



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:56 AM UTC

PDB ID : 5VFP / pdb_00005vfp
EMDB ID : EMD-8663
Title : Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome
Authors : Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.
Deposited on : 2017-04-09
Resolution : 4.20 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:

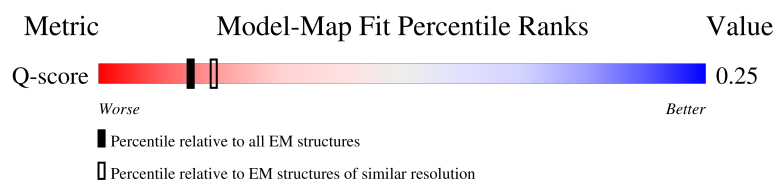
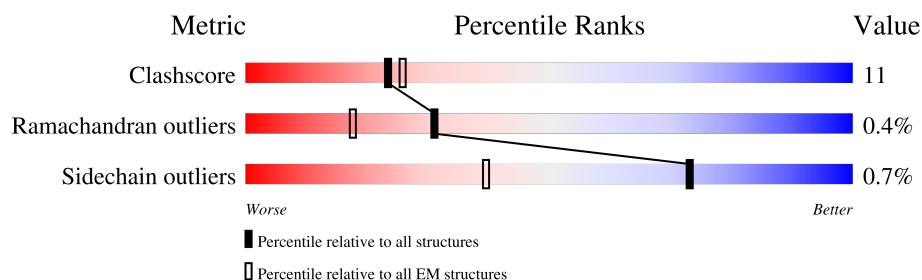
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.20 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	5410 (3.70 - 4.70)

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	G	240	25% 85% 14% .
1	g	240	40% 83% 16%
2	H	232	26% 76% 23% .
2	h	232	42% 82% 18%

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Mol	Chain	Length	Quality of chain
3	I	250	
3	i	250	
4	J	243	
4	j	243	
5	K	234	
5	k	234	
6	L	238	
6	l	238	
7	M	245	
7	m	245	
8	N	191	
8	n	191	
9	O	220	
9	o	220	
10	P	204	
10	p	204	
11	Q	199	
11	q	199	
12	R	201	
12	r	201	
13	S	213	
13	s	213	
14	T	215	
14	t	215	
15	U	911	

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Mol	Chain	Length	Quality of chain
16	V	480	81% 64% 33% ..
17	W	456	74% 65% 35% .
18	Y	378	63% 68% 31% .
19	Z	286	72% 75% 23% .
20	a	373	80% 68% 31% .
21	b	191	87% 69% 30% ..
22	c	287	63% 69% 27% ..
23	d	257	90% 68% 31% .
24	e	70	51% 30% 27% 43%
25	X	380	72% 77% 22% .
26	A	399	58% 71% 24% . 5%
27	B	389	71% 75% 20% 5%
28	C	392	67% 73% 19% . 7%
29	D	380	72% 73% 26% .
30	E	375	61% 81% 19%
31	F	396	56% 75% 19% . 5%
32	f	908	68% 40% 33% . 24%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	AGS	E	401	-	-	X	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 101342 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 alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
1	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	230	Total	C	N	O	S	0	0
			1688	1070	284	329	5		
2	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
3	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
4	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	228	Total	C	N	O	S	0	0
			1729	1086	284	349	10		
5	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
6	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
7	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
8	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
9	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
11	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
12	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
13	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
14	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	473	Total	C	N	O	S	0	0
			3808	2418	676	700	14		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 24 is a protein called sem1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	380	Total	C	N	O	S	0	0
			2893	1817	515	543	18		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	370	Total	C	N	O	S	0	0
			2806	1763	478	553	12		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	363	Total	C	N	O	S	0	0
			2859	1804	513	525	17		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	376	Total	C	N	O	S	0	0
			2859	1802	496	546	15		

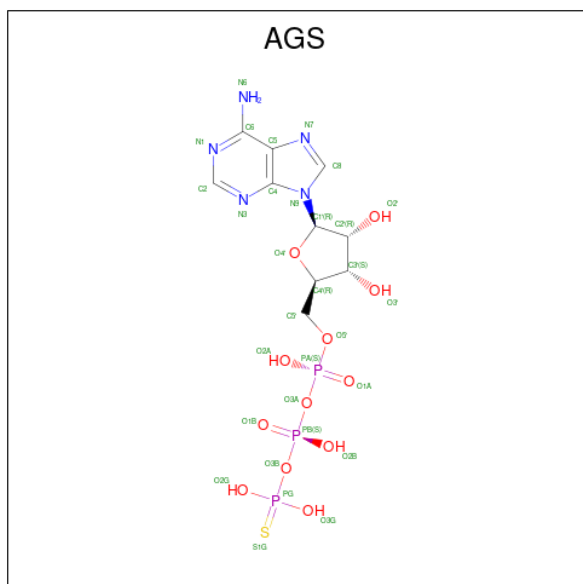
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	689	Total	C	N	O	S	0	0
			5319	3343	904	1037	35		

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	c	1	Total	Zn	0
			1	1	

- Molecule 34 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



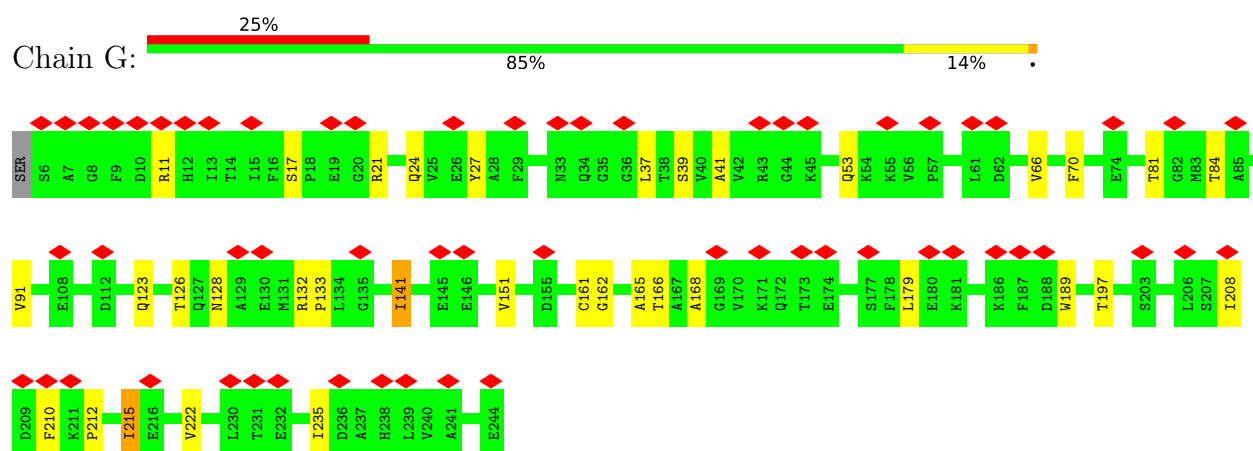
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Mol	Chain	Residues	Atoms						AltConf
34	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

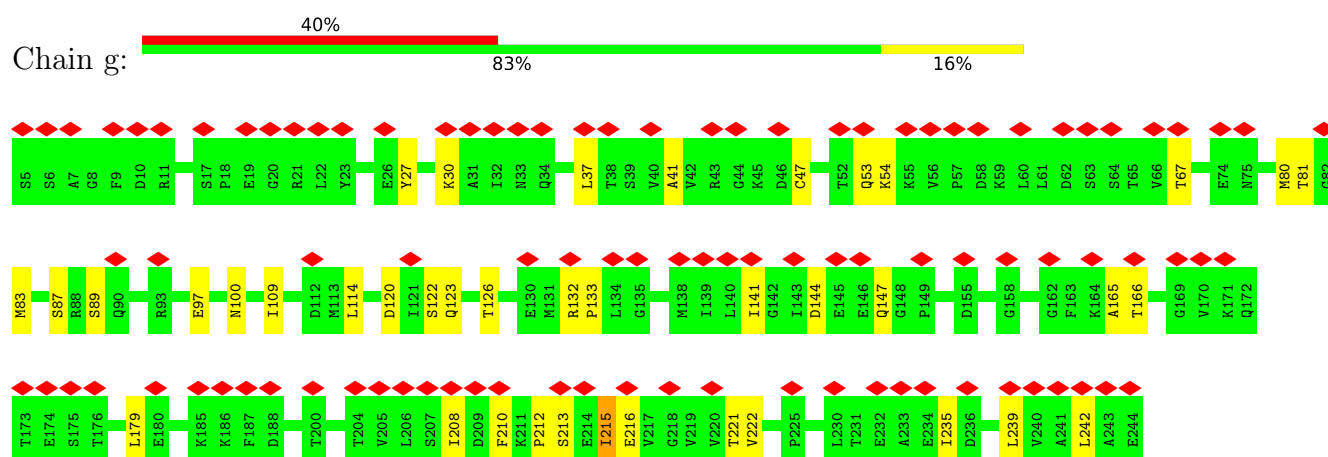
3 Residue-property plots [i](#)

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

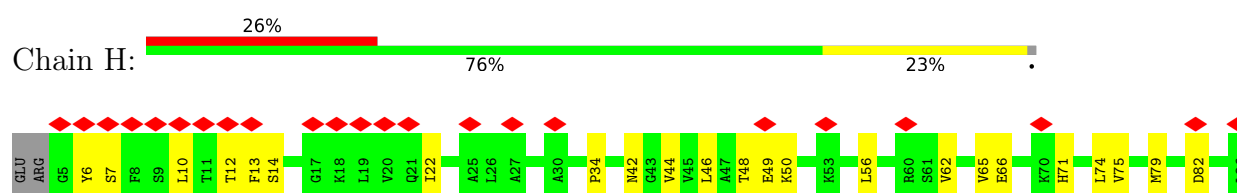
- Molecule 1: Proteasome subunit alpha type-6

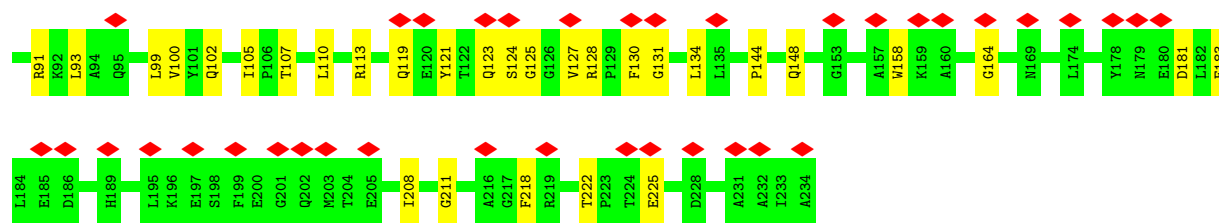


- Molecule 1: Proteasome subunit alpha type-6

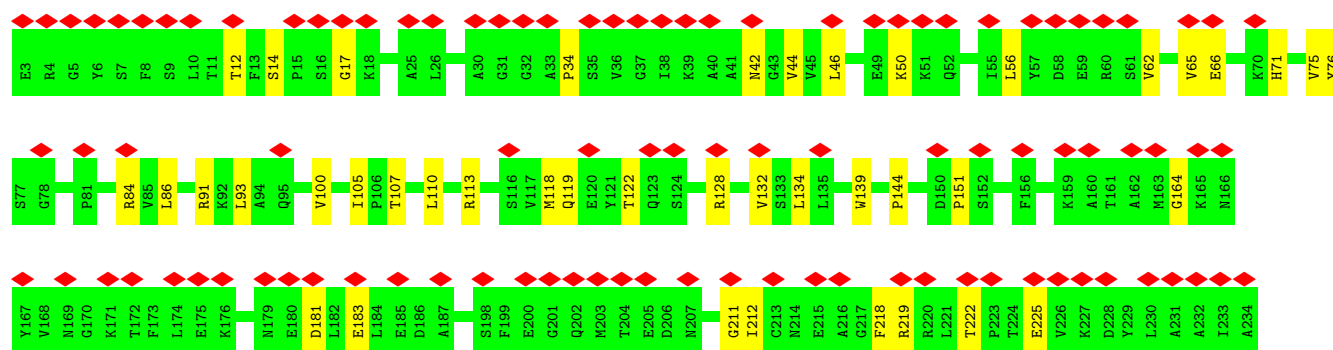
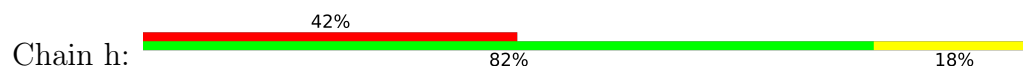


- Molecule 2: Proteasome subunit alpha type-2

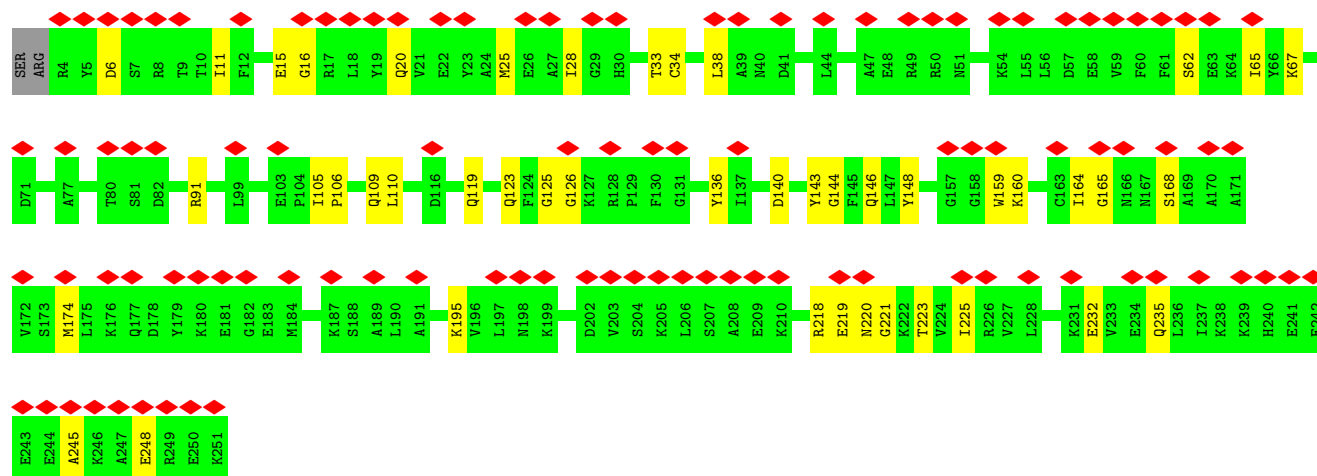
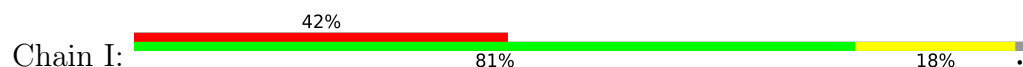




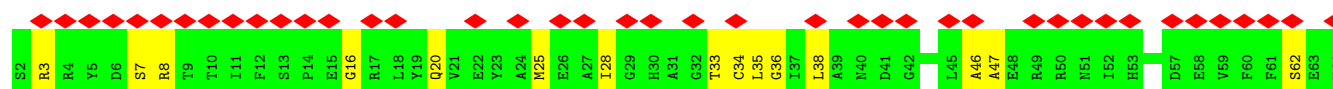
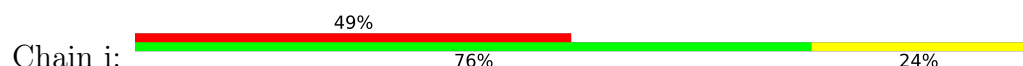
• Molecule 2: Proteasome subunit alpha type-2

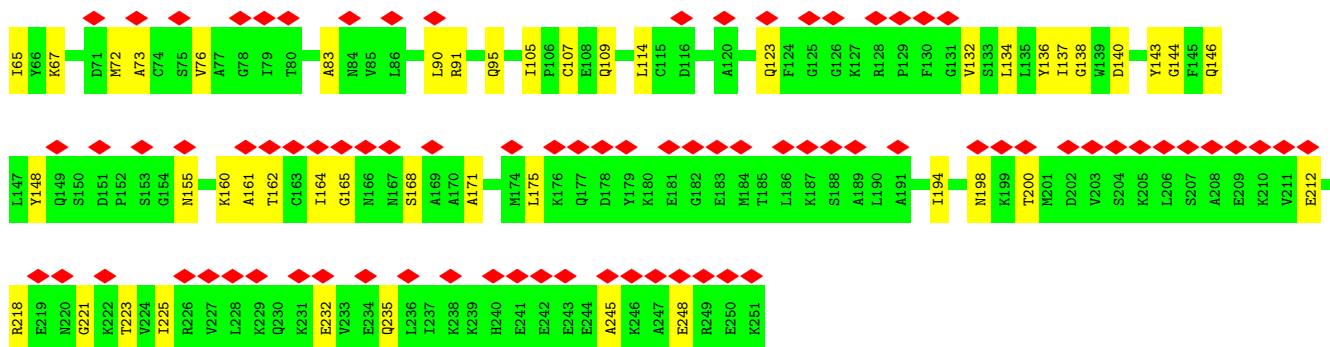


• Molecule 3: Proteasome subunit alpha type-4

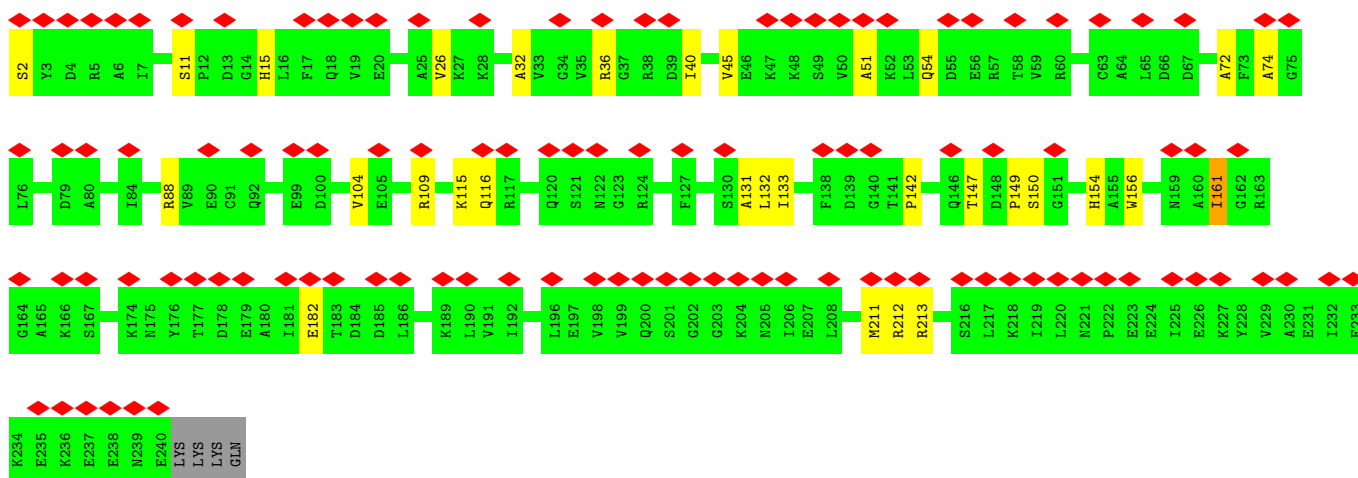
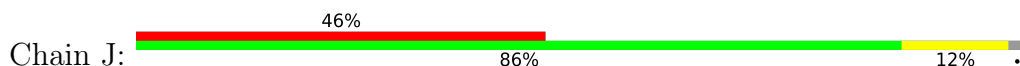


• Molecule 3: Proteasome subunit alpha type-4

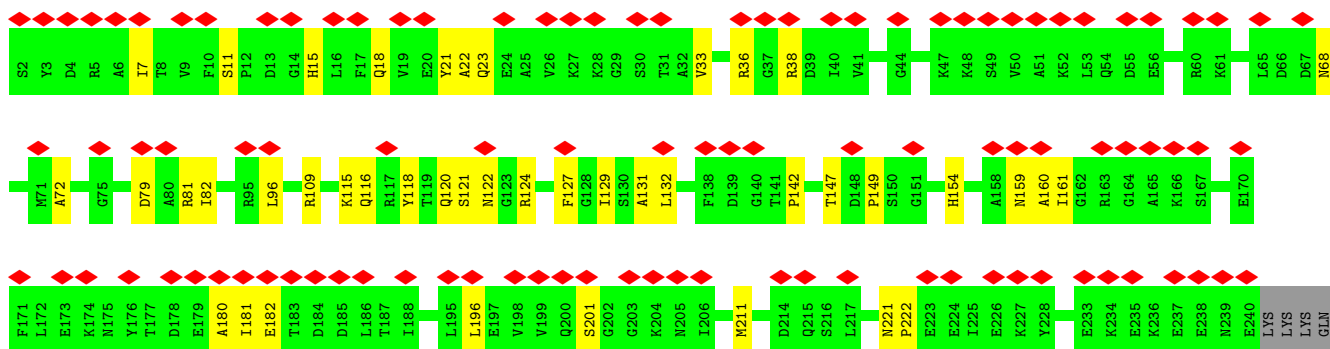
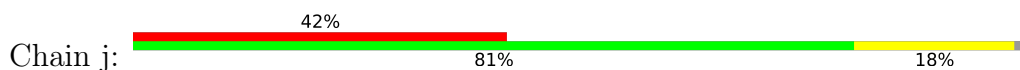




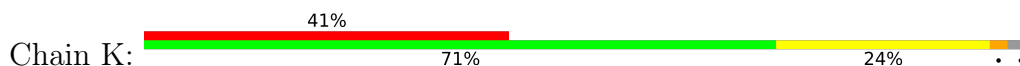
• Molecule 4: Proteasome subunit alpha type-7

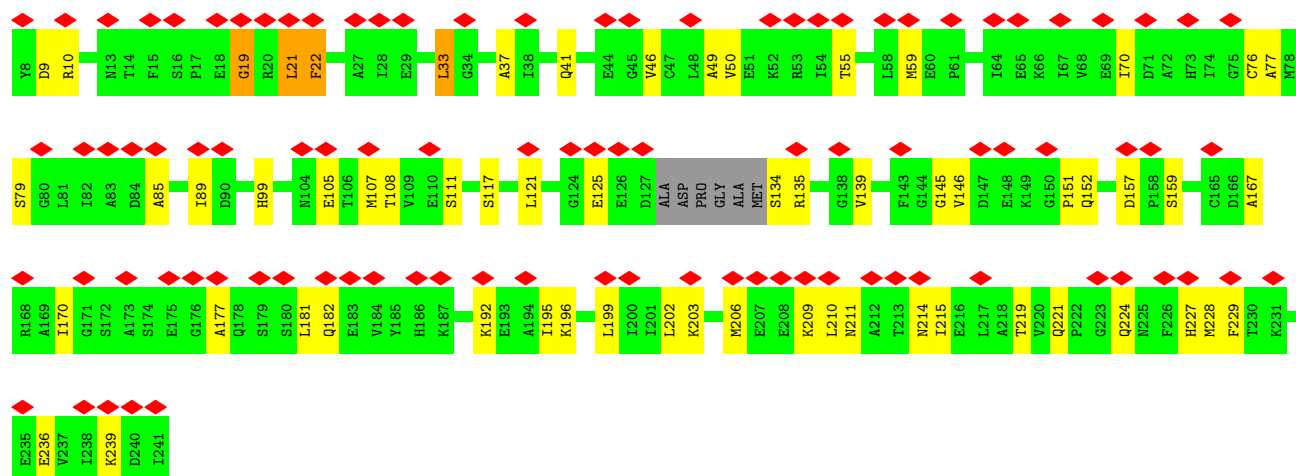


• Molecule 4: Proteasome subunit alpha type-7

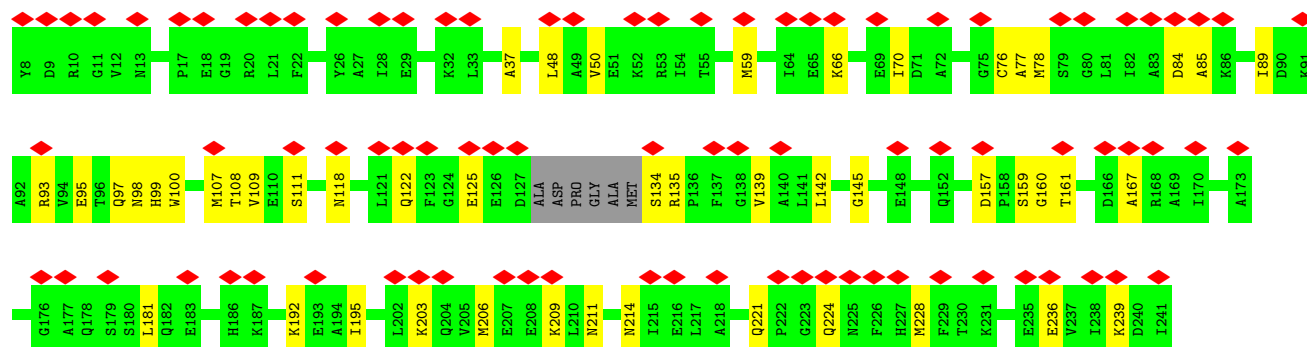
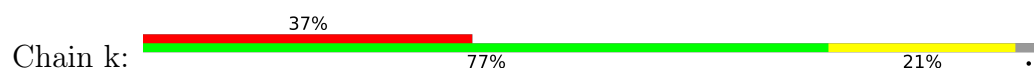


• Molecule 5: Proteasome subunit alpha type-5

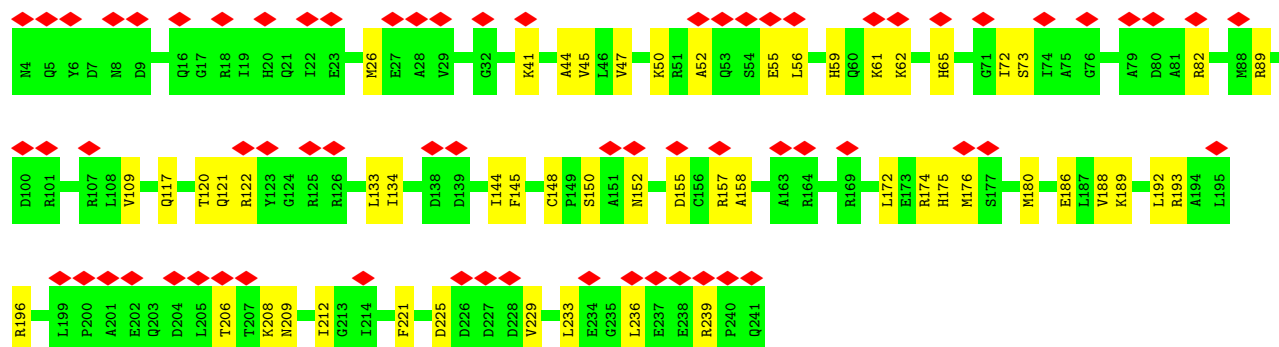
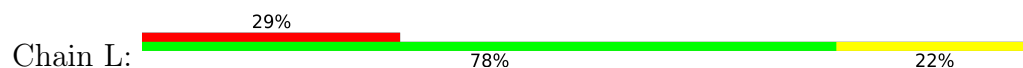




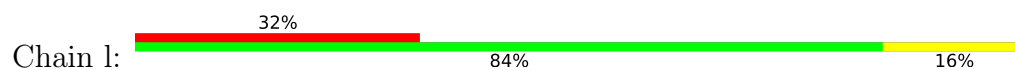
- Molecule 5: Proteasome subunit alpha type-5

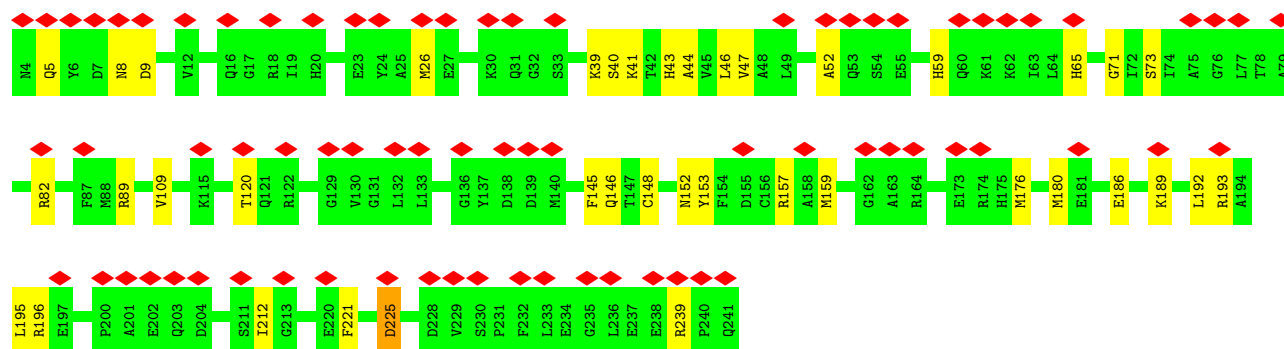


- Molecule 6: Proteasome subunit alpha type-1

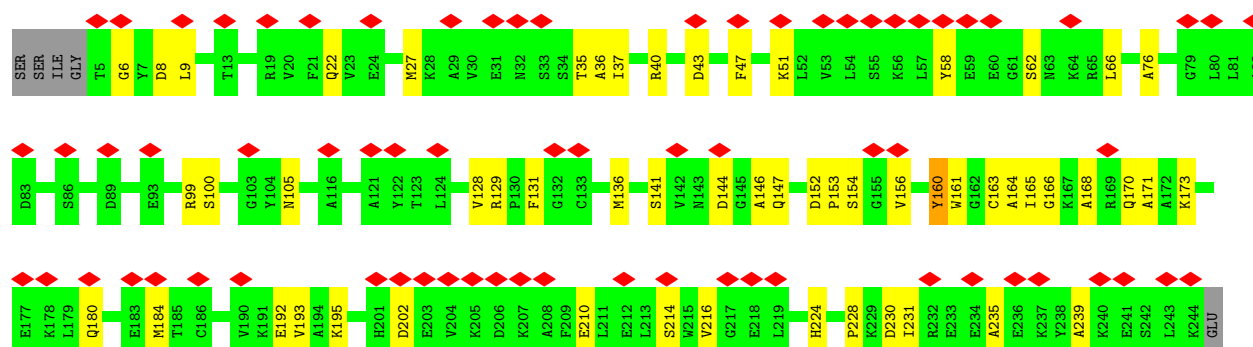
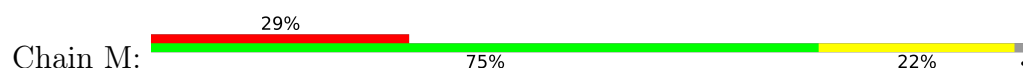


- Molecule 6: Proteasome subunit alpha type-1

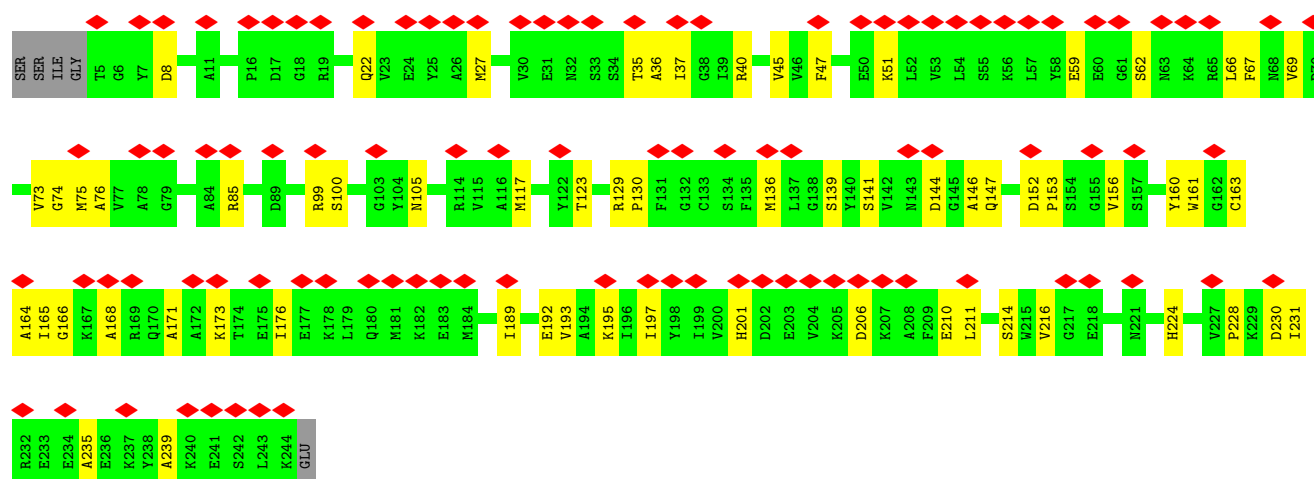
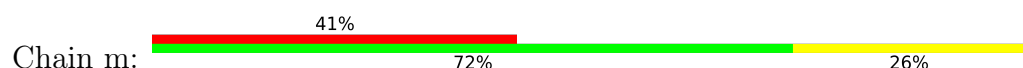




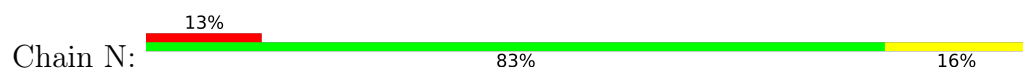
• Molecule 7: Proteasome subunit alpha type-3

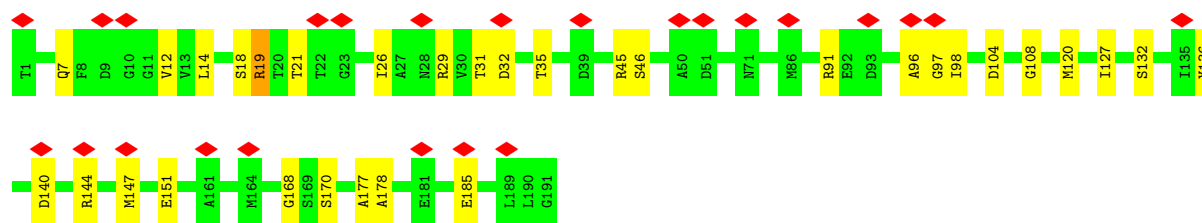


• Molecule 7: Proteasome subunit alpha type-3

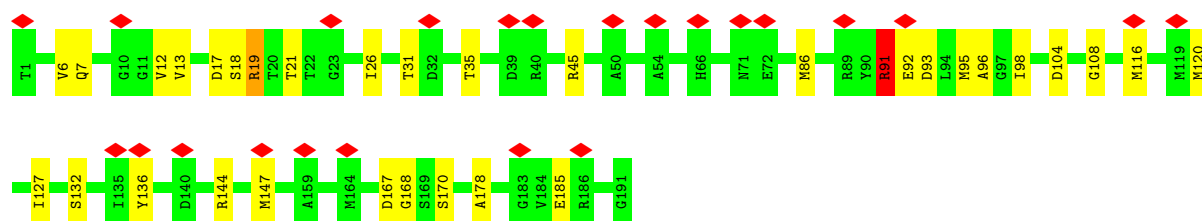
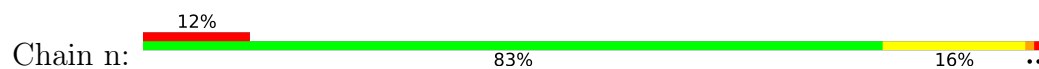


• Molecule 8: Proteasome subunit beta type-6

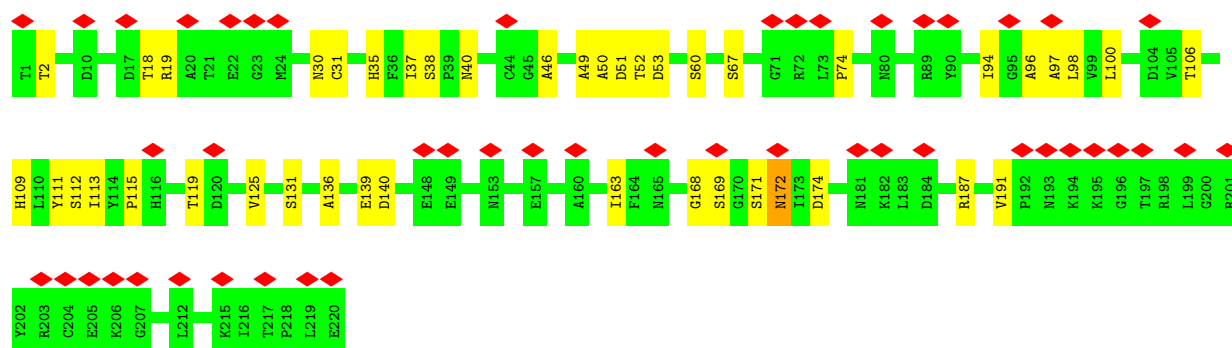
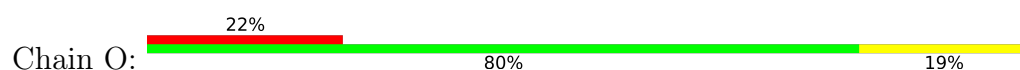




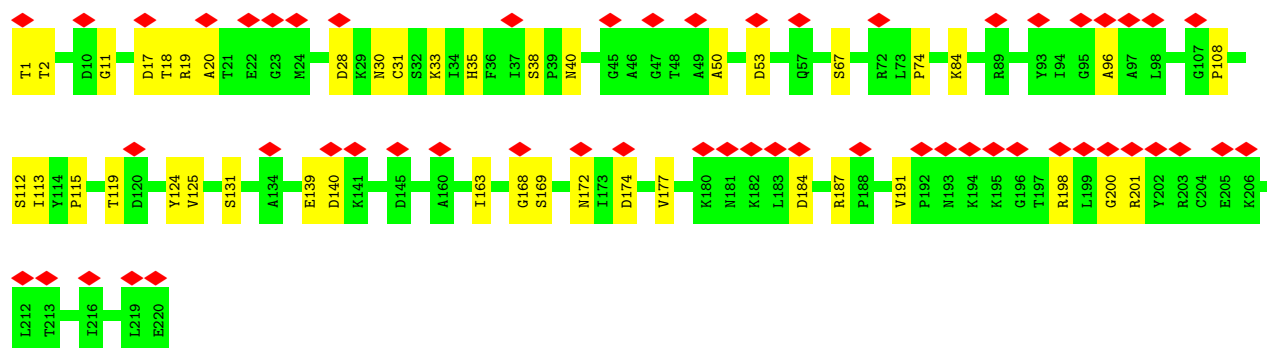
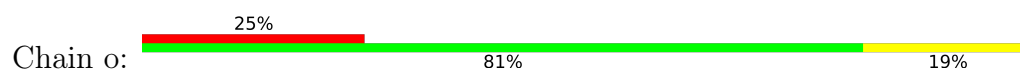
• Molecule 8: Proteasome subunit beta type-6



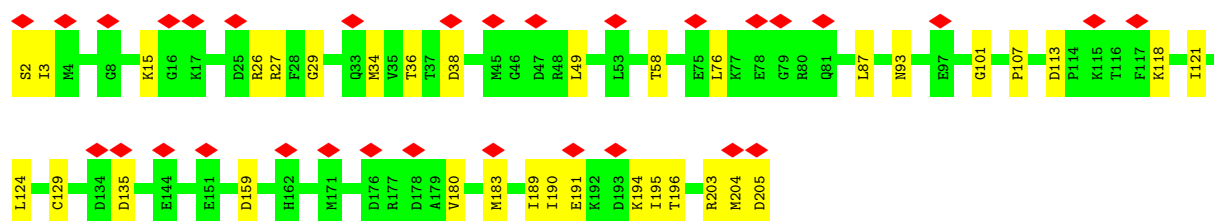
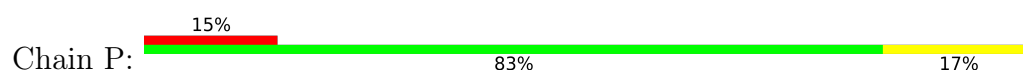
• Molecule 9: Proteasome subunit beta type-7



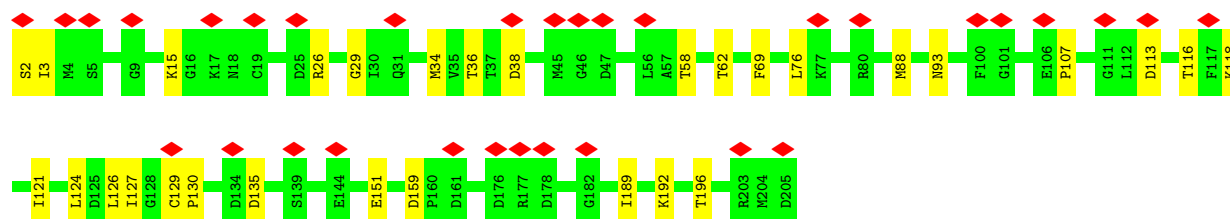
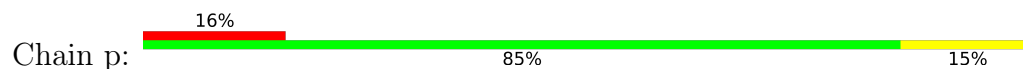
• Molecule 9: Proteasome subunit beta type-7



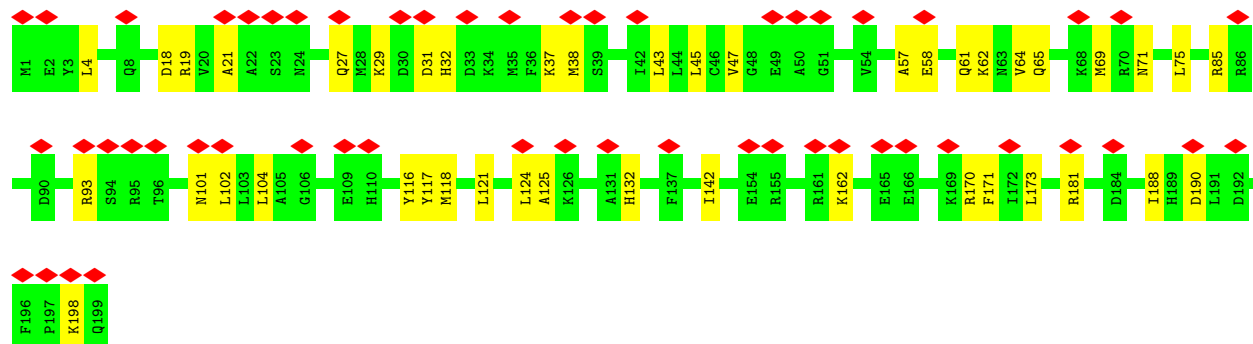
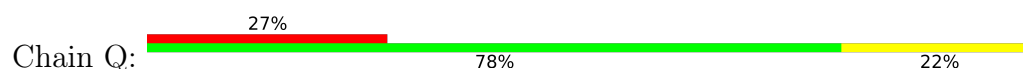
• Molecule 10: Proteasome subunit beta type-3



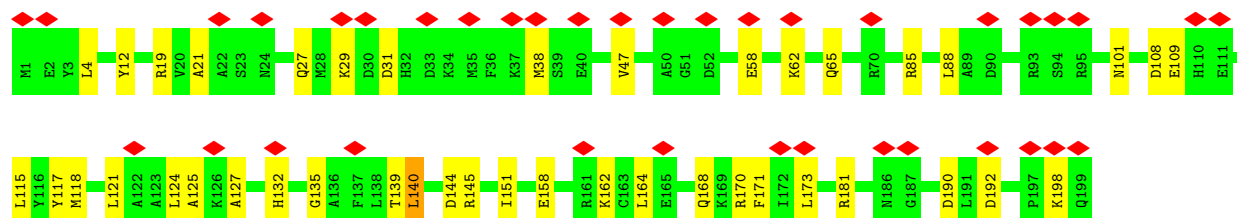
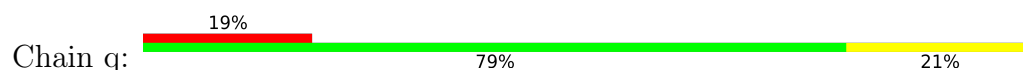
• Molecule 10: Proteasome subunit beta type-3



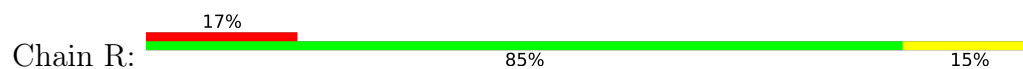
• Molecule 11: Proteasome subunit beta type-2

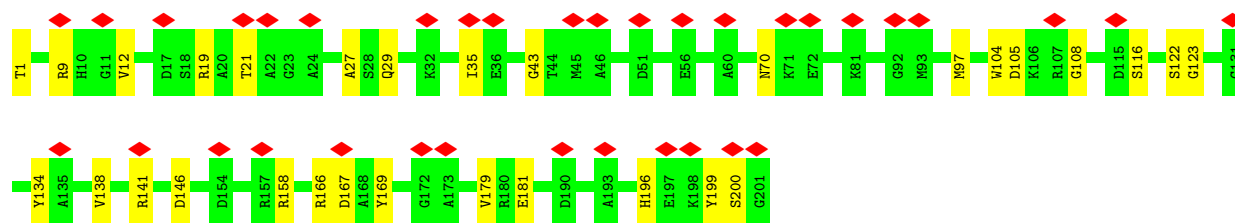


• Molecule 11: Proteasome subunit beta type-2

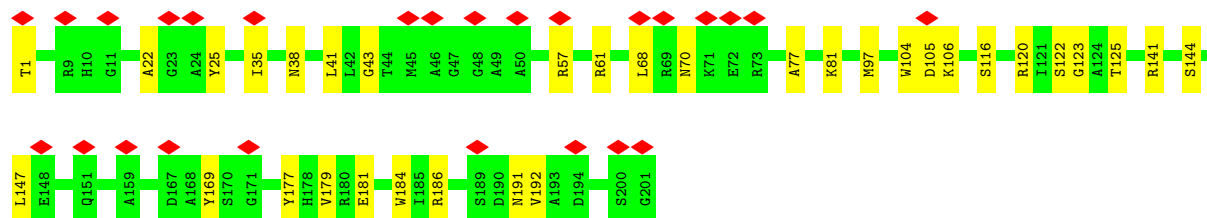
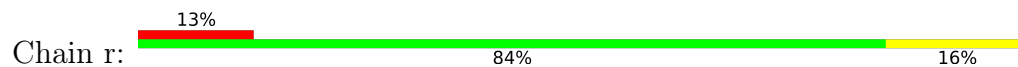


• Molecule 12: Proteasome subunit beta type-5

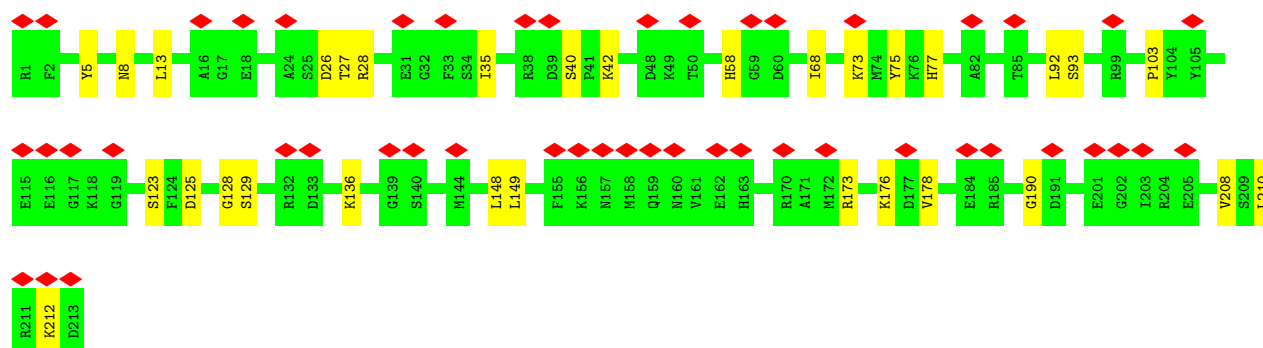
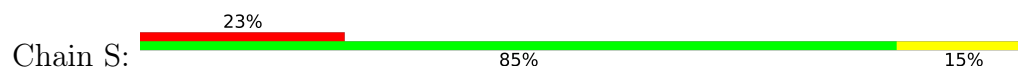




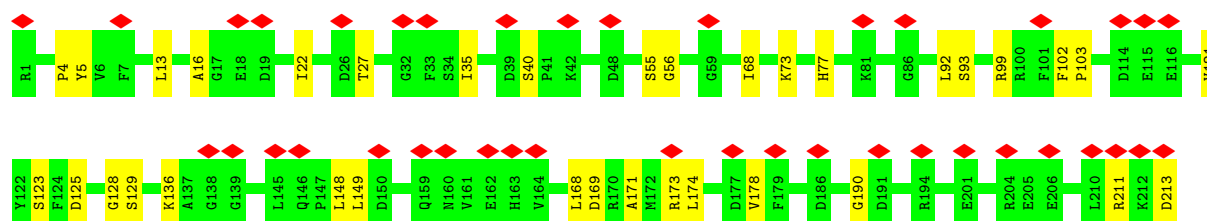
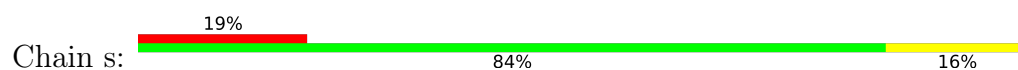
- Molecule 12: Proteasome subunit beta type-5



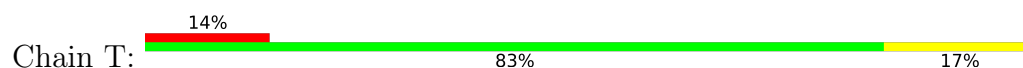
- Molecule 13: Proteasome subunit beta type-1

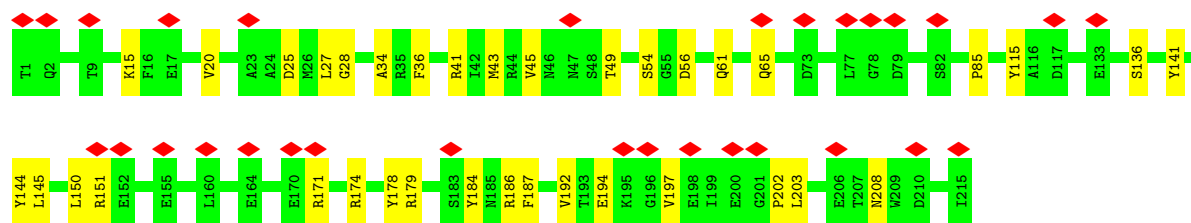


- Molecule 13: Proteasome subunit beta type-1

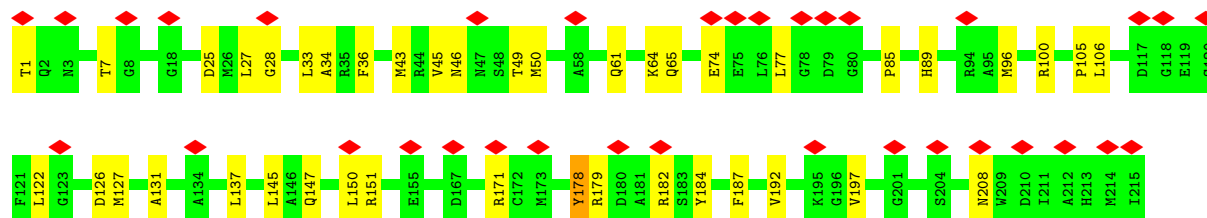
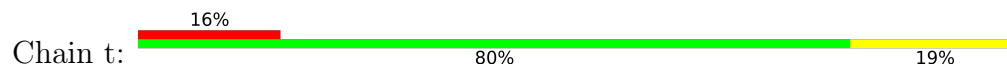


- Molecule 14: Proteasome subunit beta type-4

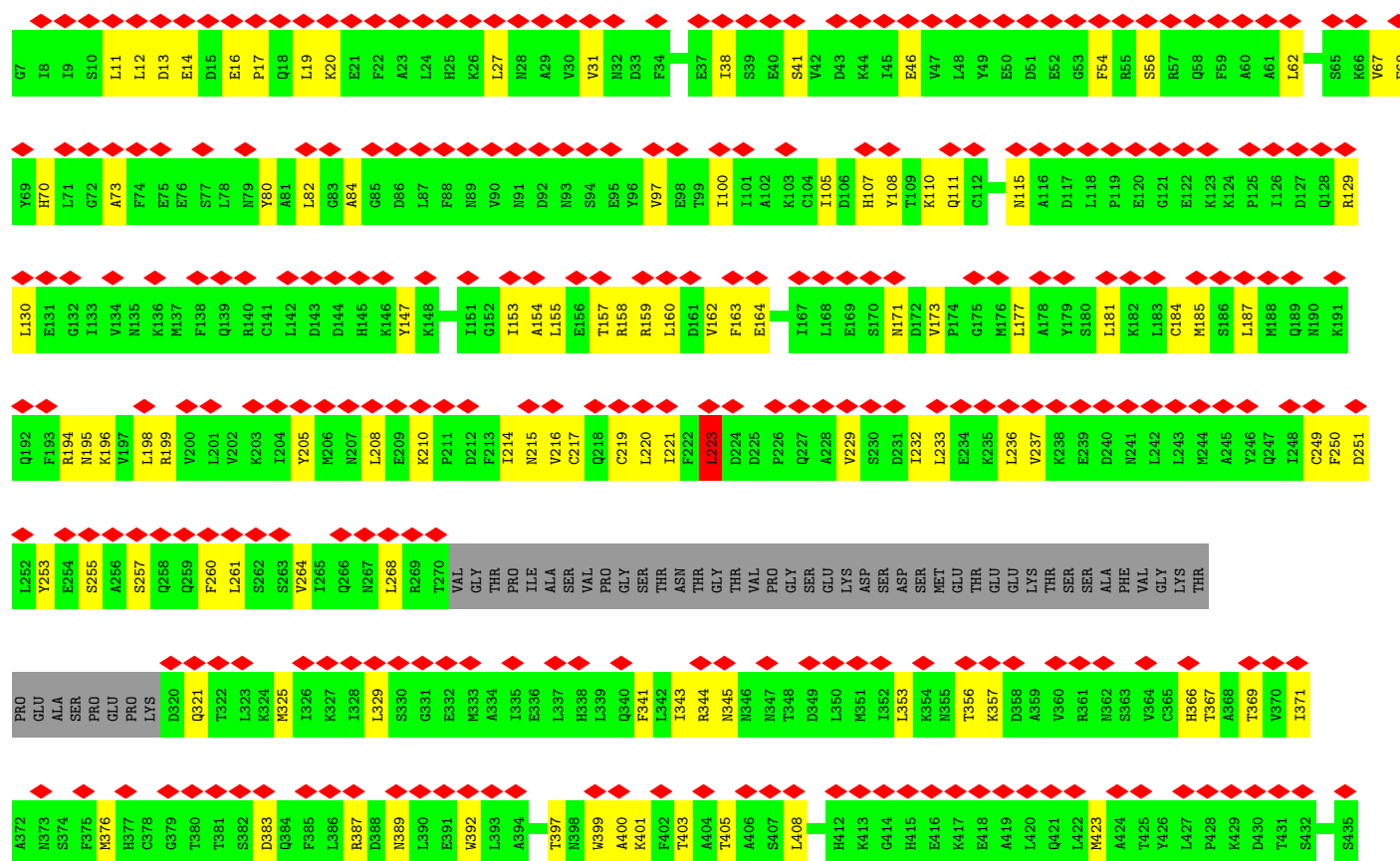


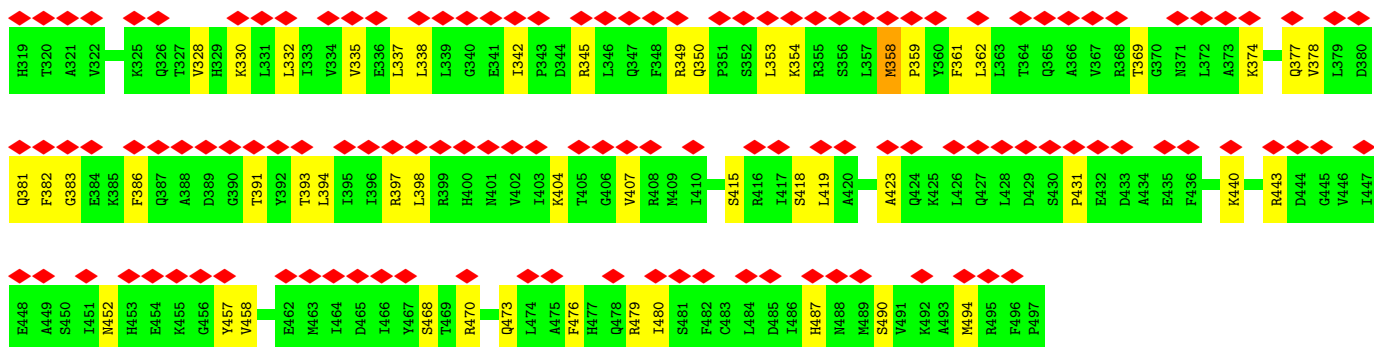


• Molecule 14: Proteasome subunit beta type-4

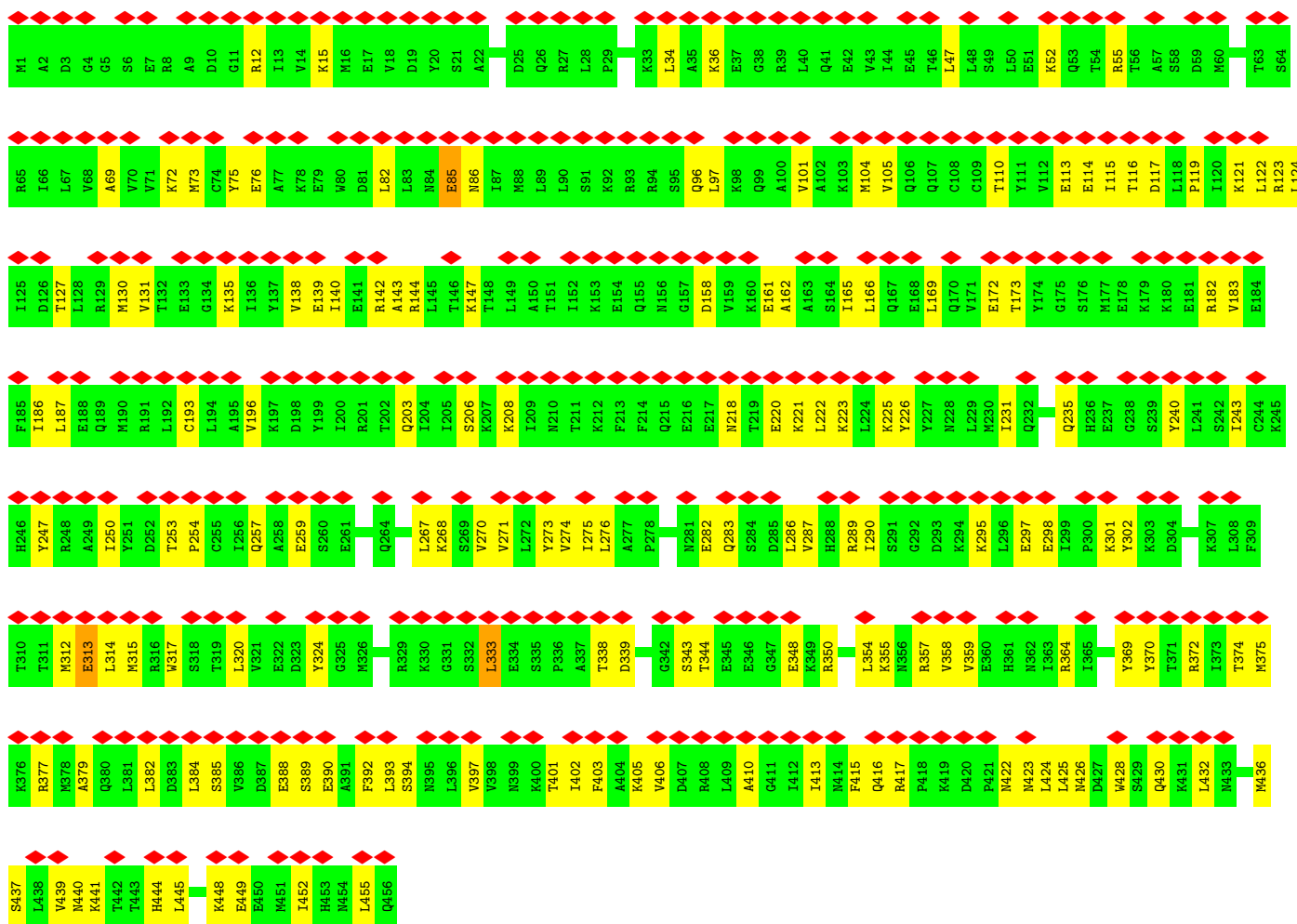
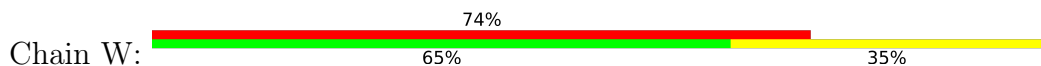


• Molecule 15: 26S proteasome non-ATPase regulatory subunit 1



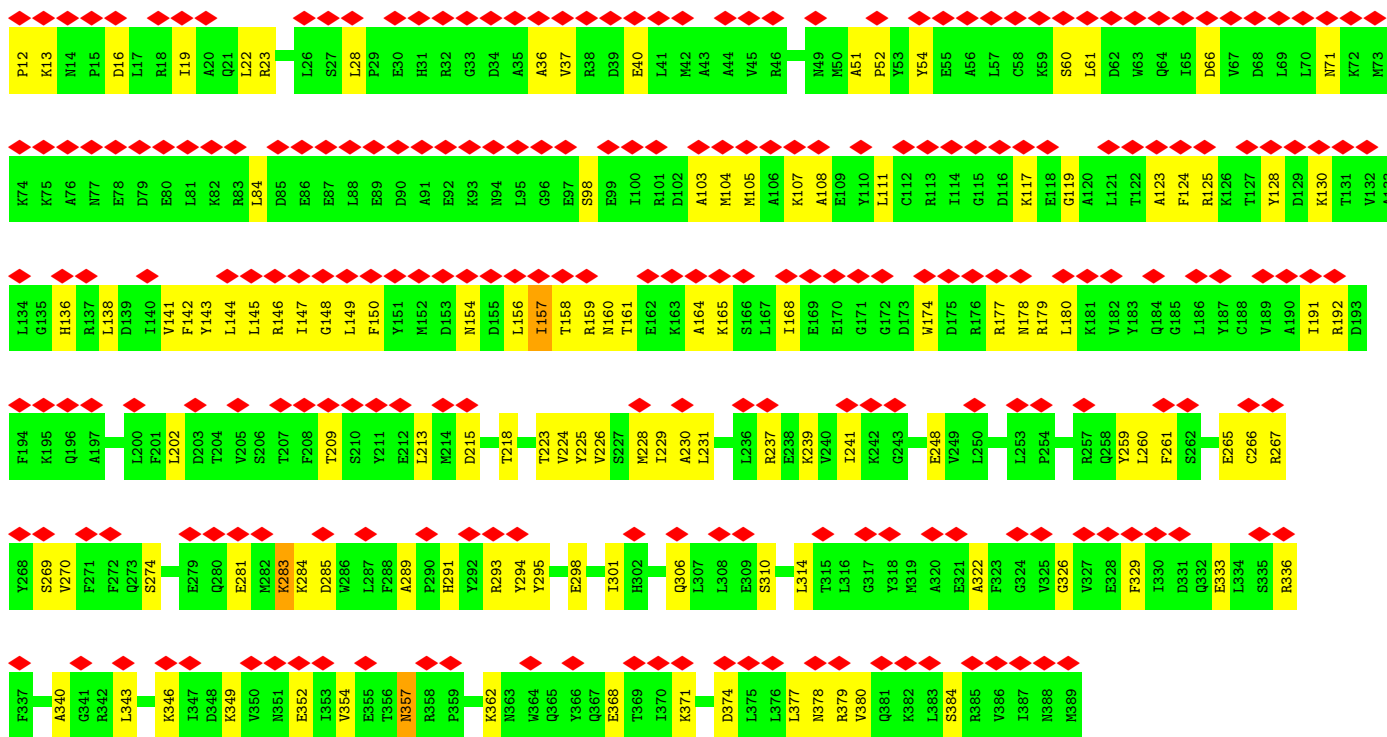


• Molecule 17: 26S proteasome non-ATPase regulatory subunit 12



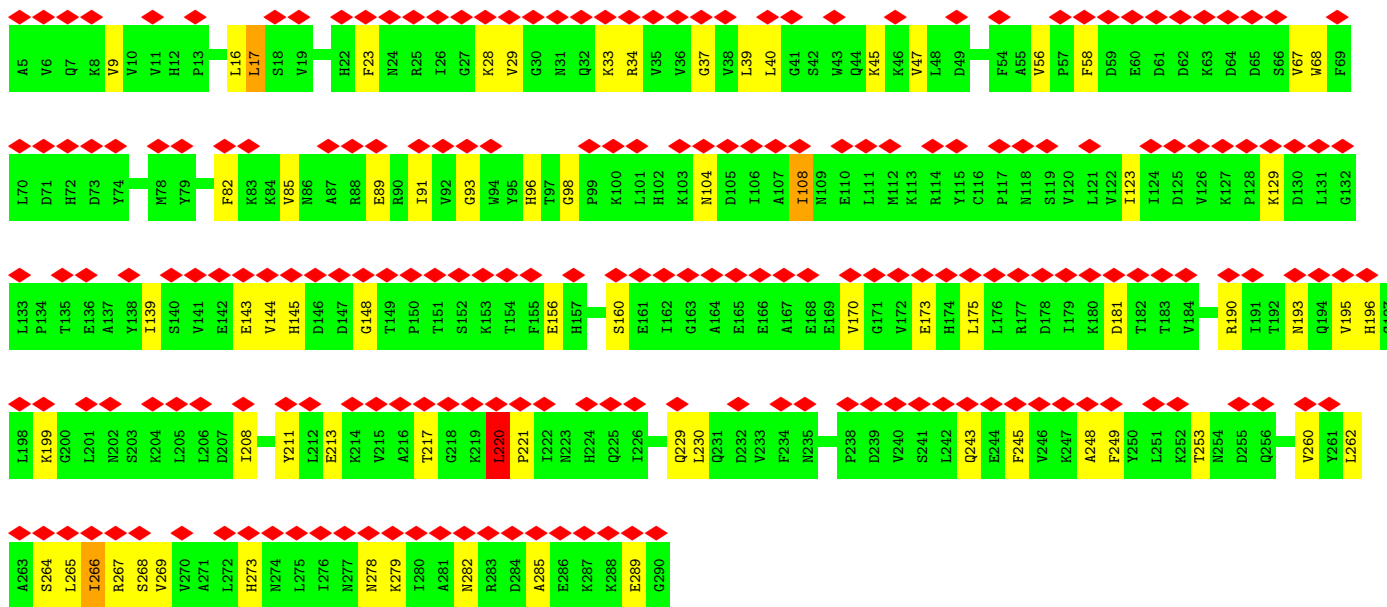
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 6





• Molecule 19: 26S proteasome non-ATPase regulatory subunit 7

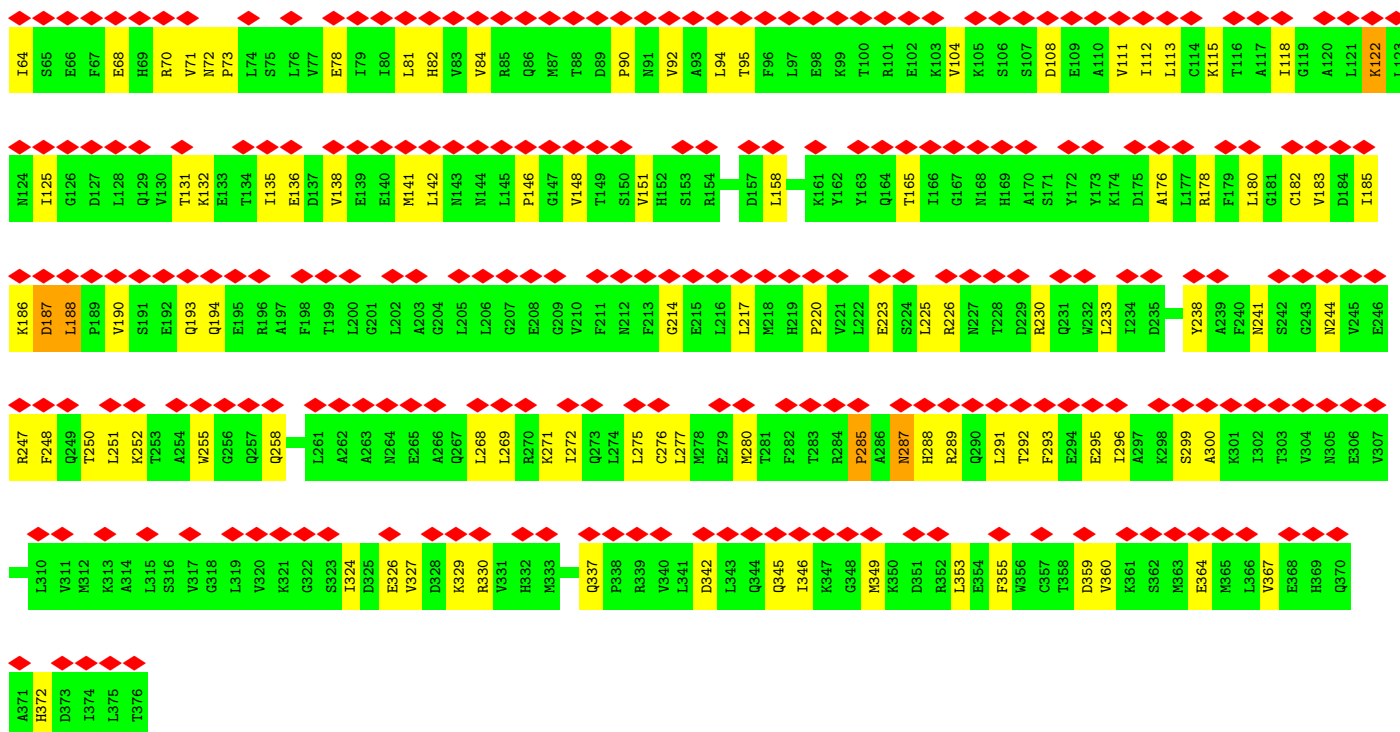
Chain Z: .



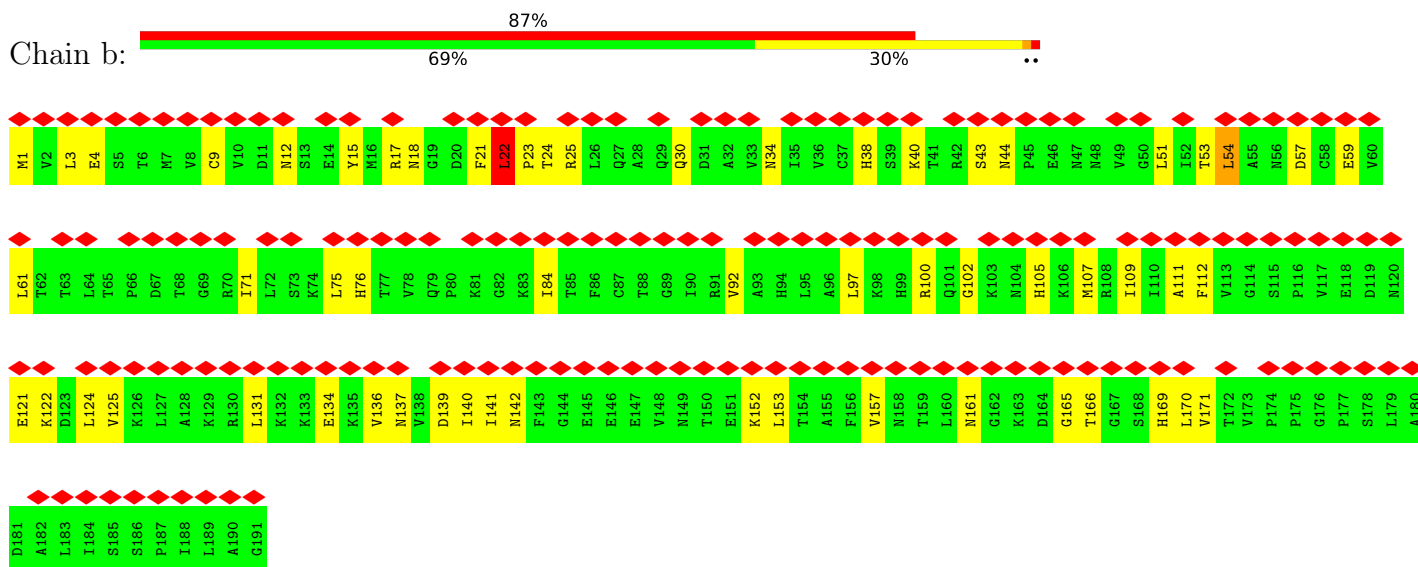
• Molecule 20: 26S proteasome non-ATPase regulatory subunit 13

Chain a: .

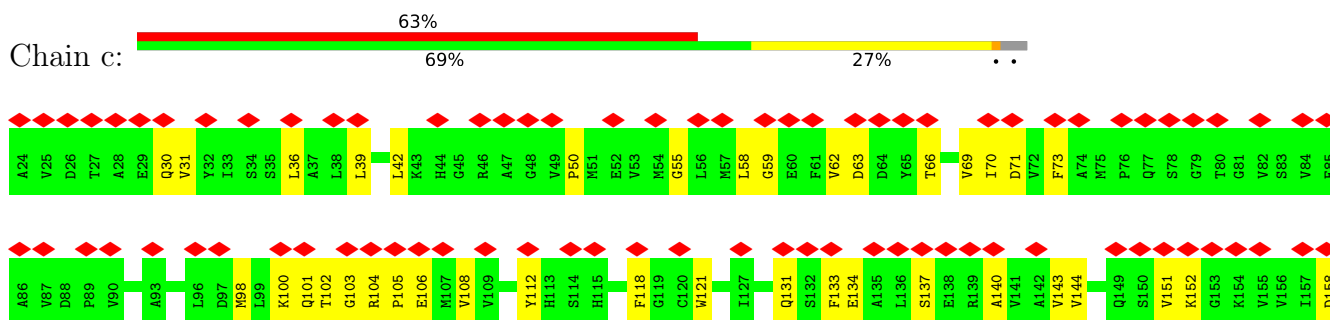


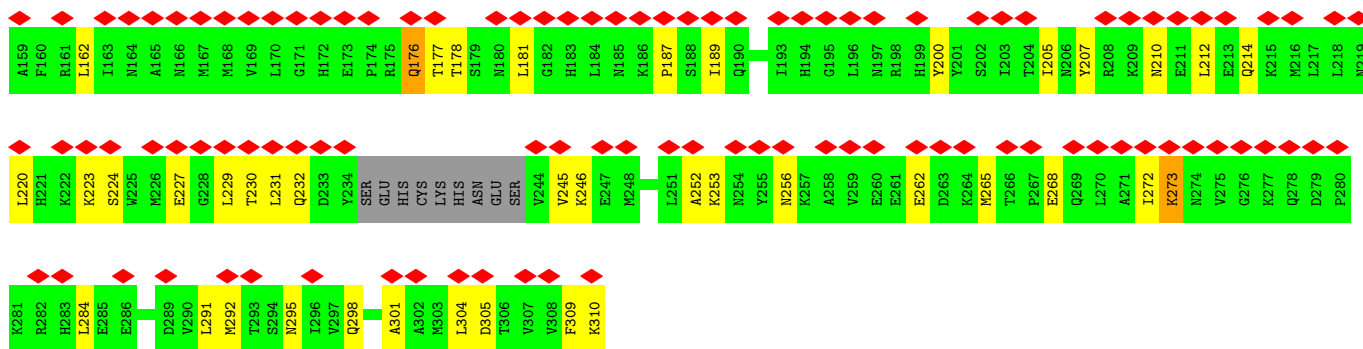


• Molecule 21: 26S proteasome non-ATPase regulatory subunit 4

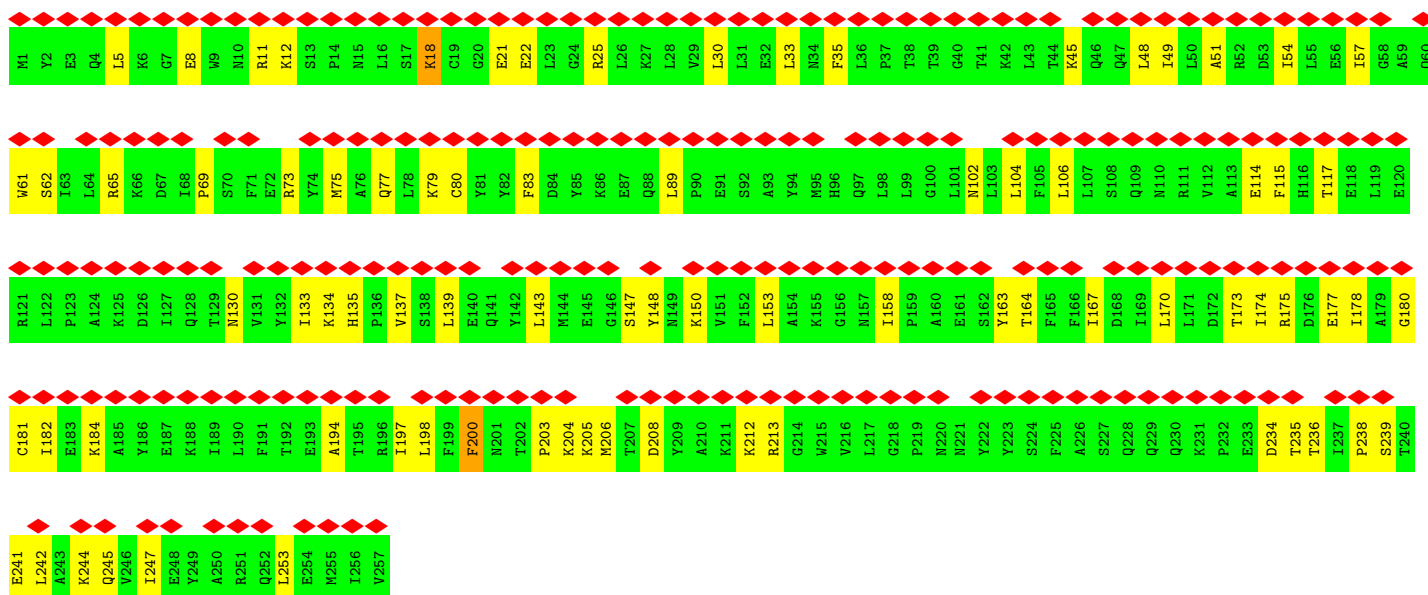


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 14

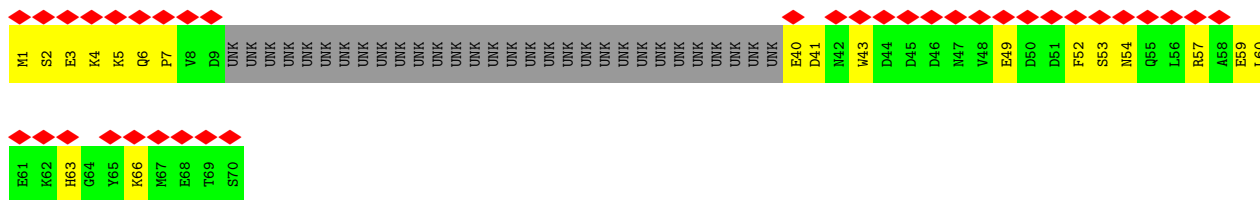
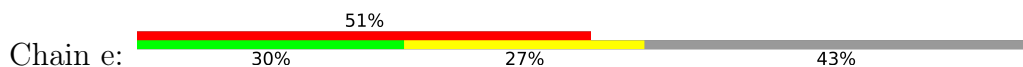




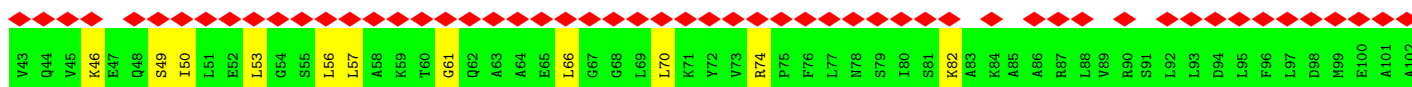
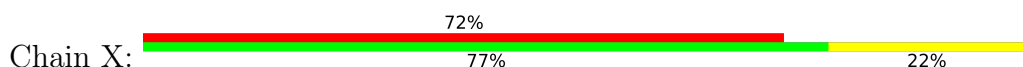
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 8

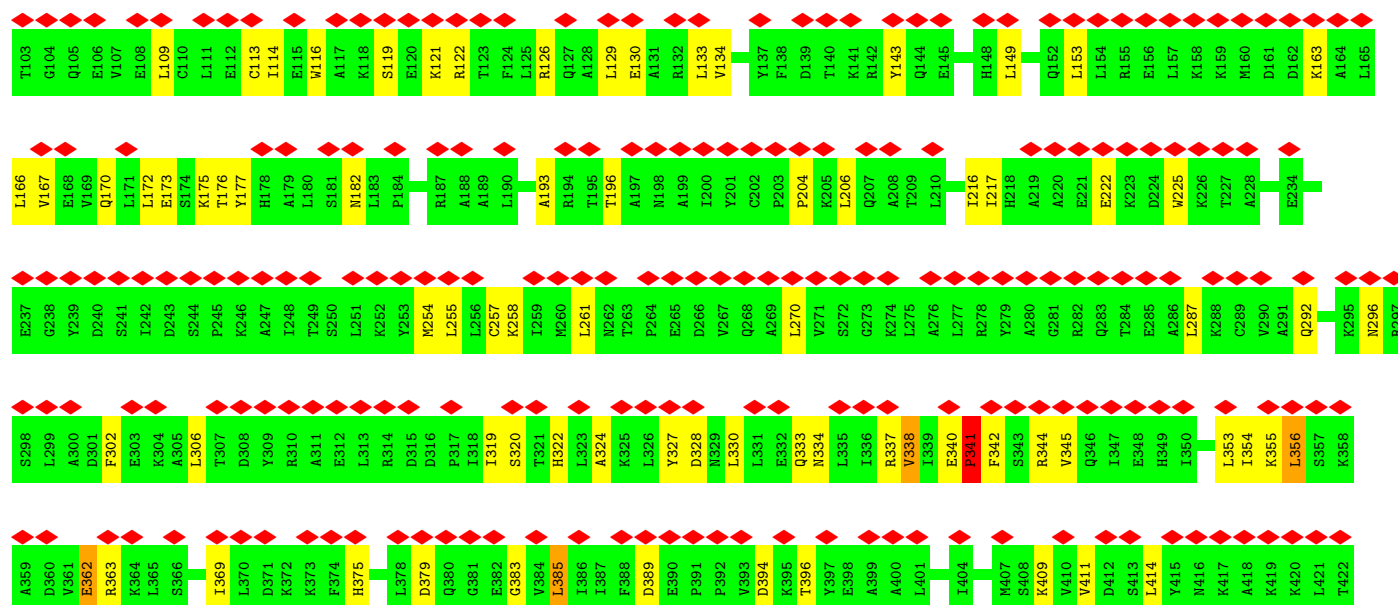


• Molecule 24: sem1

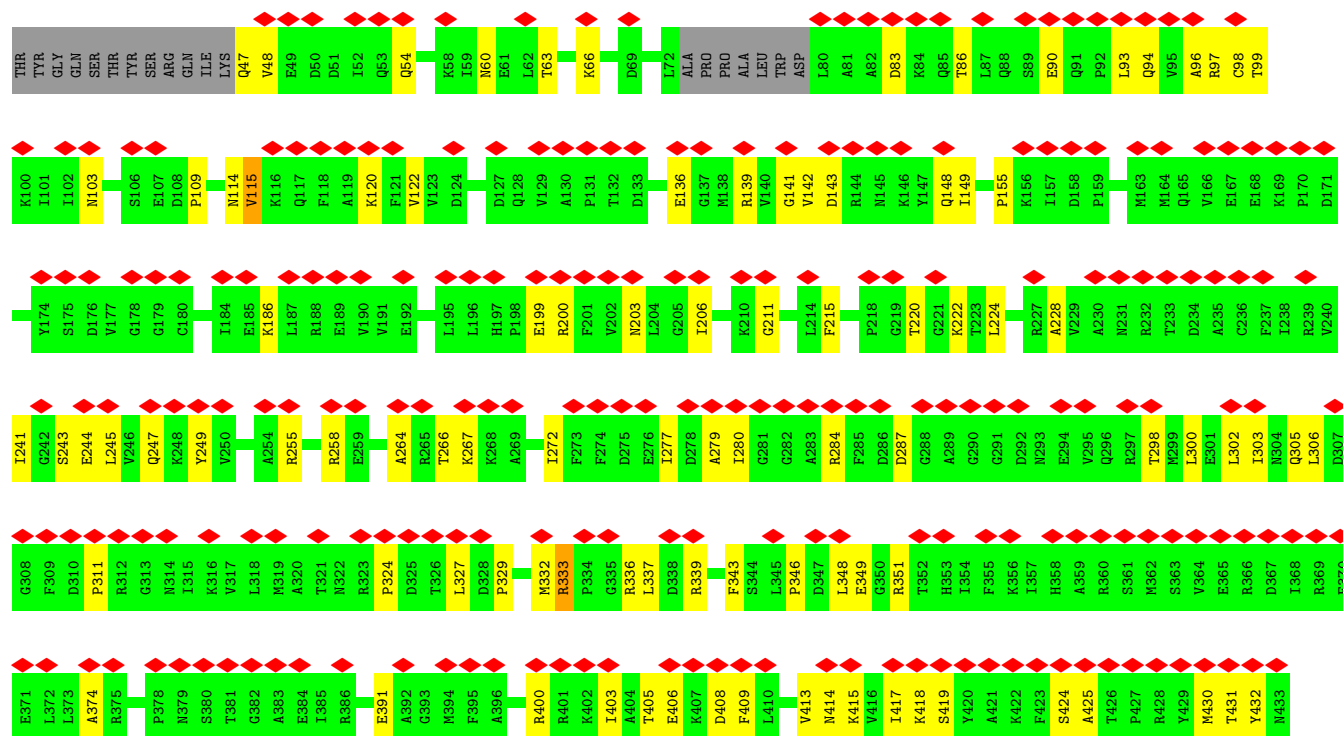


• Molecule 25: 26S proteasome non-ATPase regulatory subunit 11

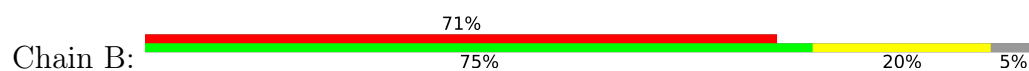




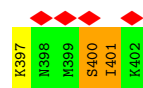
• Molecule 26: 26S proteasome regulatory subunit 7



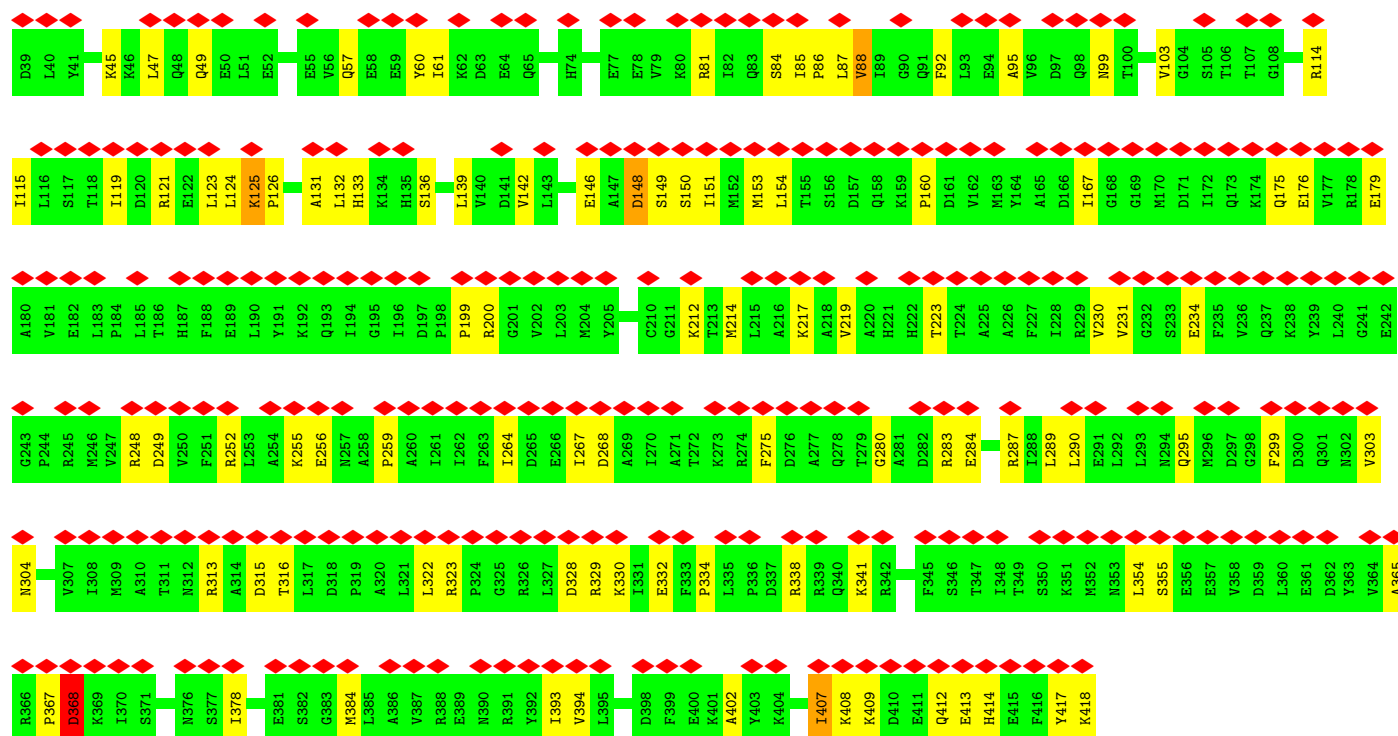
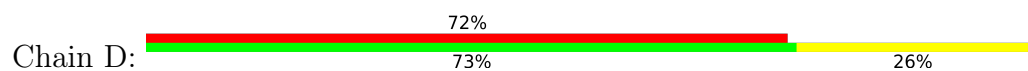
• Molecule 27: 26S proteasome regulatory subunit 4



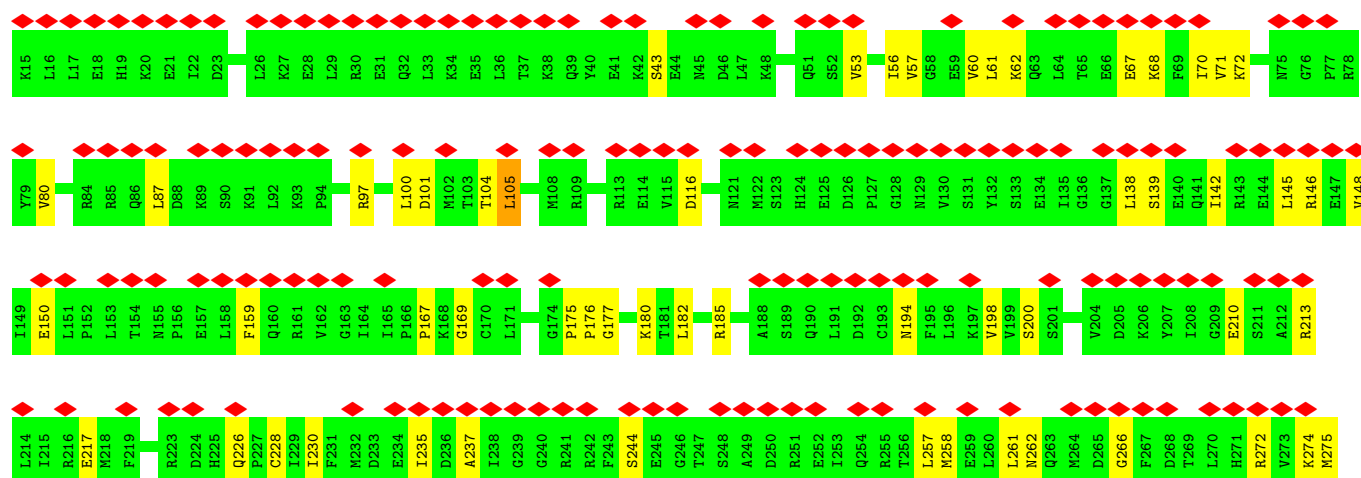
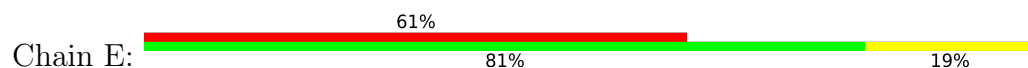


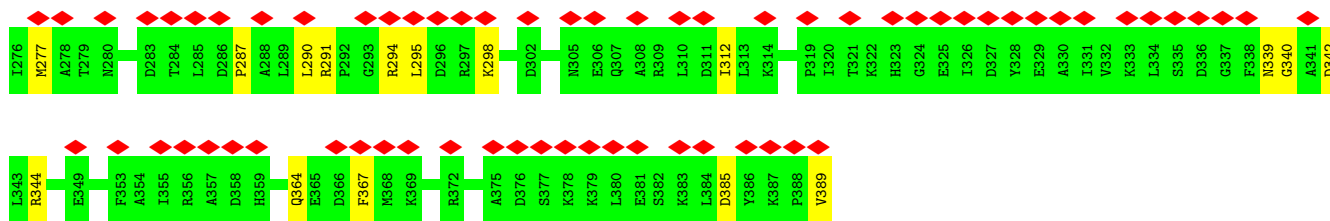


- Molecule 29: 26S proteasome regulatory subunit 6B

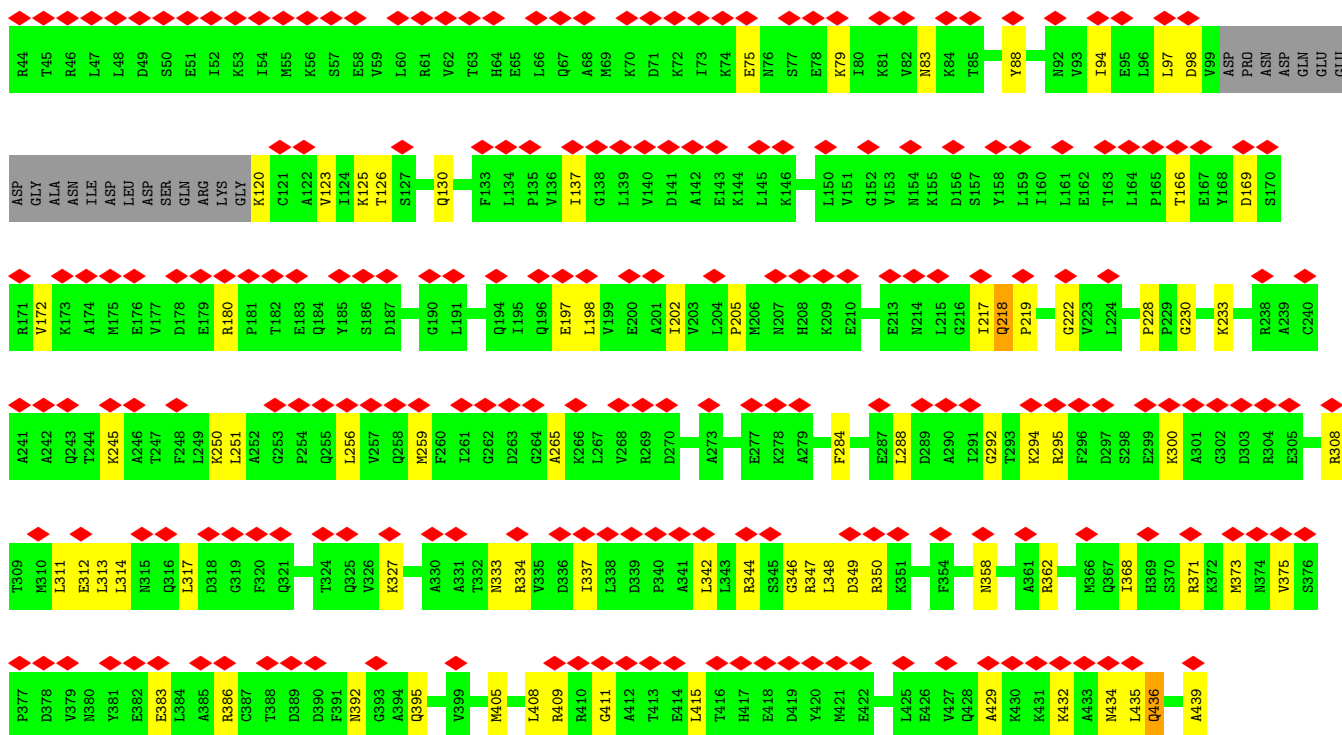
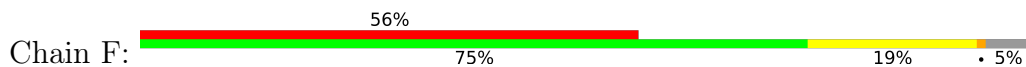


- Molecule 30: 26S proteasome regulatory subunit 10B





• Molecule 31: 26S proteasome regulatory subunit 6A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66246	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	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	0.023	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	G	0.31	0/1853	0.65	0/2515
1	g	0.29	0/1859	0.61	0/2523
2	H	0.31	0/1723	0.63	3/2346 (0.1%)
2	h	0.26	0/1743	0.53	0/2372
3	I	0.32	0/1925	0.68	0/2606
3	i	0.30	0/1942	0.66	0/2628
4	J	0.32	0/1728	0.66	2/2358 (0.1%)
4	j	0.29	0/1728	0.60	0/2358
5	K	0.30	0/1755	0.72	4/2375 (0.2%)
5	k	0.29	0/1747	0.57	0/2364
6	L	0.32	0/1885	0.59	0/2552
6	l	0.30	0/1885	0.58	2/2552 (0.1%)
7	M	0.31	0/1891	0.63	2/2552 (0.1%)
7	m	0.29	0/1891	0.61	2/2552 (0.1%)
8	N	0.32	0/1454	0.57	0/1967
8	n	0.31	0/1454	0.61	2/1967 (0.1%)
9	O	0.30	0/1670	0.57	0/2265
9	o	0.31	0/1670	0.54	0/2265
10	P	0.29	0/1614	0.52	0/2177
10	p	0.29	0/1614	0.52	0/2177
11	Q	0.34	0/1603	0.62	0/2174
11	q	0.36	0/1603	0.64	0/2174
12	R	0.31	0/1579	0.50	0/2134
12	r	0.30	0/1579	0.49	0/2134
13	S	0.30	0/1671	0.52	2/2253 (0.1%)
13	s	0.31	0/1671	0.54	2/2253 (0.1%)
14	T	0.32	0/1700	0.56	0/2305
14	t	0.30	0/1700	0.56	2/2305 (0.1%)
15	U	0.29	0/6396	0.70	3/8646 (0.0%)
16	V	0.36	1/3883 (0.0%)	0.84	10/5247 (0.2%)
17	W	0.31	0/3751	0.80	3/5042 (0.1%)
18	Y	0.32	0/3173	0.76	0/4273

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Z	0.32	0/2324	0.77	0/3150
20	a	0.30	0/3053	0.74	2/4133 (0.0%)
21	b	0.29	0/1478	0.75	5/2001 (0.2%)
22	c	0.32	0/2226	0.79	2/3007 (0.1%)
23	d	0.31	0/2162	0.83	4/2919 (0.1%)
24	e	0.35	0/338	0.94	0/450
25	X	0.29	0/3053	0.68	0/4115
26	A	0.30	0/2939	0.68	0/3970
27	B	0.28	0/2844	0.70	3/3846 (0.1%)
28	C	0.29	0/2896	0.73	6/3895 (0.2%)
29	D	0.33	0/3090	0.84	13/4168 (0.3%)
30	E	0.27	0/2904	0.62	0/3924
31	F	0.29	0/2897	0.75	9/3912 (0.2%)
32	f	0.33	1/5393 (0.0%)	0.87	19/7271 (0.3%)
All	All	0.31	2/102937 (0.0%)	0.69	102/139172 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	g	0	1
3	I	0	1
4	J	0	1
4	j	0	1
5	K	0	4
7	M	0	1
8	n	0	1
9	O	0	1
15	U	0	2
16	V	0	3
19	Z	0	2
20	a	0	2
21	b	0	1
23	d	0	2
25	X	0	2
26	A	0	1
28	C	0	2
29	D	0	6
All	All	0	35

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	358	MET	C-N	6.66	1.39	1.33
32	f	494	ARG	CA-C	5.23	1.59	1.52

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	368	ASP	CA-C-N	10.80	141.14	121.70
29	D	368	ASP	C-N-CA	10.80	141.14	121.70
32	f	488	ALA	N-CA-C	10.54	122.85	111.36
5	K	21	LEU	CA-C-N	9.27	138.39	121.70
5	K	21	LEU	C-N-CA	9.27	138.39	121.70
31	F	434	ASN	CA-C-N	8.84	137.62	121.70
31	F	434	ASN	C-N-CA	8.84	137.62	121.70
16	V	77	GLU	CA-C-N	8.76	138.28	121.54
16	V	77	GLU	C-N-CA	8.76	138.28	121.54
21	b	21	PHE	CA-C-N	8.25	141.92	121.80
21	b	21	PHE	C-N-CA	8.25	141.92	121.80
31	F	429	ALA	CA-C-N	8.14	136.36	121.70
31	F	429	ALA	C-N-CA	8.14	136.36	121.70
7	M	6	GLY	CA-C-N	7.93	135.97	121.70
7	M	6	GLY	C-N-CA	7.93	135.97	121.70
2	H	22	ILE	N-CA-C	-7.85	105.52	112.12
29	D	407	ILE	CA-C-N	7.68	135.53	121.70
29	D	407	ILE	C-N-CA	7.68	135.53	121.70
5	K	19	GLY	CA-C-N	7.58	135.35	121.70
5	K	19	GLY	C-N-CA	7.58	135.35	121.70
2	H	7	SER	CA-C-N	7.50	135.19	121.70
2	H	7	SER	C-N-CA	7.50	135.19	121.70
32	f	493	ASN	N-CA-C	-6.99	95.91	110.80
32	f	472	HIS	CA-C-N	6.93	130.42	120.79
32	f	472	HIS	C-N-CA	6.93	130.42	120.79
32	f	493	ASN	CA-C-N	-6.91	111.08	120.82
32	f	493	ASN	C-N-CA	-6.91	111.08	120.82
28	C	401	ILE	N-CA-C	6.88	123.65	109.34
31	F	432	LYS	CA-C-N	6.75	133.86	121.70
31	F	432	LYS	C-N-CA	6.75	133.86	121.70
17	W	313	GLU	CA-C-N	6.69	134.32	121.54
17	W	313	GLU	C-N-CA	6.69	134.32	121.54
28	C	401	ILE	CA-C-N	6.61	133.60	121.70
28	C	401	ILE	C-N-CA	6.61	133.60	121.70
22	c	273	LYS	CA-C-N	6.60	130.72	120.82
22	c	273	LYS	C-N-CA	6.60	130.72	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	21	PHE	N-CA-C	-6.44	98.76	109.46
15	U	457	ILE	N-CA-C	-6.41	106.27	112.29
32	f	492	SER	N-CA-C	-6.33	104.38	111.28
17	W	423	ASN	N-CA-C	-6.22	104.45	114.09
32	f	370	MET	N-CA-C	-6.15	104.65	111.36
32	f	663	GLY	N-CA-C	6.12	121.35	110.95
31	F	436	GLN	N-CA-C	6.11	123.81	110.80
32	f	324	VAL	CA-C-N	6.07	133.13	121.54
32	f	324	VAL	C-N-CA	6.07	133.13	121.54
4	J	182	GLU	CA-C-N	5.98	132.47	121.70
4	J	182	GLU	C-N-CA	5.98	132.47	121.70
32	f	489	TYR	N-CA-C	5.96	118.47	109.23
8	n	17	ASP	CA-C-N	-5.90	114.46	121.90
8	n	17	ASP	C-N-CA	-5.90	114.46	121.90
23	d	200	PHE	CA-C-N	5.86	132.74	121.54
23	d	200	PHE	C-N-CA	5.86	132.74	121.54
32	f	365	VAL	N-CA-C	5.80	121.41	109.34
16	V	261	TYR	CA-C-N	5.78	132.57	121.54
16	V	261	TYR	C-N-CA	5.78	132.57	121.54
16	V	244	ALA	CA-C-N	5.73	132.48	121.54
16	V	244	ALA	C-N-CA	5.73	132.48	121.54
32	f	374	SER	CA-C-N	-5.68	112.67	120.28
32	f	374	SER	C-N-CA	-5.68	112.67	120.28
28	C	396	GLU	CA-CB-CG	5.65	125.40	114.10
32	f	379	GLY	CA-C-N	-5.62	113.50	122.66
32	f	379	GLY	C-N-CA	-5.62	113.50	122.66
28	C	400	SER	CA-C-N	5.55	131.96	121.97
28	C	400	SER	C-N-CA	5.55	131.96	121.97
23	d	234	ASP	CA-C-N	5.53	129.98	121.19
23	d	234	ASP	C-N-CA	5.53	129.98	121.19
32	f	337	LEU	N-CA-C	5.52	122.55	110.80
16	V	28	PRO	N-CA-C	5.48	117.39	110.70
31	F	435	LEU	CA-C-N	5.45	131.96	121.54
31	F	435	LEU	C-N-CA	5.45	131.96	121.54
29	D	368	ASP	N-CA-C	5.44	126.23	111.00
13	s	190	GLY	CA-C-N	5.38	131.82	121.54
13	s	190	GLY	C-N-CA	5.38	131.82	121.54
20	a	287	ASN	CA-C-N	5.37	131.80	121.54
20	a	287	ASN	C-N-CA	5.37	131.80	121.54
27	B	138	PHE	N-CA-C	-5.32	107.80	114.56
29	D	154	LEU	CA-C-N	5.27	131.60	121.54
29	D	154	LEU	C-N-CA	5.27	131.60	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	84	LYS	CA-C-N	-5.26	115.27	121.90
16	V	84	LYS	C-N-CA	-5.26	115.27	121.90
21	b	76	HIS	CA-C-N	5.24	129.85	122.46
21	b	76	HIS	C-N-CA	5.24	129.85	122.46
14	t	178	TYR	CA-C-N	-5.15	113.53	122.14
14	t	178	TYR	C-N-CA	-5.15	113.53	122.14
27	B	437	GLY	CA-C-N	5.13	130.94	121.70
27	B	437	GLY	C-N-CA	5.13	130.94	121.70
29	D	151	ILE	CA-C-N	5.13	131.34	121.54
29	D	151	ILE	C-N-CA	5.13	131.34	121.54
15	U	223	LEU	CA-C-N	5.08	130.03	122.82
15	U	223	LEU	C-N-CA	5.08	130.03	122.82
29	D	149	SER	CA-C-N	5.07	131.23	121.54
29	D	149	SER	C-N-CA	5.07	131.23	121.54
6	l	225	ASP	CA-C-N	5.04	131.18	121.54
6	l	225	ASP	C-N-CA	5.04	131.18	121.54
13	S	190	GLY	CA-C-N	5.04	131.17	121.54
13	S	190	GLY	C-N-CA	5.04	131.17	121.54
16	V	29	PRO	N-CA-C	5.04	116.84	110.70
29	D	414	HIS	CA-C-N	5.04	131.16	121.54
29	D	414	HIS	C-N-CA	5.04	131.16	121.54
7	m	62	SER	CA-C-N	5.02	129.54	122.46
7	m	62	SER	C-N-CA	5.02	129.54	122.46
32	f	404	ASP	N-CA-C	5.01	117.14	111.02

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A	333	ARG	Sidechain
28	C	397	LYS	Peptide
28	C	400	SER	Peptide
29	D	124	LEU	Peptide
29	D	125	LYS	Peptide
29	D	150	SER	Peptide
29	D	368	ASP	Peptide
29	D	407	ILE	Peptide
29	D	86	PRO	Peptide
1	G	222	VAL	Peptide
3	I	6	ASP	Peptide
4	J	2	SER	Peptide
5	K	121	LEU	Peptide

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Mol	Chain	Res	Type	Group
5	K	19	GLY	Peptide
5	K	22	PHE	Peptide
5	K	9	ASP	Peptide
7	M	160	TYR	Peptide
9	O	172	ASN	Peptide
15	U	561	GLU	Peptide
15	U	793	LYS	Peptide
16	V	77	GLU	Peptide
16	V	78	HIS	Mainchain
16	V	79	VAL	Peptide
25	X	362	GLU	Peptide
25	X	385	LEU	Peptide
19	Z	143	GLU	Peptide
19	Z	220	LEU	Peptide
20	a	165	THR	Peptide
20	a	285	PRO	Peptide
21	b	22	LEU	Peptide
23	d	200	PHE	Peptide
23	d	33	LEU	Peptide
1	g	222	VAL	Peptide
4	j	180	ALA	Peptide
8	n	91	ARG	Peptide

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	G	1820	0	1791	21	0
1	g	1826	0	1796	23	0
2	H	1688	0	1575	33	0
2	h	1708	0	1594	25	0
3	I	1895	0	1833	26	0
3	i	1912	0	1851	35	0
4	J	1704	0	1517	19	0
4	j	1704	0	1517	29	0
5	K	1729	0	1680	40	0
5	k	1722	0	1673	32	0
6	L	1850	0	1822	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	l	1850	0	1822	29	0
7	M	1856	0	1814	40	0
7	m	1856	0	1814	40	0
8	N	1430	0	1398	20	0
8	n	1430	0	1398	20	0
9	O	1643	0	1644	25	0
9	o	1643	0	1644	25	0
10	P	1585	0	1598	24	0
10	p	1585	0	1598	24	0
11	Q	1570	0	1547	33	0
11	q	1570	0	1547	28	0
12	R	1548	0	1499	20	0
12	r	1548	0	1499	23	0
13	S	1641	0	1618	17	0
13	s	1641	0	1618	18	0
14	T	1667	0	1628	22	0
14	t	1667	0	1628	27	0
15	U	6287	0	6338	164	0
16	V	3808	0	3855	119	0
17	W	3703	0	3822	116	0
18	Y	3115	0	3120	89	0
19	Z	2281	0	2312	53	0
20	a	2995	0	3012	95	0
21	b	1458	0	1505	39	0
22	c	2187	0	2214	56	0
23	d	2116	0	2146	53	0
24	e	334	0	294	17	0
25	X	3009	0	3113	54	0
26	A	2893	0	2843	75	0
27	B	2806	0	2770	47	0
28	C	2859	0	2971	45	0
29	D	3040	0	3076	58	0
30	E	2860	0	2828	53	0
31	F	2859	0	2853	50	0
32	f	5319	0	5329	469	0
33	c	1	0	0	0	0
34	A	31	0	12	3	0
34	D	31	0	12	3	0
34	E	31	0	12	16	0
34	F	31	0	12	4	0
All	All	101342	0	100412	2212	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 11.

All (2212) 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)
30:E:340:GLY:HA3	34:E:401:AGS:N7	1.32	1.37
32:f:796:LEU:O	32:f:799:VAL:HG22	1.30	1.31
32:f:753:ALA:O	32:f:754:LYS:HE2	1.27	1.25
32:f:494:ARG:HD3	32:f:496:ASP:OD1	1.26	1.24
32:f:742:ALA:HA	32:f:745:LEU:CD2	1.66	1.23
32:f:376:PHE:CE1	32:f:798:THR:CG2	2.23	1.22
32:f:471:LEU:CG	32:f:509:LYS:HE3	1.73	1.19
32:f:494:ARG:HH21	32:f:495:GLU:HG2	1.02	1.17
32:f:494:ARG:HE	32:f:495:GLU:N	1.44	1.16
32:f:696:LEU:HD13	32:f:752:HIS:CD2	1.80	1.16
32:f:311:VAL:HB	32:f:490:ALA:HB1	1.17	1.15
32:f:692:LEU:HD12	32:f:748:LEU:HD21	1.19	1.15
26:A:48:VAL:CB	32:f:231:LEU:HD13	1.79	1.13
30:E:340:GLY:HA3	34:E:401:AGS:C8	1.77	1.12
32:f:494:ARG:NH2	32:f:495:GLU:HG2	1.64	1.12
32:f:389:LYS:CG	32:f:418:LEU:HD21	1.79	1.12
32:f:479:LEU:CD2	32:f:513:GLU:HB2	1.79	1.11
32:f:479:LEU:HD21	32:f:513:GLU:CB	1.80	1.11
32:f:692:LEU:HD12	32:f:748:LEU:CD2	1.82	1.09
32:f:471:LEU:HG	32:f:509:LYS:CE	1.83	1.08
32:f:483:PHE:CE2	32:f:799:VAL:HB	1.88	1.08
32:f:742:ALA:O	32:f:745:LEU:HG	1.54	1.07
32:f:389:LYS:HG2	32:f:418:LEU:HD21	1.29	1.07
26:A:66:LYS:CB	32:f:613:LEU:HD13	1.85	1.06
32:f:376:PHE:CE1	32:f:798:THR:HG21	1.85	1.06
30:E:340:GLY:CA	34:E:401:AGS:N7	2.20	1.05
32:f:471:LEU:HD12	32:f:509:LYS:CG	1.87	1.03
32:f:494:ARG:CD	32:f:496:ASP:OD1	2.06	1.03
32:f:780:PRO:HB3	32:f:800:LEU:HA	1.37	1.02
32:f:753:ALA:O	32:f:754:LYS:CE	2.08	1.01
32:f:337:LEU:HD13	32:f:420:TRP:HZ3	1.26	1.00
32:f:696:LEU:HD13	32:f:752:HIS:HD2	1.14	0.99
32:f:494:ARG:HG3	32:f:497:VAL:HG12	1.43	0.99
32:f:479:LEU:HD21	32:f:513:GLU:HB2	0.99	0.99
18:Y:283:LYS:O	18:Y:289:ALA:HB2	1.64	0.97
32:f:359:GLY:O	32:f:363:SER:HB3	1.63	0.97
32:f:692:LEU:CD1	32:f:748:LEU:HD21	1.93	0.96
32:f:742:ALA:HA	32:f:745:LEU:HD23	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:372:LEU:HD11	32:f:406:GLY:HA3	1.47	0.96
32:f:456:ARG:HB3	32:f:489:TYR:CE2	2.00	0.96
32:f:376:PHE:CD1	32:f:416:MET:HE1	2.01	0.95
32:f:471:LEU:HG	32:f:509:LYS:HE3	0.96	0.94
32:f:780:PRO:CB	32:f:800:LEU:HA	1.96	0.94
32:f:311:VAL:HB	32:f:490:ALA:CB	1.96	0.94
32:f:358:PHE:CZ	32:f:381:VAL:HG21	2.03	0.94
32:f:376:PHE:CE1	32:f:416:MET:HE1	2.03	0.93
32:f:691:PRO:CB	32:f:749:ALA:HB2	1.99	0.93
32:f:95:PRO:O	32:f:99:LEU:HB2	1.67	0.93
32:f:224:ASN:O	32:f:228:LYS:HB3	1.66	0.93
18:Y:374:ASP:O	18:Y:378:ASN:HB2	1.70	0.92
32:f:388:ASP:OD2	32:f:390:LEU:HB2	1.67	0.92
18:Y:225:TYR:OH	18:Y:281:GLU:HG2	1.70	0.91
19:Z:278:ASN:O	19:Z:282:ASN:HB2	1.70	0.91
32:f:483:PHE:CZ	32:f:799:VAL:HB	2.06	0.91
32:f:742:ALA:HA	32:f:745:LEU:HD21	1.53	0.90
32:f:315:GLU:HG2	32:f:491:GLY:HA2	1.51	0.90
32:f:366:ASP:OD1	32:f:367:SER:N	2.04	0.90
32:f:376:PHE:CE1	32:f:798:THR:CB	2.55	0.90
32:f:376:PHE:CE1	32:f:798:THR:HB	2.06	0.89
32:f:369:ARG:HB3	32:f:370:MET:SD	2.13	0.89
32:f:363:SER:O	32:f:365:VAL:N	2.04	0.89
18:Y:28:LEU:HD21	18:Y:283:LYS:HD2	1.52	0.89
16:V:394:LEU:O	16:V:398:LEU:HB2	1.71	0.88
32:f:223:GLU:O	32:f:227:ALA:HB3	1.73	0.88
32:f:318:THR:O	32:f:322:SER:HB3	1.74	0.88
32:f:378:ASN:HB3	32:f:391:LEU:HG	1.56	0.88
32:f:389:LYS:HG2	32:f:418:LEU:CD2	2.02	0.88
32:f:494:ARG:HE	32:f:495:GLU:H	1.16	0.87
32:f:337:LEU:HD13	32:f:420:TRP:CZ3	2.10	0.87
32:f:122:ALA:O	32:f:126:ILE:HB	1.72	0.87
20:a:131:THR:O	20:a:135:ILE:HB	1.74	0.87
32:f:311:VAL:CB	32:f:490:ALA:HB1	2.03	0.87
32:f:471:LEU:HD12	32:f:509:LYS:HG2	1.58	0.86
32:f:123:ALA:O	32:f:127:SER:HB2	1.76	0.86
32:f:691:PRO:HB2	32:f:749:ALA:HB2	1.58	0.86
32:f:376:PHE:HE1	32:f:798:THR:CG2	1.89	0.85
32:f:129:LEU:O	32:f:133:MET:HB3	1.75	0.85
32:f:378:ASN:HB3	32:f:391:LEU:CG	2.05	0.85
32:f:88:SER:CB	32:f:92:VAL:HG23	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:126:ILE:O	32:f:130:ALA:HB3	1.77	0.85
32:f:301:HIS:O	32:f:305:LEU:HB2	1.77	0.85
32:f:695:ALA:HB3	32:f:752:HIS:HB2	1.59	0.84
32:f:696:LEU:CD1	32:f:752:HIS:HD2	1.90	0.84
15:U:27:LEU:O	15:U:31:VAL:HB	1.76	0.84
32:f:336:GLU:HG3	32:f:337:LEU:HD22	1.60	0.84
26:A:333:ARG:HH12	26:A:336:ARG:HH21	1.23	0.83
32:f:796:LEU:O	32:f:799:VAL:CG2	2.22	0.83
32:f:494:ARG:HH21	32:f:495:GLU:CG	1.88	0.83
32:f:376:PHE:HE1	32:f:798:THR:CB	1.91	0.83
32:f:714:SER:O	32:f:718:ASP:HB2	1.78	0.83
16:V:187:ILE:O	16:V:191:LEU:HB2	1.79	0.83
17:W:97:LEU:O	17:W:101:VAL:HB	1.79	0.82
32:f:225:ALA:O	32:f:229:VAL:HB	1.79	0.82
15:U:341:PHE:O	15:U:345:ASN:HB2	1.79	0.81
32:f:494:ARG:NE	32:f:495:GLU:N	2.26	0.81
32:f:376:PHE:CZ	32:f:416:MET:SD	2.73	0.81
26:A:333:ARG:HH12	26:A:336:ARG:NH2	1.77	0.81
32:f:378:ASN:O	32:f:381:VAL:HG12	1.80	0.81
32:f:471:LEU:HD12	32:f:509:LYS:HG3	1.62	0.81
32:f:376:PHE:CE1	32:f:416:MET:CE	2.64	0.81
32:f:88:SER:HB2	32:f:92:VAL:HG23	1.63	0.80
32:f:742:ALA:C	32:f:745:LEU:HG	2.06	0.80
20:a:178:ARG:O	20:a:182:CYS:HB3	1.81	0.80
32:f:503:PRO:O	32:f:507:ASP:HB2	1.82	0.80
32:f:494:ARG:NE	32:f:495:GLU:H	1.80	0.80
32:f:612:LEU:O	32:f:616:CYS:HB2	1.83	0.79
19:Z:285:ALA:O	19:Z:289:GLU:HB2	1.83	0.79
32:f:232:TYR:O	32:f:236:CYS:HB2	1.82	0.79
15:U:325:MET:O	15:U:329:LEU:HB2	1.82	0.79
15:U:496:LEU:O	15:U:500:ASN:HB2	1.83	0.79
30:E:340:GLY:HA3	34:E:401:AGS:C5	2.13	0.79
32:f:184:LEU:HG	32:f:185:LEU:N	1.98	0.79
15:U:399:TRP:HE1	22:c:177:THR:HG22	1.48	0.79
32:f:745:LEU:HD12	32:f:746:ARG:N	1.99	0.78
32:f:456:ARG:HB3	32:f:489:TYR:HE2	1.47	0.78
32:f:392:THR:HG22	32:f:417:ILE:CD1	2.14	0.78
32:f:479:LEU:CD2	32:f:513:GLU:CB	2.50	0.78
32:f:635:LYS:HZ3	32:f:641:GLU:CD	1.92	0.78
32:f:370:MET:SD	32:f:370:MET:N	2.57	0.78
18:Y:28:LEU:CD2	18:Y:283:LYS:HD2	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:494:ARG:HE	32:f:494:ARG:C	1.92	0.77
32:f:635:LYS:HZ2	32:f:641:GLU:HG3	1.49	0.77
32:f:784:ASP:HB2	32:f:800:LEU:HD21	1.66	0.77
20:a:8:LEU:O	20:a:12:GLN:HB3	1.83	0.77
32:f:389:LYS:CG	32:f:418:LEU:CD2	2.63	0.77
15:U:456:ASP:O	15:U:460:TYR:HB3	1.85	0.77
32:f:695:ALA:C	32:f:752:HIS:HB3	2.09	0.77
32:f:478:ARG:HD3	32:f:504:VAL:HG13	1.68	0.76
32:f:376:PHE:CE1	32:f:798:THR:HG22	2.20	0.76
32:f:691:PRO:HB3	32:f:749:ALA:HB2	1.66	0.76
32:f:796:LEU:HG	32:f:799:VAL:HG21	1.66	0.76
22:c:305:ASP:O	22:c:309:PHE:HB3	1.86	0.75
32:f:376:PHE:CZ	32:f:798:THR:HB	2.22	0.75
32:f:675:PHE:O	32:f:679:LEU:HB2	1.85	0.75
32:f:358:PHE:O	32:f:362:GLY:HA3	1.87	0.75
32:f:357:ARG:O	32:f:361:SER:HB2	1.87	0.75
32:f:494:ARG:NH2	32:f:495:GLU:CG	2.48	0.74
32:f:494:ARG:CG	32:f:497:VAL:HG12	2.16	0.74
32:f:471:LEU:CD1	32:f:509:LYS:CE	2.65	0.74
32:f:635:LYS:NZ	32:f:641:GLU:CG	2.50	0.74
32:f:684:PRO:O	32:f:688:ARG:HB2	1.87	0.73
32:f:742:ALA:HA	32:f:745:LEU:CG	2.18	0.73
32:f:691:PRO:HG2	32:f:745:LEU:HD13	1.70	0.73
6:L:186:GLU:HA	6:L:189:LYS:HG2	1.71	0.73
16:V:227:VAL:O	16:V:231:LEU:HB2	1.89	0.73
32:f:211:ILE:O	32:f:215:ASP:HB2	1.88	0.73
17:W:82:LEU:O	17:W:86:ASN:HB2	1.88	0.72
28:C:330:LYS:O	28:C:334:ARG:HB2	1.88	0.72
32:f:664:GLU:HB3	32:f:696:LEU:HG	1.69	0.72
32:f:315:GLU:CG	32:f:491:GLY:HA2	2.20	0.72
17:W:441:LYS:O	17:W:445:LEU:HB2	1.89	0.72
25:X:163:LYS:HG3	25:X:196:THR:HG23	1.72	0.71
32:f:392:THR:CG2	32:f:417:ILE:HG21	2.18	0.71
20:a:14:SER:H	20:a:18:GLN:HG2	1.55	0.71
16:V:378:VAL:O	16:V:382:PHE:HB2	1.91	0.71
32:f:337:LEU:CD1	32:f:420:TRP:CZ3	2.74	0.71
18:Y:237:ARG:O	18:Y:241:ILE:HB	1.90	0.71
17:W:124:LEU:HD13	17:W:147:LYS:HB2	1.72	0.71
13:S:27:THR:HB	13:S:40:SER:H	1.54	0.71
32:f:625:LYS:O	32:f:629:LYS:HB2	1.91	0.71
20:a:118:ILE:O	20:a:122:LYS:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:311:VAL:O	32:f:490:ALA:O	2.09	0.71
18:Y:261:PHE:O	18:Y:265:GLU:HB2	1.91	0.70
30:E:340:GLY:CA	34:E:401:AGS:C5	2.68	0.70
32:f:494:ARG:HD3	32:f:496:ASP:CG	2.16	0.70
32:f:389:LYS:HG2	32:f:418:LEU:HD11	1.72	0.70
32:f:389:LYS:CD	32:f:418:LEU:HD21	2.20	0.70
32:f:797:LEU:O	32:f:800:LEU:HD13	1.91	0.70
3:I:143:TYR:HB2	3:I:146:GLN:HE21	1.55	0.70
11:Q:57:ALA:O	11:Q:61:GLN:HB3	1.92	0.70
26:A:244:GLU:HA	27:B:268:ARG:HH12	1.56	0.70
18:Y:301:ILE:HG13	18:Y:343:LEU:HD12	1.74	0.70
18:Y:283:LYS:O	18:Y:285:ASP:N	2.23	0.69
32:f:130:ALA:O	32:f:134:SER:HB3	1.92	0.69
32:f:311:VAL:CG2	32:f:527:VAL:O	2.39	0.69
32:f:88:SER:HB3	32:f:92:VAL:HG23	1.72	0.69
21:b:15:TYR:O	21:b:25:ARG:NH1	2.25	0.69
32:f:222:ASP:O	32:f:226:TYR:HB3	1.91	0.69
32:f:376:PHE:CD1	32:f:798:THR:HG21	2.27	0.69
32:f:664:GLU:O	32:f:665:GLU:O	2.10	0.69
16:V:328:VAL:O	16:V:332:LEU:HB2	1.93	0.69
29:D:259:PRO:HB3	29:D:304:ASN:HB2	1.74	0.69
28:C:78:ARG:HH12	28:C:80:MET:HE3	1.57	0.69
32:f:392:THR:HG22	32:f:417:ILE:HD12	1.74	0.69
32:f:353:LEU:HG	32:f:387:GLN:HG3	1.75	0.69
32:f:372:LEU:O	32:f:372:LEU:HD23	1.93	0.69
18:Y:283:LYS:C	18:Y:285:ASP:H	2.01	0.69
16:V:227:VAL:HA	16:V:230:PHE:HB3	1.74	0.69
32:f:695:ALA:HB3	32:f:752:HIS:CB	2.23	0.69
18:Y:125:ARG:HA	18:Y:128:TYR:HB3	1.76	0.68
17:W:372:ARG:H	17:W:415:PHE:HB2	1.58	0.68
32:f:688:ARG:HA	32:f:745:LEU:HD22	1.75	0.68
23:d:194:ALA:O	23:d:198:LEU:HB2	1.94	0.68
17:W:312:MET:HE1	17:W:364:ARG:HE	1.57	0.68
7:M:192:GLU:HA	7:M:195:LYS:HE3	1.76	0.68
17:W:243:ILE:HD12	17:W:273:TYR:HB2	1.75	0.68
3:I:106:PRO:HD2	3:I:109:GLN:HE21	1.59	0.68
32:f:376:PHE:HE1	32:f:798:THR:HG21	1.49	0.68
32:f:367:SER:HB3	32:f:370:MET:SD	2.34	0.68
15:U:70:HIS:HA	16:V:236:ARG:HH12	1.59	0.67
17:W:86:ASN:ND2	17:W:96:GLN:OE1	2.27	0.67
3:i:155:ASN:HA	4:j:81:ARG:HH22	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:315:GLU:HG2	32:f:491:GLY:CA	2.24	0.67
19:Z:262:LEU:O	19:Z:266:ILE:HB	1.93	0.67
32:f:478:ARG:O	32:f:482:ILE:HB	1.94	0.67
32:f:800:LEU:HD12	32:f:800:LEU:N	2.10	0.67
32:f:372:LEU:HD23	32:f:372:LEU:C	2.20	0.67
32:f:804:LEU:H	32:f:804:LEU:HD12	1.60	0.67
15:U:14:GLU:O	15:U:20:LYS:NZ	2.28	0.67
20:a:176:ALA:O	20:a:180:LEU:HB3	1.94	0.67
32:f:376:PHE:CE1	32:f:416:MET:SD	2.88	0.67
15:U:895:PRO:HG2	15:U:901:GLN:HG2	1.77	0.67
18:Y:267:ARG:HB2	18:Y:270:VAL:HG12	1.76	0.67
23:d:8:GLU:HB3	23:d:11:ARG:HB3	1.77	0.66
32:f:625:LYS:HA	32:f:657:ILE:HD11	1.75	0.66
4:J:51:ALA:HB3	4:J:54:GLN:HE22	1.60	0.66
16:V:415:SER:HB2	18:Y:346:LYS:HB3	1.76	0.66
24:e:2:SER:O	24:e:6:GLN:NE2	2.29	0.66
32:f:578:ALA:O	32:f:582:VAL:HB	1.95	0.66
26:A:241:ILE:HG22	26:A:243:SER:H	1.60	0.66
23:d:177:GLU:O	23:d:181:CYS:HB2	1.96	0.66
6:l:186:GLU:HA	6:l:189:LYS:HG2	1.75	0.66
32:f:80:ARG:HB3	32:f:95:PRO:HB2	1.78	0.66
32:f:337:LEU:HD11	32:f:422:VAL:HG21	1.77	0.66
3:I:119:GLN:HE21	3:I:123:GLN:HE22	1.43	0.66
23:d:203:PRO:HB2	23:d:205:LYS:H	1.60	0.66
31:F:79:LYS:O	31:F:83:ASN:HB2	1.96	0.66
32:f:628:ASP:HB2	32:f:657:ILE:HD13	1.77	0.66
32:f:742:ALA:O	32:f:745:LEU:CG	2.38	0.66
19:Z:45:LYS:HB3	19:Z:47:VAL:HG12	1.77	0.66
19:Z:190:ARG:HH22	20:a:372:HIS:HA	1.61	0.66
15:U:401:LYS:HE2	15:U:437:TYR:HB2	1.78	0.65
28:C:69:GLN:HG3	28:C:118:ASN:HD21	1.61	0.65
18:Y:310:SER:HB3	25:X:369:ILE:HG22	1.79	0.65
20:a:34:TRP:H	21:b:18:ASN:HD22	1.44	0.65
23:d:178:ILE:O	23:d:213:ARG:NH2	2.29	0.65
16:V:337:LEU:HD23	16:V:342:ILE:HG21	1.79	0.65
9:o:172:ASN:HB3	9:o:191:VAL:HG22	1.79	0.65
32:f:804:LEU:HD12	32:f:804:LEU:N	2.12	0.65
15:U:807:LYS:HA	15:U:836:THR:HB	1.77	0.65
32:f:311:VAL:HG21	32:f:527:VAL:O	1.95	0.65
32:f:471:LEU:CD1	32:f:509:LYS:HE3	2.26	0.65
9:o:96:ALA:H	9:o:115:PRO:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:82:LYS:HB3	25:X:122:ARG:HH12	1.60	0.65
32:f:379:GLY:O	32:f:417:ILE:HG12	1.97	0.65
22:c:245:VAL:HG13	22:c:246:LYS:HG3	1.77	0.64
26:A:114:ASN:HB3	26:A:120:LYS:HG2	1.77	0.64
32:f:635:LYS:HZ2	32:f:641:GLU:CG	2.07	0.64
9:O:18:THR:HB	9:O:31:CYS:H	1.62	0.64
22:c:104:ARG:HE	22:c:106:GLU:HB3	1.63	0.64
25:X:334:ASN:O	25:X:338:VAL:HB	1.96	0.64
32:f:389:LYS:HG2	32:f:418:LEU:CG	2.27	0.64
21:b:54:LEU:HD13	21:b:84:ILE:HG13	1.78	0.64
28:C:161:ILE:HA	28:C:164:VAL:HG12	1.79	0.64
28:C:193:GLY:HA3	28:C:355:SER:HB2	1.80	0.64
32:f:138:GLU:O	32:f:142:TYR:HB2	1.97	0.64
32:f:366:ASP:O	32:f:367:SER:HB2	1.97	0.64
32:f:804:LEU:H	32:f:804:LEU:CD1	2.11	0.64
4:J:72:ALA:HB3	4:J:132:LEU:HB2	1.78	0.64
15:U:643:SER:O	15:U:649:ARG:NH1	2.31	0.64
11:q:118:MET:HE1	11:q:124:LEU:HD23	1.79	0.64
32:f:313:GLU:O	32:f:317:LEU:HB2	1.98	0.64
20:a:248:PHE:O	20:a:252:LYS:HB2	1.98	0.64
28:C:190:GLY:HA3	28:C:317:PHE:HB2	1.80	0.64
3:I:38:LEU:HG	3:I:160:LYS:HB3	1.80	0.64
5:k:77:ALA:HB3	5:k:142:LEU:HB2	1.80	0.64
32:f:93:PRO:HB2	32:f:137:ARG:HE	1.63	0.64
8:N:21:THR:HG22	8:N:26:ILE:HG13	1.80	0.64
16:V:311:ASN:O	16:V:315:LYS:HB2	1.98	0.64
1:g:41:ALA:HB3	1:g:166:THR:HB	1.80	0.64
26:A:103:ASN:ND2	31:F:166:THR:OG1	2.31	0.63
32:f:460:ASP:N	32:f:460:ASP:OD1	2.29	0.63
6:L:206:THR:H	6:L:209:ASN:HD21	1.46	0.63
26:A:400:ARG:O	26:A:400:ARG:HG3	1.99	0.63
23:d:135:HIS:O	23:d:139:LEU:HB2	1.99	0.63
26:A:122:VAL:HB	31:F:88:TYR:HB2	1.80	0.63
26:A:284:ARG:HH12	31:F:333:ASN:HB2	1.63	0.63
32:f:376:PHE:HE1	32:f:798:THR:HB	1.53	0.63
32:f:471:LEU:CG	32:f:509:LYS:CE	2.56	0.63
32:f:692:LEU:HG	32:f:752:HIS:CE1	2.32	0.63
2:H:50:LYS:NZ	2:H:62:VAL:O	2.31	0.63
15:U:62:LEU:HD12	15:U:84:ALA:HB1	1.80	0.63
17:W:203:GLN:HA	17:W:206:SER:HB3	1.80	0.63
24:e:3:GLU:HB2	24:e:7:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:167:LEU:HD12	16:V:169:LEU:H	1.64	0.63
32:f:494:ARG:HH21	32:f:495:GLU:H	1.46	0.63
5:K:76:CYS:SG	5:K:77:ALA:N	2.72	0.63
27:B:181:GLN:O	27:B:241:ASN:ND2	2.32	0.63
31:F:375:VAL:HG22	31:F:415:LEU:HD12	1.78	0.63
15:U:80:TYR:O	15:U:84:ALA:HB2	1.99	0.63
29:D:115:ILE:HG22	29:D:139:LEU:HD12	1.79	0.63
29:D:200:ARG:NH1	29:D:303:VAL:O	2.32	0.63
32:f:687:ARG:HH21	32:f:742:ALA:HB2	1.64	0.63
15:U:155:LEU:O	15:U:158:ARG:NH1	2.31	0.62
15:U:251:ASP:O	15:U:255:SER:HB3	1.99	0.62
16:V:393:THR:O	16:V:397:ARG:NH2	2.32	0.62
17:W:274:VAL:O	17:W:283:GLN:NE2	2.32	0.62
16:V:419:LEU:O	16:V:423:ALA:HB3	1.98	0.62
20:a:247:ARG:O	20:a:251:LEU:HB3	1.99	0.62
9:o:198:ARG:NH2	10:p:151:GLU:O	2.32	0.62
32:f:392:THR:HG23	32:f:417:ILE:HG21	1.81	0.62
7:M:141:SER:HB3	7:M:144:ASP:HB2	1.82	0.62
20:a:244:ASN:HB2	20:a:272:ILE:HB	1.80	0.62
5:k:76:CYS:SG	5:k:77:ALA:N	2.73	0.62
26:A:413:VAL:HG13	26:A:417:ILE:HD12	1.80	0.62
19:Z:249:PHE:HB3	23:d:235:THR:HG23	1.81	0.62
16:V:148:ARG:NH2	16:V:189:ASP:OD1	2.32	0.62
17:W:130:MET:SD	17:W:130:MET:N	2.73	0.62
7:M:163:CYS:SG	7:M:164:ALA:N	2.73	0.62
15:U:229:VAL:HG13	15:U:268:LEU:HD11	1.81	0.62
19:Z:17:LEU:HD22	22:c:36:LEU:HB3	1.80	0.62
3:i:34:CYS:H	3:i:164:ILE:HG13	1.65	0.62
1:G:41:ALA:HB3	1:G:166:THR:HB	1.81	0.62
15:U:579:ARG:NH1	15:U:609:ASP:OD2	2.30	0.62
10:p:29:GLY:HA3	10:p:34:MET:HA	1.82	0.62
26:A:244:GLU:O	26:A:247:GLN:NE2	2.33	0.62
32:f:664:GLU:HA	32:f:697:ILE:HA	1.80	0.62
18:Y:225:TYR:CZ	18:Y:281:GLU:HG2	2.34	0.62
26:A:103:ASN:HA	26:A:136:GLU:HG2	1.82	0.62
10:p:15:LYS:HE3	10:p:121:ILE:HG12	1.82	0.61
13:s:27:THR:HB	13:s:40:SER:H	1.65	0.61
32:f:389:LYS:HD3	32:f:389:LYS:N	2.15	0.61
23:d:80:CYS:HA	23:d:83:PHE:HB3	1.82	0.61
26:A:60:ASN:HA	32:f:641:GLU:OE2	1.99	0.61
29:D:341:LYS:NZ	29:D:368:ASP:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:234:THR:O	32:f:238:ASN:HB2	2.00	0.61
32:f:483:PHE:CE2	32:f:799:VAL:CB	2.75	0.61
30:E:344:ARG:NH1	34:E:401:AGS:O2'	2.33	0.61
31:F:98:ASP:OD1	31:F:120:LYS:N	2.33	0.61
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.81	0.61
15:U:625:ILE:HG13	15:U:626:LEU:HG	1.81	0.61
16:V:349:ARG:HB3	24:e:43:TRP:HE1	1.65	0.61
3:I:15:GLU:H	3:I:16:GLY:HA2	1.65	0.61
16:V:369:THR:HG22	24:e:54:ASN:HD22	1.64	0.61
17:W:282:GLU:O	17:W:286:LEU:HB2	2.00	0.61
16:V:468:SER:OG	18:Y:362:LYS:NZ	2.34	0.61
26:A:333:ARG:NH2	34:F:501:AGS:O1A	2.33	0.61
32:f:339:ILE:HG23	32:f:340:MET:HG2	1.81	0.61
32:f:471:LEU:CD1	32:f:509:LYS:HE2	2.30	0.61
32:f:494:ARG:NE	32:f:496:ASP:H	1.99	0.61
5:K:203:LYS:HA	5:K:206:MET:HG2	1.83	0.61
9:O:96:ALA:H	9:O:115:PRO:HB3	1.66	0.61
23:d:208:ASP:O	23:d:212:LYS:HB2	2.00	0.61
27:B:122:ILE:HD11	27:B:130:GLU:HB3	1.83	0.61
28:C:80:MET:HE1	28:C:86:LEU:HB2	1.82	0.61
32:f:378:ASN:HB2	32:f:391:LEU:HD11	1.82	0.61
10:P:49:LEU:HD21	10:P:87:LEU:HD22	1.81	0.60
23:d:204:LYS:O	23:d:208:ASP:HB2	2.00	0.60
32:f:376:PHE:CG	32:f:416:MET:HE1	2.35	0.60
32:f:380:PHE:CB	32:f:751:TYR:HE2	2.14	0.60
7:M:47:PHE:HB2	7:M:214:SER:HB3	1.82	0.60
8:N:46:SER:HB2	8:N:97:GLY:HA3	1.82	0.60
15:U:609:ASP:O	15:U:615:ARG:NH1	2.34	0.60
4:J:109:ARG:NH2	12:R:70:ASN:OD1	2.34	0.60
5:K:117:SER:O	6:L:82:ARG:NH2	2.34	0.60
15:U:571:CYS:SG	15:U:601:ARG:NH2	2.72	0.60
21:b:157:VAL:HG21	21:b:170:LEU:HB2	1.82	0.60
32:f:471:LEU:O	32:f:471:LEU:HD23	2.01	0.60
11:q:21:ALA:HB3	11:q:29:LYS:HB3	1.82	0.60
15:U:519:VAL:HG23	15:U:520:MET:HG2	1.83	0.60
18:Y:23:ARG:HH21	18:Y:52:PRO:HA	1.65	0.60
8:N:32:ASP:O	8:N:45:ARG:NH1	2.34	0.60
10:P:189:ILE:HG23	10:P:196:THR:HB	1.84	0.60
11:Q:181:ARG:NH1	11:Q:190:ASP:OD1	2.35	0.60
32:f:477:MET:O	32:f:481:SER:HB2	2.02	0.60
32:f:501:LEU:HD22	32:f:518:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:5:GLN:O	6:l:8:ASN:ND2	2.35	0.60
7:m:141:SER:HB3	7:m:144:ASP:HB2	1.83	0.60
26:A:333:ARG:HE	31:F:230:GLY:HA2	1.65	0.60
32:f:129:LEU:O	32:f:133:MET:CB	2.50	0.60
5:K:209:LYS:O	5:K:214:ASN:ND2	2.34	0.60
12:R:1:THR:N	12:R:169:TYR:O	2.34	0.60
15:U:216:VAL:O	15:U:220:LEU:HB2	2.01	0.60
21:b:100:ARG:NH1	21:b:102:GLY:O	2.34	0.60
7:m:192:GLU:HA	7:m:195:LYS:HE3	1.83	0.60
29:D:332:GLU:HG3	29:D:334:PRO:HD3	1.84	0.60
32:f:315:GLU:CB	32:f:491:GLY:HA2	2.31	0.60
32:f:801:VAL:HG13	32:f:801:VAL:O	2.01	0.60
15:U:185:MET:SD	15:U:194:ARG:NH2	2.75	0.59
22:c:178:THR:HA	22:c:181:LEU:HB2	1.83	0.59
32:f:232:TYR:O	32:f:236:CYS:CB	2.49	0.59
32:f:376:PHE:CZ	32:f:416:MET:HE1	2.36	0.59
20:a:188:LEU:HG	20:a:193:GLN:HE21	1.67	0.59
23:d:235:THR:HG22	23:d:236:THR:HG23	1.83	0.59
5:k:221:GLN:HB2	5:k:224:GLN:HB3	1.84	0.59
10:p:58:THR:O	11:q:85:ARG:NH2	2.34	0.59
27:B:196:GLU:OE1	27:B:349:ARG:NH1	2.35	0.59
32:f:494:ARG:NH2	32:f:495:GLU:H	2.00	0.59
15:U:583:MET:SD	15:U:601:ARG:NH1	2.75	0.59
5:k:99:HIS:HB2	5:k:107:MET:HE3	1.84	0.59
9:o:18:THR:HB	9:o:31:CYS:H	1.67	0.59
11:Q:21:ALA:HB3	11:Q:29:LYS:HB3	1.84	0.59
14:T:43:MET:HE3	14:T:45:VAL:HG22	1.85	0.59
7:m:47:PHE:HB2	7:m:214:SER:HB3	1.85	0.59
10:p:107:PRO:HG2	10:p:124:LEU:HB2	1.84	0.59
18:Y:98:SER:HB3	18:Y:130:LYS:HE2	1.83	0.59
3:i:16:GLY:N	4:j:21:TYR:OH	2.33	0.59
30:E:290:LEU:O	30:E:298:LYS:NZ	2.31	0.59
7:M:170:GLN:HA	7:M:173:LYS:HE2	1.84	0.59
20:a:349:MET:O	20:a:353:LEU:HB2	2.03	0.59
29:D:92:PHE:HA	29:D:103:VAL:HG12	1.83	0.59
29:D:231:VAL:HB	29:D:234:GLU:HB2	1.84	0.59
32:f:389:LYS:HG2	32:f:418:LEU:CD1	2.32	0.59
5:K:70:ILE:HD11	5:K:89:ILE:HD12	1.85	0.59
8:N:7:GLN:HA	8:N:12:VAL:HA	1.85	0.59
15:U:742:HIS:O	15:U:883:ARG:NH2	2.35	0.59
18:Y:248:GLU:O	25:X:143:TYR:OH	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:176:GLN:HG3	22:c:177:THR:HG23	1.83	0.59
8:n:91:ARG:O	8:n:93:ASP:N	2.35	0.59
26:A:222:LYS:NZ	34:A:501:AGS:S1G	2.76	0.59
28:C:141:GLU:O	29:D:323:ARG:NH1	2.36	0.59
10:P:191:GLU:OE2	10:P:194:LYS:NZ	2.35	0.59
11:Q:104:LEU:HB2	11:Q:116:TYR:HB2	1.82	0.59
15:U:12:LEU:HB3	15:U:20:LYS:HE3	1.85	0.59
15:U:221:ILE:HD13	15:U:754:HIS:HB2	1.85	0.59
16:V:37:MET:HE3	16:V:41:ALA:HB2	1.84	0.58
17:W:385:SER:O	17:W:389:SER:N	2.35	0.58
17:W:389:SER:O	17:W:393:LEU:HB2	2.02	0.58
21:b:142:ASN:HD21	21:b:153:LEU:HD22	1.68	0.58
32:f:456:ARG:HD3	32:f:489:TYR:OH	2.03	0.58
20:a:268:LEU:HD23	20:a:271:LYS:HD3	1.86	0.58
13:s:148:LEU:HD23	13:s:178:VAL:HG12	1.85	0.58
32:f:438:ASP:N	32:f:438:ASP:OD1	2.35	0.58
32:f:782:HIS:HA	32:f:785:ARG:HG2	1.83	0.58
32:f:541:THR:O	32:f:545:LYS:HB2	2.02	0.58
32:f:494:ARG:CZ	32:f:496:ASP:H	2.16	0.58
32:f:618:GLU:HG2	32:f:623:LYS:HD2	1.85	0.58
8:N:178:ALA:HB3	8:N:185:GLU:HB2	1.85	0.58
13:S:148:LEU:HD23	13:S:178:VAL:HG12	1.85	0.58
16:V:197:THR:HB	16:V:200:ARG:HG3	1.85	0.58
18:Y:141:VAL:HG13	18:Y:160:ASN:HB2	1.84	0.58
18:Y:165:LYS:HG2	18:Y:168:ILE:HD12	1.86	0.58
28:C:160:GLU:OE1	28:C:313:ARG:NH2	2.32	0.58
32:f:378:ASN:O	32:f:381:VAL:CG1	2.49	0.58
16:V:440:LYS:NZ	23:d:143:LEU:O	2.36	0.58
18:Y:66:ASP:O	18:Y:71:ASN:N	2.29	0.58
2:h:222:THR:OG1	2:h:225:GLU:OE1	2.21	0.58
8:n:120:MET:H	14:t:61:GLN:HE22	1.51	0.58
1:G:11:ARG:O	1:G:24:GLN:NE2	2.35	0.58
17:W:110:THR:O	17:W:114:GLU:HB3	2.04	0.58
32:f:337:LEU:HD22	32:f:337:LEU:N	2.17	0.58
10:P:58:THR:OG1	11:Q:121:LEU:O	2.15	0.58
17:W:36:LYS:HE3	17:W:85:GLU:HB2	1.85	0.58
26:A:333:ARG:NH1	26:A:336:ARG:HH21	1.99	0.58
15:U:107:HIS:HA	15:U:110:LYS:HE3	1.86	0.58
16:V:99:ARG:HH22	16:V:151:THR:HG23	1.68	0.58
18:Y:225:TYR:HA	18:Y:228:MET:HE3	1.86	0.58
27:B:109:VAL:HG11	28:C:94:LYS:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:182:GLN:HE21	28:C:287:LYS:HG3	1.67	0.58
32:f:89:MET:HG2	32:f:90:THR:HG23	1.84	0.58
32:f:378:ASN:CB	32:f:391:LEU:HD11	2.33	0.58
16:V:473:GLN:HE22	19:Z:253:THR:HG23	1.69	0.58
16:V:476:PHE:HA	16:V:479:ARG:HB2	1.86	0.58
17:W:439:VAL:HB	22:c:229:LEU:HD13	1.86	0.58
18:Y:174:TRP:O	18:Y:178:ASN:ND2	2.37	0.58
25:X:130:GLU:HB3	25:X:153:LEU:HD21	1.86	0.58
2:H:10:LEU:HD23	2:H:125:GLY:HA2	1.86	0.57
16:V:106:ARG:O	16:V:110:HIS:ND1	2.36	0.57
17:W:257:GLN:HG3	17:W:259:GLU:H	1.69	0.57
17:W:440:ASN:O	17:W:444:HIS:ND1	2.37	0.57
18:Y:119:GLY:O	18:Y:123:ALA:HB3	2.03	0.57
7:m:163:CYS:SG	7:m:164:ALA:N	2.76	0.57
16:V:314:ARG:O	18:Y:379:ARG:NH1	2.31	0.57
17:W:172:GLU:OE1	17:W:182:ARG:NH2	2.37	0.57
17:W:375:MET:HB2	17:W:413:ILE:HG23	1.87	0.57
20:a:148:VAL:HB	20:a:151:VAL:HG12	1.85	0.57
20:a:247:ARG:HE	20:a:251:LEU:HB2	1.69	0.57
2:h:34:PRO:HA	2:h:164:GLY:HA3	1.86	0.57
5:k:70:ILE:HD11	5:k:89:ILE:HD12	1.85	0.57
11:q:140:LEU:O	11:q:144:ASP:HB2	2.04	0.57
34:E:401:AGS:O1A	31:F:344:ARG:NH1	2.37	0.57
32:f:780:PRO:O	32:f:800:LEU:HG	2.03	0.57
18:Y:156:LEU:HD23	18:Y:159:ARG:HD3	1.86	0.57
9:o:174:ASP:OD2	9:o:187:ARG:NH1	2.38	0.57
26:A:63:THR:HA	32:f:613:LEU:HD11	1.86	0.57
32:f:358:PHE:CE1	32:f:381:VAL:HG21	2.40	0.57
11:q:117:TYR:HB3	11:q:125:ALA:HB3	1.86	0.57
27:B:253:SER:O	28:C:271:ARG:NH1	2.38	0.57
30:E:340:GLY:CA	34:E:401:AGS:C8	2.68	0.57
32:f:22:GLY:O	32:f:26:GLU:HB2	2.04	0.57
10:P:107:PRO:HG2	10:P:124:LEU:HB2	1.86	0.57
23:d:164:THR:HA	23:d:167:ILE:HG12	1.85	0.57
6:l:189:LYS:HA	6:l:192:LEU:HG	1.87	0.57
27:B:133:VAL:HB	27:B:158:ALA:HA	1.85	0.57
30:E:56:ILE:HB	30:E:100:LEU:HB2	1.87	0.57
30:E:339:ASN:H	30:E:342:ASP:HB2	1.68	0.57
32:f:337:LEU:CD1	32:f:420:TRP:HZ3	2.04	0.57
32:f:378:ASN:HB3	32:f:391:LEU:CD2	2.34	0.57
7:M:35:THR:HA	7:M:166:GLY:HA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:159:ASP:N	10:P:159:ASP:OD1	2.36	0.57
3:i:143:TYR:HB2	3:i:146:GLN:HE21	1.69	0.57
6:l:41:LYS:NZ	6:l:180:MET:O	2.35	0.57
4:j:109:ARG:NH2	12:r:70:ASN:OD1	2.37	0.57
25:X:167:VAL:HA	25:X:170:GLN:HB2	1.86	0.57
32:f:127:SER:O	32:f:131:MET:CB	2.52	0.57
32:f:353:LEU:H	32:f:387:GLN:HG2	1.68	0.57
32:f:695:ALA:CB	32:f:752:HIS:CB	2.82	0.57
7:M:180:GLN:HB3	7:M:184:MET:HE3	1.86	0.57
10:P:15:LYS:HE3	10:P:121:ILE:HG12	1.86	0.57
15:U:646:PRO:O	15:U:650:TYR:HB2	2.04	0.57
34:D:501:AGS:S1G	30:E:291:ARG:NH2	2.77	0.57
32:f:780:PRO:HB2	32:f:800:LEU:HB3	1.86	0.57
10:P:26:ARG:HH21	10:P:38:ASP:HA	1.70	0.57
15:U:549:ALA:HB1	15:U:581:SER:HB2	1.86	0.57
20:a:54:ASP:HA	20:a:57:ILE:HG22	1.85	0.57
5:k:203:LYS:HA	5:k:206:MET:HG2	1.85	0.57
4:J:74:ALA:HB2	4:J:161:ILE:HD13	1.86	0.57
5:K:125:GLU:HG3	5:K:134:SER:HB2	1.86	0.57
10:P:27:ARG:NH1	10:P:180:VAL:O	2.38	0.57
17:W:428:TRP:O	17:W:432:LEU:HB2	2.03	0.57
9:o:112:SER:HB3	9:o:125:VAL:HG11	1.87	0.57
12:R:138:VAL:HG23	11:q:145:ARG:HD2	1.85	0.56
2:h:212:ILE:HD11	2:h:219:ARG:HD3	1.86	0.56
1:G:70:PHE:HD2	1:G:91:VAL:HG21	1.70	0.56
2:H:65:VAL:HG11	2:H:211:GLY:HA3	1.88	0.56
16:V:148:ARG:HH22	16:V:197:THR:HG21	1.69	0.56
23:d:75:MET:HE2	23:d:102:ASN:HB2	1.87	0.56
1:g:120:ASP:OD1	2:h:84:ARG:NH1	2.38	0.56
28:C:66:LEU:HD23	29:D:114:ARG:HE	1.70	0.56
4:J:116:GLN:NE2	4:J:150:SER:O	2.38	0.56
8:N:18:SER:HB2	8:N:31:THR:H	1.70	0.56
15:U:376:MET:HA	15:U:739:ALA:HA	1.87	0.56
16:V:86:VAL:HG12	16:V:118:GLN:HG2	1.87	0.56
16:V:330:LYS:HG3	16:V:358:MET:HB3	1.87	0.56
17:W:52:LYS:NZ	17:W:96:GLN:O	2.35	0.56
17:W:388:GLU:O	17:W:392:PHE:HB2	2.05	0.56
18:Y:154:ASN:ND2	24:e:41:ASP:OD1	2.38	0.56
20:a:70:ARG:HG2	21:b:17:ARG:HB3	1.87	0.56
32:f:140:LEU:O	32:f:144:LEU:HB2	2.04	0.56
32:f:269:ALA:HB2	32:f:277:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:456:ARG:HB3	32:f:489:TYR:CZ	2.39	0.56
32:f:487:LEU:HD23	32:f:524:MET:HE1	1.85	0.56
32:f:742:ALA:CA	32:f:745:LEU:HD21	2.32	0.56
16:V:470:ARG:HD3	16:V:473:GLN:HE21	1.71	0.56
20:a:217:LEU:O	20:a:226:ARG:NH1	2.38	0.56
22:c:220:LEU:O	22:c:224:SER:HB2	2.05	0.56
3:i:123:GLN:NE2	4:j:79:ASP:OD1	2.38	0.56
4:j:115:LYS:HE2	4:j:149:PRO:HA	1.88	0.56
32:f:226:TYR:O	32:f:230:CYS:CB	2.53	0.56
32:f:494:ARG:CZ	32:f:495:GLU:H	2.17	0.56
32:f:684:PRO:O	32:f:688:ARG:CB	2.54	0.56
32:f:780:PRO:HB2	32:f:800:LEU:CB	2.36	0.56
6:L:157:ARG:HD2	6:L:176:MET:HE3	1.87	0.56
14:T:27:LEU:HD22	14:T:184:TYR:HB2	1.87	0.56
6:l:26:MET:HE1	6:l:148:CYS:HB2	1.86	0.56
14:t:27:LEU:HD22	14:t:184:TYR:HB2	1.88	0.56
25:X:292:GLN:OE1	25:X:296:ASN:ND2	2.39	0.56
30:E:194:ASN:ND2	30:E:228:CYS:SG	2.79	0.56
30:E:287:PRO:HA	30:E:290:LEU:HB2	1.86	0.56
32:f:380:PHE:CG	32:f:751:TYR:HE2	2.24	0.56
2:H:12:THR:OG1	3:I:20:GLN:NE2	2.38	0.56
26:A:241:ILE:HB	26:A:244:GLU:HG3	1.87	0.56
26:A:302:LEU:O	26:A:306:LEU:HB2	2.05	0.56
29:D:87:LEU:HB2	30:E:80:VAL:HB	1.88	0.56
32:f:88:SER:HB2	32:f:92:VAL:CG2	2.33	0.56
32:f:742:ALA:CA	32:f:745:LEU:CD2	2.61	0.56
17:W:104:MET:SD	17:W:123:ARG:NH2	2.78	0.56
23:d:5:LEU:HD22	23:d:25:ARG:HG2	1.87	0.56
29:D:45:LYS:O	29:D:49:GLN:NE2	2.38	0.56
10:P:29:GLY:HA3	10:P:34:MET:HA	1.88	0.56
13:S:73:LYS:O	13:S:77:HIS:ND1	2.36	0.56
16:V:57:ALA:H	28:C:38:LYS:HE2	1.70	0.56
32:f:317:LEU:O	32:f:321:MET:HB2	2.05	0.56
32:f:471:LEU:HD12	32:f:509:LYS:CE	2.36	0.56
32:f:536:SER:O	32:f:540:GLN:HB2	2.05	0.56
32:f:688:ARG:HH12	32:f:788:MET:HA	1.71	0.56
5:k:160:GLY:O	6:l:82:ARG:NH2	2.38	0.56
12:r:177:TYR:OH	12:r:186:ARG:NH2	2.37	0.56
32:f:695:ALA:CB	32:f:752:HIS:HB2	2.31	0.56
1:G:128:ASN:HA	2:H:127:VAL:HG12	1.86	0.56
7:M:99:ARG:NH2	7:M:105:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:383:GLY:HA2	16:V:386:PHE:HB2	1.86	0.56
22:c:59:GLY:HA2	22:c:70:ILE:HG22	1.88	0.56
5:k:228:MET:N	5:k:228:MET:SD	2.79	0.56
17:W:390:GLU:HB3	25:X:344:ARG:HD3	1.88	0.55
17:W:401:THR:HG23	17:W:402:ILE:HD12	1.88	0.55
24:e:3:GLU:HG2	24:e:4:LYS:H	1.71	0.55
1:g:27:TYR:HA	1:g:30:LYS:HZ3	1.70	0.55
4:J:32:ALA:HB2	4:J:45:VAL:HG23	1.87	0.55
13:S:210:LEU:O	13:S:212:LYS:NZ	2.34	0.55
17:W:439:VAL:HG11	22:c:232:GLN:HG2	1.87	0.55
21:b:51:LEU:HD11	21:b:61:LEU:HB2	1.89	0.55
3:i:38:LEU:HG	3:i:160:LYS:HB3	1.88	0.55
8:n:35:THR:OG1	8:n:45:ARG:NH2	2.39	0.55
32:f:623:LYS:O	32:f:627:GLU:CB	2.54	0.55
32:f:692:LEU:HD12	32:f:748:LEU:HD23	1.84	0.55
32:f:742:ALA:HA	32:f:745:LEU:HG	1.87	0.55
32:f:742:ALA:CA	32:f:745:LEU:HG	2.35	0.55
5:K:46:VAL:HG23	5:K:151:PRO:HB2	1.89	0.55
14:T:178:TYR:OH	14:T:208:ASN:N	2.35	0.55
15:U:68:PHE:HB3	15:U:73:ALA:HB3	1.88	0.55
15:U:465:LEU:O	15:U:474:ARG:NH1	2.39	0.55
28:C:113:ARG:NH2	28:C:129:ASN:O	2.40	0.55
32:f:376:PHE:CD1	32:f:416:MET:CE	2.83	0.55
3:I:25:MET:HA	3:I:28:ILE:HD12	1.89	0.55
15:U:46:GLU:OE2	15:U:80:TYR:OH	2.24	0.55
24:e:63:HIS:HA	24:e:66:LYS:HG3	1.87	0.55
2:h:42:ASN:ND2	2:h:183:GLU:OE1	2.38	0.55
32:f:80:ARG:O	32:f:84:SER:HB3	2.07	0.55
32:f:426:LEU:O	32:f:430:ASP:HB3	2.07	0.55
2:H:181:ASP:OD1	2:H:181:ASP:N	2.38	0.55
7:M:214:SER:OG	7:M:224:HIS:NE2	2.39	0.55
9:O:140:ASP:OD1	14:t:171:ARG:NH2	2.40	0.55
17:W:222:LEU:O	17:W:226:TYR:N	2.39	0.55
1:g:47:CYS:HA	1:g:221:THR:HA	1.89	0.55
3:i:161:ALA:HB1	3:i:175:LEU:HD13	1.89	0.55
13:s:5:TYR:OH	13:s:103:PRO:O	2.24	0.55
32:f:575:ALA:O	32:f:579:ALA:HB2	2.07	0.55
13:S:68:ILE:HD11	13:S:92:LEU:HD13	1.88	0.55
15:U:325:MET:HB2	15:U:329:LEU:HD12	1.87	0.55
16:V:259:LEU:HD13	16:V:294:ARG:HH21	1.72	0.55
16:V:391:THR:HG23	16:V:394:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:426:ASN:O	17:W:430:GLN:HB3	2.06	0.55
2:H:222:THR:OG1	2:H:225:GLU:OE1	2.21	0.55
19:Z:195:VAL:O	19:Z:199:LYS:HB2	2.06	0.55
21:b:57:ASP:HB3	21:b:59:GLU:HG3	1.89	0.55
4:j:115:LYS:NZ	4:j:129:ILE:O	2.40	0.55
7:m:67:PHE:HB2	7:m:75:MET:HB2	1.87	0.55
7:m:201:HIS:HE1	7:m:206:ASP:HB2	1.72	0.55
27:B:362:LYS:HE2	27:B:380:LEU:HB2	1.87	0.55
3:I:91:ARG:NH1	10:P:76:LEU:O	2.40	0.55
1:g:83:MET:SD	1:g:132:ARG:NH1	2.73	0.55
29:D:280:GLY:HA2	29:D:283:ARG:HE	1.71	0.55
30:E:146:ARG:NH1	30:E:150:GLU:OE1	2.40	0.55
22:c:144:VAL:HB	22:c:158:ASP:HB3	1.88	0.55
23:d:238:PRO:HA	23:d:241:GLU:HG2	1.88	0.55
11:q:181:ARG:NH1	11:q:190:ASP:OD1	2.40	0.55
32:f:278:VAL:HA	32:f:281:ILE:HG22	1.89	0.55
32:f:353:LEU:HG	32:f:387:GLN:CG	2.36	0.55
32:f:780:PRO:CB	32:f:800:LEU:CA	2.79	0.55
19:Z:181:ASP:OD1	19:Z:181:ASP:N	2.39	0.55
9:o:1:THR:HG23	9:o:33:LYS:HE3	1.90	0.55
10:p:62:THR:OG1	11:q:85:ARG:NH2	2.40	0.55
25:X:324:ALA:O	25:X:328:ASP:HB2	2.07	0.55
27:B:254:GLU:O	27:B:257:GLN:NE2	2.40	0.55
15:U:229:VAL:HG22	15:U:268:LEU:HD21	1.87	0.54
15:U:522:GLY:O	15:U:559:ARG:NH2	2.40	0.54
16:V:137:GLU:HA	16:V:140:ASP:HB2	1.89	0.54
18:Y:283:LYS:C	18:Y:285:ASP:N	2.65	0.54
18:Y:294:TYR:O	18:Y:298:GLU:HB2	2.06	0.54
6:l:39:LYS:HE2	6:l:157:ARG:HA	1.89	0.54
32:f:8:LYS:O	32:f:12:GLN:HB2	2.08	0.54
4:J:36:ARG:NH1	4:J:142:PRO:O	2.39	0.54
9:O:172:ASN:HB3	9:O:191:VAL:HG22	1.90	0.54
12:R:141:ARG:HH12	11:q:162:LYS:HB3	1.71	0.54
3:i:140:ASP:OD1	3:i:144:GLY:N	2.41	0.54
5:k:209:LYS:O	5:k:214:ASN:ND2	2.40	0.54
14:t:1:THR:N	14:t:105:PRO:O	2.39	0.54
32:f:586:PRO:HA	32:f:589:SER:HB2	1.89	0.54
3:I:136:TYR:HB2	3:I:148:TYR:HB2	1.89	0.54
10:P:190:ILE:HG22	10:P:195:ILE:HG23	1.88	0.54
15:U:789:ILE:HG22	15:U:791:LEU:HB2	1.88	0.54
19:Z:40:LEU:HA	19:Z:91:ILE:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:210:ASN:O	22:c:214:GLN:N	2.38	0.54
22:c:268:GLU:HG3	25:X:409:LYS:HE3	1.88	0.54
26:A:245:LEU:HD12	26:A:280:ILE:HG12	1.89	0.54
32:f:229:VAL:O	32:f:233:LEU:HB2	2.06	0.54
17:W:82:LEU:O	17:W:86:ASN:CB	2.53	0.54
20:a:70:ARG:HH21	21:b:17:ARG:HD2	1.73	0.54
20:a:90:PRO:O	20:a:94:LEU:N	2.39	0.54
20:a:186:LYS:O	20:a:193:GLN:NE2	2.40	0.54
21:b:137:ASN:ND2	21:b:165:GLY:O	2.39	0.54
4:j:115:LYS:HE3	4:j:127:PHE:HB2	1.89	0.54
26:A:47:GLN:N	32:f:185:LEU:CD1	2.70	0.54
26:A:284:ARG:HD2	31:F:334:ARG:HD3	1.90	0.54
32:f:229:VAL:O	32:f:233:LEU:CB	2.56	0.54
32:f:281:ILE:O	32:f:285:CYS:CB	2.56	0.54
32:f:714:SER:C	32:f:718:ASP:HB2	2.33	0.54
6:L:158:ALA:HB1	6:L:172:LEU:HD22	1.90	0.54
7:M:37:ILE:HD11	7:M:193:VAL:HG13	1.89	0.54
8:N:96:ALA:HB1	8:N:98:ILE:HG12	1.89	0.54
18:Y:215:ASP:O	18:Y:218:THR:OG1	2.25	0.54
18:Y:293:ARG:HH12	24:e:57:ARG:HG3	1.72	0.54
7:m:173:LYS:HA	7:m:176:ILE:HB	1.89	0.54
15:U:733:ALA:O	15:U:737:LEU:HB2	2.07	0.54
17:W:339:ASP:O	17:W:350:ARG:NH1	2.41	0.54
20:a:214:GLY:HA2	20:a:217:LEU:HD13	1.89	0.54
8:n:127:ILE:HB	8:n:132:SER:HB2	1.89	0.54
10:p:58:THR:OG1	11:q:121:LEU:O	2.22	0.54
30:E:226:GLN:HG3	30:E:272:ARG:HD2	1.89	0.54
32:f:358:PHE:HZ	32:f:381:VAL:HG21	1.66	0.54
32:f:377:VAL:HG22	32:f:751:TYR:HB2	1.88	0.54
32:f:663:GLY:O	32:f:697:ILE:HB	2.07	0.54
15:U:494:TYR:O	15:U:498:LYS:NZ	2.36	0.54
18:Y:326:GLY:HA2	18:Y:329:PHE:HB2	1.89	0.54
19:Z:82:PHE:HA	19:Z:85:VAL:HG12	1.90	0.54
23:d:175:ARG:HD3	23:d:178:ILE:HD12	1.89	0.54
23:d:178:ILE:HG21	23:d:198:LEU:HD21	1.90	0.54
5:k:48:LEU:HD21	5:k:77:ALA:HB2	1.88	0.54
10:p:189:ILE:HG23	10:p:196:THR:HB	1.89	0.54
26:A:54:GLN:CB	27:B:69:LYS:CB	2.86	0.54
29:D:412:GLN:H	29:D:413:GLU:HA	1.73	0.54
30:E:60:VAL:HA	30:E:71:VAL:HG12	1.90	0.54
32:f:8:LYS:O	32:f:12:GLN:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:15:GLN:NE2	32:f:47:GLU:OE1	2.41	0.54
32:f:253:LEU:O	32:f:257:ARG:HB2	2.07	0.54
32:f:273:ASN:ND2	32:f:310:ASP:OD2	2.41	0.54
32:f:403:LYS:O	32:f:407:MET:N	2.40	0.54
15:U:623:GLY:HA3	15:U:658:ILE:HG13	1.90	0.54
15:U:639:LEU:HD21	28:C:50:ASN:HB3	1.90	0.54
16:V:452:ASN:HB3	16:V:457:TYR:HB2	1.90	0.54
17:W:135:LYS:HA	17:W:140:ILE:HB	1.89	0.54
17:W:403:PHE:HD2	17:W:417:ARG:HB2	1.72	0.54
28:C:78:ARG:NH1	28:C:79:ALA:O	2.41	0.54
30:E:182:LEU:HD22	34:E:401:AGS:H2'	1.88	0.54
32:f:688:ARG:HA	32:f:745:LEU:CD2	2.38	0.54
4:J:131:ALA:H	4:J:147:THR:HG1	1.54	0.54
15:U:524:LYS:NZ	15:U:562:GLU:O	2.34	0.54
15:U:584:TYR:OH	15:U:768:GLN:NE2	2.41	0.54
16:V:443:ARG:NH2	23:d:181:CYS:SG	2.81	0.54
7:m:123:THR:HG22	7:m:130:PRO:HB3	1.89	0.54
9:o:124:TYR:OH	9:o:139:GLU:OE1	2.25	0.54
25:X:379:ASP:H	25:X:385:LEU:HD13	1.73	0.54
31:F:94:ILE:HD11	31:F:125:LYS:HB2	1.90	0.54
10:p:2:SER:OG	10:p:3:ILE:N	2.38	0.54
29:D:248:ARG:HG2	29:D:295:GLN:HE22	1.73	0.54
30:E:244:SER:HB2	31:F:300:LYS:HA	1.90	0.54
32:f:211:ILE:O	32:f:215:ASP:CB	2.56	0.54
30:E:210:GLU:OE2	30:E:213:ARG:NH2	2.39	0.53
32:f:80:ARG:O	32:f:84:SER:CB	2.57	0.53
4:j:120:GLN:HE22	5:k:135:ARG:HG2	1.74	0.53
9:o:35:HIS:NE2	9:o:53:ASP:OD1	2.41	0.53
32:f:314:TYR:CE1	32:f:490:ALA:HB3	2.43	0.53
2:H:66:GLU:OE2	2:H:91:ARG:NH2	2.41	0.53
2:H:119:GLN:NE2	2:H:123:GLN:OE1	2.40	0.53
9:O:174:ASP:OD2	9:O:187:ARG:NH1	2.40	0.53
15:U:455:GLY:H	15:U:457:ILE:HG12	1.73	0.53
20:a:244:ASN:HB3	20:a:275:LEU:HB3	1.89	0.53
23:d:203:PRO:HD2	23:d:206:MET:HG2	1.91	0.53
4:j:116:GLN:NE2	5:k:84:ASP:OD1	2.40	0.53
7:m:37:ILE:HD11	7:m:193:VAL:HG13	1.91	0.53
25:X:163:LYS:HA	25:X:166:LEU:HD13	1.91	0.53
32:f:76:GLU:OE1	32:f:79:ARG:NH2	2.41	0.53
32:f:138:GLU:O	32:f:142:TYR:CB	2.55	0.53
3:I:62:SER:OG	3:I:65:ILE:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:50:LYS:HE2	6:L:61:LYS:HA	1.91	0.53
7:M:235:ALA:O	7:M:239:ALA:N	2.39	0.53
13:S:125:ASP:OD1	13:S:129:SER:N	2.41	0.53
14:T:171:ARG:NH2	9:o:140:ASP:OD1	2.41	0.53
18:Y:209:THR:HA	18:Y:213:LEU:HD12	1.90	0.53
20:a:49:CYS:SG	20:a:50:PHE:N	2.82	0.53
3:i:62:SER:OG	3:i:65:ILE:O	2.27	0.53
26:A:90:GLU:HA	26:A:93:LEU:HD23	1.89	0.53
28:C:132:ASP:HB3	28:C:135:VAL:HB	1.90	0.53
32:f:313:GLU:O	32:f:317:LEU:CB	2.55	0.53
32:f:515:ALA:HB1	32:f:558:LEU:HD21	1.91	0.53
5:K:221:GLN:HB2	5:K:224:GLN:HB3	1.89	0.53
15:U:444:TYR:HB2	15:U:476:GLY:HA3	1.91	0.53
16:V:89:LYS:HD3	16:V:92:ARG:HH11	1.74	0.53
1:g:53:GLN:HA	1:g:215:ILE:HA	1.90	0.53
2:h:118:MET:HE2	2:h:151:PRO:HA	1.91	0.53
29:D:367:PRO:HD2	29:D:413:GLU:HG3	1.91	0.53
32:f:336:GLU:CG	32:f:337:LEU:HD22	2.36	0.53
32:f:477:MET:O	32:f:481:SER:CB	2.56	0.53
5:K:55:THR:HG21	26:A:430:MET:HE2	1.89	0.53
5:K:228:MET:N	5:K:228:MET:SD	2.81	0.53
18:Y:336:ARG:O	18:Y:340:ALA:HB2	2.08	0.53
7:m:214:SER:OG	7:m:224:HIS:NE2	2.42	0.53
26:A:48:VAL:HA	32:f:188:VAL:HG21	1.90	0.53
6:L:72:ILE:HG22	6:L:134:ILE:HG12	1.90	0.53
7:M:51:LYS:O	7:M:210:GLU:N	2.39	0.53
9:O:112:SER:HB3	9:O:125:VAL:HG11	1.90	0.53
15:U:607:VAL:O	15:U:615:ARG:NH1	2.41	0.53
15:U:765:VAL:HG13	15:U:775:LEU:HD22	1.90	0.53
5:k:93:ARG:NH1	12:r:68:LEU:O	2.41	0.53
5:k:167:ALA:HB3	5:k:181:LEU:HD21	1.90	0.53
6:l:148:CYS:SG	6:l:152:ASN:N	2.81	0.53
32:f:311:VAL:CB	32:f:490:ALA:CB	2.77	0.53
32:f:366:ASP:O	32:f:367:SER:CB	2.57	0.53
19:Z:229:GLN:NE2	20:a:337:GLN:OE1	2.42	0.53
21:b:30:GLN:HG3	21:b:75:LEU:HD22	1.91	0.53
3:i:218:ARG:NH1	3:i:223:THR:OG1	2.35	0.53
6:l:65:HIS:O	6:l:89:ARG:NH2	2.42	0.53
30:E:67:GLU:HG3	30:E:68:LYS:HG3	1.90	0.53
18:Y:333:GLU:HA	18:Y:336:ARG:HH21	1.74	0.53
20:a:73:PRO:HG3	20:a:104:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:122:SER:O	1:g:126:THR:OG1	2.25	0.53
13:s:125:ASP:OD1	13:s:129:SER:N	2.40	0.53
25:X:126:ARG:NH2	25:X:130:GLU:OE2	2.42	0.53
27:B:317:ASP:HB2	27:B:346:ARG:HG2	1.91	0.53
32:f:24:THR:HG22	32:f:71:TYR:HB2	1.91	0.53
32:f:306:GLU:HB3	32:f:339:ILE:HD12	1.91	0.53
11:Q:171:PHE:HB3	11:Q:173:LEU:H	1.74	0.53
18:Y:191:ILE:HG21	24:e:40:GLU:HB3	1.91	0.53
23:d:45:LYS:HG2	23:d:48:LEU:HD12	1.90	0.53
5:k:37:ALA:HB2	5:k:50:VAL:HG23	1.91	0.53
8:n:144:ARG:H	8:n:147:MET:HE3	1.73	0.53
32:f:479:LEU:CD2	32:f:513:GLU:HB3	2.39	0.53
32:f:691:PRO:HB3	32:f:749:ALA:CB	2.39	0.53
5:K:85:ALA:HB2	5:K:139:VAL:HG21	1.90	0.52
6:L:26:MET:HE1	6:L:148:CYS:HB2	1.91	0.52
15:U:731:ILE:HD12	15:U:734:GLN:HB2	1.89	0.52
16:V:237:THR:OG1	16:V:241:ARG:NH2	2.35	0.52
17:W:320:LEU:HD21	17:W:354:LEU:HD21	1.91	0.52
3:i:47:ALA:HB3	3:i:212:GLU:HB3	1.91	0.52
29:D:212:LYS:NZ	34:D:501:AGS:O3G	2.42	0.52
32:f:600:TYR:HB3	32:f:608:LYS:HE2	1.91	0.52
4:J:88:ARG:NH1	11:Q:69:MET:O	2.43	0.52
6:L:73:SER:HB3	6:L:133:LEU:HB2	1.91	0.52
14:T:28:GLY:HA3	14:T:36:PHE:HB2	1.89	0.52
16:V:267:ALA:HA	16:V:270:LEU:HG	1.91	0.52
19:Z:173:GLU:HB2	22:c:152:LYS:HB2	1.91	0.52
20:a:34:TRP:HD1	21:b:18:ASN:HB2	1.74	0.52
21:b:161:ASN:HD22	21:b:166:THR:HA	1.75	0.52
32:f:537:THR:OG1	32:f:538:ILE:N	2.42	0.52
3:I:105:ILE:HD11	3:I:109:GLN:HG3	1.92	0.52
15:U:82:LEU:O	15:U:129:ARG:NH1	2.42	0.52
18:Y:192:ARG:NH2	18:Y:291:HIS:O	2.42	0.52
4:j:7:ILE:HG22	4:j:18:GLN:HG3	1.90	0.52
14:t:28:GLY:HA3	14:t:36:PHE:HB2	1.91	0.52
25:X:119:SER:O	25:X:121:LYS:NZ	2.38	0.52
30:E:340:GLY:HA2	34:E:401:AGS:C5	2.39	0.52
31:F:230:GLY:HA3	31:F:392:ASN:HD22	1.75	0.52
7:M:8:ASP:O	7:M:22:GLN:NE2	2.35	0.52
17:W:372:ARG:O	20:a:327:VAL:N	2.42	0.52
31:F:180:ARG:HH22	31:F:245:LYS:HG2	1.73	0.52
15:U:462:LEU:HD23	15:U:481:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:349:MET:O	20:a:353:LEU:CB	2.57	0.52
27:B:125:THR:OG1	27:B:126:SER:N	2.42	0.52
32:f:612:LEU:O	32:f:616:CYS:CB	2.56	0.52
1:G:141:ILE:HG22	1:G:151:VAL:HG22	1.91	0.52
5:K:37:ALA:HB2	5:K:50:VAL:HG23	1.90	0.52
18:Y:12:PRO:O	18:Y:146:ARG:NH1	2.36	0.52
18:Y:147:ILE:HA	18:Y:150:PHE:HD2	1.73	0.52
22:c:253:LYS:NZ	25:X:394:ASP:OD1	2.42	0.52
22:c:301:ALA:HA	22:c:304:LEU:HG	1.91	0.52
32:f:632:LYS:HD2	32:f:661:ALA:HA	1.92	0.52
8:N:14:LEU:HB2	8:N:177:ALA:HB3	1.92	0.52
15:U:389:ASN:HB3	15:U:392:TRP:HE3	1.75	0.52
15:U:688:LEU:HD22	15:U:713:TYR:HE1	1.75	0.52
23:d:5:LEU:HD21	23:d:54:ILE:HG21	1.92	0.52
2:h:86:LEU:HD13	2:h:134:LEU:HD11	1.92	0.52
7:m:235:ALA:O	7:m:239:ALA:N	2.40	0.52
26:A:414:ASN:HA	26:A:418:LYS:HD3	1.92	0.52
32:f:641:GLU:HG3	32:f:641:GLU:O	2.09	0.52
5:K:41:GLN:NE2	5:K:151:PRO:O	2.42	0.52
15:U:14:GLU:HG2	15:U:16:GLU:H	1.74	0.52
17:W:72:LYS:HD2	17:W:123:ARG:HD3	1.91	0.52
19:Z:265:LEU:O	19:Z:268:SER:OG	2.27	0.52
25:X:70:LEU:HD22	25:X:109:LEU:HD23	1.91	0.52
32:f:262:PHE:HB3	32:f:281:ILE:HD11	1.91	0.52
10:P:58:THR:O	11:Q:85:ARG:NH2	2.43	0.52
15:U:456:ASP:O	15:U:460:TYR:CB	2.56	0.52
15:U:490:ARG:HE	15:U:492:ASP:H	1.57	0.52
16:V:153:LYS:O	16:V:157:THR:OG1	2.28	0.52
19:Z:170:VAL:HA	22:c:152:LYS:HA	1.92	0.52
32:f:127:SER:O	32:f:131:MET:HB3	2.10	0.52
32:f:378:ASN:HB3	32:f:391:LEU:CD1	2.39	0.52
32:f:392:THR:HG22	32:f:417:ILE:HD13	1.92	0.52
15:U:661:ALA:HA	15:U:694:ILE:HD12	1.91	0.52
16:V:82:LEU:HA	16:V:87:SER:HB2	1.92	0.52
18:Y:51:ALA:HA	18:Y:54:TYR:HB3	1.92	0.52
9:o:2:THR:HG23	9:o:131:SER:HA	1.92	0.52
25:X:324:ALA:HA	25:X:327:TYR:HB3	1.90	0.52
28:C:147:THR:OG1	28:C:206:HIS:NE2	2.38	0.52
32:f:647:GLY:HA2	32:f:655:LEU:HG	1.92	0.52
13:S:5:TYR:OH	13:S:103:PRO:O	2.27	0.51
10:p:26:ARG:HH21	10:p:38:ASP:HA	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:295:ARG:HH22	31:F:311:LEU:HD21	1.73	0.51
32:f:463:LEU:HD22	32:f:466:LEU:CD1	2.40	0.51
32:f:485:LEU:HD12	32:f:488:ALA:HB3	1.92	0.51
32:f:523:GLY:O	32:f:527:VAL:N	2.43	0.51
18:Y:228:MET:SD	18:Y:295:TYR:OH	2.69	0.51
22:c:36:LEU:HD11	22:c:71:ASP:HA	1.92	0.51
6:l:65:HIS:HA	6:l:221:PHE:HE2	1.75	0.51
28:C:325:ARG:HD3	28:C:353:GLY:HA2	1.90	0.51
29:D:167:ILE:HG12	29:D:214:MET:HE3	1.93	0.51
29:D:384:MET:HE2	30:E:159:PHE:HD1	1.75	0.51
32:f:268:LEU:O	32:f:272:LEU:HB2	2.10	0.51
32:f:800:LEU:N	32:f:800:LEU:CD1	2.73	0.51
4:J:211:MET:HG2	4:J:213:ARG:H	1.75	0.51
11:Q:38:MET:O	11:Q:65:GLN:NE2	2.43	0.51
23:d:150:LYS:HD2	23:d:153:LEU:HB2	1.92	0.51
12:R:158:ARG:HG2	11:q:145:ARG:HE	1.75	0.51
16:V:285:TRP:HD1	16:V:315:LYS:HE2	1.76	0.51
22:c:187:PRO:HG2	22:c:189:ILE:HB	1.91	0.51
34:F:501:AGS:O1B	34:F:501:AGS:O2G	2.27	0.51
32:f:336:GLU:HG3	32:f:337:LEU:H	1.76	0.51
12:R:158:ARG:HH12	12:R:199:TYR:HB3	1.76	0.51
9:o:113:ILE:HG12	9:o:119:THR:HG22	1.92	0.51
14:t:43:MET:HE3	14:t:45:VAL:HG22	1.93	0.51
25:X:345:VAL:HG23	25:X:353:LEU:HD21	1.93	0.51
28:C:131:VAL:HG13	28:C:133:PRO:HD3	1.91	0.51
17:W:139:GLU:O	17:W:143:ALA:N	2.40	0.51
18:Y:266:CYS:SG	18:Y:306:GLN:NE2	2.83	0.51
3:i:91:ARG:NH1	10:p:76:LEU:O	2.44	0.51
30:E:262:ASN:O	30:E:266:GLY:N	2.44	0.51
32:f:301:HIS:O	32:f:305:LEU:CB	2.53	0.51
32:f:623:LYS:O	32:f:627:GLU:HB2	2.11	0.51
16:V:159:LEU:HD12	16:V:178:SER:HB3	1.93	0.51
16:V:345:ARG:HD3	16:V:361:PHE:HA	1.93	0.51
17:W:379:ALA:HA	17:W:382:LEU:HD12	1.92	0.51
7:m:152:ASP:OD1	7:m:156:VAL:N	2.42	0.51
25:X:337:ARG:NH2	25:X:353:LEU:O	2.41	0.51
34:E:401:AGS:O2G	34:E:401:AGS:O2B	2.28	0.51
31:F:202:ILE:HG23	31:F:327:LYS:HD3	1.93	0.51
31:F:408:LEU:HD12	31:F:411:GLY:HA2	1.93	0.51
32:f:468:ASP:OD2	32:f:475:ASN:N	2.42	0.51
32:f:502:LEU:HG	32:f:540:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:635:LYS:HZ3	32:f:641:GLU:CG	2.21	0.51
6:L:50:LYS:HB3	6:L:59:HIS:HB3	1.91	0.51
15:U:249:CYS:O	15:U:253:TYR:HB2	2.10	0.51
25:X:375:HIS:ND1	25:X:389:ASP:OD2	2.41	0.51
28:C:338:LEU:HD13	28:C:342:ILE:HG21	1.93	0.51
29:D:255:LYS:HA	29:D:303:VAL:HG11	1.91	0.51
32:f:531:ASN:HA	32:f:569:LYS:HA	1.93	0.51
32:f:556:ARG:NH1	32:f:786:GLN:OE1	2.44	0.51
4:J:115:LYS:HE2	4:J:149:PRO:HA	1.92	0.51
11:Q:4:LEU:HD12	11:Q:45:LEU:HB3	1.93	0.51
15:U:147:TYR:OH	15:U:171:ASN:OD1	2.27	0.51
16:V:187:ILE:HA	16:V:191:LEU:HD13	1.91	0.51
22:c:252:ALA:O	22:c:256:ASN:ND2	2.44	0.51
23:d:236:THR:O	23:d:239:SER:OG	2.21	0.51
6:l:120:THR:O	7:m:129:ARG:NH1	2.28	0.51
14:t:96:MET:HE1	14:t:106:LEU:HB2	1.93	0.51
25:X:222:GLU:HA	25:X:225:TRP:HE1	1.76	0.51
31:F:313:LEU:O	31:F:317:LEU:HB2	2.11	0.51
32:f:343:LYS:NZ	32:f:804:LEU:HD23	2.26	0.51
32:f:380:PHE:CG	32:f:751:TYR:CE2	2.99	0.51
5:K:219:THR:HB	5:K:221:GLN:HE22	1.75	0.51
15:U:541:HIS:HB2	15:U:544:ILE:HG22	1.93	0.51
17:W:124:LEU:HD22	17:W:147:LYS:HD2	1.92	0.51
22:c:98:MET:O	22:c:102:THR:OG1	2.25	0.51
13:s:169:ASP:OD2	13:s:173:ARG:NH1	2.44	0.51
34:A:501:AGS:O1B	34:A:501:AGS:O2A	2.28	0.51
27:B:315:GLN:OE1	27:B:322:ARG:NH1	2.42	0.51
31:F:251:LEU:HD11	31:F:256:LEU:HD21	1.92	0.51
32:f:440:ILE:O	32:f:444:ALA:HB2	2.10	0.51
5:K:33:LEU:HD13	26:A:432:TYR:CG	2.46	0.50
14:T:141:TYR:HA	14:T:144:TYR:HD2	1.75	0.50
16:V:235:LEU:O	16:V:239:THR:OG1	2.25	0.50
17:W:55:ARG:HH11	17:W:75:TYR:HB3	1.76	0.50
17:W:186:ILE:HD11	17:W:208:LYS:HG3	1.93	0.50
21:b:22:LEU:O	21:b:24:THR:N	2.44	0.50
6:l:109:VAL:HG21	6:l:145:PHE:HD2	1.75	0.50
10:p:113:ASP:HB2	10:p:118:LYS:HB3	1.93	0.50
32:f:804:LEU:N	32:f:804:LEU:CD1	2.74	0.50
1:G:53:GLN:HA	1:G:215:ILE:HA	1.93	0.50
4:J:11:SER:OG	4:J:15:HIS:N	2.44	0.50
7:M:36:ALA:O	7:M:165:ILE:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:13:LEU:HD11	13:S:149:LEU:HD11	1.93	0.50
15:U:772:TRP:HD1	15:U:775:LEU:HG	1.76	0.50
16:V:80:LYS:HE2	16:V:118:GLN:HE22	1.75	0.50
16:V:418:SER:HA	16:V:458:VAL:HB	1.93	0.50
25:X:134:VAL:HB	25:X:149:LEU:HD23	1.92	0.50
26:A:143:ASP:HB3	26:A:148:GLN:H	1.75	0.50
31:F:294:LYS:N	31:F:337:ILE:O	2.44	0.50
32:f:463:LEU:HD22	32:f:466:LEU:HD11	1.93	0.50
32:f:536:SER:HA	32:f:539:LEU:HB3	1.93	0.50
2:H:99:LEU:O	2:H:102:GLN:NE2	2.45	0.50
5:K:99:HIS:HB2	5:K:107:MET:HE3	1.94	0.50
11:Q:37:LYS:O	11:Q:61:GLN:NE2	2.38	0.50
15:U:685:GLN:NE2	15:U:725:MET:O	2.44	0.50
16:V:126:ALA:HB1	16:V:130:PHE:HB2	1.92	0.50
16:V:309:MET:HE3	16:V:332:LEU:HG	1.93	0.50
19:Z:269:VAL:O	19:Z:273:HIS:ND1	2.41	0.50
8:n:167:ASP:HB3	8:n:170:SER:HB2	1.92	0.50
28:C:246:ILE:HB	28:C:291:VAL:HG12	1.92	0.50
9:O:163:ILE:HA	9:O:168:GLY:HA3	1.93	0.50
12:R:196:HIS:O	12:R:200:SER:CB	2.60	0.50
17:W:422:ASN:HD21	17:W:425:LEU:HB3	1.76	0.50
21:b:53:THR:HG22	21:b:59:GLU:H	1.77	0.50
3:i:90:LEU:HD12	3:i:114:LEU:HD22	1.93	0.50
3:i:171:ALA:HB2	3:i:200:THR:HG21	1.94	0.50
4:j:11:SER:OG	4:j:15:HIS:N	2.40	0.50
9:o:84:LYS:HE2	9:o:119:THR:HG21	1.93	0.50
26:A:48:VAL:CB	32:f:231:LEU:CD1	2.72	0.50
29:D:408:LYS:HE3	30:E:389:VAL:HB	1.92	0.50
32:f:337:LEU:N	32:f:337:LEU:CD2	2.73	0.50
32:f:343:LYS:O	32:f:347:ASP:N	2.40	0.50
32:f:455:VAL:HG12	32:f:457:ASN:H	1.76	0.50
32:f:691:PRO:HA	32:f:694:LEU:HB3	1.93	0.50
10:P:203:ARG:HH12	12:r:191:ASN:HD21	1.60	0.50
18:Y:13:LYS:HG2	18:Y:143:TYR:HE1	1.77	0.50
7:m:40:ARG:HA	7:m:45:VAL:HA	1.94	0.50
29:D:88:VAL:HG23	29:D:132:LEU:HB2	1.93	0.50
32:f:517:VAL:O	32:f:521:ALA:CB	2.60	0.50
15:U:493:VAL:HA	15:U:497:LEU:HD13	1.94	0.50
16:V:283:ASN:ND2	24:e:1:MET:O	2.44	0.50
17:W:406:VAL:HA	17:W:413:ILE:HB	1.94	0.50
18:Y:142:PHE:HA	18:Y:145:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:294:TYR:HB2	24:e:52:PHE:HZ	1.75	0.50
22:c:55:GLY:HA3	22:c:112:TYR:CZ	2.47	0.50
23:d:170:LEU:HA	23:d:173:THR:HG22	1.94	0.50
25:X:46:LYS:HD3	25:X:49:SER:HB3	1.93	0.50
26:A:333:ARG:CZ	34:F:501:AGS:O1A	2.59	0.50
30:E:180:LYS:NZ	34:E:401:AGS:O1B	2.45	0.50
30:E:237:ALA:HB1	31:F:308:ARG:HG3	1.94	0.50
32:f:745:LEU:HD12	32:f:745:LEU:C	2.36	0.50
7:M:144:ASP:O	7:M:147:GLN:NE2	2.43	0.50
16:V:179:LYS:HD2	16:V:214:HIS:CD2	2.46	0.50
19:Z:33:LYS:HE2	19:Z:34:ARG:HG2	1.92	0.50
20:a:72:ASN:ND2	20:a:108:ASP:OD2	2.45	0.50
22:c:39:LEU:HD23	22:c:42:LEU:HD21	1.93	0.50
13:s:68:ILE:HD11	13:s:92:LEU:HD13	1.93	0.50
27:B:411:ARG:NH2	27:B:418:ASP:OD2	2.45	0.50
30:E:57:VAL:HG13	30:E:97:ARG:HD3	1.94	0.50
32:f:347:ASP:O	32:f:351:THR:OG1	2.25	0.50
32:f:479:LEU:HA	32:f:517:VAL:HG21	1.93	0.50
15:U:237:VAL:HA	15:U:321:GLN:HE21	1.76	0.50
16:V:227:VAL:O	16:V:231:LEU:CB	2.59	0.50
17:W:169:LEU:O	17:W:208:LYS:NZ	2.45	0.50
19:Z:265:LEU:HD21	25:X:396:THR:HG23	1.93	0.50
20:a:25:LEU:HD13	20:a:40:GLN:HG2	1.93	0.50
20:a:122:LYS:HA	20:a:125:ILE:HG12	1.93	0.50
1:g:97:GLU:HA	1:g:100:ASN:HD22	1.77	0.50
26:A:245:LEU:HB3	26:A:298:THR:HG21	1.94	0.50
31:F:169:ASP:HB2	31:F:172:VAL:HG23	1.94	0.50
32:f:337:LEU:HD22	32:f:337:LEU:H	1.75	0.50
32:f:790:GLN:HG3	32:f:792:ALA:H	1.75	0.50
6:L:189:LYS:HG3	6:L:193:ARG:HH12	1.77	0.50
10:P:113:ASP:HB2	10:P:118:LYS:HB3	1.93	0.50
14:T:136:SER:HB2	14:T:150:LEU:HD13	1.94	0.50
15:U:11:LEU:HA	23:d:73:ARG:HD2	1.94	0.50
15:U:261:LEU:HA	15:U:264:VAL:HG12	1.93	0.50
3:i:7:SER:OG	3:i:8:ARG:N	2.45	0.50
7:m:76:ALA:HB3	7:m:136:MET:HB2	1.94	0.50
11:q:135:GLY:O	11:q:139:THR:OG1	2.27	0.50
31:F:392:ASN:OD1	31:F:395:GLN:N	2.41	0.50
32:f:392:THR:CG2	32:f:417:ILE:HD13	2.42	0.50
2:H:148:GLN:OE1	2:H:158:TRP:NE1	2.45	0.49
16:V:185:GLN:O	16:V:189:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:234:ARG:HG3	16:V:250:LEU:HD11	1.93	0.49
17:W:105:VAL:HG11	17:W:143:ALA:HB1	1.94	0.49
17:W:268:LYS:HA	17:W:271:VAL:HG12	1.94	0.49
22:c:262:GLU:HA	22:c:265:MET:HG2	1.93	0.49
3:i:25:MET:HA	3:i:28:ILE:HD12	1.94	0.49
4:j:36:ARG:HB2	4:j:142:PRO:HB2	1.94	0.49
29:D:199:PRO:HB3	29:D:328:ASP:HB2	1.93	0.49
30:E:177:GLY:HA2	31:F:344:ARG:HH11	1.76	0.49
32:f:226:TYR:O	32:f:230:CYS:HB2	2.11	0.49
32:f:376:PHE:CZ	32:f:798:THR:CB	2.91	0.49
9:O:30:ASN:OD1	9:O:187:ARG:NH2	2.45	0.49
13:S:123:SER:HB3	13:S:136:LYS:HG3	1.95	0.49
15:U:82:LEU:HD21	15:U:130:LEU:HD23	1.93	0.49
15:U:205:TYR:HD2	15:U:215:ASN:HB3	1.77	0.49
15:U:465:LEU:HD11	15:U:477:GLY:HA3	1.95	0.49
16:V:131:LEU:HD23	16:V:134:PHE:HD2	1.77	0.49
16:V:239:THR:HG22	16:V:240:LEU:HG	1.94	0.49
16:V:335:VAL:HA	16:V:338:LEU:HB2	1.94	0.49
3:i:232:GLU:HA	3:i:235:GLN:HG2	1.94	0.49
27:B:223:ILE:HD12	27:B:350:LYS:HG3	1.93	0.49
31:F:368:ILE:HG12	31:F:371:ARG:HH22	1.77	0.49
9:O:50:ALA:HB2	10:P:129:CYS:HB2	1.93	0.49
9:O:98:LEU:HB2	9:O:113:ILE:HB	1.94	0.49
17:W:425:LEU:HA	17:W:428:TRP:HB2	1.94	0.49
3:i:3:ARG:NH2	6:l:9:ASP:OD1	2.45	0.49
8:n:127:ILE:HG21	8:n:136:TYR:HB2	1.94	0.49
26:A:406:GLU:HA	26:A:409:PHE:HD2	1.77	0.49
30:E:43:SER:OG	31:F:75:GLU:OE1	2.21	0.49
32:f:234:THR:HG23	32:f:637:LYS:HE2	1.94	0.49
32:f:376:PHE:CZ	32:f:416:MET:CE	2.95	0.49
32:f:478:ARG:NE	32:f:504:VAL:HG22	2.27	0.49
32:f:517:VAL:O	32:f:521:ALA:HB3	2.12	0.49
2:H:100:VAL:HG13	10:P:93:ASN:HD22	1.76	0.49
7:M:168:ALA:HB1	7:M:171:ALA:HB3	1.94	0.49
14:T:145:LEU:HB3	14:T:179:ARG:HH21	1.77	0.49
15:U:366:HIS:O	15:U:369:THR:OG1	2.29	0.49
17:W:317:TRP:HD1	17:W:358:VAL:HG11	1.77	0.49
12:r:122:SER:OG	12:r:123:GLY:N	2.45	0.49
30:E:139:SER:HA	30:E:142:ILE:HD12	1.95	0.49
15:U:616:ARG:HH21	15:U:647:HIS:HA	1.76	0.49
16:V:132:LEU:HD23	16:V:135:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:139:GLU:HB3	17:W:142:ARG:HB2	1.94	0.49
17:W:374:THR:HG23	20:a:327:VAL:HA	1.94	0.49
8:n:96:ALA:HB1	8:n:98:ILE:HG12	1.93	0.49
11:q:19:ARG:HH21	11:q:31:ASP:HB2	1.76	0.49
11:q:47:VAL:O	11:q:101:ASN:N	2.44	0.49
25:X:337:ARG:NH1	25:X:340:GLU:OE1	2.44	0.49
25:X:389:ASP:OD1	25:X:389:ASP:N	2.45	0.49
28:C:210:THR:N	28:C:243:PRO:O	2.39	0.49
32:f:336:GLU:HB3	32:f:337:LEU:HD23	1.95	0.49
32:f:691:PRO:HG2	32:f:745:LEU:CD1	2.41	0.49
2:H:10:LEU:O	2:H:124:SER:OG	2.23	0.49
15:U:13:ASP:OD2	23:d:73:ARG:NH1	2.45	0.49
16:V:90:GLU:HB3	16:V:131:LEU:HD21	1.94	0.49
19:Z:67:VAL:HG13	21:b:92:VAL:HG23	1.93	0.49
19:Z:139:ILE:O	19:Z:156:GLU:N	2.44	0.49
10:p:159:ASP:N	10:p:159:ASP:OD1	2.46	0.49
26:A:249:TYR:HB3	31:F:259:MET:HG3	1.94	0.49
32:f:389:LYS:HD2	32:f:418:LEU:HD21	1.92	0.49
2:H:71:HIS:HA	2:H:218:PHE:H	1.77	0.49
10:P:101:GLY:O	11:Q:93:ARG:NH1	2.46	0.49
16:V:42:ALA:O	16:V:62:HIS:ND1	2.46	0.49
21:b:122:LYS:HA	21:b:125:VAL:HG12	1.94	0.49
7:M:36:ALA:N	7:M:165:ILE:O	2.41	0.49
7:M:202:ASP:N	7:M:202:ASP:OD1	2.46	0.49
7:M:228:PRO:HB2	7:M:231:ILE:HB	1.95	0.49
10:P:2:SER:OG	10:P:3:ILE:N	2.46	0.49
16:V:283:ASN:HD21	24:e:2:SER:HA	1.78	0.49
17:W:315:MET:HE1	17:W:320:LEU:HD13	1.95	0.49
21:b:1:MET:HB3	21:b:44:ASN:HB2	1.93	0.49
9:o:19:ARG:HB2	9:o:169:SER:HA	1.94	0.49
32:f:343:LYS:HZ2	32:f:804:LEU:HD23	1.77	0.49
5:K:182:GLN:NE2	6:L:55:GLU:OE1	2.46	0.49
5:K:210:LEU:HD11	5:K:215:ILE:HG12	1.94	0.49
16:V:377:GLN:O	16:V:381:GLN:HB3	2.13	0.49
17:W:97:LEU:HD11	17:W:130:MET:HB3	1.95	0.49
17:W:235:GLN:NE2	17:W:339:ASP:OD2	2.45	0.49
12:r:38:ASN:HD22	12:r:41:LEU:HD12	1.77	0.49
26:A:94:GLN:NE2	26:A:143:ASP:OD1	2.43	0.49
27:B:303:ARG:O	27:B:307:ARG:NH2	2.46	0.49
27:B:361:LYS:HD2	27:B:384:ILE:HG12	1.93	0.49
29:D:175:GLN:NE2	29:D:179:GLU:OE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:94:LYS:HA	32:f:97:LYS:HG2	1.94	0.49
5:K:177:ALA:O	5:K:181:LEU:HB2	2.13	0.49
9:O:37:ILE:HD13	9:O:60:SER:HB2	1.94	0.49
12:R:97:MET:O	12:R:116:SER:N	2.43	0.49
15:U:895:PRO:HD2	15:U:902:PRO:HD2	1.93	0.49
17:W:34:LEU:HD22	17:W:47:LEU:HD13	1.95	0.49
20:a:220:PRO:HA	20:a:223:GLU:HG2	1.94	0.49
4:j:33:VAL:HG12	4:j:160:ALA:HA	1.95	0.49
6:l:46:LEU:HD13	6:l:73:SER:HB2	1.94	0.49
28:C:217:SER:HB3	28:C:220:VAL:HG23	1.95	0.49
32:f:597:VAL:HG22	32:f:630:ASP:HB2	1.95	0.49
3:I:232:GLU:HA	3:I:235:GLN:HG2	1.95	0.48
14:T:187:PHE:O	14:T:203:LEU:N	2.45	0.48
17:W:144:ARG:HA	17:W:147:LYS:HE2	1.93	0.48
20:a:214:GLY:O	20:a:241:ASN:ND2	2.46	0.48
25:X:411:VAL:HA	25:X:414:LEU:HD12	1.94	0.48
29:D:119:ILE:O	29:D:121:ARG:NH1	2.45	0.48
8:N:29:ARG:NH1	9:O:139:GLU:OE1	2.39	0.48
15:U:661:ALA:HB3	15:U:746:ILE:HD11	1.95	0.48
16:V:353:LEU:HD11	16:V:359:PRO:HD3	1.94	0.48
17:W:273:TYR:HA	17:W:276:LEU:HD13	1.95	0.48
5:k:157:ASP:OD2	5:k:159:SER:OG	2.30	0.48
29:D:313:ARG:HG3	29:D:315:ASP:H	1.77	0.48
32:f:372:LEU:C	32:f:372:LEU:CD2	2.86	0.48
32:f:387:GLN:N	32:f:387:GLN:NE2	2.60	0.48
32:f:657:ILE:HA	32:f:660:ILE:HD12	1.94	0.48
6:L:44:ALA:HB1	6:L:144:ILE:HD11	1.95	0.48
12:R:9:ARG:NH2	12:R:146:ASP:OD1	2.33	0.48
17:W:382:LEU:HB3	17:W:384:LEU:HG	1.95	0.48
18:Y:177:ARG:HA	18:Y:180:LEU:HD13	1.95	0.48
19:Z:213:GLU:O	19:Z:217:THR:C	2.55	0.48
32:f:140:LEU:O	32:f:144:LEU:CB	2.61	0.48
32:f:487:LEU:HD22	32:f:801:VAL:HG11	1.95	0.48
8:N:127:ILE:HD13	8:N:136:TYR:HB2	1.95	0.48
14:T:115:TYR:HE2	14:T:194:GLU:HB3	1.78	0.48
17:W:69:ALA:HB1	17:W:73:MET:HE3	1.95	0.48
17:W:428:TRP:HA	17:W:432:LEU:HD13	1.96	0.48
19:Z:266:ILE:HG21	22:c:291:LEU:HD22	1.95	0.48
20:a:277:LEU:HA	20:a:280:MET:HE3	1.94	0.48
2:h:93:LEU:HD11	2:h:113:ARG:HB3	1.95	0.48
7:m:35:THR:HA	7:m:166:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:178:ALA:HB3	8:n:185:GLU:HB2	1.94	0.48
29:D:268:ASP:OD1	29:D:316:THR:OG1	2.30	0.48
31:F:222:GLY:HA3	31:F:348:LEU:HA	1.94	0.48
3:I:245:ALA:HA	3:I:248:GLU:HG2	1.96	0.48
5:K:211:ASN:OD1	5:K:214:ASN:ND2	2.47	0.48
8:N:104:ASP:N	8:N:108:GLY:O	2.43	0.48
9:O:2:THR:HG23	9:O:131:SER:HA	1.95	0.48
11:Q:117:TYR:HB3	11:Q:125:ALA:HB3	1.95	0.48
15:U:710:ARG:HG2	15:U:737:LEU:HD21	1.94	0.48
17:W:267:LEU:HA	17:W:270:VAL:HG12	1.94	0.48
20:a:226:ARG:NH2	20:a:238:TYR:OH	2.47	0.48
6:l:189:LYS:HZ2	6:l:193:ARG:HH12	1.59	0.48
25:X:330:LEU:HA	25:X:333:GLN:HB2	1.96	0.48
26:A:200:ARG:HD3	31:F:408:LEU:HD11	1.96	0.48
26:A:415:LYS:O	26:A:419:SER:HB2	2.13	0.48
32:f:30:GLY:O	32:f:34:ARG:HB2	2.14	0.48
11:Q:4:LEU:HD22	11:Q:18:ASP:H	1.78	0.48
15:U:598:ALA:O	15:U:602:LEU:HB2	2.14	0.48
16:V:112:VAL:HA	16:V:115:LYS:HE3	1.95	0.48
23:d:244:LYS:HA	23:d:247:ILE:HD12	1.95	0.48
6:l:225:ASP:OD1	6:l:225:ASP:N	2.46	0.48
11:q:164:LEU:O	11:q:168:GLN:NE2	2.46	0.48
30:E:275:MET:HB3	30:E:277:MET:HE2	1.95	0.48
32:f:253:LEU:O	32:f:257:ARG:CB	2.61	0.48
32:f:389:LYS:HB3	32:f:392:THR:HG21	1.95	0.48
32:f:453:SER:O	32:f:488:ALA:O	2.31	0.48
12:R:166:ARG:NH2	10:p:34:MET:O	2.47	0.48
16:V:102:PRO:O	16:V:105:SER:OG	2.31	0.48
18:Y:103:ALA:O	18:Y:107:LYS:NZ	2.41	0.48
24:e:49:GLU:OE2	24:e:53:SER:OG	2.32	0.48
5:k:211:ASN:OD1	5:k:214:ASN:ND2	2.47	0.48
9:o:30:ASN:OD1	9:o:187:ARG:NH2	2.46	0.48
26:A:329:PRO:HA	26:A:332:MET:HB2	1.96	0.48
27:B:201:VAL:HG21	27:B:328:ILE:HD11	1.95	0.48
32:f:127:SER:O	32:f:131:MET:HB2	2.13	0.48
11:Q:19:ARG:HH21	11:Q:31:ASP:HB2	1.79	0.48
15:U:353:LEU:O	15:U:357:LYS:HB2	2.13	0.48
6:l:52:ALA:HB2	6:l:59:HIS:CD2	2.48	0.48
9:o:163:ILE:HA	9:o:168:GLY:HA3	1.94	0.48
12:r:97:MET:O	12:r:116:SER:N	2.45	0.48
25:X:177:TYR:O	25:X:182:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:236:GLU:HG3	5:K:239:LYS:HE3	1.95	0.48
6:L:189:LYS:HA	6:L:192:LEU:HG	1.94	0.48
9:O:113:ILE:HG12	9:O:119:THR:HG22	1.94	0.48
16:V:393:THR:HB	16:V:397:ARG:HH22	1.78	0.48
22:c:227:GLU:HB2	22:c:230:THR:HA	1.95	0.48
26:A:96:ALA:HB3	27:B:132:TYR:HB2	1.95	0.48
29:D:176:GLU:OE2	29:D:329:ARG:NH1	2.47	0.48
32:f:336:GLU:CG	32:f:337:LEU:CD2	2.92	0.48
32:f:456:ARG:HD3	32:f:489:TYR:CZ	2.49	0.48
8:N:35:THR:OG1	8:N:45:ARG:NH2	2.46	0.48
12:R:97:MET:HB3	12:R:116:SER:HB3	1.96	0.48
15:U:249:CYS:O	15:U:253:TYR:CB	2.62	0.48
15:U:341:PHE:O	15:U:345:ASN:CB	2.57	0.48
15:U:701:ILE:HG21	15:U:810:THR:HG22	1.96	0.48
17:W:247:TYR:HA	17:W:250:ILE:HG23	1.94	0.48
24:e:59:GLU:HG3	24:e:60:LEU:HD22	1.95	0.48
3:i:83:ALA:HB2	3:i:132:VAL:HG11	1.96	0.48
7:m:197:ILE:HG21	7:m:211:LEU:HD13	1.95	0.48
14:t:145:LEU:HB3	14:t:179:ARG:HH21	1.79	0.48
26:A:97:ARG:HE	27:B:131:HIS:HE1	1.62	0.48
32:f:252:ALA:O	32:f:256:PHE:HB2	2.14	0.48
6:L:59:HIS:ND1	6:L:208:LYS:O	2.39	0.47
12:R:19:ARG:HH21	12:R:29:GLN:HE22	1.62	0.47
16:V:88:GLY:H	16:V:118:GLN:HE21	1.62	0.47
23:d:134:LYS:HA	23:d:137:VAL:HG22	1.96	0.47
8:n:7:GLN:HA	8:n:12:VAL:HA	1.96	0.47
14:t:25:ASP:HA	14:t:187:PHE:HA	1.96	0.47
32:f:178:LYS:NZ	32:f:215:ASP:O	2.42	0.47
32:f:315:GLU:HA	32:f:318:THR:HG22	1.95	0.47
32:f:559:PRO:HA	32:f:562:LEU:HB2	1.96	0.47
32:f:688:ARG:CA	32:f:745:LEU:HD22	2.44	0.47
7:M:230:ASP:OD1	7:M:230:ASP:N	2.46	0.47
16:V:362:LEU:HD21	16:V:374:LYS:HE3	1.96	0.47
17:W:218:ASN:ND2	17:W:220:GLU:O	2.46	0.47
1:g:165:ALA:HB3	2:h:56:LEU:HD22	1.96	0.47
2:h:139:TRP:HA	2:h:144:PRO:HA	1.96	0.47
26:A:211:GLY:HA3	26:A:337:LEU:HA	1.96	0.47
32:f:675:PHE:O	32:f:679:LEU:CB	2.59	0.47
2:H:6:TYR:OH	2:H:13:PHE:O	2.31	0.47
11:Q:118:MET:HE1	11:Q:124:LEU:HD23	1.95	0.47
17:W:124:LEU:HA	17:W:127:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:161:GLU:CD	17:W:162:ALA:H	2.22	0.47
20:a:293:PHE:HB3	20:a:329:LYS:HB3	1.96	0.47
2:h:50:LYS:NZ	2:h:62:VAL:O	2.47	0.47
5:k:98:ASN:OD1	12:r:61:ARG:NH2	2.38	0.47
26:A:391:GLU:OE1	27:B:349:ARG:NE	2.48	0.47
32:f:209:MET:SD	32:f:213:GLN:NE2	2.87	0.47
32:f:445:LEU:HG	32:f:462:ALA:HB2	1.95	0.47
15:U:520:MET:HG3	15:U:525:ASN:ND2	2.29	0.47
15:U:571:CYS:HA	15:U:579:ARG:HG2	1.97	0.47
15:U:622:LEU:HD23	15:U:625:ILE:HD11	1.96	0.47
18:Y:16:ASP:HB3	18:Y:146:ARG:HH21	1.79	0.47
20:a:255:TRP:O	20:a:258:GLN:NE2	2.44	0.47
1:g:212:PRO:HB3	1:g:235:ILE:HG22	1.96	0.47
25:X:74:ARG:HH22	25:X:116:TRP:HB2	1.79	0.47
28:C:85:VAL:HG21	28:C:123:LEU:HD11	1.96	0.47
32:f:333:LEU:HA	32:f:338:ASP:HB2	1.94	0.47
32:f:645:ASP:HB3	32:f:648:ALA:HB3	1.95	0.47
5:K:157:ASP:OD2	5:K:159:SER:OG	2.31	0.47
5:K:206:MET:HE1	5:K:210:LEU:HD13	1.97	0.47
19:Z:243:GLN:HE22	22:c:310:LYS:HE2	1.79	0.47
19:Z:278:ASN:O	19:Z:282:ASN:CB	2.55	0.47
20:a:7:PHE:HE2	20:a:57:ILE:HD12	1.78	0.47
21:b:4:GLU:OE2	21:b:40:LYS:NZ	2.47	0.47
22:c:229:LEU:HD23	22:c:231:LEU:HD13	1.94	0.47
23:d:18:LYS:HA	23:d:21:GLU:HB3	1.95	0.47
5:k:84:ASP:OD2	5:k:135:ARG:NH2	2.36	0.47
9:o:11:GLY:HA2	9:o:108:PRO:HB3	1.96	0.47
10:p:113:ASP:N	10:p:118:LYS:O	2.47	0.47
13:s:55:SER:OG	13:s:56:GLY:N	2.48	0.47
14:t:192:VAL:HG12	14:t:197:VAL:HG22	1.97	0.47
28:C:43:ARG:HH21	29:D:57:GLN:HB2	1.78	0.47
29:D:84:SER:OG	29:D:85:ILE:N	2.47	0.47
32:f:166:VAL:O	32:f:170:TRP:HB2	2.14	0.47
32:f:392:THR:HA	32:f:414:LEU:CD2	2.44	0.47
5:K:145:GLY:O	5:K:152:GLN:N	2.36	0.47
6:L:225:ASP:OD1	6:L:225:ASP:N	2.44	0.47
15:U:801:GLN:HA	15:U:841:LYS:HB2	1.97	0.47
2:h:66:GLU:OE2	2:h:91:ARG:NH2	2.48	0.47
7:m:8:ASP:O	7:m:22:GLN:NE2	2.42	0.47
8:n:104:ASP:N	8:n:108:GLY:O	2.44	0.47
30:E:101:ASP:HB3	30:E:105:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:626:GLU:OE1	32:f:782:HIS:NE2	2.47	0.47
3:I:174:MET:SD	3:I:195:LYS:NZ	2.88	0.47
15:U:105:ILE:HA	15:U:108:TYR:HB3	1.97	0.47
15:U:367:THR:HB	15:U:403:THR:HG21	1.97	0.47
15:U:644:TYR:HB3	28:C:57:ARG:NE	2.30	0.47
16:V:234:ARG:HA	16:V:237:THR:HG22	1.97	0.47
16:V:350:GLN:HB3	16:V:353:LEU:HB3	1.97	0.47
19:Z:28:LYS:HG3	19:Z:29:VAL:HG13	1.96	0.47
20:a:73:PRO:HG2	20:a:113:LEU:HD11	1.97	0.47
20:a:285:PRO:HG2	20:a:288:HIS:CE1	2.49	0.47
22:c:30:GLN:HB3	22:c:66:THR:HG22	1.96	0.47
23:d:148:TYR:HE1	23:d:174:ILE:HG23	1.79	0.47
1:g:89:SER:OG	7:m:117:MET:SD	2.64	0.47
4:j:96:LEU:HA	11:q:62:LYS:HE3	1.96	0.47
6:l:157:ARG:HD2	6:l:176:MET:HE3	1.95	0.47
10:p:36:THR:OG1	10:p:38:ASP:OD1	2.26	0.47
10:p:88:MET:HG3	10:p:124:LEU:HD11	1.97	0.47
25:X:173:GLU:HA	25:X:176:THR:HG22	1.96	0.47
29:D:87:LEU:HD22	29:D:131:ALA:HB1	1.96	0.47
29:D:99:ASN:HA	29:D:115:ILE:HG13	1.95	0.47
29:D:249:ASP:OD1	29:D:252:ARG:NH2	2.48	0.47
29:D:284:GLU:HA	29:D:287:ARG:HG2	1.97	0.47
31:F:383:GLU:HG2	31:F:386:ARG:HH22	1.80	0.47
32:f:797:LEU:HD22	32:f:797:LEU:HA	1.76	0.47
6:L:122:ARG:HG2	7:M:128:VAL:HG12	1.97	0.47
9:O:46:ALA:HB3	9:O:97:ALA:HB3	1.96	0.47
15:U:678:ASP:O	15:U:684:ARG:NH1	2.43	0.47
26:A:142:VAL:HG22	26:A:149:ILE:HG12	1.97	0.47
30:E:235:ILE:HD11	30:E:277:MET:HB3	1.96	0.47
32:f:248:LEU:O	32:f:252:ALA:CB	2.62	0.47
7:M:152:ASP:OD2	7:M:154:SER:OG	2.29	0.47
7:M:152:ASP:OD1	7:M:156:VAL:N	2.48	0.47
16:V:78:HIS:HB2	16:V:81:GLN:HG3	1.97	0.47
17:W:187:LEU:HB3	17:W:226:TYR:HE1	1.80	0.47
22:c:73:PHE:O	22:c:112:TYR:OH	2.22	0.47
7:m:27:MET:HA	7:m:153:PRO:HG2	1.97	0.47
7:m:228:PRO:HB2	7:m:231:ILE:HB	1.97	0.47
9:o:17:ASP:OD1	9:o:17:ASP:N	2.47	0.47
26:A:186:LYS:HE2	31:F:409:ARG:HH22	1.79	0.47
34:E:401:AGS:O1A	34:E:401:AGS:O3B	2.33	0.47
32:f:331:LEU:O	32:f:335:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:338:THR:O	17:W:343:SER:N	2.45	0.47
18:Y:314:LEU:HB3	18:Y:354:VAL:HB	1.97	0.47
20:a:185:ILE:HD12	20:a:187:ASP:HB3	1.96	0.47
13:s:123:SER:HB3	13:s:136:LYS:HG3	1.97	0.47
14:t:7:THR:OG1	14:t:182:ARG:NH2	2.45	0.47
25:X:257:CYS:O	25:X:261:LEU:N	2.48	0.47
30:E:385:ASP:OD1	30:E:385:ASP:N	2.46	0.47
32:f:695:ALA:CB	32:f:752:HIS:HB3	2.44	0.47
2:H:107:THR:HA	2:H:110:LEU:HD13	1.97	0.46
13:S:173:ARG:NH1	9:o:200:GLY:O	2.48	0.46
15:U:576:PRO:HG2	15:U:577:ILE:HG12	1.97	0.46
20:a:111:VAL:HG21	20:a:141:MET:HE2	1.97	0.46
21:b:112:PHE:HE1	21:b:141:ILE:HD12	1.80	0.46
21:b:140:ILE:HG21	21:b:153:LEU:HD23	1.98	0.46
3:i:136:TYR:HB2	3:i:148:TYR:HB2	1.97	0.46
25:X:258:LYS:HE3	25:X:270:LEU:HD12	1.97	0.46
26:A:324:PRO:HA	26:A:327:LEU:HD23	1.97	0.46
31:F:313:LEU:O	31:F:317:LEU:CB	2.64	0.46
32:f:79:ARG:HE	32:f:95:PRO:HG3	1.80	0.46
7:M:66:LEU:HD13	7:M:214:SER:HB2	1.97	0.46
9:O:38:SER:OG	9:O:40:ASN:OD1	2.22	0.46
15:U:525:ASN:O	15:U:529:ILE:N	2.42	0.46
18:Y:124:PHE:O	18:Y:128:TYR:HB2	2.15	0.46
23:d:49:ILE:HD11	23:d:89:LEU:HD22	1.97	0.46
1:g:37:LEU:HD23	1:g:81:THR:HA	1.96	0.46
5:k:109:VAL:HG21	5:k:145:GLY:HA3	1.97	0.46
11:q:115:LEU:HD23	11:q:127:ALA:HB3	1.97	0.46
26:A:199:GLU:O	26:A:203:ASN:ND2	2.37	0.46
26:A:255:ARG:HA	26:A:258:ARG:HD2	1.97	0.46
27:B:170:LEU:HB3	27:B:174:MET:HE2	1.98	0.46
32:f:675:PHE:CG	32:f:694:LEU:HD23	2.51	0.46
5:K:134:SER:OG	5:K:135:ARG:N	2.46	0.46
20:a:182:CYS:SG	20:a:183:VAL:N	2.88	0.46
1:g:215:ILE:H	1:g:215:ILE:HG13	1.53	0.46
4:j:38:ARG:NH1	4:j:182:GLU:O	2.40	0.46
13:s:171:ALA:HA	13:s:174:LEU:HD12	1.97	0.46
30:E:198:VAL:HG12	30:E:200:SER:H	1.80	0.46
31:F:250:LYS:HA	31:F:284:PHE:HB3	1.97	0.46
32:f:193:PRO:C	32:f:208:LEU:HD12	2.40	0.46
1:G:84:THR:HB	7:M:156:VAL:HG22	1.98	0.46
12:R:134:TYR:HE2	12:R:167:ASP:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:182:LYS:HB3	16:V:182:LYS:HE3	1.82	0.46
17:W:406:VAL:HG21	25:X:344:ARG:HA	1.98	0.46
18:Y:144:LEU:HA	18:Y:147:ILE:HG22	1.96	0.46
20:a:230:ARG:HE	20:a:233:LEU:HD22	1.81	0.46
20:a:252:LYS:HA	20:a:255:TRP:HB2	1.96	0.46
20:a:292:THR:HA	20:a:330:ARG:HA	1.97	0.46
22:c:100:LYS:HG2	22:c:105:PRO:HB3	1.96	0.46
23:d:106:LEU:HD21	23:d:115:PHE:HA	1.97	0.46
23:d:158:ILE:HG21	23:d:163:TYR:HB2	1.97	0.46
23:d:180:GLY:HA2	23:d:184:LYS:HE3	1.96	0.46
7:m:73:VAL:HG22	7:m:139:SER:HB2	1.97	0.46
7:m:99:ARG:NH2	7:m:105:ASN:OD1	2.48	0.46
7:m:160:TYR:HD2	7:m:163:CYS:HB2	1.80	0.46
26:A:224:LEU:O	26:A:228:ALA:HB2	2.16	0.46
34:E:401:AGS:H8	34:E:401:AGS:H5'1	1.97	0.46
31:F:346:GLY:HA2	31:F:349:ASP:HA	1.97	0.46
32:f:281:ILE:O	32:f:285:CYS:HB3	2.15	0.46
18:Y:377:LEU:HA	18:Y:380:VAL:HG22	1.98	0.46
20:a:296:ILE:O	20:a:300:ALA:CB	2.64	0.46
2:h:65:VAL:HG11	2:h:211:GLY:HA3	1.97	0.46
14:t:122:LEU:HG	14:t:137:LEU:HD12	1.98	0.46
26:A:277:ILE:HG22	26:A:280:ILE:HD12	1.98	0.46
28:C:99:VAL:HB	28:C:103:ILE:HD11	1.97	0.46
29:D:92:PHE:HZ	29:D:95:ALA:HB2	1.80	0.46
32:f:392:THR:HB	32:f:414:LEU:HD22	1.97	0.46
32:f:475:ASN:O	32:f:478:ARG:HB3	2.15	0.46
1:G:208:ILE:HB	1:G:210:PHE:HD2	1.81	0.46
3:I:105:ILE:HG12	3:I:110:LEU:HB2	1.98	0.46
6:L:52:ALA:HB2	6:L:59:HIS:CD2	2.51	0.46
7:M:216:VAL:HB	7:M:224:HIS:CD2	2.50	0.46
15:U:723:ASP:HB3	15:U:726:ALA:HB2	1.96	0.46
15:U:885:MET:HB3	15:U:888:GLN:HB2	1.97	0.46
18:Y:380:VAL:HG12	25:X:414:LEU:HD21	1.96	0.46
19:Z:193:ASN:HA	19:Z:196:HIS:CE1	2.51	0.46
22:c:151:VAL:H	29:D:81:ARG:HH22	1.63	0.46
25:X:320:SER:O	25:X:324:ALA:CB	2.64	0.46
26:A:346:PRO:O	26:A:351:ARG:NH1	2.48	0.46
32:f:479:LEU:HD23	32:f:513:GLU:CB	2.42	0.46
32:f:538:ILE:HA	32:f:541:THR:HG22	1.97	0.46
3:I:33:THR:HG23	3:I:168:SER:HB2	1.97	0.46
3:I:67:LYS:HG3	3:I:225:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:67:SER:HB3	9:O:74:PRO:HG3	1.97	0.46
15:U:397:THR:H	15:U:400:ALA:HB3	1.81	0.46
16:V:179:LYS:HE3	16:V:214:HIS:HA	1.98	0.46
16:V:404:LYS:HA	16:V:407:VAL:HG12	1.98	0.46
17:W:221:LYS:O	17:W:225:LYS:N	2.48	0.46
20:a:194:GLN:HA	20:a:225:LEU:HB3	1.98	0.46
1:g:165:ALA:HB1	1:g:179:LEU:HD13	1.97	0.46
3:i:73:ALA:HB3	3:i:137:ILE:HD11	1.98	0.46
4:j:68:ASN:HA	4:j:211:MET:HE1	1.98	0.46
7:m:144:ASP:O	7:m:147:GLN:NE2	2.45	0.46
26:A:300:LEU:HD23	26:A:303:ILE:HD12	1.98	0.46
34:E:401:AGS:O2B	34:E:401:AGS:O2A	2.34	0.46
32:f:695:ALA:O	32:f:752:HIS:HB3	2.15	0.46
5:K:79:SER:HB2	5:K:170:ILE:HD13	1.98	0.46
9:O:35:HIS:NE2	9:O:53:ASP:OD1	2.48	0.46
10:P:205:ASP:HB3	12:r:192:VAL:HG11	1.98	0.46
12:R:104:TRP:CD2	12:R:181:GLU:HA	2.50	0.46
15:U:383:ASP:O	15:U:387:ARG:NH1	2.48	0.46
16:V:94:VAL:HG11	16:V:134:PHE:HB3	1.97	0.46
18:Y:104:MET:O	18:Y:108:ALA:CB	2.64	0.46
5:k:125:GLU:HG3	5:k:134:SER:HB2	1.97	0.46
8:n:6:VAL:O	8:n:13:VAL:N	2.41	0.46
25:X:167:VAL:HG21	25:X:193:ALA:HA	1.97	0.46
32:f:353:LEU:H	32:f:387:GLN:CG	2.29	0.46
32:f:424:GLY:HA2	32:f:427:THR:HG22	1.96	0.46
12:R:35:ILE:N	12:R:43:GLY:O	2.49	0.46
16:V:51:ALA:HB3	16:V:147:PHE:HE1	1.81	0.46
17:W:320:LEU:HD11	17:W:354:LEU:HD11	1.97	0.46
20:a:132:LYS:O	20:a:136:GLU:HB3	2.16	0.46
4:j:159:ASN:OD1	4:j:160:ALA:N	2.49	0.46
26:A:258:ARG:HG2	26:A:305:GLN:HE22	1.80	0.46
29:D:378:ILE:HG23	29:D:402:ALA:HB1	1.98	0.46
32:f:125:ILE:HA	32:f:129:LEU:HD12	1.98	0.46
32:f:541:THR:O	32:f:545:LYS:CB	2.63	0.46
32:f:635:LYS:NZ	32:f:641:GLU:HG3	2.16	0.46
5:K:192:LYS:HA	5:K:195:ILE:HD12	1.98	0.46
15:U:599:ILE:HG13	29:D:60:TYR:HE2	1.80	0.46
20:a:64:ILE:O	20:a:68:GLU:CB	2.64	0.46
20:a:112:ILE:HB	20:a:151:VAL:HG21	1.98	0.46
20:a:142:LEU:HG	20:a:146:PRO:HB3	1.98	0.46
21:b:131:LEU:HD22	21:b:136:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:220:THR:HG21	26:A:343:PHE:HB3	1.97	0.46
30:E:258:MET:HG2	30:E:261:LEU:HD12	1.98	0.46
1:G:189:TRP:HZ3	1:G:197:THR:HG21	1.81	0.45
3:I:159:TRP:HA	4:J:54:GLN:HB2	1.98	0.45
11:Q:58:GLU:O	11:Q:62:LYS:HB2	2.16	0.45
15:U:748:LEU:HD23	15:U:760:VAL:HG22	1.98	0.45
16:V:46:GLY:HA3	16:V:62:HIS:HD1	1.81	0.45
17:W:116:THR:OG1	17:W:117:ASP:N	2.49	0.45
1:g:109:ILE:HD13	1:g:114:LEU:HD12	1.98	0.45
25:X:57:LEU:HA	25:X:61:GLY:HA3	1.98	0.45
27:B:357:ASP:OD1	27:B:360:THR:OG1	2.24	0.45
8:N:144:ARG:H	8:N:147:MET:HE3	1.82	0.45
15:U:477:GLY:O	15:U:481:LEU:HB2	2.16	0.45
16:V:101:LEU:O	16:V:103:SER:N	2.49	0.45
17:W:377:ARG:HE	20:a:326:GLU:HB3	1.81	0.45
20:a:21:VAL:O	20:a:25:LEU:HB2	2.16	0.45
20:a:176:ALA:O	20:a:180:LEU:CB	2.64	0.45
2:h:76:TYR:HB2	2:h:132:VAL:HG13	1.97	0.45
12:r:144:SER:H	12:r:147:LEU:HD11	1.81	0.45
28:C:168:PRO:HG3	28:C:175:PHE:HE2	1.81	0.45
29:D:355:SER:HB3	29:D:393:ILE:HG23	1.98	0.45
15:U:441:GLY:HA2	15:U:444:TYR:HB3	1.97	0.45
32:f:226:TYR:O	32:f:230:CYS:HB3	2.16	0.45
32:f:376:PHE:CZ	32:f:798:THR:HG22	2.50	0.45
32:f:378:ASN:HB3	32:f:391:LEU:HD21	1.97	0.45
32:f:796:LEU:HD12	32:f:799:VAL:HG11	1.98	0.45
3:I:219:GLU:OE2	3:I:220:ASN:ND2	2.48	0.45
12:R:12:VAL:HB	12:R:179:VAL:HB	1.98	0.45
12:R:196:HIS:O	12:R:200:SER:HB3	2.16	0.45
15:U:195:ASN:HB2	15:U:223:LEU:HD23	1.98	0.45
15:U:697:GLN:NE2	15:U:742:HIS:O	2.50	0.45
15:U:800:VAL:HG21	15:U:914:LEU:HD21	1.97	0.45
15:U:904:LYS:HB3	15:U:913:ILE:HG12	1.97	0.45
20:a:81:LEU:HA	20:a:84:VAL:HG12	1.99	0.45
21:b:121:GLU:HA	21:b:124:LEU:HG	1.99	0.45
23:d:182:ILE:HG22	23:d:213:ARG:NH2	2.32	0.45
23:d:203:PRO:HG2	23:d:205:LYS:HE2	1.98	0.45
1:g:123:GLN:OE1	2:h:128:ARG:NH2	2.49	0.45
7:m:40:ARG:NH1	7:m:146:ALA:O	2.48	0.45
7:m:40:ARG:HE	7:m:161:TRP:CD1	2.33	0.45
25:X:113:CYS:HB3	25:X:129:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:509:LYS:HB3	32:f:514:VAL:HG21	1.99	0.45
32:f:533:ASP:OD1	32:f:565:ASN:ND2	2.50	0.45
6:L:45:VAL:HG11	6:L:188:VAL:HG22	1.98	0.45
7:M:40:ARG:HE	7:M:161:TRP:CD1	2.34	0.45
7:M:160:TYR:HD2	7:M:163:CYS:HB2	1.81	0.45
9:O:136:ALA:HB2	14:t:179:ARG:HH22	1.81	0.45
15:U:559:ARG:NH1	15:U:562:GLU:OE1	2.49	0.45
17:W:253:THR:O	17:W:257:GLN:N	2.45	0.45
26:A:400:ARG:O	26:A:400:ARG:CG	2.65	0.45
32:f:45:LEU:HD22	32:f:86:THR:HG21	1.99	0.45
32:f:664:GLU:HB3	32:f:696:LEU:CG	2.43	0.45
5:K:167:ALA:H	6:L:56:LEU:HD13	1.82	0.45
8:N:120:MET:H	14:T:61:GLN:HE22	1.65	0.45
13:S:26:ASP:OD1	13:S:26:ASP:N	2.47	0.45
15:U:898:CYS:SG	15:U:899:ARG:N	2.89	0.45
17:W:183:VAL:HG21	17:W:223:LYS:HE3	1.98	0.45
20:a:92:VAL:O	20:a:95:THR:OG1	2.31	0.45
27:B:222:VAL:HG13	27:B:351:ILE:HD12	1.99	0.45
28:C:375:ARG:HH21	28:C:377:HIS:HB2	1.81	0.45
29:D:45:LYS:HD3	29:D:45:LYS:HA	1.80	0.45
29:D:338:ARG:HH12	29:D:365:ALA:HA	1.80	0.45
31:F:97:LEU:O	31:F:120:LYS:N	2.49	0.45
32:f:664:GLU:C	32:f:665:GLU:O	2.59	0.45
32:f:688:ARG:HG3	32:f:745:LEU:HB3	1.99	0.45
3:I:140:ASP:OD1	3:I:144:GLY:N	2.48	0.45
6:L:41:LYS:NZ	6:L:180:MET:O	2.47	0.45
8:N:19:ARG:NH1	8:N:170:SER:O	2.49	0.45
11:Q:19:ARG:HE	11:Q:31:ASP:HA	1.82	0.45
15:U:111:GLN:OE1	15:U:115:ASN:ND2	2.50	0.45
17:W:275:ILE:O	17:W:357:ARG:NE	2.50	0.45
23:d:114:GLU:HA	23:d:117:THR:HG22	1.98	0.45
8:n:19:ARG:NH1	8:n:170:SER:O	2.50	0.45
11:q:101:ASN:HB3	11:q:132:HIS:CD2	2.51	0.45
14:t:49:THR:HB	14:t:85:PRO:HG3	1.98	0.45
26:A:351:ARG:HE	26:A:374:ALA:HB1	1.82	0.45
34:D:501:AGS:S1G	34:D:501:AGS:O2B	2.75	0.45
32:f:714:SER:O	32:f:718:ASP:CB	2.55	0.45
7:M:43:ASP:N	7:M:43:ASP:OD1	2.50	0.45
7:M:76:ALA:HB3	7:M:136:MET:HB2	1.99	0.45
19:Z:40:LEU:HD13	19:Z:89:GLU:HG2	1.98	0.45
25:X:354:ILE:HG23	25:X:356:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:28:ARG:O	13:S:42:LYS:NZ	2.48	0.45
15:U:808:PRO:HA	15:U:811:PHE:HD2	1.82	0.45
20:a:244:ASN:HD21	20:a:299:SER:HB3	1.82	0.45
5:k:108:THR:O	5:k:111:SER:OG	2.30	0.45
7:m:69:VAL:H	7:m:74:GLY:HA2	1.81	0.45
9:o:200:GLY:HA3	9:o:201:ARG:HA	1.60	0.45
13:s:73:LYS:O	13:s:77:HIS:ND1	2.35	0.45
32:f:420:TRP:CG	32:f:421:ASP:H	2.34	0.45
1:G:123:GLN:NE2	2:H:82:ASP:OD1	2.50	0.45
3:I:34:CYS:H	3:I:164:ILE:HG13	1.82	0.45
6:L:65:HIS:O	6:L:89:ARG:NH2	2.50	0.45
6:L:120:THR:O	7:M:129:ARG:NH1	2.40	0.45
11:Q:31:ASP:N	11:Q:31:ASP:OD1	2.50	0.45
15:U:208:LEU:HD23	15:U:210:LYS:H	1.80	0.45
16:V:78:HIS:H	16:V:81:GLN:HG3	1.82	0.45
16:V:291:TYR:HD1	16:V:294:ARG:HH12	1.65	0.45
18:Y:141:VAL:HG21	18:Y:164:ALA:HB2	1.99	0.45
2:h:181:ASP:OD1	2:h:181:ASP:N	2.44	0.45
4:j:121:SER:OG	4:j:122:ASN:N	2.50	0.45
8:N:144:ARG:NH2	8:N:151:GLU:OE1	2.50	0.44
11:Q:198:LYS:H	11:q:198:LYS:H	1.65	0.44
15:U:681:ASN:HB2	15:U:723:ASP:HB2	1.98	0.44
16:V:227:VAL:HG13	16:V:230:PHE:HD2	1.82	0.44
17:W:131:VAL:HG13	17:W:140:ILE:HG22	1.98	0.44
17:W:231:ILE:HG21	17:W:250:ILE:HG22	1.99	0.44
18:Y:259:TYR:CD1	18:Y:274:SER:HB2	2.53	0.44
21:b:131:LEU:HA	21:b:134:GLU:HB2	1.99	0.44
2:h:12:THR:OG1	3:i:20:GLN:NE2	2.50	0.44
13:s:99:ARG:HH21	13:s:102:PHE:HD2	1.66	0.44
32:f:359:GLY:O	32:f:363:SER:CB	2.50	0.44
32:f:638:ASP:OD1	32:f:638:ASP:N	2.50	0.44
1:G:165:ALA:HB1	1:G:179:LEU:HD13	1.99	0.44
2:H:42:ASN:ND2	2:H:183:GLU:OE1	2.51	0.44
6:L:157:ARG:NH2	7:M:58:TYR:O	2.51	0.44
15:U:160:LEU:O	15:U:164:GLU:HB2	2.17	0.44
18:Y:157:ILE:H	18:Y:157:ILE:HG13	1.52	0.44
19:Z:96:HIS:CE1	19:Z:123:ILE:HG12	2.52	0.44
22:c:102:THR:HG22	22:c:103:GLY:H	1.82	0.44
1:g:67:THR:HG23	1:g:216:GLU:HG2	1.99	0.44
4:j:131:ALA:H	4:j:147:THR:HG1	1.61	0.44
7:m:66:LEU:HD13	7:m:214:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:13:LEU:HD11	13:s:149:LEU:HD11	1.99	0.44
32:f:354:GLU:HG3	32:f:355:ASN:H	1.82	0.44
32:f:664:GLU:O	32:f:665:GLU:C	2.57	0.44
11:Q:57:ALA:O	11:Q:61:GLN:CB	2.62	0.44
11:Q:64:VAL:HG13	11:Q:75:LEU:HD12	2.00	0.44
14:T:186:ARG:HE	14:T:202:PRO:HB2	1.82	0.44
16:V:256:ARG:HD2	24:e:5:LYS:HB2	1.98	0.44
16:V:256:ARG:HG3	24:e:5:LYS:HD3	1.99	0.44
16:V:350:GLN:H	16:V:353:LEU:HD23	1.82	0.44
16:V:419:LEU:HD13	16:V:431:PRO:HB3	1.99	0.44
17:W:139:GLU:HG2	17:W:142:ARG:HD2	1.99	0.44
17:W:301:LYS:HB3	17:W:324:TYR:HE1	1.82	0.44
20:a:342:ASP:H	20:a:345:GLN:HB2	1.82	0.44
22:c:137:SER:HB3	22:c:140:ALA:HB2	2.00	0.44
34:A:501:AGS:PG	27:B:343:ARG:HH12	2.40	0.44
28:C:50:ASN:HD22	29:D:61:ILE:HD12	1.82	0.44
29:D:230:VAL:HB	29:D:264:ILE:HG12	1.99	0.44
32:f:379:GLY:O	32:f:417:ILE:CG1	2.65	0.44
32:f:646:MET:HA	32:f:649:HIS:HD1	1.82	0.44
11:Q:101:ASN:HB3	11:Q:132:HIS:CD2	2.52	0.44
17:W:315:MET:HE3	17:W:315:MET:HB2	1.82	0.44
19:Z:37:GLY:HA2	19:Z:56:VAL:HG12	1.98	0.44
3:i:245:ALA:HA	3:i:248:GLU:HG2	1.99	0.44
4:j:72:ALA:HB3	4:j:132:LEU:HB2	1.99	0.44
6:l:47:VAL:HG13	6:l:212:ILE:HG13	1.99	0.44
25:X:114:ILE:HD11	25:X:133:LEU:HD22	1.99	0.44
26:A:264:ALA:HB2	26:A:272:ILE:HD11	1.98	0.44
32:f:22:GLY:O	32:f:26:GLU:CB	2.66	0.44
5:K:108:THR:O	5:K:111:SER:OG	2.34	0.44
16:V:494:MET:HG2	28:C:49:ARG:NH2	2.32	0.44
17:W:369:TYR:HB3	20:a:324:ILE:HD13	2.00	0.44
17:W:370:TYR:H	20:a:324:ILE:HD13	1.83	0.44
18:Y:329:PHE:HB3	24:e:66:LYS:HD3	1.99	0.44
20:a:367:VAL:HG13	23:d:244:LYS:HE3	1.99	0.44
22:c:112:TYR:HA	22:c:143:VAL:HB	2.00	0.44
4:j:118:TYR:HE1	4:j:124:ARG:HH21	1.66	0.44
9:o:38:SER:OG	9:o:40:ASN:OD1	2.26	0.44
11:q:192:ASP:OD1	11:q:192:ASP:N	2.50	0.44
28:C:86:LEU:HD21	28:C:94:LYS:HB3	1.99	0.44
30:E:237:ALA:HB2	31:F:311:LEU:HD12	2.00	0.44
32:f:130:ALA:O	32:f:134:SER:CB	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:281:ILE:O	32:f:285:CYS:HB2	2.18	0.44
32:f:316:ASP:HA	32:f:319:GLU:HG2	1.99	0.44
15:U:38:ILE:HB	15:U:67:VAL:HG21	1.99	0.44
15:U:638:SER:HB2	15:U:671:LEU:HD13	1.98	0.44
18:Y:269:SER:OG	18:Y:322:ALA:O	2.25	0.44
19:Z:129:LYS:O	22:c:223:LYS:NZ	2.50	0.44
21:b:34:ASN:O	21:b:38:HIS:ND1	2.37	0.44
23:d:130:ASN:ND2	23:d:133:ILE:HG12	2.33	0.44
10:p:126:LEU:HD12	10:p:127:ILE:HG23	1.98	0.44
11:q:171:PHE:CE2	11:q:173:LEU:HB2	2.53	0.44
26:A:327:LEU:HD13	26:A:327:LEU:HA	1.85	0.44
27:B:438:LEU:HA	27:B:439:TYR:HA	1.81	0.44
32:f:378:ASN:CB	32:f:391:LEU:CD1	2.94	0.44
32:f:608:LYS:HA	32:f:611:GLN:HB3	1.99	0.44
32:f:780:PRO:HB2	32:f:800:LEU:HA	1.94	0.44
2:H:48:THR:OG1	2:H:49:GLU:N	2.46	0.44
15:U:250:PHE:HA	15:U:253:TYR:HB3	1.99	0.44
15:U:646:PRO:O	15:U:650:TYR:CB	2.66	0.44
16:V:60:ALA:HB1	16:V:63:SER:HB2	2.00	0.44
17:W:110:THR:HA	17:W:113:GLU:HG2	2.00	0.44
19:Z:34:ARG:HD3	19:Z:96:HIS:HB2	1.99	0.44
19:Z:267:ARG:HH12	22:c:295:ASN:HB2	1.83	0.44
20:a:287:ASN:HD21	20:a:289:ARG:HE	1.64	0.44
22:c:118:PHE:HE2	22:c:121:TRP:H	1.64	0.44
23:d:51:ALA:HA	23:d:54:ILE:HG12	1.99	0.44
11:q:38:MET:O	11:q:65:GLN:NE2	2.50	0.44
28:C:147:THR:HG23	28:C:149:GLU:HG3	2.00	0.44
28:C:193:GLY:O	28:C:356:GLY:N	2.47	0.44
32:f:536:SER:O	32:f:540:GLN:CB	2.66	0.44
2:H:6:TYR:HE2	2:H:14:SER:HA	1.83	0.44
2:H:44:VAL:HG23	2:H:144:PRO:HB2	1.99	0.44
6:L:121:GLN:HE22	7:M:131:PHE:HE1	1.63	0.44
7:M:58:TYR:OH	7:M:62:SER:O	2.35	0.44
15:U:214:ILE:HA	15:U:217:CYS:HB3	2.00	0.44
15:U:408:LEU:HD23	15:U:423:MET:HE2	2.00	0.44
17:W:158:ASP:OD1	17:W:158:ASP:N	2.45	0.44
17:W:218:ASN:ND2	17:W:223:LYS:H	2.16	0.44
17:W:301:LYS:O	17:W:324:TYR:OH	2.25	0.44
18:Y:36:ALA:O	18:Y:40:GLU:HB2	2.17	0.44
20:a:248:PHE:O	20:a:252:LYS:CB	2.64	0.44
8:n:19:ARG:NH2	8:n:168:GLY:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:83:ASP:O	26:A:86:THR:OG1	2.31	0.44
31:F:94:ILE:HD12	31:F:123:VAL:HG12	1.99	0.44
32:f:355:ASN:HA	32:f:358:PHE:HD2	1.83	0.44
32:f:380:PHE:CB	32:f:751:TYR:CE2	2.99	0.44
32:f:690:VAL:O	32:f:694:LEU:HB2	2.18	0.44
1:G:165:ALA:HB3	2:H:56:LEU:HD22	1.98	0.44
1:G:212:PRO:HB3	1:G:235:ILE:HG22	2.00	0.44
3:I:125:GLY:HA2	3:I:126:GLY:HA2	1.76	0.44
5:K:196:LYS:HA	5:K:199:LEU:HG	2.00	0.44
15:U:612:ASP:HA	15:U:615:ARG:HD3	1.99	0.44
17:W:286:LEU:HA	17:W:289:ARG:HH11	1.83	0.44
1:g:80:MET:HE2	1:g:87:SER:HA	1.99	0.44
2:h:71:HIS:HA	2:h:218:PHE:H	1.83	0.44
3:i:105:ILE:HD11	3:i:109:GLN:HG3	2.00	0.44
6:l:47:VAL:HG22	6:l:212:ILE:HG23	2.00	0.44
8:n:18:SER:HB2	8:n:31:THR:H	1.83	0.44
12:r:77:ALA:O	12:r:120:ARG:NH2	2.46	0.44
25:X:362:GLU:HB3	25:X:363:ARG:H	1.63	0.44
28:C:188:LEU:HD13	28:C:317:PHE:HZ	1.83	0.44
31:F:265:ALA:HA	31:F:312:GLU:HG2	2.00	0.44
32:f:380:PHE:CD2	32:f:380:PHE:O	2.70	0.44
32:f:623:LYS:O	32:f:627:GLU:HB3	2.17	0.44
32:f:692:LEU:HG	32:f:752:HIS:HE1	1.77	0.44
4:J:154:HIS:HE1	5:K:59:MET:HE3	1.82	0.43
6:L:196:ARG:HH21	6:L:239:ARG:HG3	1.83	0.43
15:U:559:ARG:HD2	15:U:562:GLU:HB2	1.99	0.43
16:V:215:ALA:O	16:V:219:GLU:HB2	2.18	0.43
16:V:350:GLN:O	16:V:354:LYS:N	2.51	0.43
17:W:297:GLU:HA	17:W:302:TYR:HD2	1.83	0.43
12:r:22:ALA:N	12:r:25:TYR:O	2.41	0.43
14:t:27:LEU:HD11	14:t:34:ALA:HB1	1.99	0.43
27:B:112:LEU:HD23	27:B:123:VAL:HG12	2.00	0.43
30:E:61:LEU:HD12	30:E:70:ILE:HG22	2.00	0.43
32:f:303:VAL:HG22	32:f:339:ILE:HA	2.00	0.43
32:f:357:ARG:NH2	32:f:754:LYS:HG3	2.33	0.43
32:f:376:PHE:CZ	32:f:798:THR:CG2	2.91	0.43
1:G:37:LEU:HD23	1:G:81:THR:HG22	1.99	0.43
1:G:215:ILE:H	1:G:215:ILE:HG13	1.65	0.43
11:Q:27:GLN:O	11:q:170:ARG:NH1	2.51	0.43
15:U:471:ASP:HB2	15:U:508:THR:HG21	1.98	0.43
15:U:581:SER:O	15:U:585:THR:OG1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:173:THR:HG23	17:W:182:ARG:HH11	1.83	0.43
18:Y:384:SER:HB2	19:Z:279:LYS:HE3	2.00	0.43
21:b:40:LYS:HA	21:b:43:SER:HB3	2.00	0.43
23:d:242:LEU:HD23	23:d:245:GLN:HG3	2.00	0.43
14:t:126:ASP:OD1	14:t:127:MET:N	2.52	0.43
31:F:358:ASN:O	31:F:362:ARG:NH1	2.51	0.43
32:f:286:LYS:HD3	32:f:326:LEU:HD23	2.00	0.43
32:f:494:ARG:HE	32:f:494:ARG:CA	2.32	0.43
5:K:105:GLU:OE2	13:S:75:TYR:OH	2.33	0.43
13:S:35:ILE:HB	14:T:151:ARG:HH12	1.84	0.43
15:U:154:ALA:HA	15:U:162:VAL:HG13	2.01	0.43
16:V:476:PHE:HD2	19:Z:260:VAL:HG12	1.83	0.43
17:W:193:CYS:HA	17:W:196:VAL:HB	1.99	0.43
18:Y:148:GLY:HA3	18:Y:157:ILE:HG23	2.00	0.43
9:o:67:SER:HB3	9:o:74:PRO:HG3	2.01	0.43
26:A:63:THR:O	32:f:613:LEU:HD21	2.19	0.43
27:B:134:SER:O	27:B:159:VAL:N	2.52	0.43
28:C:164:VAL:HG13	28:C:165:ILE:HG13	1.99	0.43
28:C:212:ILE:O	28:C:247:PHE:N	2.40	0.43
29:D:133:HIS:HD2	29:D:136:SER:H	1.66	0.43
32:f:368:ALA:O	32:f:372:LEU:HB2	2.18	0.43
1:G:11:ARG:NE	1:G:27:TYR:OH	2.52	0.43
15:U:196:LYS:HA	15:U:199:ARG:HG2	2.00	0.43
15:U:560:MET:SD	15:U:595:ASN:ND2	2.88	0.43
20:a:64:ILE:O	20:a:68:GLU:HB2	2.17	0.43
6:l:40:SER:OG	6:l:43:HIS:N	2.44	0.43
8:n:86:MET:HE2	8:n:86:MET:HB3	1.90	0.43
8:n:95:MET:HG2	8:n:116:MET:HE3	2.00	0.43
25:X:254:MET:HG3	25:X:255:LEU:HG	2.00	0.43
32:f:283:THR:O	32:f:287:ASP:HB2	2.18	0.43
1:G:132:ARG:HA	1:G:133:PRO:HD3	1.78	0.43
15:U:257:SER:HB3	15:U:260:PHE:HB2	2.00	0.43
18:Y:144:LEU:HB2	18:Y:160:ASN:HB3	2.00	0.43
18:Y:224:VAL:HG21	18:Y:260:LEU:HD11	2.01	0.43
22:c:50:PRO:HG3	30:E:53:VAL:HG11	1.99	0.43
14:t:147:GLN:HA	14:t:150:LEU:HD12	2.00	0.43
25:X:302:PHE:O	25:X:306:LEU:HB2	2.18	0.43
30:E:364:GLN:HA	30:E:367:PHE:HD2	1.83	0.43
32:f:122:ALA:HB1	32:f:126:ILE:HD12	2.01	0.43
32:f:494:ARG:NE	32:f:494:ARG:CA	2.82	0.43
2:H:74:LEU:HD21	2:H:134:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:725:MET:SD	15:U:725:MET:N	2.82	0.43
16:V:46:GLY:HA3	16:V:62:HIS:ND1	2.34	0.43
16:V:191:LEU:O	16:V:194:LYS:NZ	2.39	0.43
16:V:295:ILE:HD13	16:V:295:ILE:HA	1.89	0.43
16:V:386:PHE:HE1	16:V:394:LEU:HD11	1.83	0.43
17:W:344:THR:O	17:W:348:GLU:HB3	2.18	0.43
22:c:63:ASP:OD1	22:c:66:THR:OG1	2.29	0.43
23:d:79:LYS:O	23:d:83:PHE:N	2.44	0.43
29:D:418:LYS:HA	29:D:418:LYS:HD2	1.86	0.43
30:E:101:ASP:OD2	30:E:104:THR:N	2.42	0.43
31:F:126:THR:N	31:F:130:GLN:O	2.44	0.43
32:f:248:LEU:O	32:f:252:ALA:HB3	2.19	0.43
32:f:282:PHE:HE2	32:f:317:LEU:HD21	1.83	0.43
11:Q:29:LYS:HE3	11:Q:32:HIS:HA	1.99	0.43
13:S:93:SER:OG	13:S:128:GLY:O	2.31	0.43
13:S:176:LYS:HE2	13:S:208:VAL:HG21	2.00	0.43
15:U:233:LEU:HA	15:U:236:LEU:HG	2.01	0.43
16:V:148:ARG:O	16:V:152:GLY:N	2.41	0.43
17:W:254:PRO:HA	17:W:257:GLN:HG2	2.00	0.43
20:a:35:HIS:CE1	21:b:17:ARG:HB2	2.53	0.43
20:a:190:VAL:HA	20:a:193:GLN:HB2	2.01	0.43
20:a:252:LYS:HD3	20:a:255:TRP:HB2	1.99	0.43
1:g:132:ARG:HA	1:g:133:PRO:HD3	1.77	0.43
5:k:97:GLN:HG3	12:r:61:ARG:HG3	2.01	0.43
5:k:192:LYS:HA	5:k:195:ILE:HD12	2.01	0.43
10:p:116:THR:O	10:p:192:LYS:NZ	2.44	0.43
26:A:339:ARG:HH21	31:F:405:MET:HE3	1.83	0.43
27:B:337:LEU:HD13	27:B:337:LEU:HA	1.90	0.43
28:C:79:ALA:HB2	28:C:108:VAL:HG11	1.99	0.43
32:f:358:PHE:O	32:f:362:GLY:CA	2.63	0.43
1:G:39:SER:OG	1:G:168:ALA:O	2.29	0.43
15:U:533:VAL:O	15:U:537:GLN:NE2	2.48	0.43
22:c:58:LEU:HA	22:c:108:VAL:HA	1.99	0.43
23:d:143:LEU:HA	23:d:147:SER:HB2	2.01	0.43
14:t:49:THR:OG1	14:t:50:MET:N	2.52	0.43
25:X:204:PRO:HG2	25:X:206:LEU:HG	2.00	0.43
2:H:46:LEU:HD13	2:H:75:VAL:HG22	2.00	0.43
15:U:19:LEU:HD13	23:d:30:LEU:HD13	2.00	0.43
16:V:480:ILE:HD11	19:Z:264:SER:HA	2.00	0.43
20:a:135:ILE:HG12	20:a:158:LEU:HD13	2.00	0.43
21:b:9:CYS:HB3	21:b:111:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:208:ILE:HB	1:g:210:PHE:HD1	1.84	0.43
2:h:119:GLN:O	2:h:122:THR:OG1	2.27	0.43
4:j:82:ILE:HD13	4:j:82:ILE:HA	1.90	0.43
26:A:47:GLN:N	32:f:185:LEU:HD13	2.34	0.43
26:A:405:THR:OG1	26:A:408:ASP:N	2.52	0.43
32:f:688:ARG:HA	32:f:745:LEU:CB	2.49	0.43
32:f:794:ALA:HA	32:f:797:LEU:HB2	2.01	0.43
2:H:93:LEU:HD11	2:H:113:ARG:HB3	2.00	0.43
5:K:146:VAL:HA	5:K:151:PRO:HA	2.00	0.43
6:L:109:VAL:HG21	6:L:145:PHE:HD2	1.84	0.43
15:U:70:HIS:HB2	16:V:236:ARG:HH22	1.84	0.43
15:U:356:THR:HG21	15:U:731:ILE:HD13	2.01	0.43
16:V:89:LYS:HD3	16:V:92:ARG:NH1	2.34	0.43
17:W:287:VAL:HA	17:W:290:ILE:HG12	2.00	0.43
18:Y:104:MET:O	18:Y:108:ALA:HB2	2.19	0.43
18:Y:202:LEU:HD11	18:Y:239:LYS:HE3	2.01	0.43
2:h:107:THR:HA	2:h:110:LEU:HD13	2.01	0.43
7:m:36:ALA:N	7:m:165:ILE:O	2.41	0.43
8:n:21:THR:HG22	8:n:26:ILE:HG13	2.00	0.43
8:n:136:TYR:HE2	14:t:33:LEU:HD11	1.84	0.43
11:q:158:GLU:HG3	11:q:162:LYS:HE3	2.00	0.43
25:X:255:LEU:HD12	25:X:287:LEU:HD13	2.00	0.43
26:A:99:THR:HG22	26:A:115:VAL:HA	2.01	0.43
26:A:139:ARG:HD3	26:A:155:PRO:HA	2.01	0.43
27:B:189:GLY:HA3	27:B:356:PRO:HG2	2.00	0.43
30:E:230:ILE:HB	30:E:275:MET:HG2	2.01	0.43
32:f:389:LYS:HD3	32:f:389:LYS:H	1.81	0.43
5:K:49:ALA:HB1	5:K:202:LEU:HD11	2.01	0.42
7:M:9:LEU:O	7:M:22:GLN:NE2	2.52	0.42
7:M:40:ARG:NH1	7:M:146:ALA:O	2.52	0.42
10:P:135:ASP:OD1	10:P:135:ASP:N	2.49	0.42
15:U:345:ASN:O	15:U:743:ASN:ND2	2.43	0.42
15:U:604:HIS:O	15:U:608:SER:OG	2.27	0.42
15:U:638:SER:O	15:U:641:SER:OG	2.28	0.42
18:Y:154:ASN:HA	18:Y:157:ILE:HD11	1.99	0.42
2:h:100:VAL:HG13	10:p:93:ASN:HD22	1.82	0.42
4:j:221:ASN:HA	4:j:222:PRO:HD3	1.82	0.42
13:s:93:SER:OG	13:s:128:GLY:O	2.30	0.42
14:t:74:GLU:HG3	14:t:77:LEU:HD12	2.01	0.42
26:A:206:ILE:HG22	31:F:373:MET:HG2	2.01	0.42
32:f:207:LEU:HD13	32:f:207:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:104:VAL:HG23	4:J:133:ILE:HG22	2.01	0.42
6:L:52:ALA:HB2	6:L:59:HIS:HD2	1.84	0.42
8:N:19:ARG:NH2	8:N:168:GLY:O	2.52	0.42
12:R:122:SER:OG	12:R:123:GLY:N	2.51	0.42
14:T:171:ARG:HG2	14:T:174:ARG:HH12	1.84	0.42
15:U:475:HIS:O	15:U:478:SER:OG	2.31	0.42
16:V:48:THR:HA	16:V:147:PHE:CE1	2.54	0.42
17:W:76:GLU:OE2	17:W:123:ARG:NH1	2.52	0.42
17:W:394:SER:HA	17:W:397:VAL:HG12	2.01	0.42
17:W:415:PHE:HB3	17:W:416:GLN:H	1.61	0.42
19:Z:34:ARG:HE	19:Z:98:GLY:HA3	1.84	0.42
20:a:35:HIS:HE1	21:b:17:ARG:HB2	1.84	0.42
20:a:280:MET:HB2	20:a:291:LEU:HD13	2.01	0.42
20:a:360:VAL:HG22	22:c:310:LYS:HA	2.01	0.42
22:c:162:LEU:HD13	22:c:200:TYR:CZ	2.54	0.42
1:g:54:LYS:NZ	1:g:213:SER:O	2.46	0.42
3:i:164:ILE:HG22	3:i:165:GLY:H	1.84	0.42
4:j:18:GLN:O	4:j:22:ALA:CB	2.67	0.42
8:n:127:ILE:HD13	8:n:136:TYR:HB2	2.01	0.42
11:Q:47:VAL:O	11:Q:101:ASN:N	2.50	0.42
13:S:8:ASN:OD1	13:S:58:HIS:N	2.52	0.42
16:V:247:GLN:HB3	16:V:276:PHE:CE1	2.55	0.42
20:a:292:THR:HG23	20:a:295:GLU:H	1.83	0.42
23:d:104:LEU:HD21	23:d:167:ILE:HG23	2.01	0.42
27:B:230:THR:HG21	27:B:353:PHE:HB3	2.01	0.42
29:D:252:ARG:O	29:D:256:GLU:HB2	2.19	0.42
32:f:412:ALA:HA	32:f:447:ALA:HB2	2.00	0.42
32:f:446:LEU:HD13	32:f:480:GLY:HA2	2.00	0.42
2:H:79:MET:HE3	2:H:131:GLY:HA3	2.02	0.42
2:H:124:SER:HA	2:H:125:GLY:HA2	1.79	0.42
3:I:109:GLN:HB3	11:Q:71:ASN:HD21	1.84	0.42
6:L:148:CYS:SG	6:L:152:ASN:N	2.83	0.42
14:T:41:ARG:HH21	14:T:54:SER:HA	1.84	0.42
15:U:198:LEU:HD21	15:U:219:CYS:HA	2.01	0.42
15:U:580:ARG:NH2	15:U:768:GLN:OE1	2.52	0.42
3:i:72:MET:HE3	3:i:72:MET:HB2	1.93	0.42
3:i:72:MET:HG2	3:i:138:GLY:HA3	2.01	0.42
4:j:131:ALA:N	4:j:147:THR:OG1	2.40	0.42
26:A:287:ASP:OD1	26:A:287:ASP:N	2.52	0.42
27:B:223:ILE:HG13	27:B:347:ILE:HG21	2.02	0.42
29:D:280:GLY:HA2	29:D:283:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:80:ARG:HE	32:f:99:LEU:HD13	1.85	0.42
32:f:479:LEU:HD23	32:f:513:GLU:HB3	2.02	0.42
32:f:645:ASP:O	32:f:649:HIS:ND1	2.51	0.42
6:L:155:ASP:HB3	7:M:62:SER:HB2	2.01	0.42
8:N:127:ILE:HB	8:N:132:SER:HB2	2.00	0.42
15:U:97:VAL:HA	15:U:100:ILE:HG12	2.01	0.42
15:U:802:TYR:CZ	15:U:841:LYS:HE3	2.54	0.42
17:W:449:GLU:HA	17:W:452:ILE:HG12	2.01	0.42
21:b:97:LEU:HD22	21:b:109:ILE:HD11	2.02	0.42
25:X:53:LEU:HD23	25:X:56:LEU:HD12	2.01	0.42
26:A:266:THR:OG1	26:A:267:LYS:N	2.53	0.42
28:C:115:ALA:N	28:C:125:LYS:O	2.43	0.42
29:D:275:PHE:HZ	29:D:289:LEU:HD12	1.84	0.42
32:f:471:LEU:HD11	32:f:509:LYS:HE2	2.00	0.42
32:f:509:LYS:O	32:f:554:TYR:OH	2.36	0.42
32:f:698:SER:OG	32:f:716:ASP:OD1	2.36	0.42
1:G:17:SER:OG	1:G:21:ARG:O	2.32	0.42
5:K:21:LEU:HA	5:K:22:PHE:HB2	2.02	0.42
9:O:106:THR:OG1	9:O:109:HIS:NE2	2.35	0.42
15:U:38:ILE:HA	15:U:41:SER:HB3	2.01	0.42
16:V:131:LEU:O	16:V:135:LEU:N	2.45	0.42
16:V:148:ARG:NH2	16:V:197:THR:HG21	2.34	0.42
17:W:115:ILE:HD13	17:W:119:PRO:HG2	2.02	0.42
17:W:355:LYS:HA	17:W:358:VAL:HG22	2.02	0.42
18:Y:158:THR:O	18:Y:161:THR:OG1	2.33	0.42
3:i:95:GLN:HG3	10:p:69:PHE:CD1	2.55	0.42
3:i:105:ILE:HG13	3:i:107:CYS:H	1.85	0.42
7:m:99:ARG:HH21	7:m:105:ASN:HA	1.85	0.42
7:m:230:ASP:OD1	7:m:230:ASP:N	2.51	0.42
12:r:35:ILE:N	12:r:43:GLY:O	2.53	0.42
28:C:114:VAL:HA	28:C:127:LEU:H	1.85	0.42
34:E:401:AGS:O2G	31:F:347:ARG:NH2	2.52	0.42
32:f:86:THR:HG23	32:f:87:THR:H	1.85	0.42
32:f:311:VAL:HG22	32:f:527:VAL:O	2.19	0.42
3:I:218:ARG:NH1	3:I:223:THR:OG1	2.44	0.42
8:N:91:ARG:NH1	14:T:56:ASP:OD2	2.52	0.42
10:P:36:THR:OG1	10:P:38:ASP:OD1	2.30	0.42
14:T:49:THR:HB	14:T:85:PRO:HG3	2.01	0.42
15:U:749:GLN:HA	15:U:755:THR:HA	2.01	0.42
16:V:131:LEU:HA	16:V:134:PHE:HB2	2.02	0.42
18:Y:84:LEU:HD11	18:Y:111:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:105:MET:HE1	18:Y:136:HIS:HB3	2.01	0.42
19:Z:68:TRP:CD1	19:Z:104:ASN:HD21	2.38	0.42
19:Z:245:PHE:HB3	19:Z:248:ALA:HB3	2.01	0.42
20:a:247:ARG:NH1	20:a:250:THR:O	2.48	0.42
20:a:360:VAL:O	20:a:364:GLU:HB2	2.20	0.42
6:l:189:LYS:HZ2	6:l:193:ARG:HH22	1.67	0.42
9:o:50:ALA:HB2	10:p:129:CYS:HB2	2.02	0.42
14:t:89:HIS:CE1	14:t:131:ALA:HB1	2.55	0.42
32:f:77:GLU:O	32:f:81:GLN:HB2	2.19	0.42
1:G:161:CYS:SG	1:G:162:GLY:N	2.93	0.42
6:L:65:HIS:HA	6:L:221:PHE:HE2	1.84	0.42
16:V:104:THR:HA	16:V:107:ARG:HB2	2.02	0.42
18:Y:281:GLU:OE1	18:Y:281:GLU:HA	2.19	0.42
19:Z:269:VAL:HG12	19:Z:273:HIS:CE1	2.55	0.42
20:a:186:LYS:HB3	20:a:193:GLN:HE22	1.85	0.42
20:a:287:ASN:ND2	20:a:289:ARG:HE	2.18	0.42
21:b:97:LEU:HD23	21:b:107:MET:HG2	2.01	0.42
22:c:55:GLY:N	22:c:112:TYR:O	2.44	0.42
6:l:196:ARG:HH21	6:l:239:ARG:HG3	1.84	0.42
7:m:51:LYS:O	7:m:210:GLU:N	2.52	0.42
12:r:1:THR:N	12:r:169:TYR:O	2.50	0.42
13:s:4:PRO:O	14:t:100:ARG:NH2	2.52	0.42
26:A:279:ALA:HB2	27:B:310:LEU:HD23	2.00	0.42
27:B:112:LEU:HD11	27:B:144:LEU:HD22	2.02	0.42
31:F:217:ILE:HG13	31:F:218:GLN:H	1.85	0.42
32:f:228:LYS:O	32:f:232:TYR:HB3	2.19	0.42
32:f:512:MET:HE1	32:f:554:TYR:HA	2.02	0.42
32:f:635:LYS:HD3	32:f:641:GLU:HG2	2.01	0.42
4:J:211:MET:HE2	4:J:213:ARG:HA	2.01	0.42
7:M:100:SER:HA	14:T:65:GLN:HE21	1.85	0.42
8:N:140:ASP:OD1	8:N:140:ASP:N	2.53	0.42
15:U:798:PRO:HB3	15:U:900:TYR:CG	2.55	0.42
16:V:186:LYS:HE2	16:V:234:ARG:HH11	1.84	0.42
16:V:245:ASP:HA	16:V:276:PHE:CZ	2.55	0.42
16:V:490:SER:HB2	19:Z:278:ASN:HD22	1.85	0.42
17:W:275:ILE:HG23	17:W:357:ARG:HG3	2.01	0.42
17:W:359:VAL:HG21	17:W:392:PHE:HB3	2.01	0.42
18:Y:229:ILE:HG22	18:Y:230:ALA:H	1.83	0.42
19:Z:9:VAL:HG22	19:Z:160:SER:HA	2.02	0.42
21:b:141:ILE:HG23	21:b:171:VAL:HB	2.02	0.42
3:i:36:GLY:H	3:i:162:THR:HG22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:67:LYS:HG3	3:i:225:ILE:HD12	2.02	0.42
6:l:157:ARG:HH12	7:m:59:GLU:HA	1.85	0.42
26:A:348:LEU:HB3	26:A:349:GLU:H	1.72	0.42
29:D:367:PRO:HB2	29:D:368:ASP:HB2	2.01	0.42
32:f:8:LYS:HD3	32:f:39:LYS:HD2	2.02	0.42
32:f:629:LYS:HE2	32:f:660:ILE:HG21	2.02	0.42
32:f:632:LYS:NZ	32:f:660:ILE:O	2.46	0.42
32:f:664:GLU:HA	32:f:697:ILE:CA	2.46	0.42
2:H:105:ILE:HG12	2:H:110:LEU:HD12	2.02	0.42
9:O:51:ASP:HB3	9:O:94:ILE:HG23	2.02	0.42
14:T:27:LEU:HD11	14:T:34:ALA:HB1	2.02	0.42
17:W:333:LEU:H	17:W:333:LEU:HG	1.78	0.42
18:Y:124:PHE:O	18:Y:128:TYR:CB	2.68	0.42
19:Z:208:ILE:HG13	19:Z:211:TYR:HD2	1.85	0.42
20:a:26:GLU:O	20:a:30:THR:OG1	2.31	0.42
20:a:78:GLU:O	20:a:82:HIS:ND1	2.43	0.42
23:d:62:SER:HA	23:d:65:ARG:HG2	2.01	0.42
2:h:105:ILE:HG12	2:h:110:LEU:HD12	2.02	0.42
3:i:35:LEU:HG	3:i:46:ALA:HB3	2.01	0.42
7:m:36:ALA:O	7:m:165:ILE:N	2.46	0.42
25:X:341:PRO:HB3	25:X:383:GLY:O	2.20	0.42
29:D:160:PRO:HG2	29:D:217:LYS:HA	2.02	0.42
29:D:264:ILE:HG22	29:D:267:ILE:HG22	2.01	0.42
30:E:258:MET:HA	30:E:261:LEU:HB2	2.02	0.42
32:f:671:ALA:O	32:f:674:THR:OG1	2.26	0.42
15:U:16:GLU:HA	15:U:17:PRO:HD3	1.85	0.41
15:U:698:GLN:NE2	15:U:703:CYS:HB3	2.35	0.41
15:U:898:CYS:O	15:U:901:GLN:NE2	2.53	0.41
16:V:377:GLN:O	16:V:381:GLN:CB	2.68	0.41
17:W:295:LYS:HD3	17:W:298:GLU:HG3	2.02	0.41
17:W:422:ASN:OD1	17:W:425:LEU:N	2.50	0.41
17:W:448:LYS:HZ3	17:W:448:LYS:HG3	1.65	0.41
20:a:115:LYS:HD3	20:a:118:ILE:HD12	2.02	0.41
23:d:18:LYS:O	23:d:22:GLU:HB2	2.20	0.41
1:g:144:ASP:HB3	1:g:147:GLN:HB2	2.01	0.41
9:o:20:ALA:HB3	9:o:28:ASP:HB3	2.01	0.41
13:s:35:ILE:HB	14:t:151:ARG:HH12	1.85	0.41
25:X:172:LEU:HD12	25:X:175:LYS:HD3	2.00	0.41
29:D:354:LEU:HA	29:D:394:VAL:HB	2.02	0.41
30:E:61:LEU:HD11	30:E:72:LYS:HB2	2.02	0.41
32:f:402:ASN:OD1	32:f:403:LYS:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:478:ARG:HD3	32:f:504:VAL:CG1	2.45	0.41
32:f:620:PHE:HD2	32:f:623:LYS:HG2	1.85	0.41
32:f:635:LYS:NZ	32:f:641:GLU:CD	2.66	0.41
5:K:167:ALA:HB3	5:K:181:LEU:HD21	2.02	0.41
6:L:62:LYS:HZ1	31:F:439:ALA:HB3	1.85	0.41
15:U:181:LEU:HD11	15:U:205:TYR:HE2	1.85	0.41
15:U:343:ILE:HG23	15:U:344:ARG:HG2	2.02	0.41
15:U:575:ASP:HA	15:U:579:ARG:HH21	1.84	0.41
16:V:128:ARG:NH2	16:V:162:GLU:OE2	2.53	0.41
19:Z:58:PHE:CE1	19:Z:68:TRP:HB2	2.55	0.41
20:a:292:THR:O	20:a:296:ILE:HD12	2.21	0.41
21:b:12:ASN:OD1	21:b:53:THR:OG1	2.33	0.41
22:c:131:GLN:HA	22:c:134:GLU:HG2	2.01	0.41
1:g:239:LEU:HD12	1:g:242:LEU:HD11	2.02	0.41
10:p:135:ASP:OD1	10:p:135:ASP:N	2.45	0.41
29:D:322:LEU:HD22	29:D:330:LYS:HE2	2.02	0.41
32:f:81:GLN:O	32:f:85:SER:HB2	2.21	0.41
32:f:513:GLU:HG3	32:f:557:TRP:HZ3	1.84	0.41
4:J:26:VAL:HG13	4:J:74:ALA:HB3	2.02	0.41
5:K:227:HIS:CE1	5:K:229:PHE:HB3	2.55	0.41
9:O:19:ARG:HB2	9:O:169:SER:HA	2.01	0.41
10:P:183:MET:HE3	10:P:204:MET:HE3	2.02	0.41
11:Q:142:ILE:HG21	12:r:141:ARG:HH21	1.85	0.41
15:U:11:LEU:HD22	23:d:77:GLN:HE21	1.84	0.41
15:U:184:CYS:HA	15:U:187:LEU:HG	2.02	0.41
15:U:436:ALA:HB1	15:U:473:VAL:HG22	2.02	0.41
16:V:108:LEU:HD23	16:V:111:TYR:HD2	1.85	0.41
16:V:248:ALA:HA	16:V:251:LEU:HB3	2.01	0.41
17:W:121:LYS:HG3	17:W:122:LEU:HD12	2.02	0.41
18:Y:192:ARG:CZ	18:Y:294:TYR:HB3	2.49	0.41
20:a:115:LYS:HB3	20:a:138:VAL:HG22	2.02	0.41
20:a:355:PHE:O	20:a:359:ASP:HB2	2.20	0.41
21:b:3:LEU:HB3	21:b:105:HIS:HA	2.01	0.41
22:c:295:ASN:HA	22:c:298:GLN:HG2	2.01	0.41
2:h:14:SER:OG	2:h:17:GLY:N	2.53	0.41
11:q:12:TYR:OH	11:q:151:ILE:O	2.30	0.41
26:A:215:PHE:CG	26:A:324:PRO:HG3	2.55	0.41
31:F:205:PRO:HB3	31:F:219:PRO:HB3	2.01	0.41
32:f:40:ASP:HB3	32:f:41:LYS:H	1.69	0.41
32:f:338:ASP:HA	32:f:341:GLU:HG3	2.02	0.41
32:f:389:LYS:O	32:f:392:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:533:ASP:OD1	32:f:533:ASP:N	2.53	0.41
32:f:664:GLU:CB	32:f:696:LEU:HG	2.45	0.41
2:H:82:ASP:HB3	2:H:130:PHE:HD1	1.86	0.41
14:T:192:VAL:HG12	14:T:197:VAL:HG22	2.02	0.41
15:U:154:ALA:HB1	15:U:163:PHE:HA	2.02	0.41
16:V:251:LEU:O	16:V:255:LEU:HB2	2.19	0.41
16:V:255:LEU:HD22	16:V:291:TYR:HB3	2.02	0.41
21:b:139:ASP:OD1	21:b:169:HIS:N	2.50	0.41
5:k:95:GLU:HA	5:k:98:ASN:HD22	1.85	0.41
5:k:157:ASP:OD1	5:k:161:THR:N	2.53	0.41
7:m:100:SER:HA	14:t:65:GLN:HE21	1.86	0.41
27:B:227:PRO:O	27:B:230:THR:OG1	2.27	0.41
30:E:145:LEU:HA	30:E:148:VAL:HG12	2.01	0.41
32:f:86:THR:O	32:f:87:THR:HB	2.21	0.41
32:f:303:VAL:HG13	32:f:339:ILE:HG13	2.02	0.41
32:f:696:LEU:HA	32:f:696:LEU:HD12	1.78	0.41
15:U:645:ASN:HD21	15:U:648:VAL:HG23	1.85	0.41
18:Y:138:LEU:HD12	18:Y:141:VAL:HB	2.02	0.41
18:Y:149:LEU:HD12	18:Y:149:LEU:HA	1.86	0.41
21:b:111:ALA:HB3	21:b:140:ILE:HG23	2.02	0.41
3:i:33:THR:HG23	3:i:168:SER:HB2	2.02	0.41
6:l:153:TYR:OH	7:m:85:ARG:NH1	2.54	0.41
12:r:104:TRP:CD2	12:r:181:GLU:HA	2.55	0.41
13:s:211:ARG:NH2	13:s:213:ASP:OD2	2.46	0.41
27:B:190:LEU:HB3	27:B:191:ASP:H	1.63	0.41
27:B:255:LEU:HD13	27:B:255:LEU:HA	1.94	0.41
31:F:228:PRO:O	31:F:233:LYS:NZ	2.53	0.41
32:f:796:LEU:HG	32:f:799:VAL:CG2	2.42	0.41
2:H:93:LEU:HD21	2:H:113:ARG:HD2	2.02	0.41
3:I:164:ILE:HG22	3:I:165:GLY:H	1.86	0.41
6:L:148:CYS:SG	6:L:150:SER:OG	2.70	0.41
6:L:174:ARG:HG3	6:L:175:HIS:ND1	2.35	0.41
11:Q:170:ARG:NH1	11:q:27:GLN:O	2.54	0.41
18:Y:60:SER:OG	18:Y:61:LEU:N	2.53	0.41
19:Z:16:LEU:HD13	22:c:220:LEU:HD21	2.02	0.41
20:a:269:LEU:HA	20:a:272:ILE:HG12	2.01	0.41
4:j:23:GLN:HG2	4:j:149:PRO:HG2	2.02	0.41
6:l:146:GLN:HE22	6:l:159:MET:HE2	1.86	0.41
26:A:98:CYS:HA	26:A:141:GLY:HA2	2.03	0.41
27:B:190:LEU:HD12	27:B:194:ILE:HG12	2.02	0.41
29:D:123:LEU:HB3	29:D:142:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:182:LEU:HA	30:E:185:ARG:HB2	2.03	0.41
32:f:311:VAL:CA	32:f:490:ALA:HB1	2.48	0.41
11:Q:162:LYS:HB3	12:r:141:ARG:NH2	2.36	0.41
15:U:657:GLY:HA3	15:U:690:ALA:HB1	2.03	0.41
17:W:12:ARG:HD2	17:W:15:LYS:HG3	2.03	0.41
18:Y:19:ILE:HA	18:Y:22:LEU:HB2	2.02	0.41
18:Y:191:ILE:HD12	18:Y:291:HIS:CE1	2.55	0.41
18:Y:298:GLU:HA	18:Y:301:ILE:HG22	2.03	0.41
3:i:194:ILE:O	3:i:198:ASN:HB2	2.20	0.41
12:r:105:ASP:OD1	12:r:106:LYS:N	2.54	0.41
13:s:22:ILE:HD11	13:s:168:LEU:HD12	2.02	0.41
4:J:156:TRP:CD1	5:K:59:MET:HA	2.56	0.41
6:L:192:LEU:HD13	6:L:236:LEU:HD21	2.03	0.41
14:T:25:ASP:HA	14:T:187:PHE:HA	2.01	0.41
15:U:157:THR:HG23	15:U:159:ARG:H	1.86	0.41
15:U:465:LEU:HB3	15:U:474:ARG:CZ	2.51	0.41
16:V:224:LEU:O	16:V:228:ARG:HG2	2.21	0.41
17:W:452:ILE:HA	17:W:455:LEU:HG	2.02	0.41
18:Y:231:LEU:HD12	18:Y:231:LEU:HA	1.94	0.41
18:Y:283:LYS:HD3	18:Y:283:LYS:HA	1.96	0.41
20:a:247:ARG:O	20:a:251:LEU:CB	2.68	0.41
21:b:152:LYS:HE2	21:b:152:LYS:HB2	1.92	0.41
23:d:54:ILE:HA	23:d:57:ILE:HG22	2.02	0.41
7:m:168:ALA:HB1	7:m:171:ALA:HB3	2.02	0.41
11:q:58:GLU:OE2	12:r:81:LYS:NZ	2.39	0.41
27:B:250:VAL:HB	27:B:284:ILE:HG23	2.03	0.41
30:E:167:PRO:O	30:E:274:LYS:NZ	2.52	0.41
31:F:288:LEU:O	31:F:292:GLY:N	2.40	0.41
32:f:545:LYS:HE2	32:f:555:ALA:HA	2.03	0.41
32:f:573:ILE:HG22	32:f:576:ILE:HB	2.01	0.41
2:H:34:PRO:HA	2:H:164:GLY:HA3	2.03	0.41
9:O:49:ALA:O	9:O:52:THR:OG1	2.32	0.41
9:O:171:SER:OG	9:O:172:ASN:N	2.54	0.41
10:P:76:LEU:HD23	10:P:76:LEU:HA	1.94	0.41
11:Q:43:LEU:HD21	11:Q:188:ILE:HG12	2.03	0.41
11:Q:102:LEU:HB2	11:Q:118:MET:HG3	2.03	0.41
12:R:21:THR:HA	12:R:27:ALA:H	1.86	0.41
15:U:401:LYS:O	15:U:405:THR:HG22	2.20	0.41
15:U:602:LEU:O	15:U:606:ALA:HB2	2.21	0.41
15:U:650:TYR:HD1	15:U:683:VAL:HA	1.86	0.41
16:V:487:HIS:O	16:V:490:SER:OG	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:403:PHE:CD2	17:W:417:ARG:HB2	2.54	0.41
17:W:437:SER:O	17:W:441:LYS:HG2	2.21	0.41
19:Z:23:PHE:HD2	22:c:212:LEU:HD21	1.86	0.41
19:Z:68:TRP:CZ3	19:Z:108:ILE:HG13	2.56	0.41
20:a:4:VAL:HG12	20:a:6:GLY:H	1.85	0.41
21:b:100:ARG:NH1	21:b:105:HIS:HB2	2.35	0.41
22:c:31:VAL:HB	22:c:205:ILE:HG13	2.02	0.41
22:c:133:PHE:O	22:c:137:SER:N	2.44	0.41
23:d:69:PRO:O	23:d:73:ARG:HB2	2.21	0.41
4:j:18:GLN:O	4:j:22:ALA:HB2	2.20	0.41
5:k:66:LYS:HA	5:k:78:MET:HE3	2.03	0.41
9:o:177:VAL:HB	9:o:184:ASP:HB2	2.02	0.41
14:t:46:ASN:OD1	14:t:46:ASN:N	2.53	0.41
25:X:319:ILE:HA	25:X:322:HIS:ND1	2.36	0.41
26:A:424:SER:HA	26:A:425:ALA:HA	1.77	0.41
27:B:219:PRO:O	27:B:326:LYS:NZ	2.53	0.41
27:B:283:PHE:CE2	27:B:285:ASP:HB2	2.56	0.41
28:C:45:LEU:O	28:C:49:ARG:HG2	2.21	0.41
30:E:116:ASP:HB2	30:E:217:GLU:HG2	2.03	0.41
32:f:183:PRO:O	32:f:185:LEU:N	2.52	0.41
32:f:374:SER:O	32:f:375:SER:C	2.59	0.41
32:f:378:ASN:HB3	32:f:391:LEU:HD11	2.01	0.41
32:f:478:ARG:HD3	32:f:504:VAL:HG22	2.03	0.41
15:U:740:GLY:O	15:U:743:ASN:ND2	2.54	0.41
17:W:166:LEU:HD23	17:W:169:LEU:HD12	2.03	0.41
17:W:436:MET:HA	17:W:439:VAL:HG22	2.01	0.41
18:Y:349:LYS:O	18:Y:352:GLU:N	2.54	0.41
18:Y:368:GLU:HA	18:Y:371:LYS:HB2	2.02	0.41
22:c:98:MET:HG2	22:c:101:GLN:HE21	1.85	0.41
5:k:118:ASN:O	5:k:122:GLN:NE2	2.54	0.41
6:l:192:LEU:HA	6:l:195:LEU:HB2	2.02	0.41
12:r:179:VAL:HA	12:r:184:TRP:HA	2.03	0.41
25:X:57:LEU:HB3	25:X:66:LEU:HB2	2.03	0.41
27:B:341:LEU:HA	27:B:346:ARG:HD2	2.03	0.41
27:B:376:ASP:O	27:B:378:VAL:N	2.54	0.41
30:E:175:PRO:HA	30:E:176:PRO:HD3	1.98	0.41
32:f:170:TRP:CZ3	32:f:208:LEU:HB3	2.55	0.41
32:f:333:LEU:HD23	32:f:338:ASP:HB3	2.02	0.41
6:L:229:VAL:O	6:L:233:LEU:N	2.50	0.40
7:M:40:ARG:HH21	7:M:161:TRP:NE1	2.19	0.40
15:U:177:LEU:O	15:U:205:TYR:OH	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:160:LEU:HA	16:V:163:VAL:HG23	2.04	0.40
17:W:162:ALA:HA	17:W:165:ILE:HG22	2.03	0.40
18:Y:37:VAL:HA	18:Y:40:GLU:HB3	2.03	0.40
18:Y:357:ASN:HD22	18:Y:357:ASN:HA	1.67	0.40
19:Z:145:HIS:HB3	19:Z:148:GLY:N	2.36	0.40
19:Z:220:LEU:H	19:Z:220:LEU:HG	1.17	0.40
20:a:68:GLU:OE1	20:a:71:VAL:N	2.46	0.40
20:a:112:ILE:H	20:a:112:ILE:HG13	1.75	0.40
20:a:342:ASP:O	20:a:346:ILE:N	2.44	0.40
4:j:154:HIS:HE1	5:k:59:MET:HE3	1.85	0.40
4:j:196:LEU:O	4:j:201:SER:OG	2.26	0.40
13:s:16:ALA:HB2	13:s:121:VAL:HG23	2.02	0.40
25:X:327:TYR:O	25:X:330:LEU:N	2.53	0.40
27:B:188:GLY:HA3	27:B:364:ILE:HD11	2.02	0.40
27:B:361:LYS:HE2	27:B:390:LEU:HB3	2.03	0.40
31:F:314:LEU:HD21	31:F:342:LEU:HD23	2.01	0.40
32:f:336:GLU:HG3	32:f:337:LEU:CD2	2.38	0.40
32:f:780:PRO:HB2	32:f:800:LEU:CA	2.50	0.40
3:I:105:ILE:HA	3:I:106:PRO:HD3	1.83	0.40
4:J:40:ILE:HA	4:J:212:ARG:HA	2.03	0.40
12:R:105:ASP:N	12:R:108:GLY:O	2.40	0.40
17:W:144:ARG:HA	17:W:147:LYS:HG2	2.01	0.40
18:Y:223:THR:HA	18:Y:226:VAL:HG12	2.03	0.40
19:Z:273:HIS:HB3	22:c:284:LEU:HG	2.03	0.40
2:h:44:VAL:HG23	2:h:144:PRO:HB2	2.04	0.40
5:k:236:GLU:HG3	5:k:239:LYS:HE3	2.03	0.40
10:p:124:LEU:HG	10:p:130:PRO:HA	2.04	0.40
29:D:219:VAL:O	29:D:223:THR:N	2.54	0.40
31:F:197:GLU:HG2	31:F:350:ARG:HH21	1.87	0.40
32:f:298:LEU:HA	32:f:301:HIS:CD2	2.55	0.40
32:f:380:PHE:CD2	32:f:751:TYR:CE2	3.09	0.40
32:f:389:LYS:CD	32:f:389:LYS:N	2.83	0.40
5:K:33:LEU:H	5:K:33:LEU:HG	1.48	0.40
15:U:54:PHE:CZ	15:U:56:SER:HB2	2.57	0.40
15:U:229:VAL:HA	15:U:232:ILE:HG12	2.03	0.40
17:W:240:TYR:HD1	17:W:276:LEU:HB3	1.86	0.40
17:W:405:LYS:HA	25:X:342:PHE:HB2	2.03	0.40
19:Z:190:ARG:HA	19:Z:193:ASN:HD22	1.87	0.40
20:a:244:ASN:HD21	20:a:276:CYS:HB3	1.86	0.40
2:h:46:LEU:HD13	2:h:75:VAL:HG22	2.04	0.40
3:i:76:VAL:HG23	3:i:134:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:39:LYS:HA	6:l:44:ALA:HA	2.03	0.40
14:t:43:MET:SD	14:t:64:LYS:HG3	2.61	0.40
28:C:24:TYR:HA	28:C:27:LYS:HE2	2.04	0.40
29:D:148:ASP:OD1	29:D:148:ASP:N	2.53	0.40
30:E:261:LEU:O	30:E:294:ARG:NH2	2.37	0.40
31:F:120:LYS:HA	31:F:137:ILE:HD11	2.03	0.40
32:f:687:ARG:O	32:f:745:LEU:HD22	2.21	0.40
1:G:126:THR:O	2:H:128:ARG:NH1	2.50	0.40
2:H:79:MET:HB3	29:D:417:TYR:HB2	2.03	0.40
11:Q:170:ARG:NH2	12:r:125:THR:OG1	2.54	0.40
14:T:15:LYS:HG2	14:T:20:VAL:HG22	2.02	0.40
16:V:98:LEU:HD23	16:V:141:THR:HB	2.02	0.40
19:Z:175:LEU:HD23	22:c:207:TYR:HB3	2.03	0.40
22:c:272:ILE:HG22	22:c:273:LYS:H	1.86	0.40
22:c:292:MET:HE2	23:d:253:LEU:HD21	2.04	0.40
23:d:12:LYS:HB3	23:d:61:TRP:HE1	1.85	0.40
5:k:100:TRP:O	12:r:57:ARG:NH2	2.55	0.40
6:l:71:GLY:HA3	6:l:221:PHE:CZ	2.57	0.40
7:m:189:ILE:HA	7:m:192:GLU:HB2	2.04	0.40
7:m:216:VAL:HB	7:m:224:HIS:CD2	2.57	0.40
11:q:108:ASP:OD1	11:q:109:GLU:N	2.55	0.40
27:B:152:LEU:HD23	27:B:159:VAL:HA	2.03	0.40
28:C:219:LEU:HD22	29:D:290:LEU:HD21	2.03	0.40
30:E:169:GLY:HA3	30:E:295:LEU:HD23	2.03	0.40
5:K:117:SER:HB3	6:L:82:ARG:HH22	1.86	0.40
6:L:47:VAL:HG13	6:L:212:ILE:HG13	2.04	0.40
6:L:117:GLN:O	6:L:120:THR:OG1	2.32	0.40
7:M:27:MET:HA	7:M:153:PRO:HG2	2.04	0.40
9:O:100:LEU:HB3	9:O:111:TYR:HB2	2.02	0.40
15:U:403:THR:HG23	15:U:777:HIS:HE2	1.85	0.40
15:U:483:LEU:HD12	15:U:486:MET:HE3	2.02	0.40
16:V:99:ARG:HH21	16:V:150:ARG:NE	2.20	0.40
18:Y:179:ARG:NH2	18:Y:213:LEU:HG	2.37	0.40
19:Z:39:LEU:HB3	19:Z:93:GLY:C	2.46	0.40
20:a:33:LEU:HD13	20:a:36:GLN:HB2	2.04	0.40
20:a:275:LEU:HD12	20:a:275:LEU:HA	1.89	0.40
5:k:85:ALA:HB2	5:k:139:VAL:HG21	2.03	0.40
14:t:178:TYR:OH	14:t:208:ASN:N	2.46	0.40
27:B:353:PHE:HD1	27:B:353:PHE:HA	1.79	0.40
29:D:146:GLU:HB2	30:E:62:LYS:HD3	2.04	0.40
34:F:501:AGS:H5'1	34:F:501:AGS:H8	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:211:ILE:HA	32:f:214:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	237/240 (99%)	210 (89%)	27 (11%)	0	100	100
1	g	238/240 (99%)	218 (92%)	20 (8%)	0	100	100
2	H	228/232 (98%)	213 (93%)	15 (7%)	0	100	100
2	h	230/232 (99%)	226 (98%)	4 (2%)	0	100	100
3	I	246/250 (98%)	226 (92%)	19 (8%)	1 (0%)	30	66
3	i	248/250 (99%)	227 (92%)	20 (8%)	1 (0%)	30	66
4	J	237/243 (98%)	218 (92%)	19 (8%)	0	100	100
4	j	237/243 (98%)	216 (91%)	20 (8%)	1 (0%)	30	66
5	K	224/234 (96%)	205 (92%)	18 (8%)	1 (0%)	30	66
5	k	224/234 (96%)	206 (92%)	18 (8%)	0	100	100
6	L	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
6	l	236/238 (99%)	224 (95%)	12 (5%)	0	100	100
7	M	238/245 (97%)	221 (93%)	17 (7%)	0	100	100
7	m	238/245 (97%)	222 (93%)	16 (7%)	0	100	100
8	N	189/191 (99%)	180 (95%)	8 (4%)	1 (0%)	24	62
8	n	189/191 (99%)	178 (94%)	8 (4%)	3 (2%)	7	37
9	O	218/220 (99%)	207 (95%)	11 (5%)	0	100	100
9	o	218/220 (99%)	207 (95%)	11 (5%)	0	100	100
10	P	202/204 (99%)	193 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
11	Q	197/199 (99%)	178 (90%)	19 (10%)	0	100	100
11	q	197/199 (99%)	177 (90%)	20 (10%)	0	100	100
12	R	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
12	r	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
13	S	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	s	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
14	T	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
14	t	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
15	U	798/911 (88%)	721 (90%)	77 (10%)	0	100	100
16	V	471/480 (98%)	411 (87%)	55 (12%)	5 (1%)	11	45
17	W	454/456 (100%)	400 (88%)	51 (11%)	3 (1%)	18	54
18	Y	376/378 (100%)	325 (86%)	48 (13%)	3 (1%)	16	52
19	Z	284/286 (99%)	246 (87%)	35 (12%)	3 (1%)	11	45
20	a	371/373 (100%)	331 (89%)	39 (10%)	1 (0%)	36	71
21	b	189/191 (99%)	170 (90%)	17 (9%)	2 (1%)	11	45
22	c	274/287 (96%)	235 (86%)	38 (14%)	1 (0%)	30	66
23	d	255/257 (99%)	219 (86%)	35 (14%)	1 (0%)	30	66
24	e	36/70 (51%)	29 (81%)	7 (19%)	0	100	100
25	X	378/380 (100%)	341 (90%)	35 (9%)	2 (0%)	24	62
26	A	376/399 (94%)	327 (87%)	45 (12%)	4 (1%)	11	45
27	B	366/389 (94%)	322 (88%)	42 (12%)	2 (0%)	24	62
28	C	359/392 (92%)	320 (89%)	36 (10%)	3 (1%)	16	52
29	D	378/380 (100%)	323 (85%)	49 (13%)	6 (2%)	7	37
30	E	373/375 (100%)	340 (91%)	33 (9%)	0	100	100
31	F	372/396 (94%)	337 (91%)	33 (9%)	2 (0%)	24	62
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	10	42
All	All	12934/13558 (95%)	11738 (91%)	1142 (9%)	54 (0%)	31	66

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	78	HIS

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Mol	Chain	Res	Type
16	V	262	SER
17	W	314	LEU
18	Y	283	LYS
18	Y	284	LYS
8	n	92	GLU
29	D	148	ASP
29	D	409	LYS
32	f	337	LEU
32	f	364	GLN
32	f	367	SER
32	f	665	GLU
16	V	60	ALA
21	b	22	LEU
8	n	91	ARG
27	B	377	ASP
31	F	436	GLN
32	f	183	PRO
32	f	365	VAL
5	K	10	ARG
17	W	313	GLU
17	W	410	ALA
19	Z	220	LEU
22	c	176	GLN
23	d	35	PHE
29	D	126	PRO
32	f	184	LEU
32	f	326	LEU
16	V	54	LYS
20	a	187	ASP
4	j	181	ILE
25	X	355	LYS
26	A	431	THR
28	C	89	VAL
29	D	299	PHE
8	N	19	ARG
18	Y	117	LYS
3	i	221	GLY
8	n	19	ARG
28	C	90	HIS
3	I	221	GLY
16	V	102	PRO
26	A	109	PRO

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Mol	Chain	Res	Type
29	D	153	MET
19	Z	221	PRO
26	A	115	VAL
27	B	433	GLY
28	C	401	ILE
21	b	23	PRO
31	F	218	GLN
25	X	341	PRO
26	A	311	PRO
19	Z	144	VAL
29	D	125	LYS

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	G	192/205 (94%)	189 (98%)	3 (2%)	55	69
1	g	193/205 (94%)	191 (99%)	2 (1%)	68	75
2	H	162/190 (85%)	160 (99%)	2 (1%)	63	73
2	h	164/190 (86%)	164 (100%)	0	100	100
3	I	191/210 (91%)	190 (100%)	1 (0%)	81	81
3	i	193/210 (92%)	193 (100%)	0	100	100
4	J	152/207 (73%)	151 (99%)	1 (1%)	76	78
4	j	152/207 (73%)	151 (99%)	1 (1%)	76	78
5	K	187/196 (95%)	186 (100%)	1 (0%)	81	81
5	k	186/196 (95%)	186 (100%)	0	100	100
6	L	198/204 (97%)	198 (100%)	0	100	100
6	l	198/204 (97%)	198 (100%)	0	100	100
7	M	192/202 (95%)	192 (100%)	0	100	100
7	m	192/202 (95%)	192 (100%)	0	100	100
8	N	148/148 (100%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	n	148/148 (100%)	148 (100%)	0	100	100
9	O	177/181 (98%)	177 (100%)	0	100	100
9	o	177/181 (98%)	177 (100%)	0	100	100
10	P	172/173 (99%)	172 (100%)	0	100	100
10	p	172/173 (99%)	172 (100%)	0	100	100
11	Q	164/170 (96%)	164 (100%)	0	100	100
11	q	164/170 (96%)	161 (98%)	3 (2%)	51	66
12	R	153/156 (98%)	153 (100%)	0	100	100
12	r	153/156 (98%)	153 (100%)	0	100	100
13	S	174/178 (98%)	174 (100%)	0	100	100
13	s	174/178 (98%)	174 (100%)	0	100	100
14	T	175/178 (98%)	175 (100%)	0	100	100
14	t	175/178 (98%)	175 (100%)	0	100	100
15	U	685/779 (88%)	679 (99%)	6 (1%)	70	75
16	V	410/414 (99%)	405 (99%)	5 (1%)	63	73
17	W	416/416 (100%)	412 (99%)	4 (1%)	68	75
18	Y	334/334 (100%)	332 (99%)	2 (1%)	78	80
19	Z	257/257 (100%)	252 (98%)	5 (2%)	50	66
20	a	333/333 (100%)	331 (99%)	2 (1%)	78	80
21	b	167/167 (100%)	165 (99%)	2 (1%)	63	73
22	c	243/252 (96%)	241 (99%)	2 (1%)	73	77
23	d	231/231 (100%)	229 (99%)	2 (1%)	70	75
24	e	38/38 (100%)	38 (100%)	0	100	100
25	X	327/327 (100%)	321 (98%)	6 (2%)	51	66
26	A	298/343 (87%)	297 (100%)	1 (0%)	86	84
27	B	300/345 (87%)	300 (100%)	0	100	100
28	C	315/340 (93%)	312 (99%)	3 (1%)	68	75
29	D	333/333 (100%)	331 (99%)	2 (1%)	78	80
30	E	298/329 (91%)	293 (98%)	5 (2%)	53	67
31	F	296/340 (87%)	295 (100%)	1 (0%)	86	84
32	f	580/763 (76%)	564 (97%)	16 (3%)	38	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	10739/11537 (93%)	10661 (99%)	78 (1%)	73	78

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	66	VAL
1	G	141	ILE
1	G	215	ILE
2	H	121	TYR
2	H	208	ILE
3	I	11	ILE
4	J	161	ILE
5	K	33	LEU
15	U	153	ILE
15	U	173	VAL
15	U	223	LEU
15	U	371	ILE
15	U	529	ILE
15	U	554	LEU
16	V	40	GLU
16	V	86	VAL
16	V	224	LEU
16	V	255	LEU
16	V	275	VAL
17	W	85	GLU
17	W	138	VAL
17	W	333	LEU
17	W	424	LEU
18	Y	157	ILE
18	Y	357	ASN
19	Z	17	LEU
19	Z	108	ILE
19	Z	220	LEU
19	Z	230	LEU
19	Z	266	ILE
20	a	122	LYS
20	a	188	LEU
21	b	54	LEU
21	b	71	ILE
22	c	62	VAL
22	c	69	VAL
23	d	18	LYS

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Mol	Chain	Res	Type
23	d	197	ILE
1	g	141	ILE
1	g	215	ILE
4	j	161	ILE
11	q	4	LEU
11	q	88	LEU
11	q	140	LEU
25	X	50	ILE
25	X	216	ILE
25	X	217	ILE
25	X	338	VAL
25	X	341	PRO
25	X	356	LEU
26	A	403	ILE
28	C	57	ARG
28	C	109	THR
28	C	275	GLU
29	D	47	LEU
29	D	88	VAL
30	E	87	LEU
30	E	105	LEU
30	E	138	LEU
30	E	257	LEU
30	E	312	ILE
31	F	198	LEU
32	f	88	SER
32	f	184	LEU
32	f	207	LEU
32	f	337	LEU
32	f	370	MET
32	f	381	VAL
32	f	387	GLN
32	f	389	LYS
32	f	391	LEU
32	f	403	LYS
32	f	460	ASP
32	f	463	LEU
32	f	479	LEU
32	f	641	GLU
32	f	797	LEU
32	f	800	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151)

such sidechains are listed below:

Mol	Chain	Res	Type
1	G	68	HIS
1	G	100	ASN
1	G	123	GLN
2	H	119	GLN
2	H	123	GLN
3	I	20	GLN
3	I	102	GLN
3	I	119	GLN
3	I	146	GLN
3	I	198	ASN
4	J	15	HIS
4	J	54	GLN
4	J	85	ASN
4	J	154	HIS
4	J	175	ASN
5	K	23	GLN
5	K	41	GLN
5	K	164	GLN
5	K	214	ASN
6	L	20	HIS
6	L	121	GLN
7	M	68	ASN
7	M	110	HIS
7	M	180	GLN
8	N	110	GLN
10	P	61	GLN
10	P	93	ASN
11	Q	71	ASN
11	Q	168	GLN
12	R	10	HIS
12	R	38	ASN
13	S	159	GLN
14	T	61	GLN
14	T	65	GLN
15	U	79	ASN
15	U	452	ASN
15	U	453	HIS
15	U	491	GLN
15	U	707	ASN
15	U	718	ASN
15	U	768	GLN
16	V	81	GLN

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Mol	Chain	Res	Type
16	V	118	GLN
16	V	193	GLN
16	V	283	ASN
16	V	473	GLN
17	W	106	GLN
17	W	156	ASN
17	W	235	GLN
17	W	264	GLN
17	W	440	ASN
17	W	444	HIS
18	Y	49	ASN
18	Y	71	ASN
18	Y	178	ASN
18	Y	196	GLN
18	Y	306	GLN
18	Y	367	GLN
18	Y	388	ASN
19	Z	278	ASN
19	Z	282	ASN
20	a	9	GLN
20	a	62	ASN
20	a	169	HIS
20	a	193	GLN
20	a	370	GLN
22	c	113	HIS
22	c	128	ASN
22	c	214	GLN
22	c	254	ASN
22	c	295	ASN
23	d	77	GLN
23	d	135	HIS
24	e	6	GLN
24	e	54	ASN
24	e	55	GLN
1	g	100	ASN
3	i	88	ASN
3	i	102	GLN
3	i	146	GLN
3	i	149	GLN
3	i	167	ASN
3	i	198	ASN
4	j	18	GLN

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Mol	Chain	Res	Type
4	j	116	GLN
4	j	154	HIS
4	j	175	ASN
5	k	99	HIS
5	k	152	GLN
5	k	214	ASN
5	k	225	ASN
6	l	8	ASN
6	l	90	GLN
6	l	146	GLN
7	m	97	ASN
7	m	101	ASN
7	m	180	GLN
7	m	201	HIS
8	n	154	GLN
9	o	62	ASN
9	o	116	HIS
10	p	93	ASN
11	q	168	GLN
12	r	38	ASN
12	r	85	ASN
13	s	146	GLN
13	s	160	ASN
14	t	61	GLN
14	t	65	GLN
14	t	81	HIS
14	t	213	HIS
25	X	170	GLN
25	X	213	GLN
25	X	292	GLN
25	X	296	ASN
25	X	329	ASN
26	A	91	GLN
26	A	247	GLN
26	A	293	ASN
26	A	296	GLN
27	B	131	HIS
27	B	277	HIS
28	C	90	HIS
28	C	171	HIS
28	C	221	GLN
28	C	241	HIS

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Mol	Chain	Res	Type
28	C	278	ASN
28	C	332	HIS
28	C	398	ASN
29	D	65	GLN
29	D	133	HIS
29	D	295	GLN
29	D	304	ASN
29	D	380	GLN
30	E	86	GLN
30	E	194	ASN
30	E	339	ASN
30	E	364	GLN
31	F	83	ASN
31	F	255	GLN
31	F	417	HIS
31	F	428	GLN
32	f	102	HIS
32	f	213	GLN
32	f	352	HIS
32	f	387	GLN
32	f	473	ASN
32	f	493	ASN
32	f	540	GLN
32	f	565	ASN
32	f	650	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	AGS	F	501	-	32,33,33	1.01	2 (6%)	45,52,52	1.24	2 (4%)
34	AGS	E	401	-	32,33,33	0.94	2 (6%)	45,52,52	0.90	2 (4%)
34	AGS	D	501	-	32,33,33	0.75	2 (6%)	45,52,52	1.11	3 (6%)
34	AGS	A	501	-	32,33,33	0.78	2 (6%)	45,52,52	0.98	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	AGS	F	501	-	-	6/21/38/38	0/3/3/3
34	AGS	E	401	-	-	6/21/38/38	0/3/3/3
34	AGS	D	501	-	-	8/21/38/38	0/3/3/3
34	AGS	A	501	-	-	5/21/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	401	AGS	PA-O3A	-3.47	1.55	1.59
34	F	501	AGS	PB-O3B	-3.28	1.56	1.59
34	F	501	AGS	PB-O3A	-3.16	1.56	1.59
34	D	501	AGS	PB-O3B	-2.88	1.56	1.59
34	E	401	AGS	PB-O3A	-2.33	1.57	1.59
34	A	501	AGS	PA-O3A	-2.26	1.57	1.59
34	A	501	AGS	PG-S1G	2.03	1.95	1.90
34	D	501	AGS	PG-S1G	2.03	1.95	1.90

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	501	AGS	PB-O3B-PG	-5.95	111.39	133.17
34	D	501	AGS	PB-O3B-PG	-5.72	112.25	133.17
34	A	501	AGS	PB-O3B-PG	-4.36	117.21	133.17
34	E	401	AGS	PB-O3B-PG	-3.84	119.12	133.17
34	E	401	AGS	O3A-PA-O1A	-2.70	102.58	110.70
34	D	501	AGS	O2A-PA-O3A	2.25	113.36	107.27
34	A	501	AGS	O3B-PB-O1B	-2.17	104.18	110.70
34	F	501	AGS	O2B-PB-O3B	-2.05	101.72	107.27
34	D	501	AGS	O3G-PG-O3B	2.04	111.45	104.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

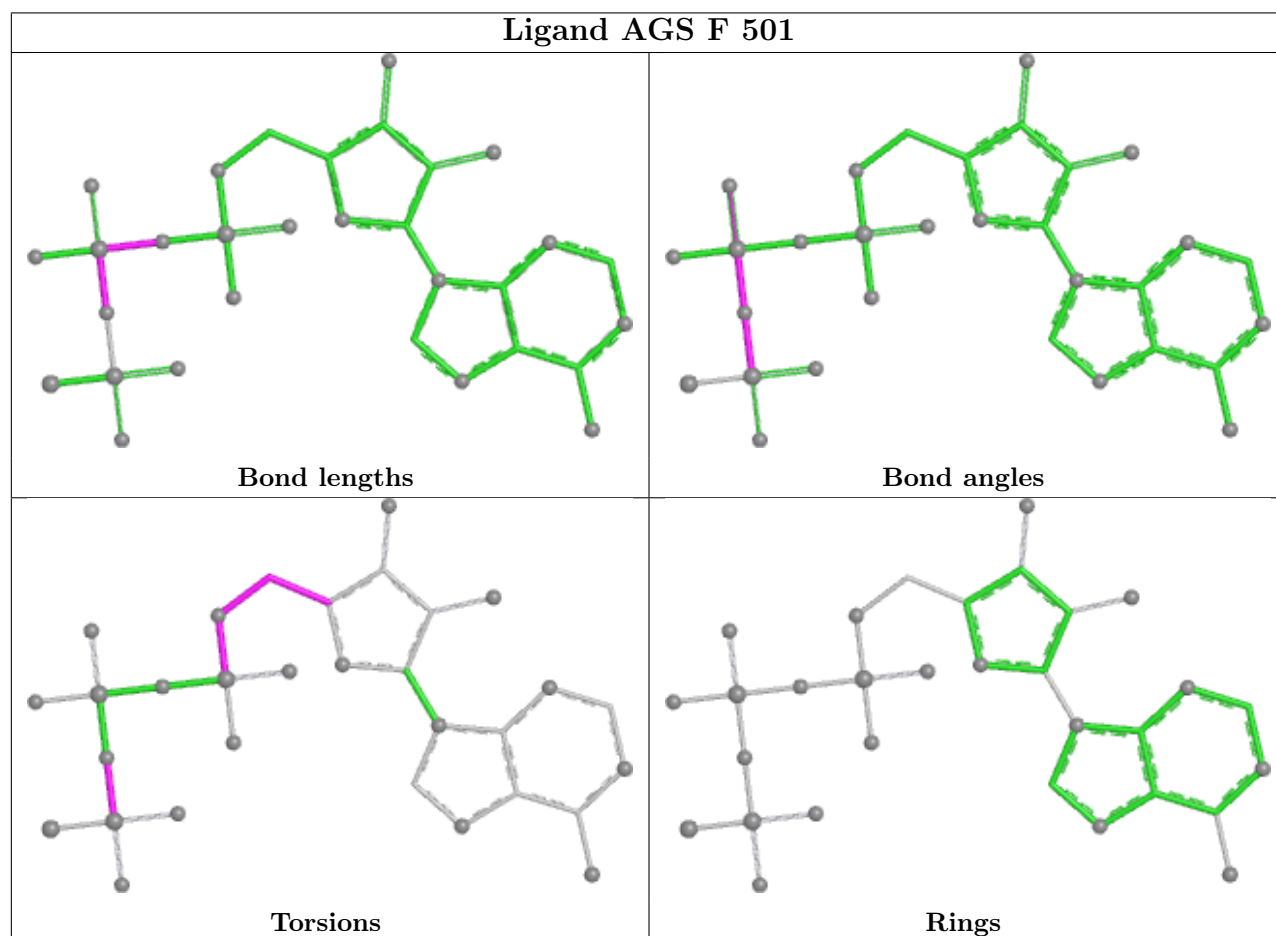
Mol	Chain	Res	Type	Atoms
34	A	501	AGS	C5'-O5'-PA-O1A
34	D	501	AGS	C5'-O5'-PA-O1A
34	D	501	AGS	C5'-O5'-PA-O3A
34	E	401	AGS	PB-O3B-PG-O2G
34	E	401	AGS	C5'-O5'-PA-O1A
34	E	401	AGS	C5'-O5'-PA-O2A
34	E	401	AGS	C5'-O5'-PA-O3A
34	F	501	AGS	PB-O3B-PG-O2G
34	F	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O3A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

There are no ring outliers.

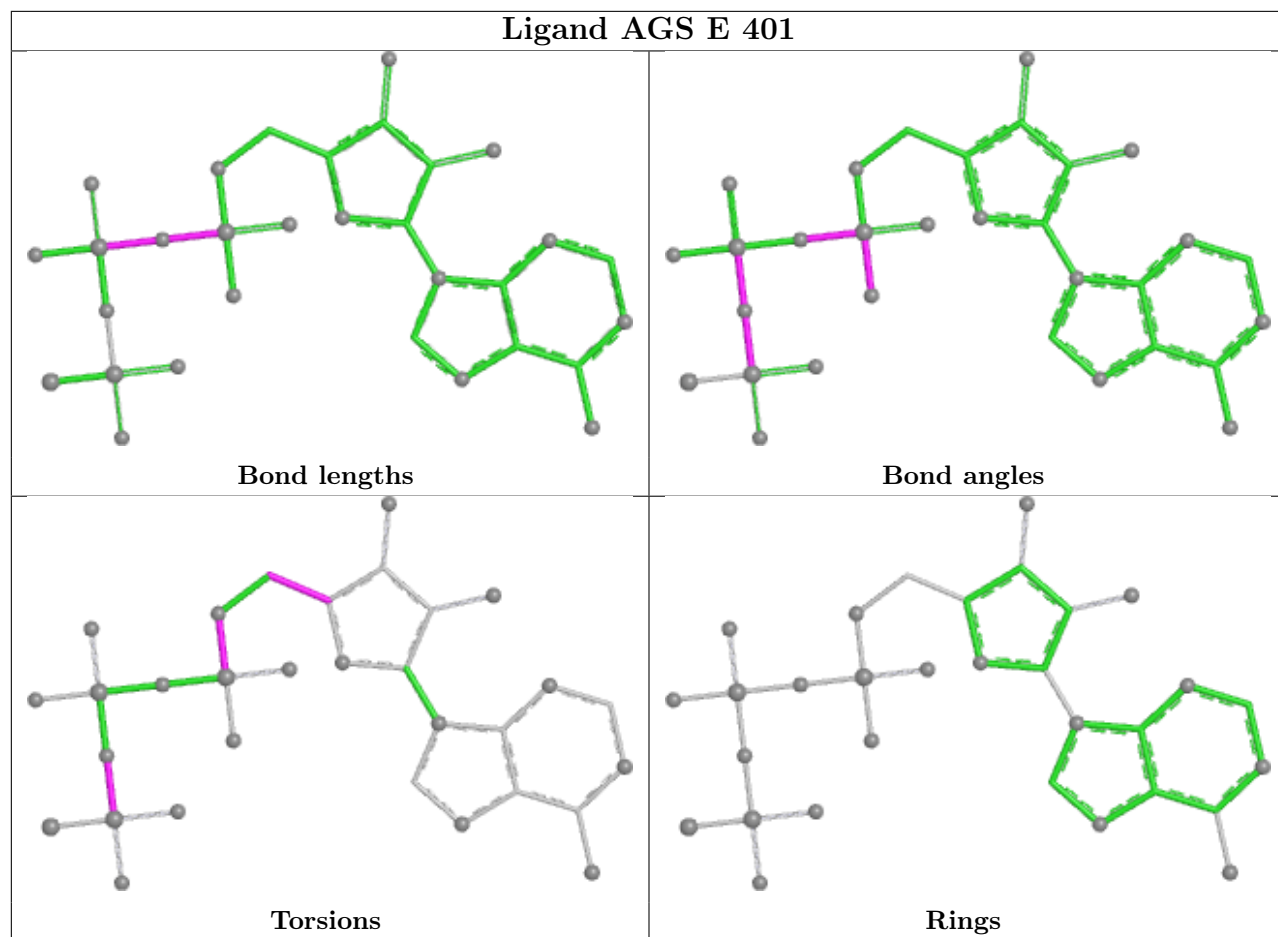
4 monomers are involved in 26 short contacts:

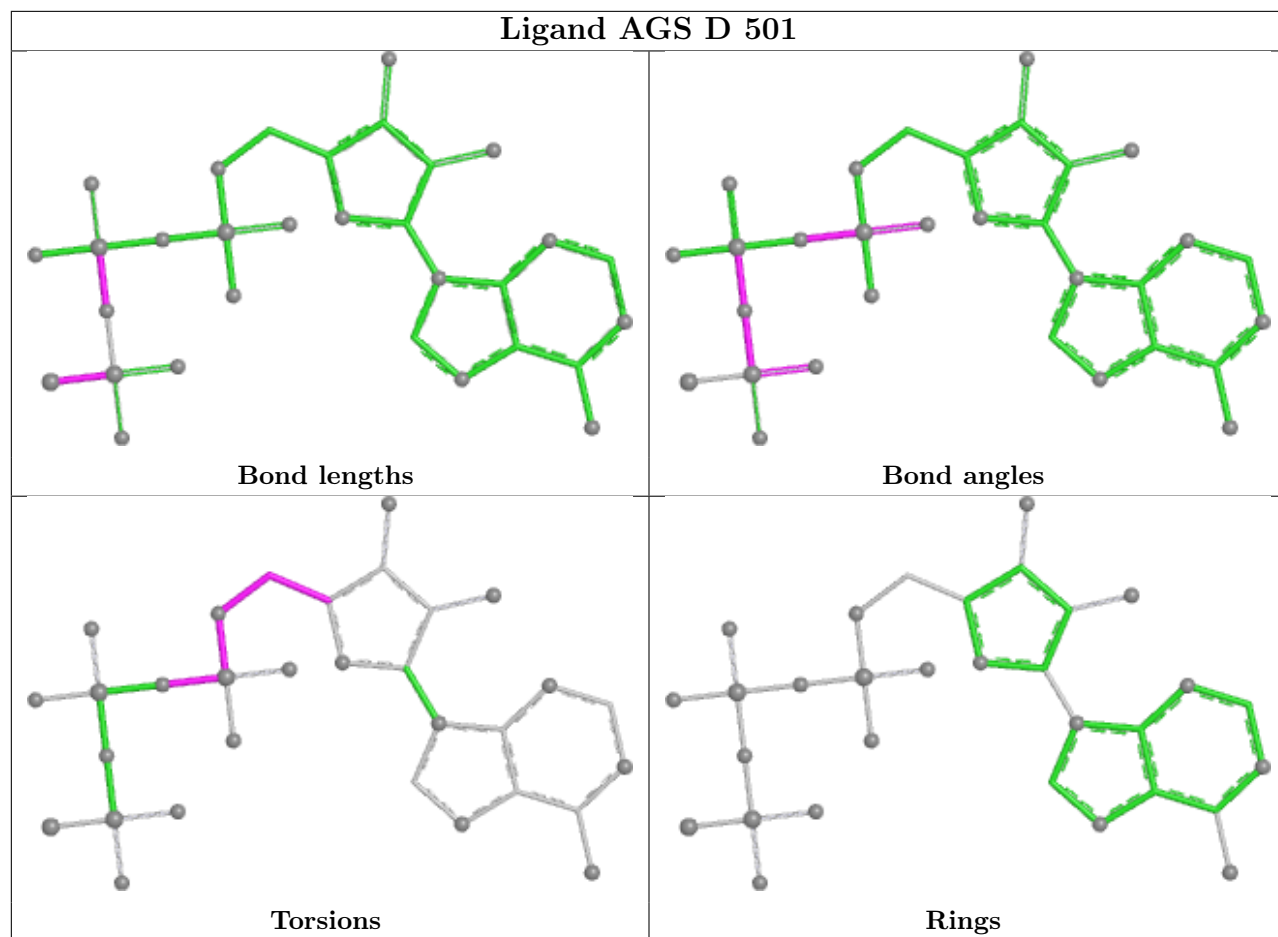
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	F	501	AGS	4	0
34	E	401	AGS	16	0
34	D	501	AGS	3	0
34	A	501	AGS	3	0

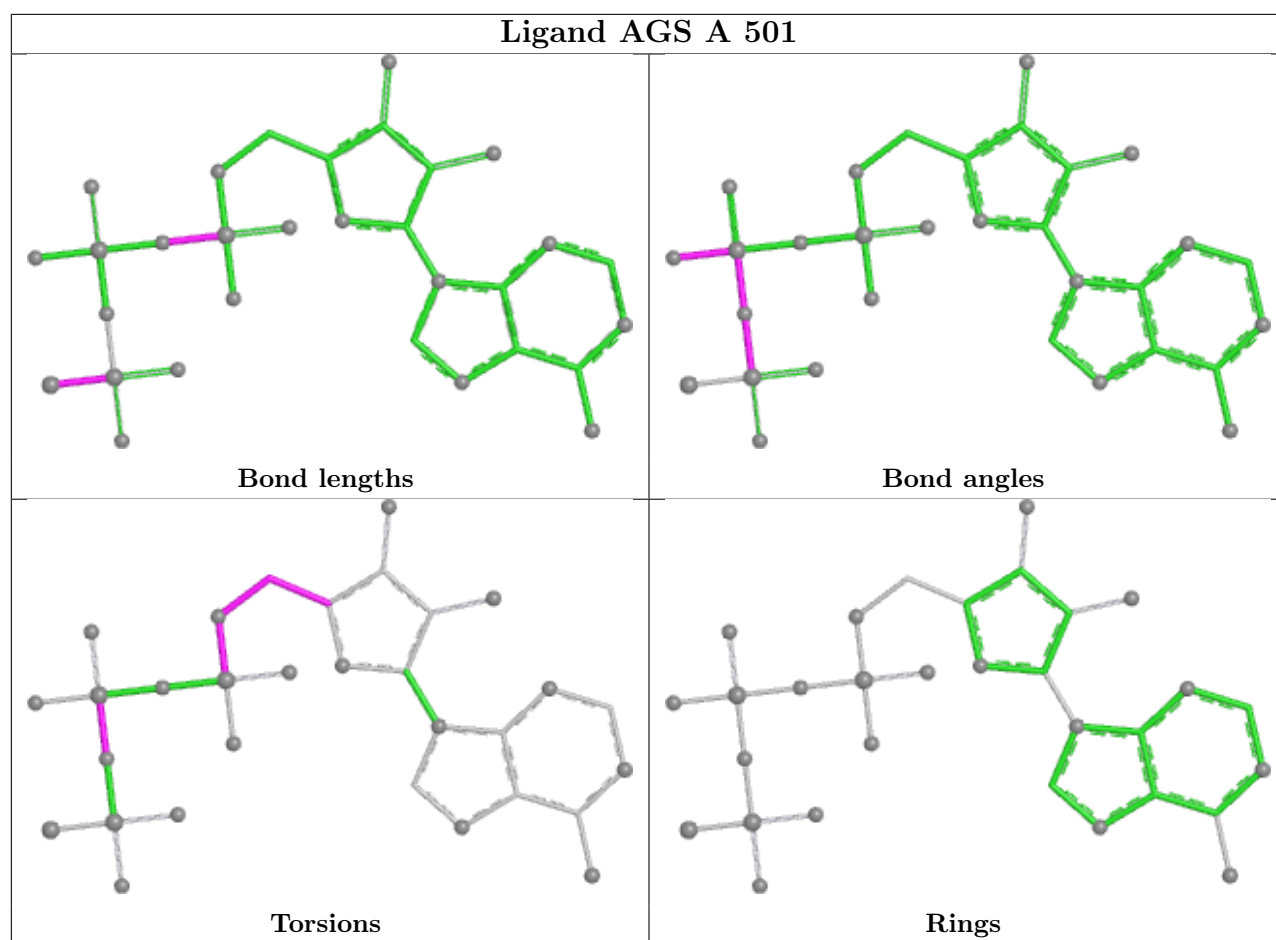
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand AGS E 401







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.

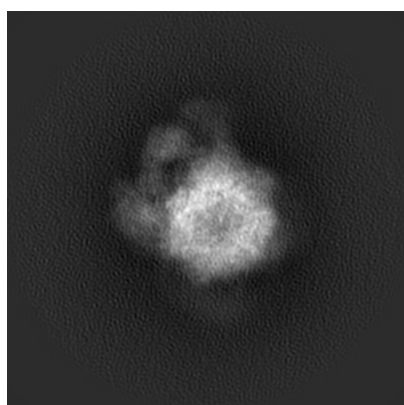
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8663. These allow visual inspection of the internal detail of the map and identification of artifacts.

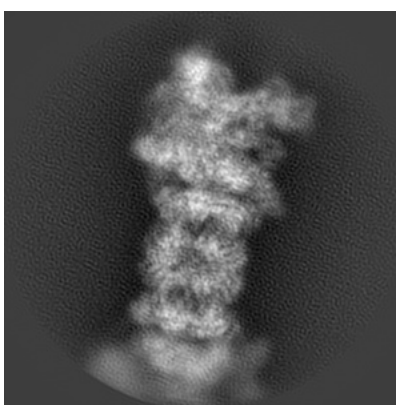
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

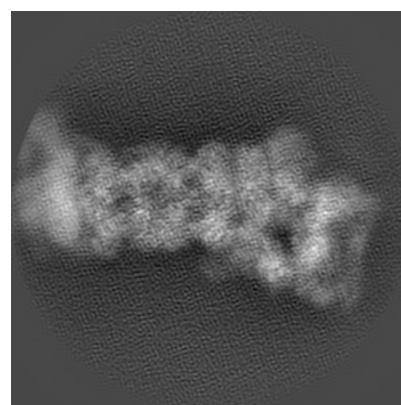
6.1.1 Primary map



X



Y

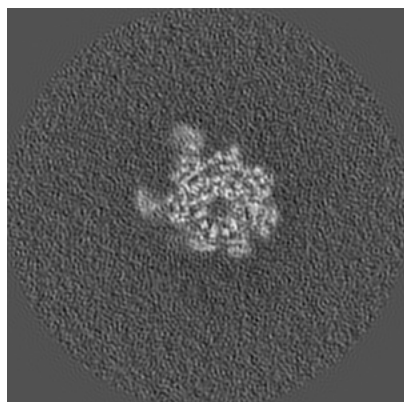


Z

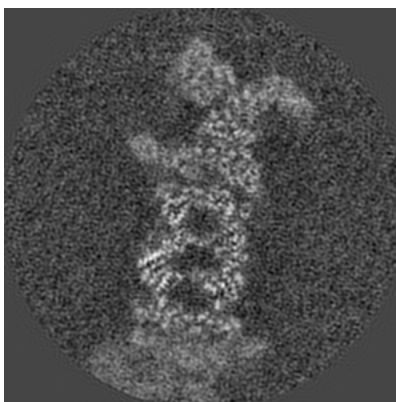
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

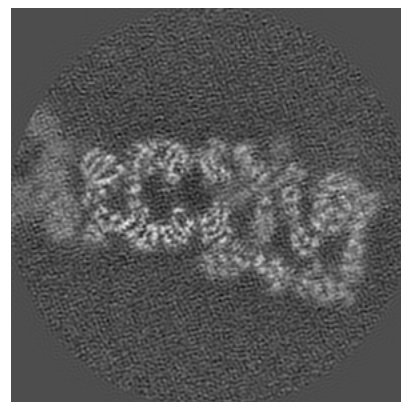
6.2.1 Primary map



X Index: 280



Y Index: 280

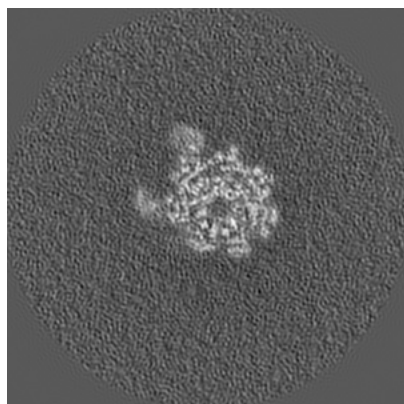


Z Index: 280

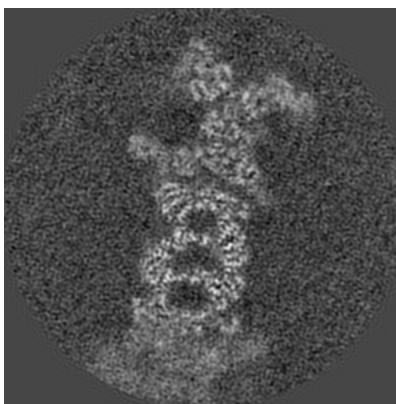
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

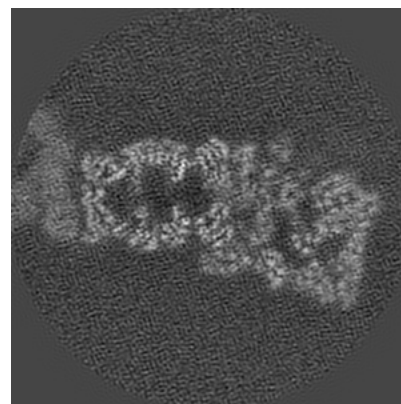
6.3.1 Primary map



X Index: 281



Y Index: 277

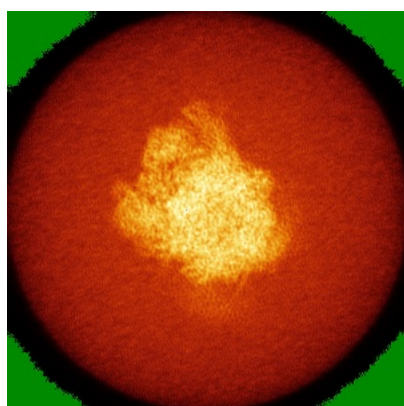


Z Index: 275

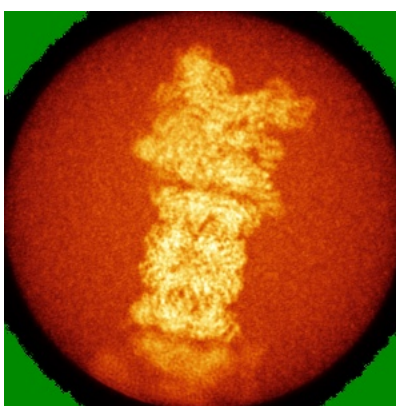
The images above show the largest variance slices of the map in three orthogonal directions.

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

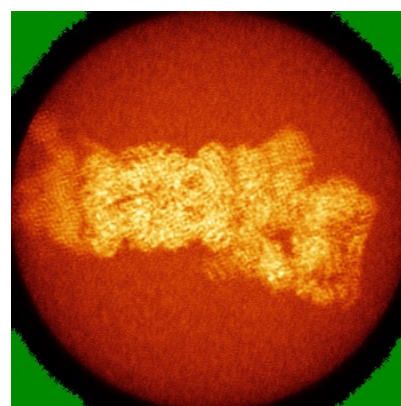
6.4.1 Primary map



X



Y

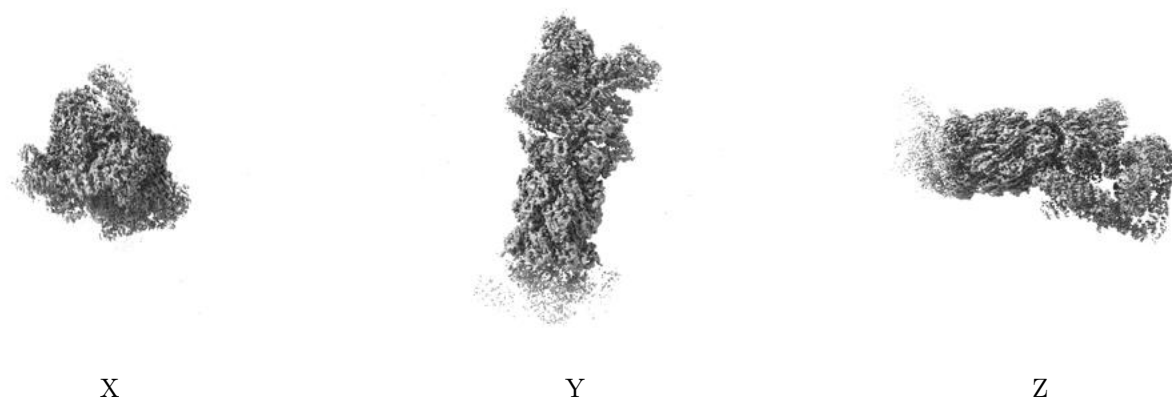


Z

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

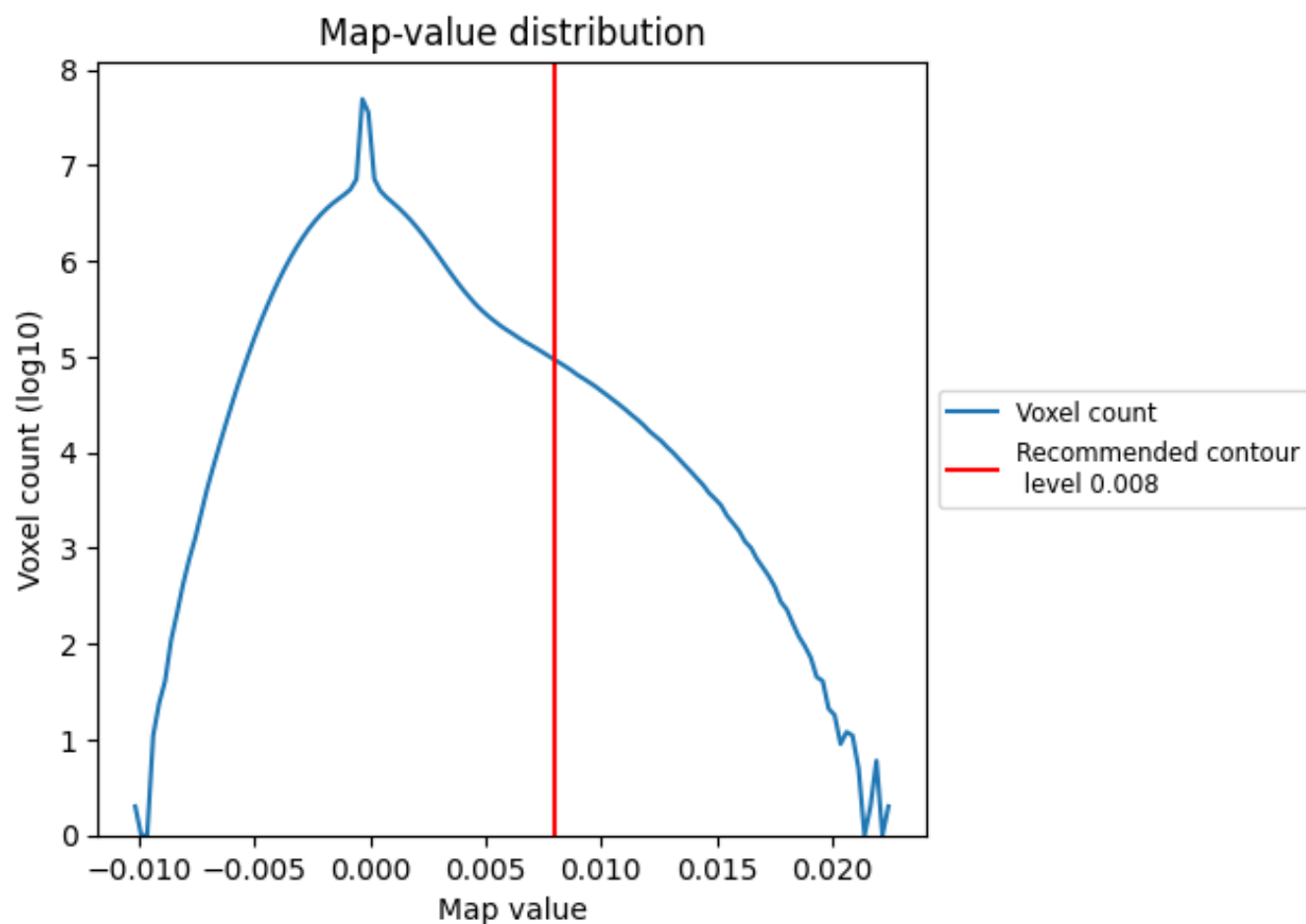
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

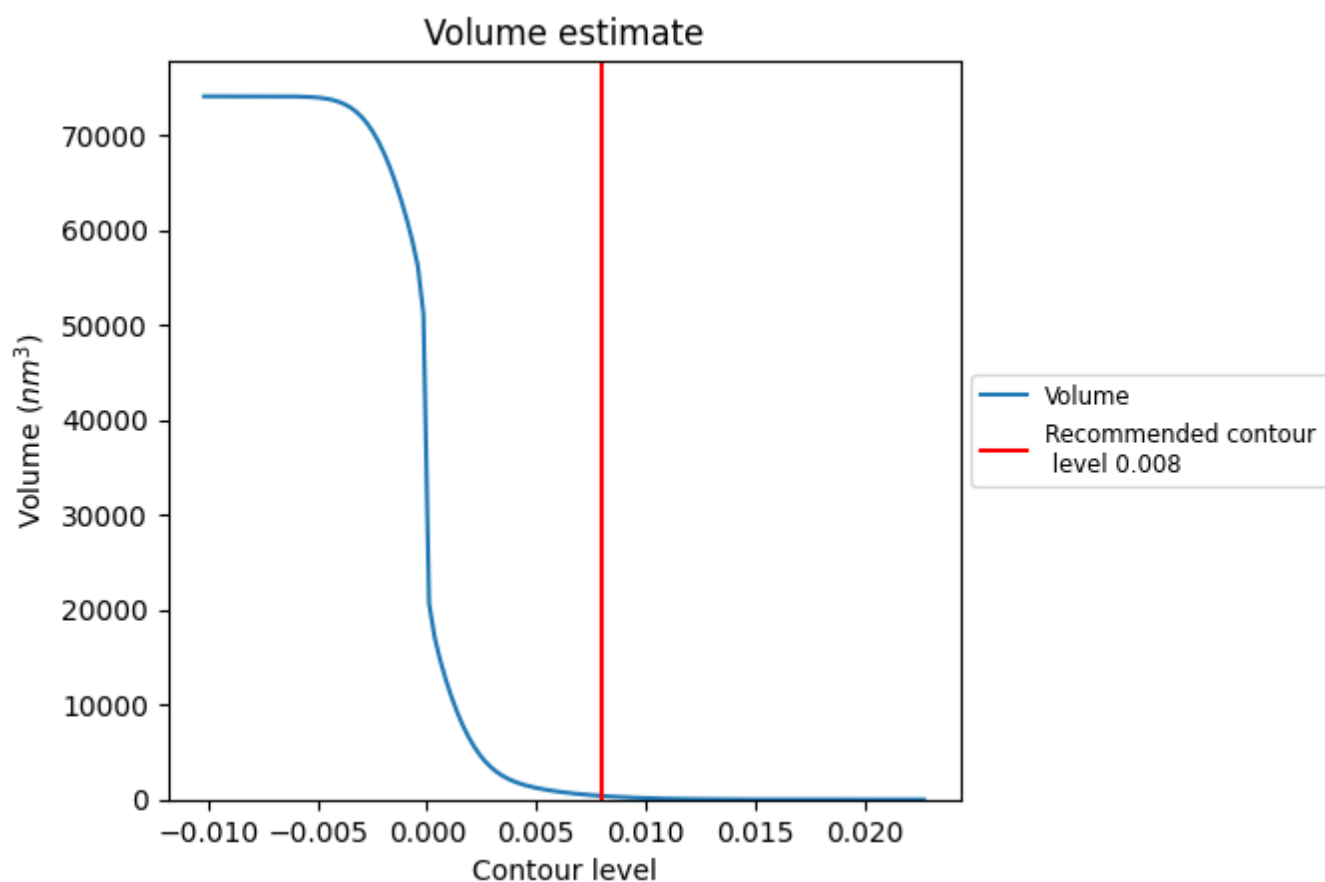
This section contains the results of statistical analysis of the map.

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.

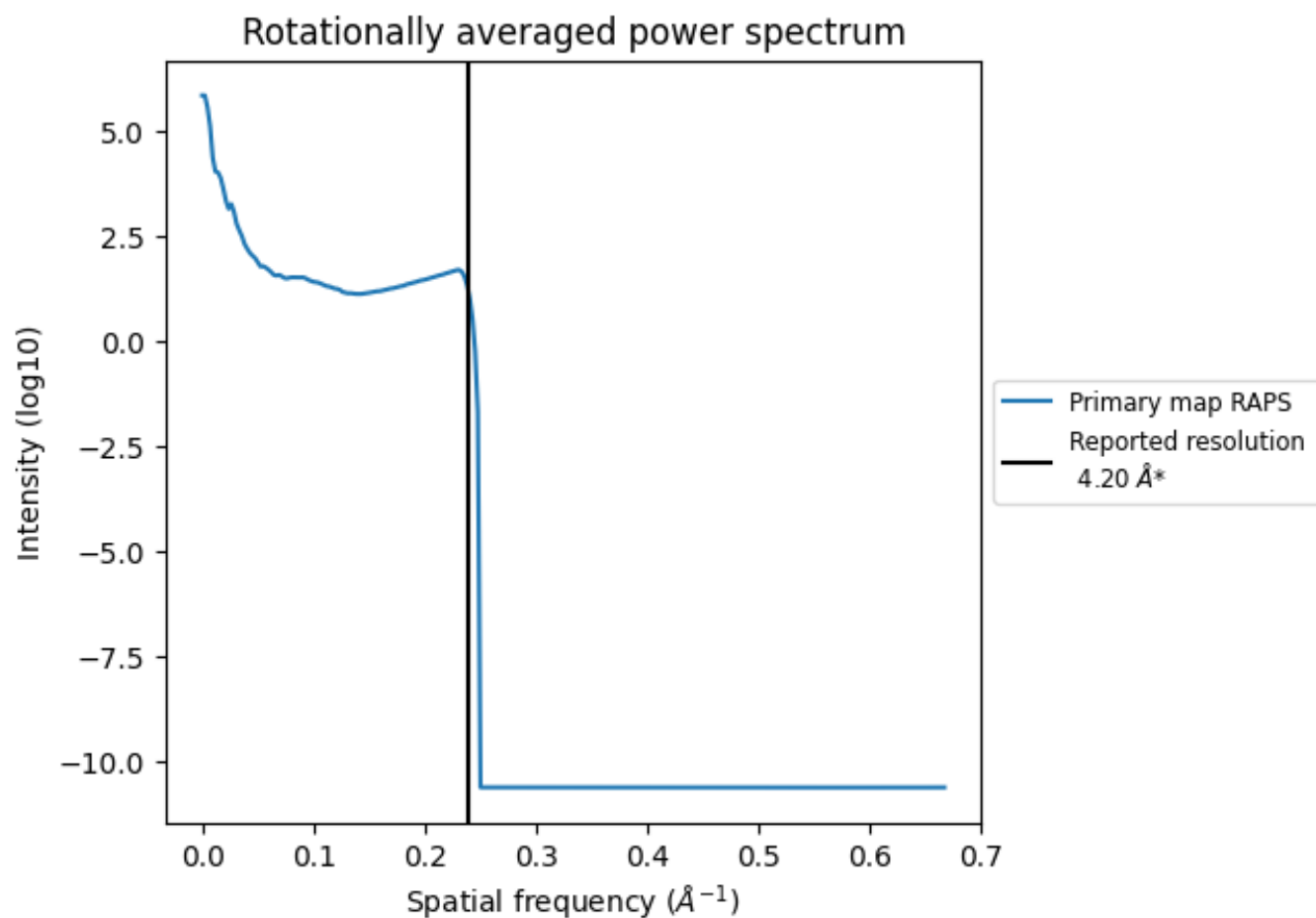
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 381 nm³; this corresponds to an approximate mass of 344 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 0.238 $\text{\AA}^{-1}$

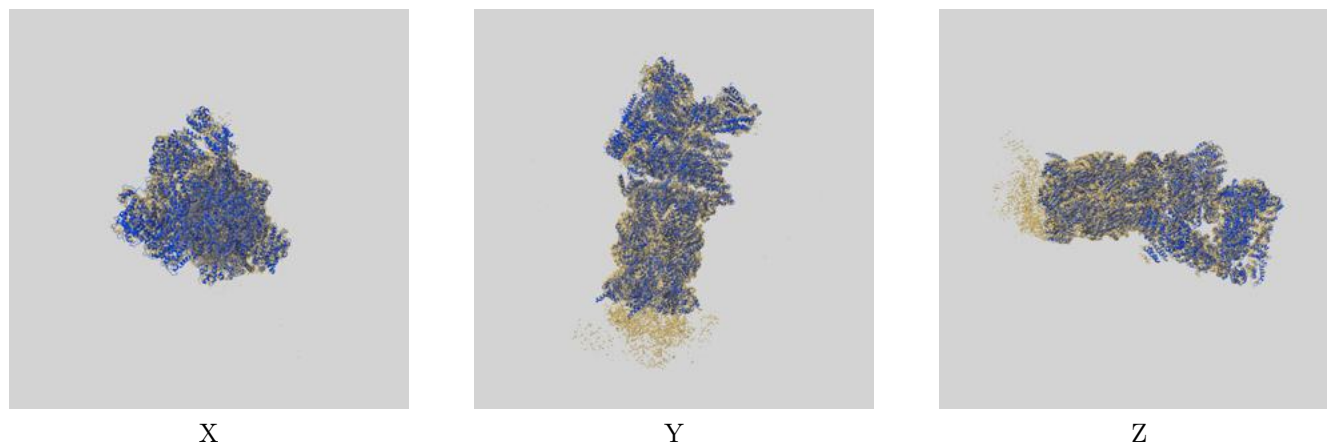
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

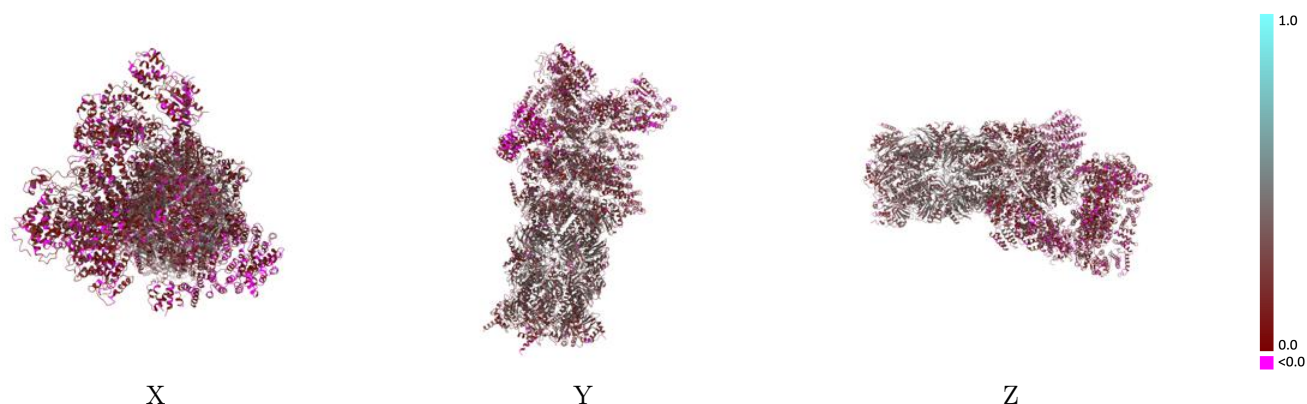
This section contains information regarding the fit between EMDB map EMD-8663 and PDB model 5VFP. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



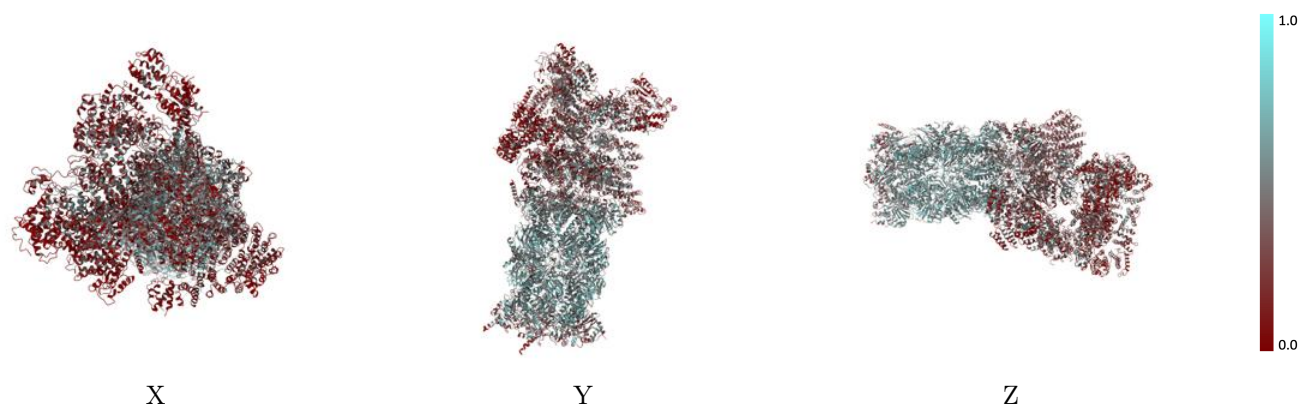
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



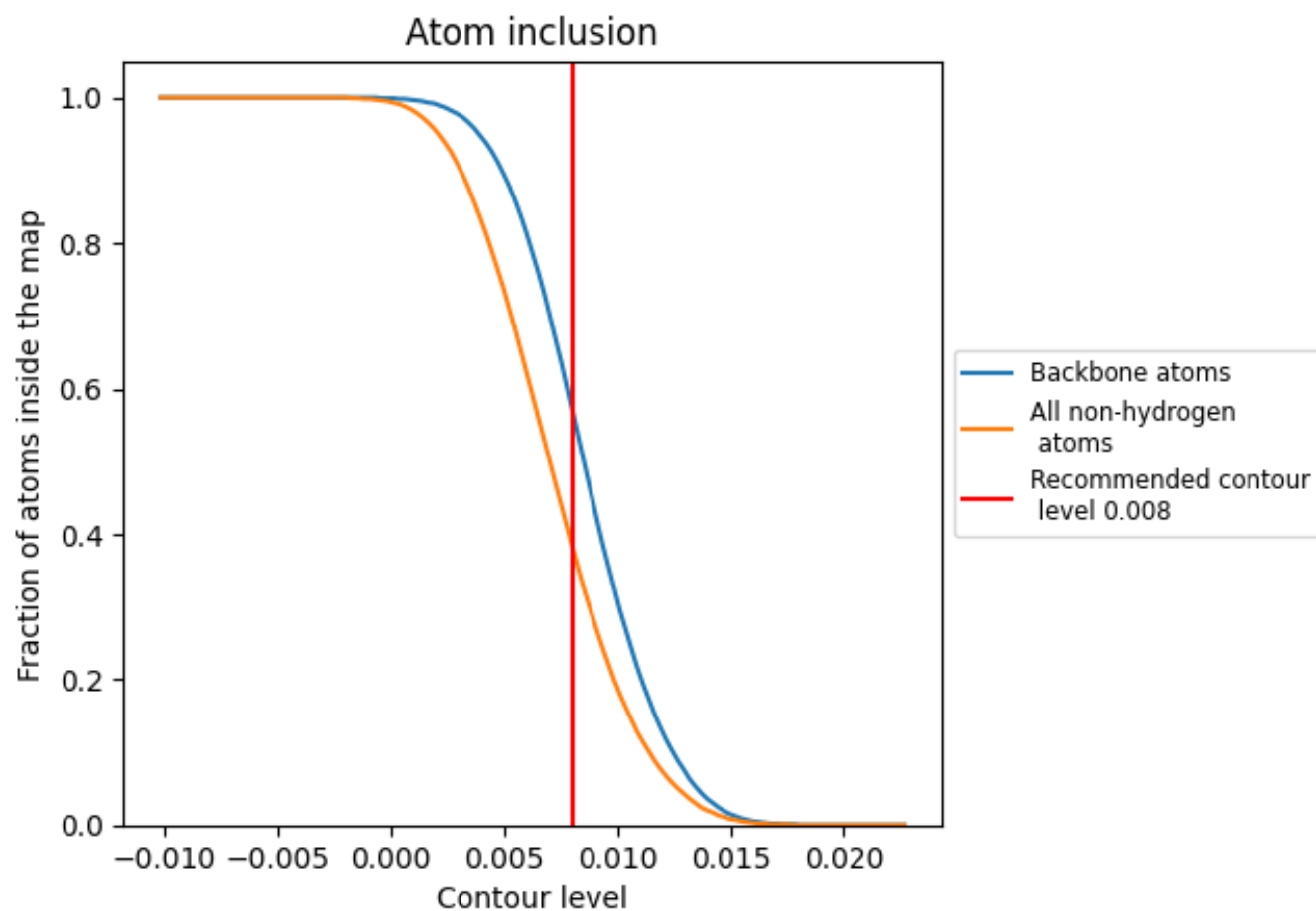
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 38% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3840	0.2500
A	0.3480	0.2590
B	0.2810	0.2520
C	0.2830	0.2300
D	0.2940	0.2570
E	0.3560	0.2650
F	0.3600	0.2590
G	0.5150	0.3320
H	0.5350	0.3240
I	0.4580	0.2840
J	0.4330	0.2700
K	0.4490	0.2760
L	0.5040	0.3020
M	0.5070	0.3020
N	0.6130	0.3610
O	0.5520	0.3400
P	0.5710	0.3530
Q	0.5420	0.3170
R	0.5980	0.3540
S	0.5440	0.3410
T	0.5950	0.3570
U	0.3000	0.1860
V	0.2060	0.1670
W	0.2570	0.1650
X	0.2740	0.2240
Y	0.3160	0.1800
Z	0.2810	0.1930
a	0.2280	0.1600
b	0.1570	0.1470
c	0.3050	0.1920
d	0.1330	0.1380
e	0.1790	0.1800
f	0.1530	0.0730
g	0.4370	0.2810
h	0.4470	0.2890



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Chain	Atom inclusion	Q-score
i	 0.4190	 0.2660
j	 0.4480	 0.2800
k	 0.4550	 0.2810
l	 0.5090	 0.2900
m	 0.4570	 0.2710
n	 0.6040	 0.3600
o	 0.5340	 0.3320
p	 0.5670	 0.3490
q	 0.5730	 0.3350
r	 0.6060	 0.3570
s	 0.5740	 0.3460
t	 0.6140	 0.3510