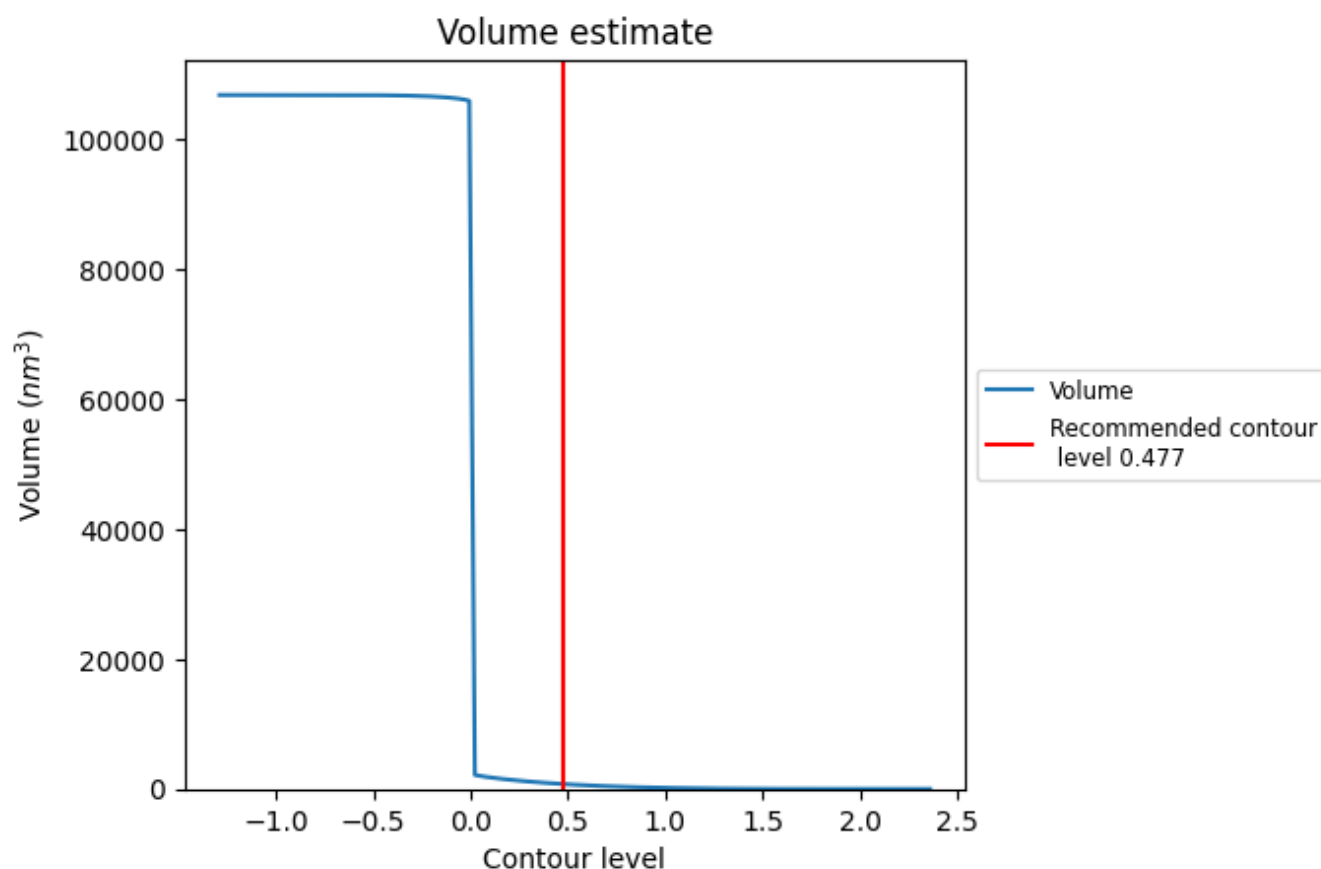
This section contains the results of statistical analysis of the map.

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.

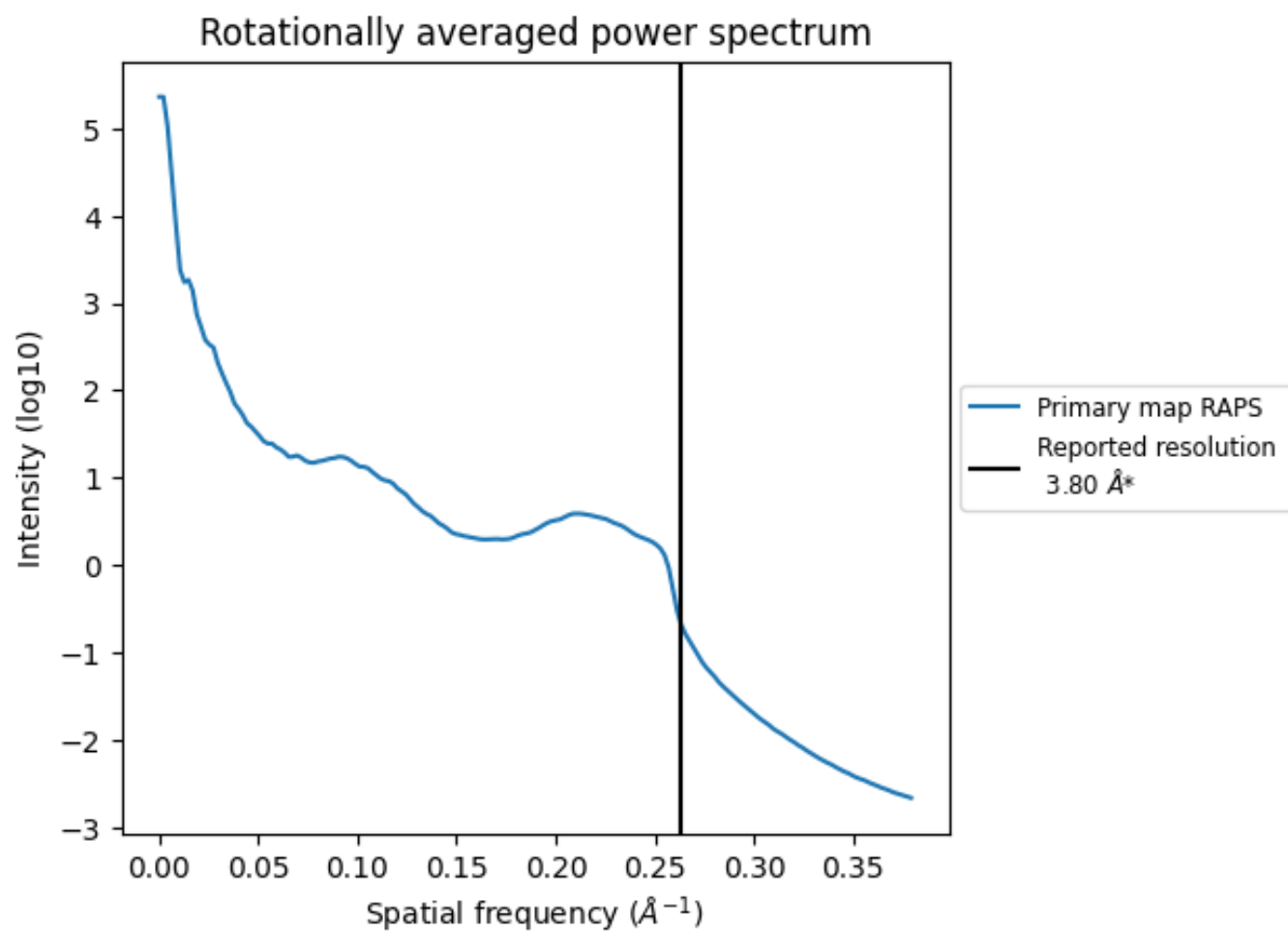
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 755 nm^3 ; this corresponds to an approximate mass of 682 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 0.263 Å⁻¹

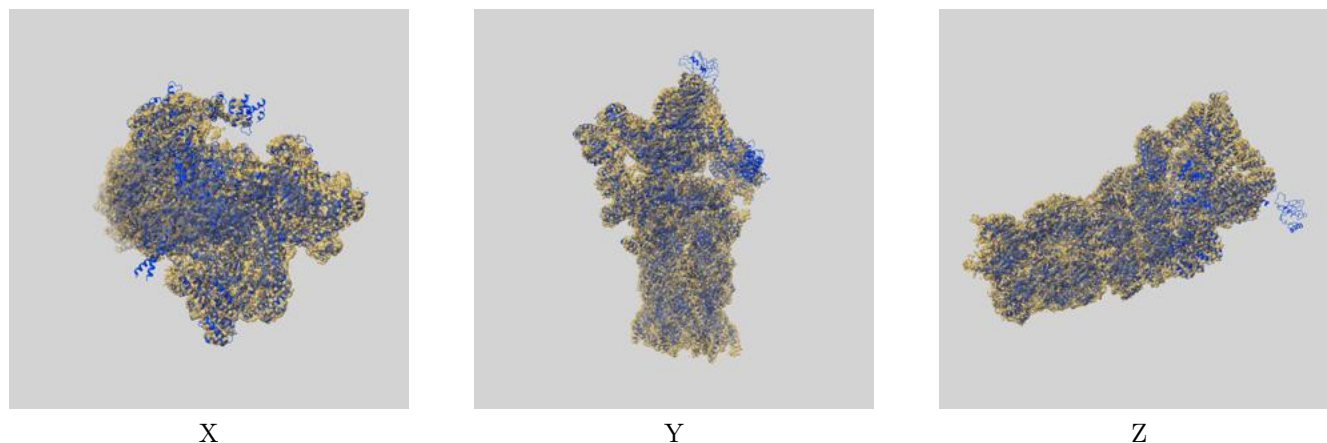
8 Fourier-Shell correlation ⓘ

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-9771 and PDB model 6J2Q. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



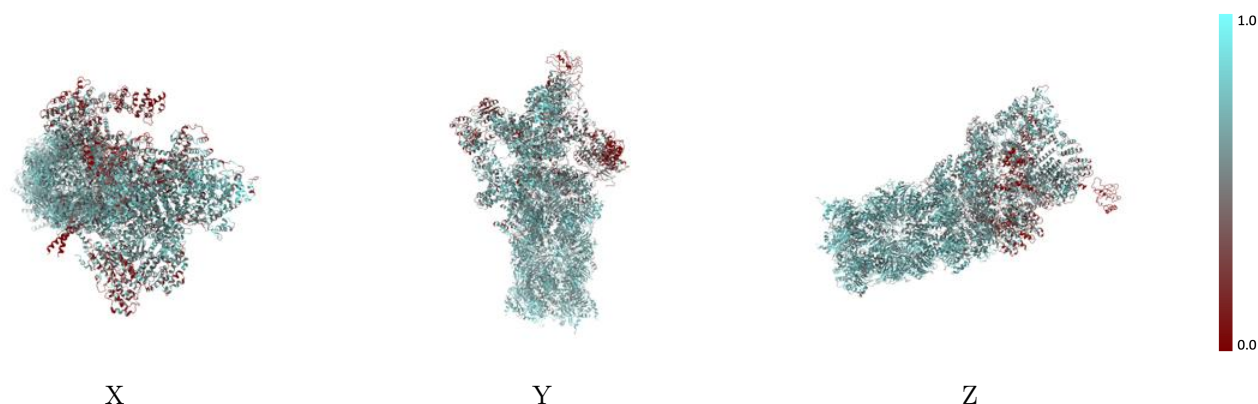
The images above show the 3D surface view of the map at the recommended contour level 0.477 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



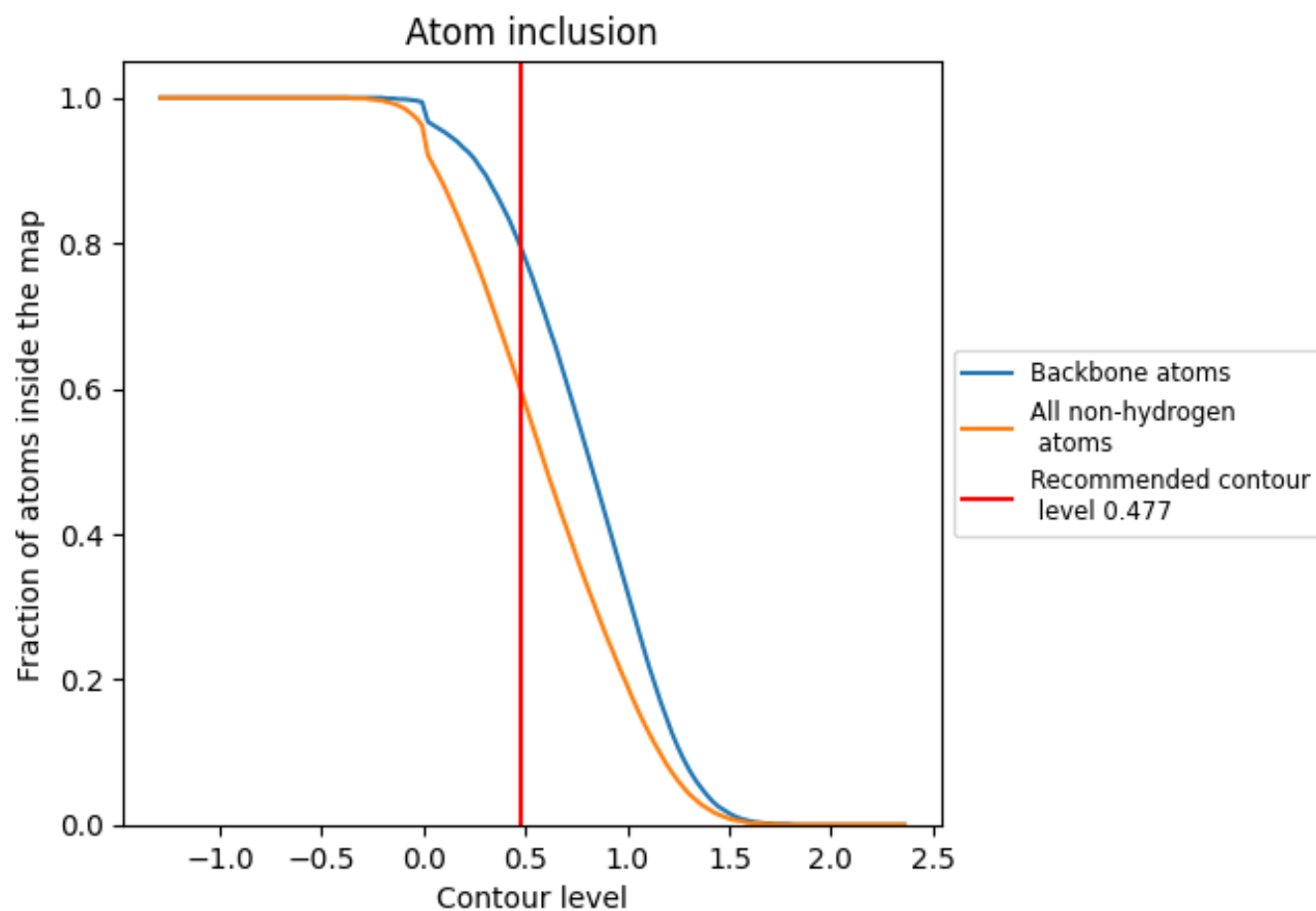
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.477).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 60% 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 (0.477) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5990	 0.2640
1	 0.6820	 0.3770
2	 0.7030	 0.3890
3	 0.6920	 0.3750
4	 0.6540	 0.3380
5	 0.7170	 0.3640
6	 0.6950	 0.3630
7	 0.7050	 0.3920
A	 0.6840	 0.3760
B	 0.6880	 0.3720
C	 0.6740	 0.3520
D	 0.7000	 0.3510
E	 0.6730	 0.3450
F	 0.6870	 0.3640
G	 0.6780	 0.3670
H	 0.5960	 0.2570
I	 0.5630	 0.2350
J	 0.5600	 0.2260
K	 0.5940	 0.2550
L	 0.5760	 0.2710
M	 0.5990	 0.2710
N	 0.5700	 0.1740
O	 0.4350	 0.1190
P	 0.5840	 0.1860
Q	 0.6100	 0.2300
R	 0.5740	 0.1730
S	 0.5350	 0.1470
T	 0.5700	 0.1630
U	 0.6080	 0.2170
V	 0.5640	 0.1920
W	 0.3270	 0.0820
X	 0.0000	 -0.0000
Y	 0.5090	 0.1080
Z	 0.2950	 0.0850
a	 0.6980	 0.3830



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Chain	Atom inclusion	Q-score
b	 0.6750	 0.3670
c	 0.6920	 0.3330
d	 0.6730	 0.3040
e	 0.6790	 0.3620
f	 0.7040	 0.3770
g	 0.6780	 0.3430
h	 0.6950	 0.3750
i	 0.6940	 0.3730
j	 0.6760	 0.3430
k	 0.7170	 0.3360
l	 0.7070	 0.3380
m	 0.6650	 0.3260
n	 0.6930	 0.3070