



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:12 PM UTC

PDB ID : 5VFQ / pdb_00005vfq
EMDB ID : EMD-8664
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:

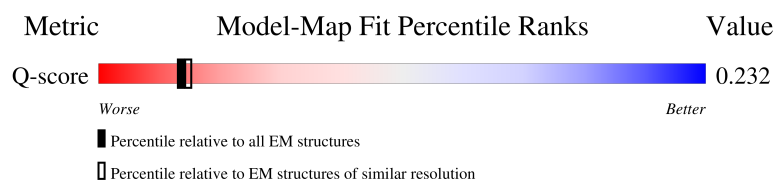
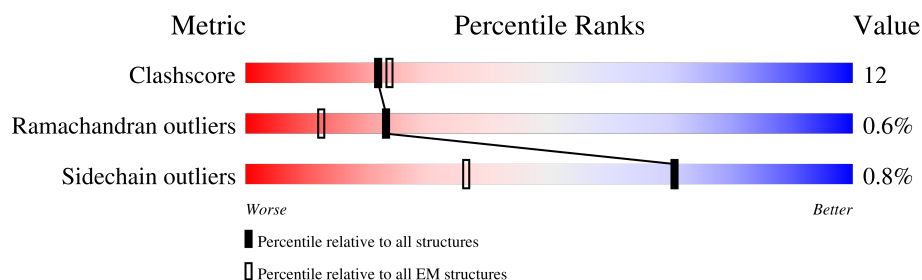
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	16% 82% 17% .
1	g	240	12% 83% 17%
2	H	232	9% 82% 17% .
2	h	232	11% 84% 16%

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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	
17	W	456	
18	X	380	
19	Y	378	
20	Z	286	
21	a	373	
22	b	191	
23	c	287	
24	d	257	
25	e	70	
26	A	399	
27	B	389	
28	C	392	
29	D	380	
30	E	375	
31	F	396	
32	f	908	

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	D	501	-	-	X	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 101134 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	447	Total	C	N	O	S	0	0
			3600	2287	639	660	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 11.

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

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 25 is a protein called Sem1.

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

- 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		

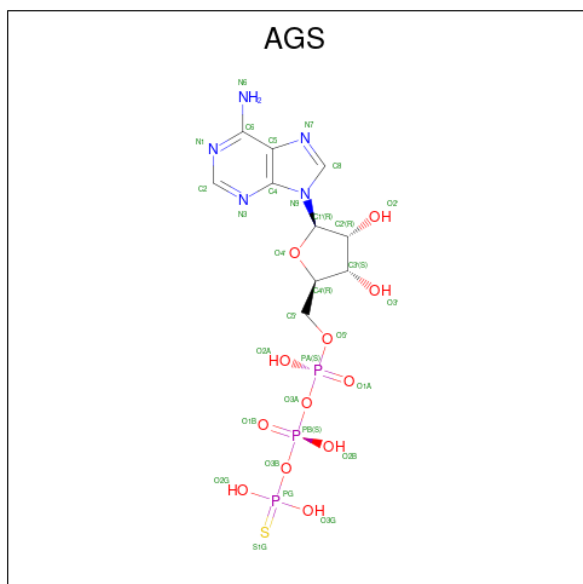
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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).



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

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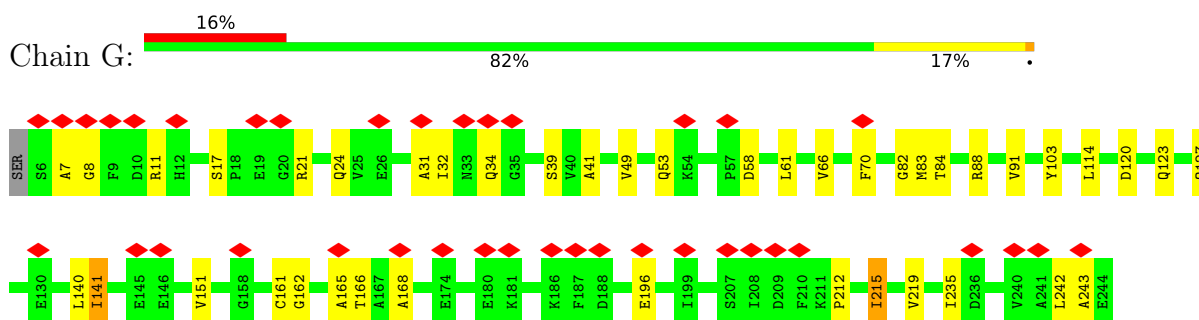
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Mol	Chain	Residues	Atoms						AltConf
34	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
34	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

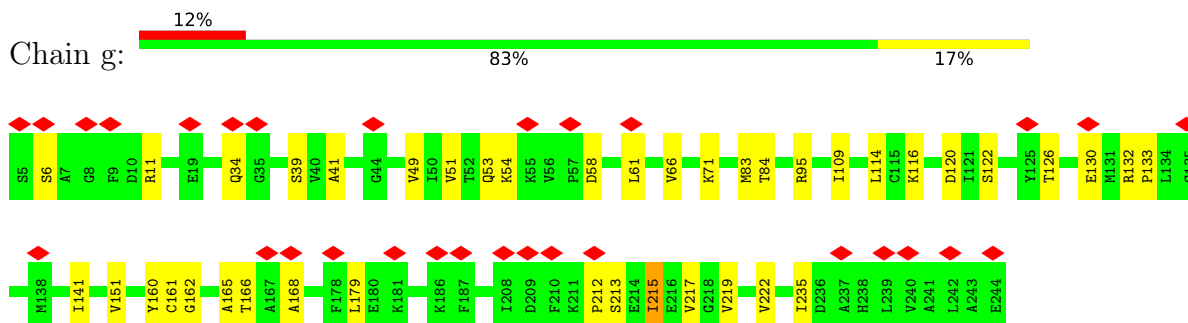
3 Residue-property plots [i](#)

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.

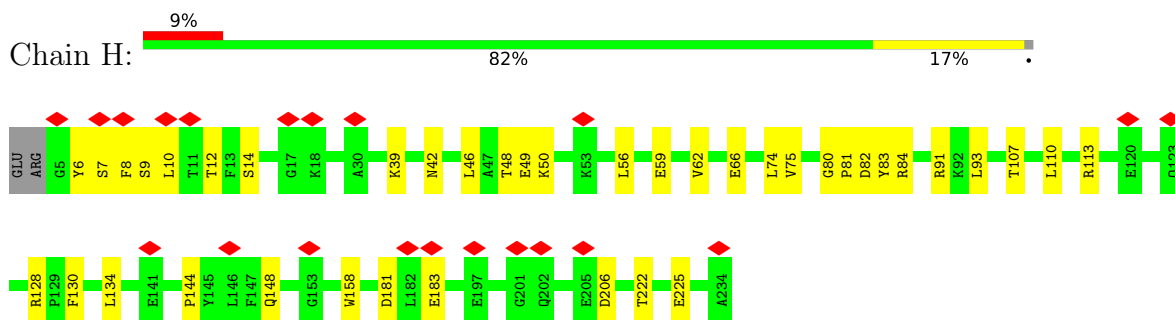
- Molecule 1: Proteasome subunit alpha type-6



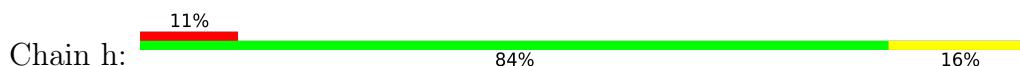
- Molecule 1: Proteasome subunit alpha type-6

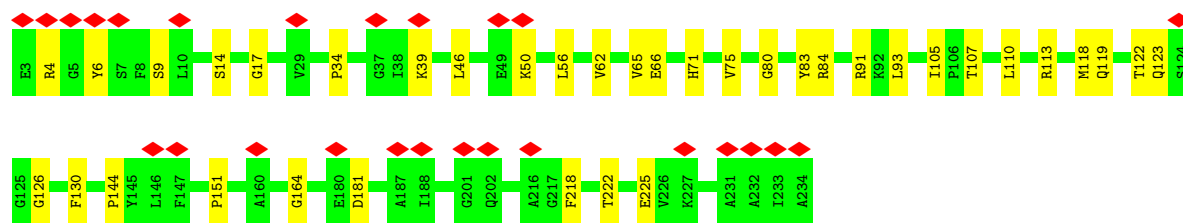


- Molecule 2: Proteasome subunit alpha type-2

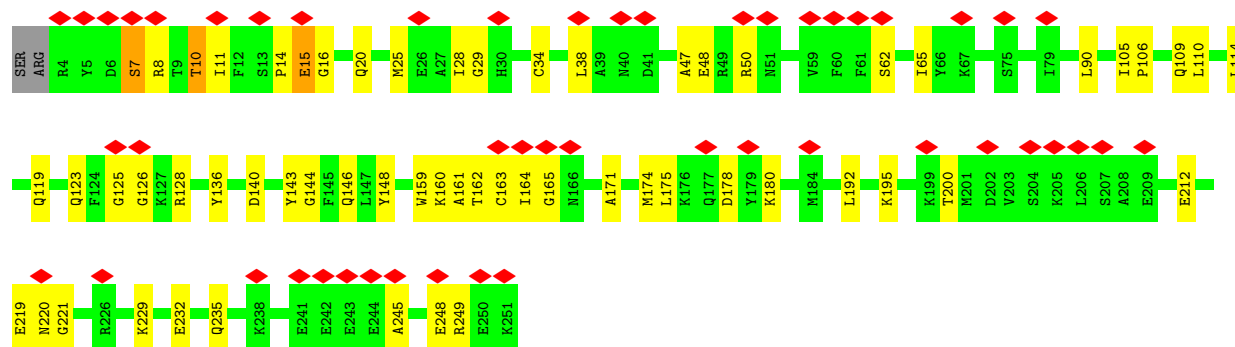
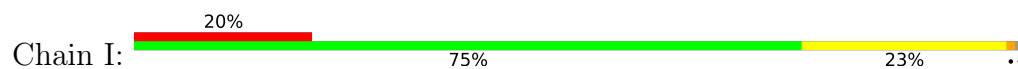


- Molecule 2: Proteasome subunit alpha type-2

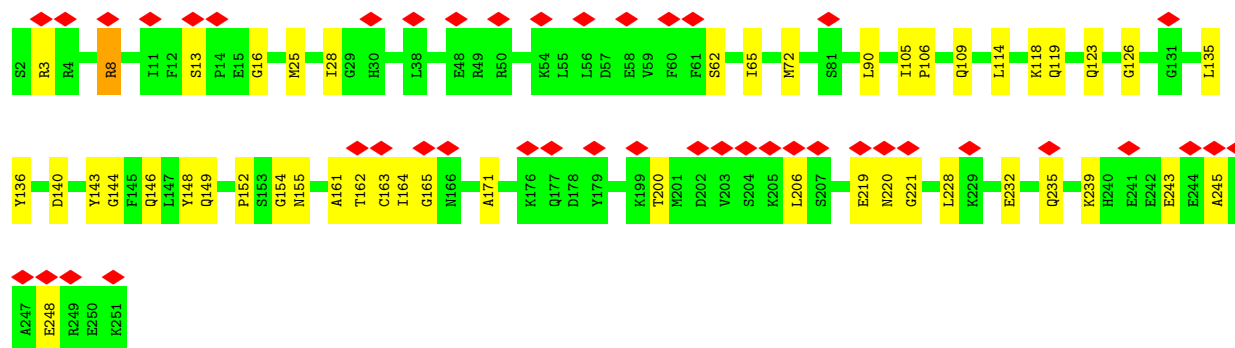
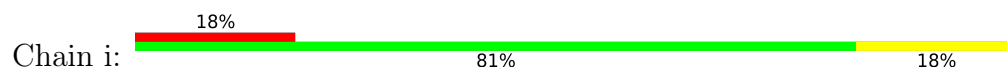




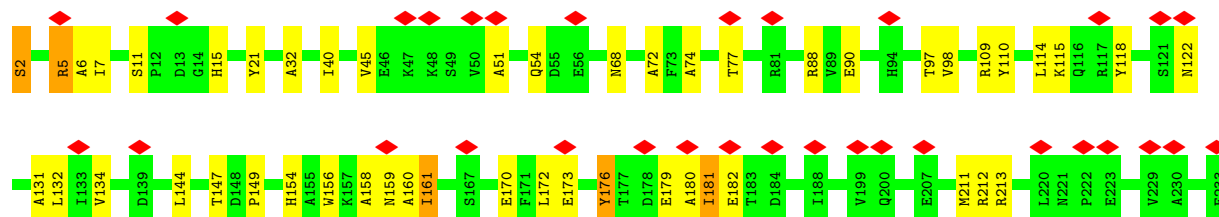
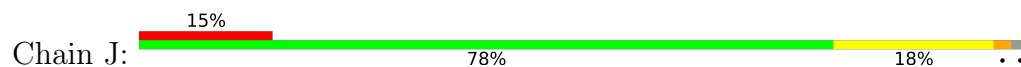
• Molecule 3: Proteasome subunit alpha type-4

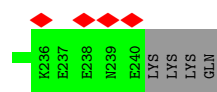


• Molecule 3: Proteasome subunit alpha type-4

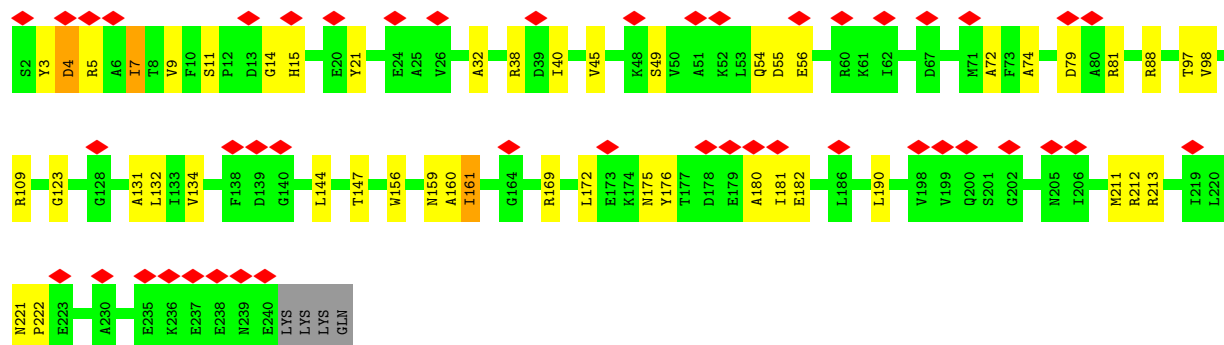
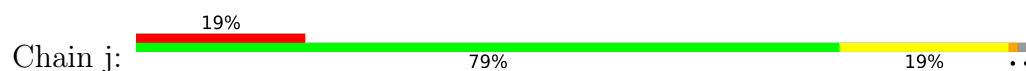


• Molecule 4: Proteasome subunit alpha type-7

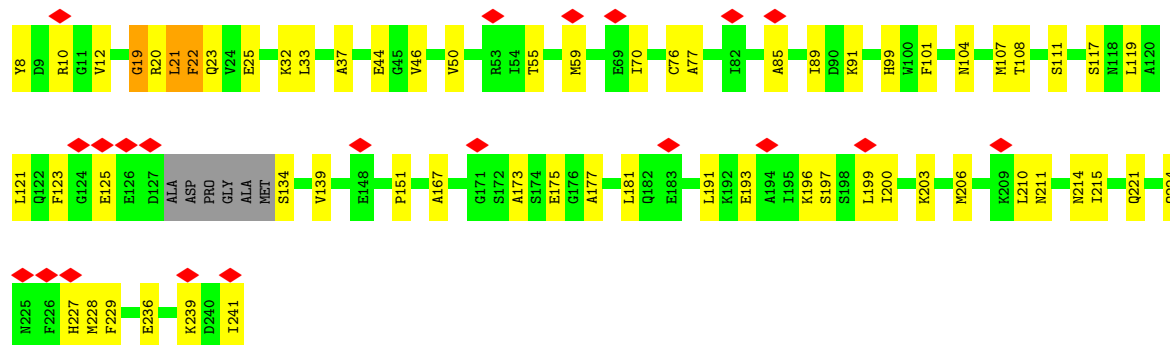




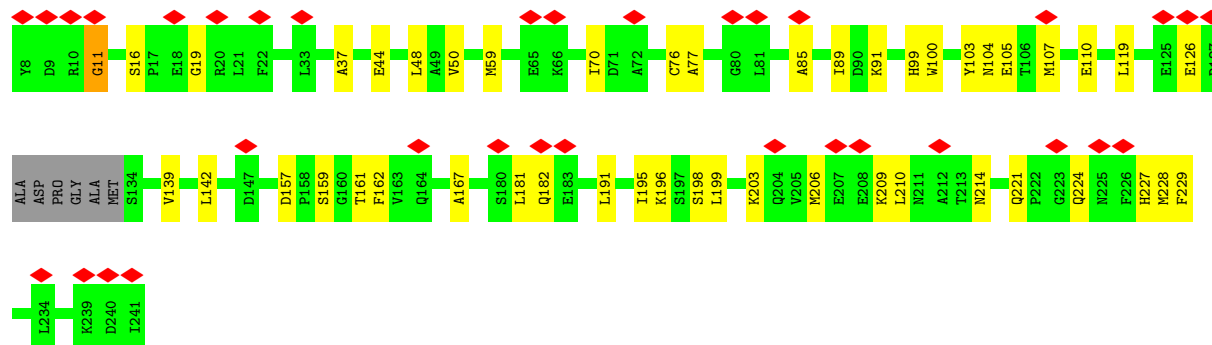
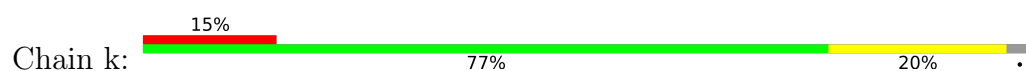
- Molecule 4: Proteasome subunit alpha type-7



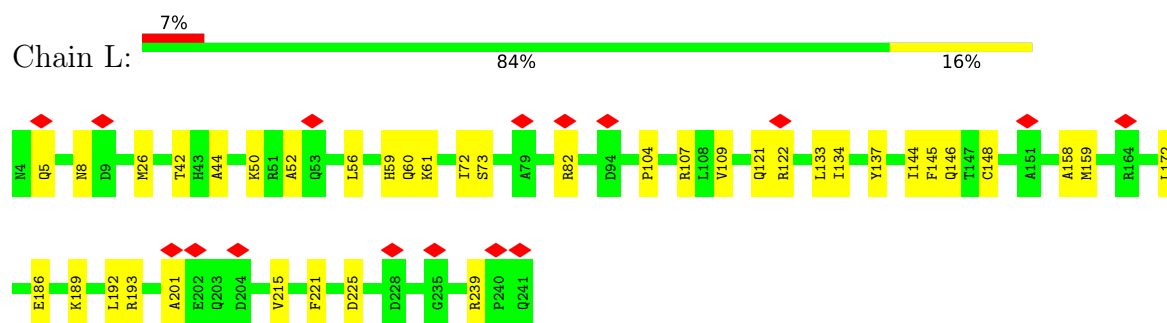
- Molecule 5: Proteasome subunit alpha type-5



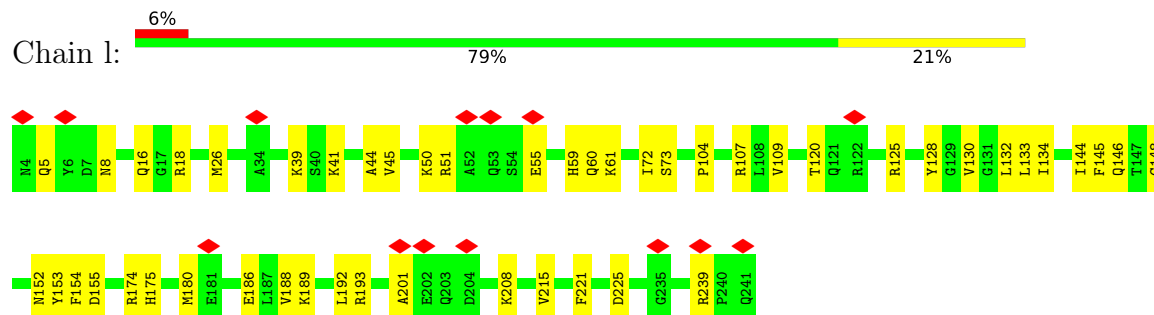
- Molecule 5: Proteasome subunit alpha type-5



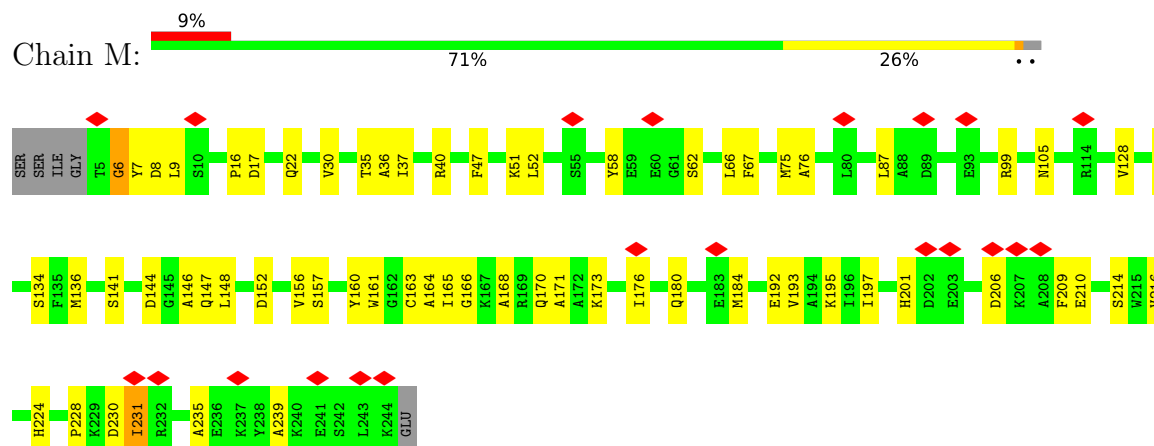
- Molecule 6: Proteasome subunit alpha type-1



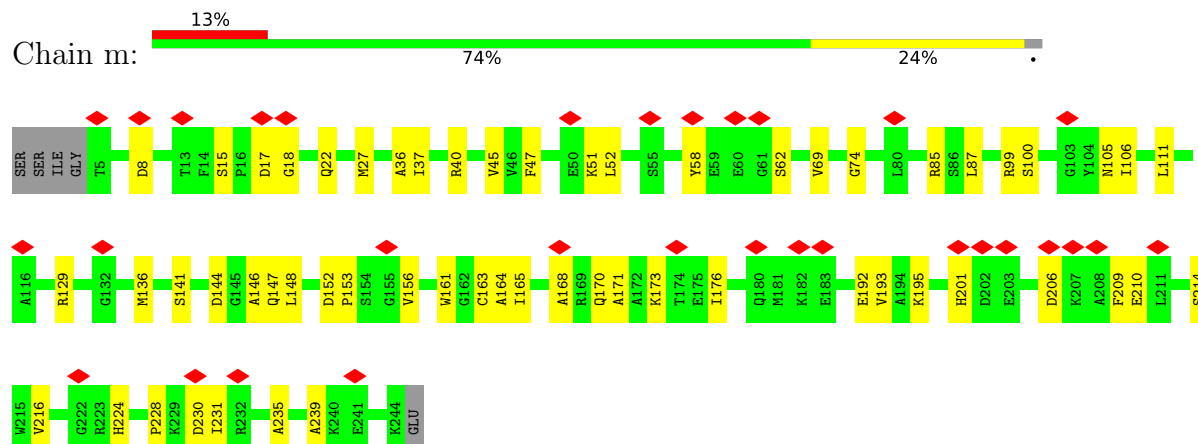
- Molecule 6: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-3

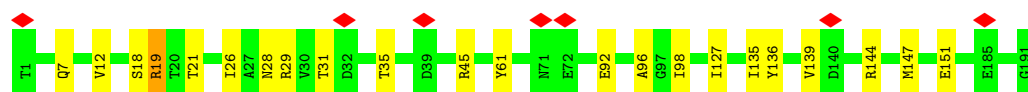


- Molecule 7: Proteasome subunit alpha type-3



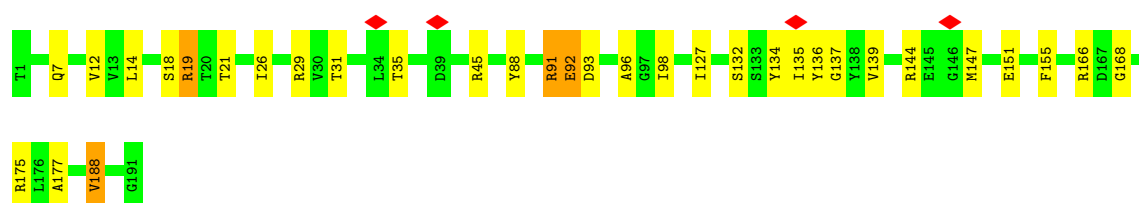
- Molecule 8: Proteasome subunit beta type-6

Chain N:  88% 11%



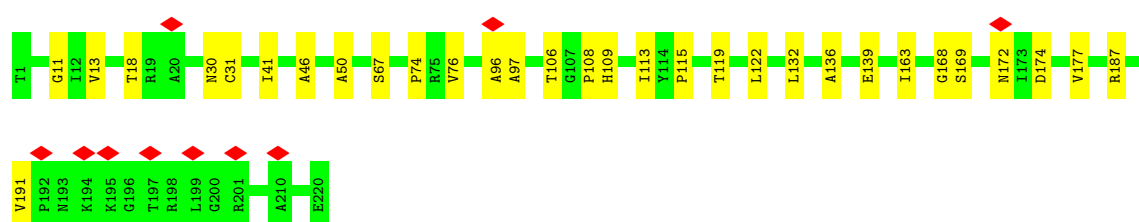
- Molecule 8: Proteasome subunit beta type-6

Chain n:  83% 15%



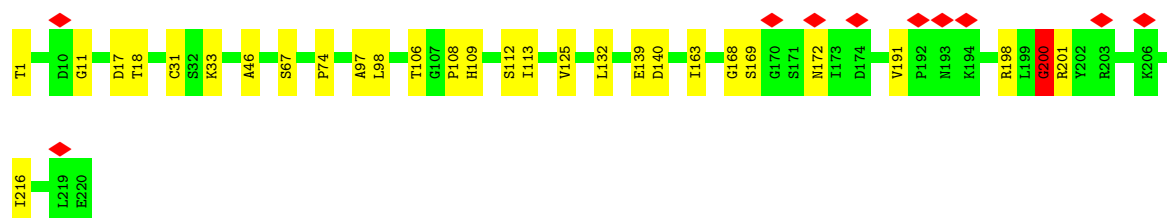
- Molecule 9: Proteasome subunit beta type-7

Chain O:  5% 86% 14%



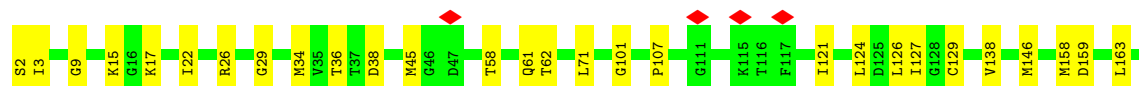
- Molecule 9: Proteasome subunit beta type-7

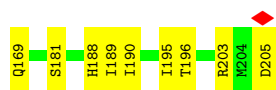
Chain o:  5% 87% 13%



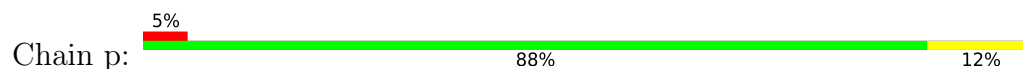
- Molecule 10: Proteasome subunit beta type-3

Chain P:  82% 18%

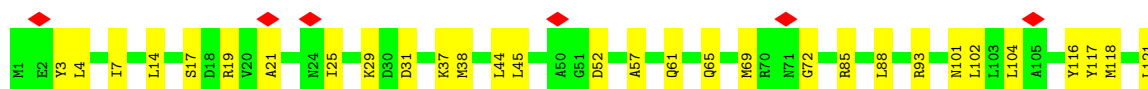
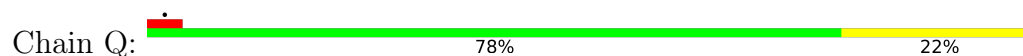




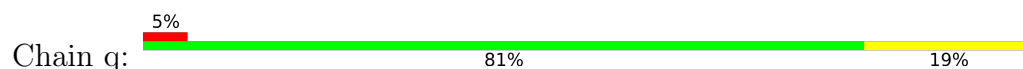
- Molecule 10: Proteasome subunit beta type-3



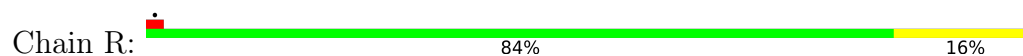
- Molecule 11: Proteasome subunit beta type-2



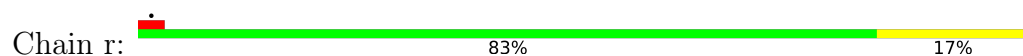
- Molecule 11: Proteasome subunit beta type-2

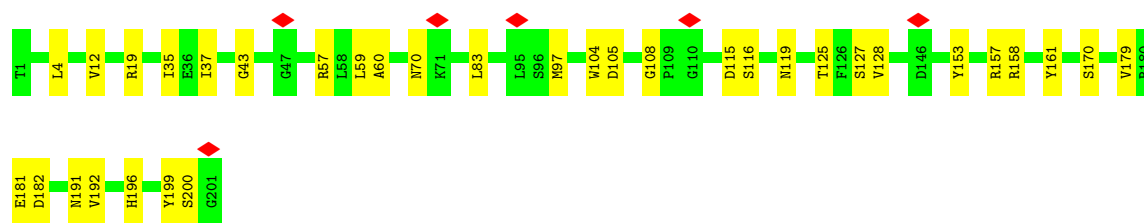


- Molecule 12: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-5

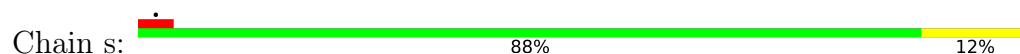




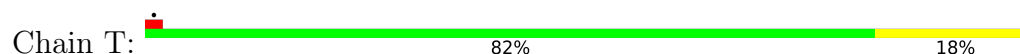
- Molecule 13: Proteasome subunit beta type-1



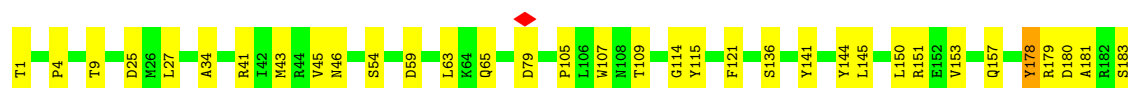
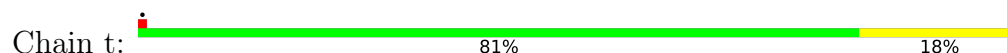
- Molecule 13: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-4

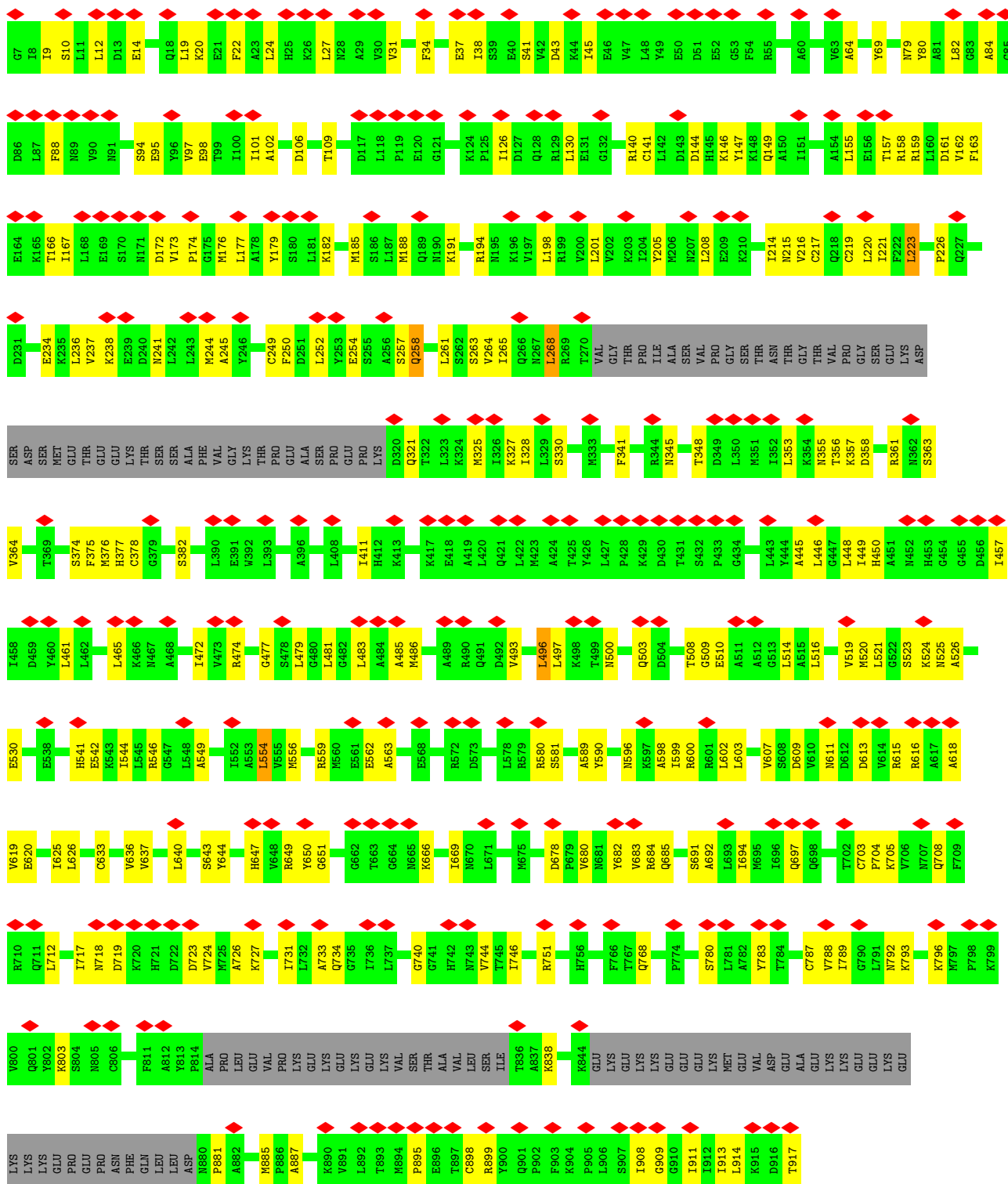


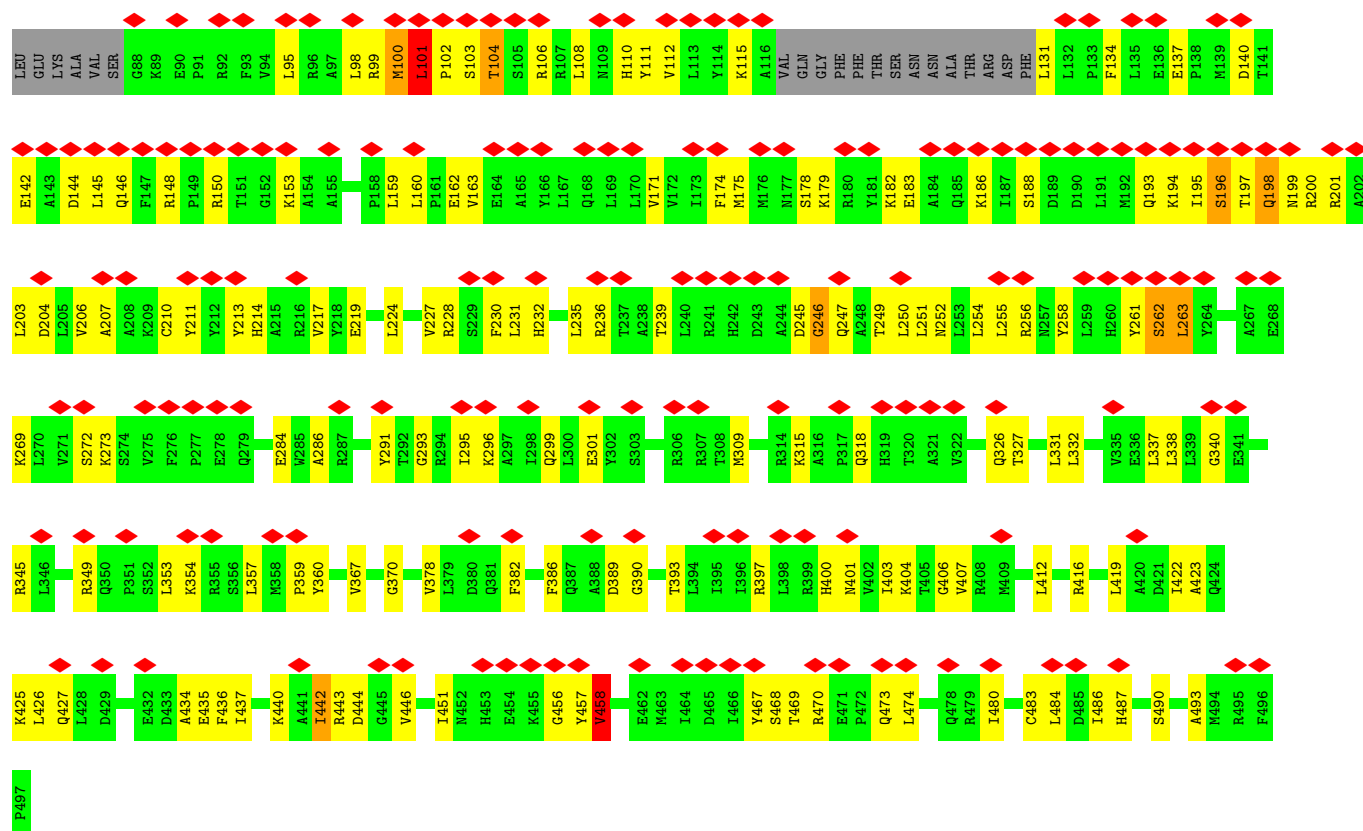
- Molecule 14: Proteasome subunit beta type-4



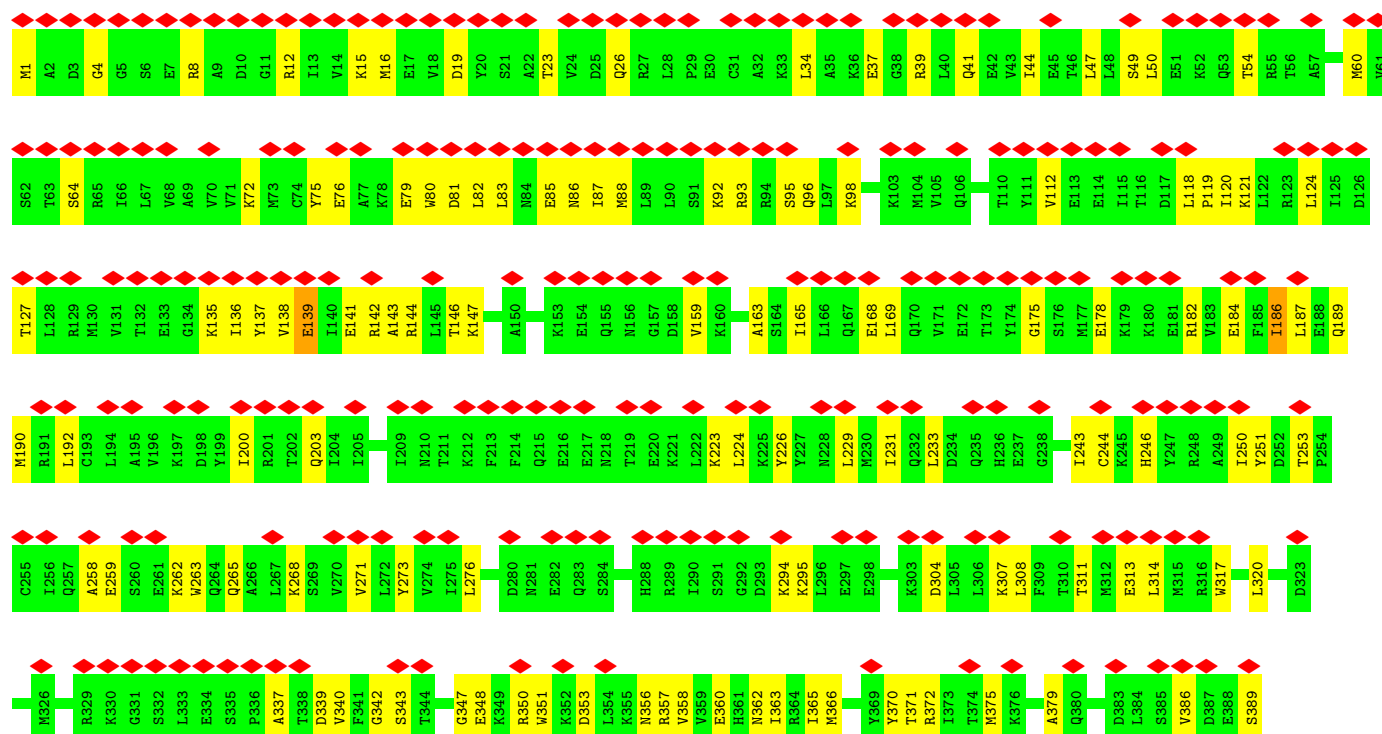
- Molecule 15: 26S proteasome non-ATPase regulatory subunit 1

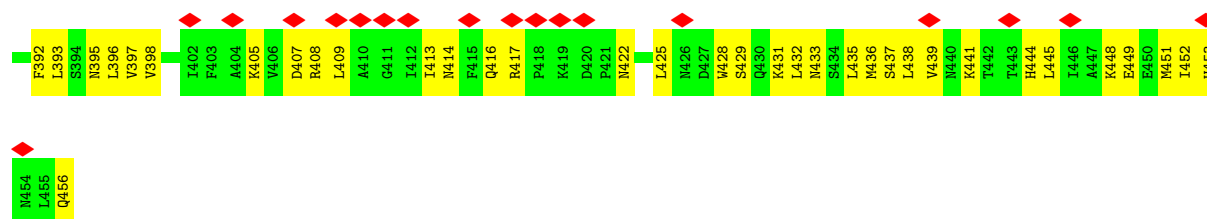




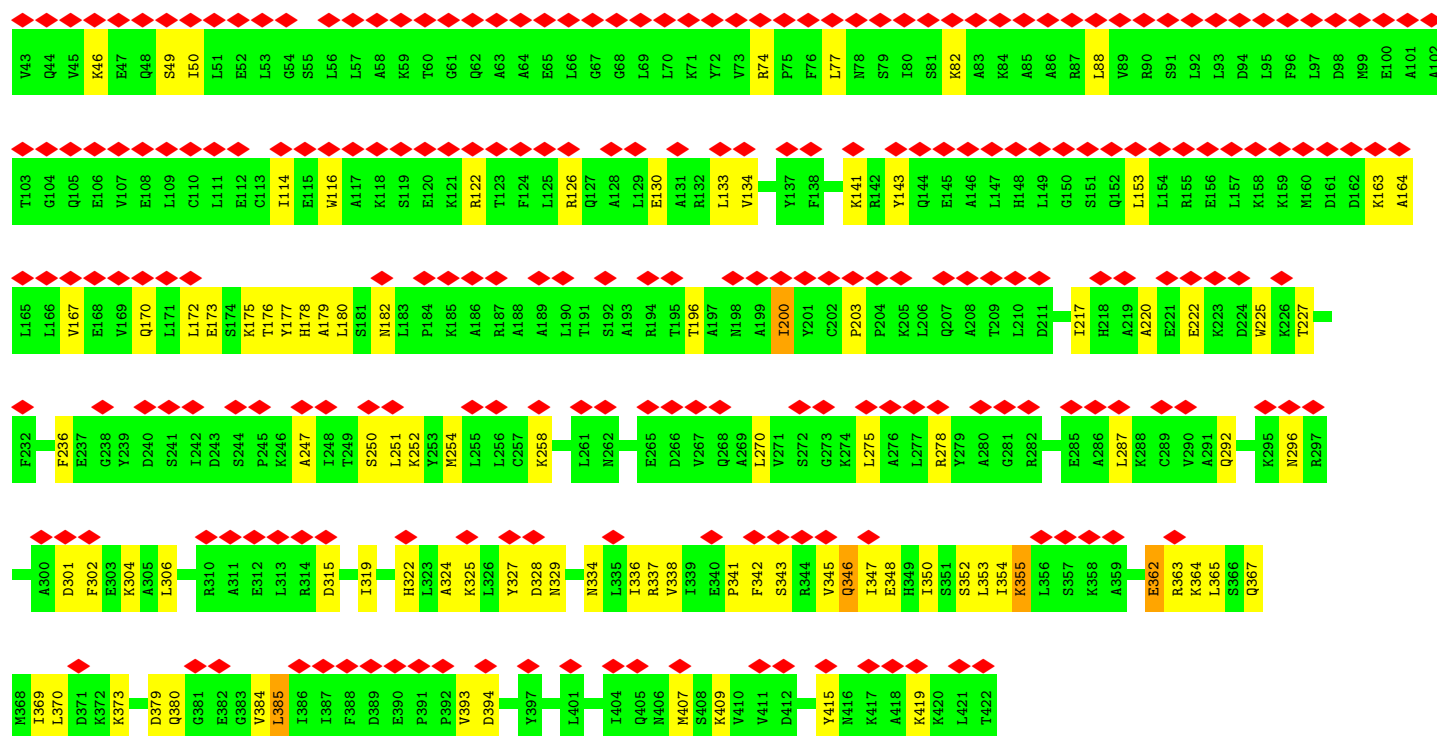
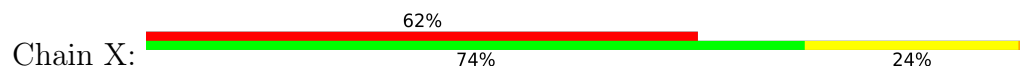


• Molecule 17: 26S proteasome non-ATPase regulatory subunit 12

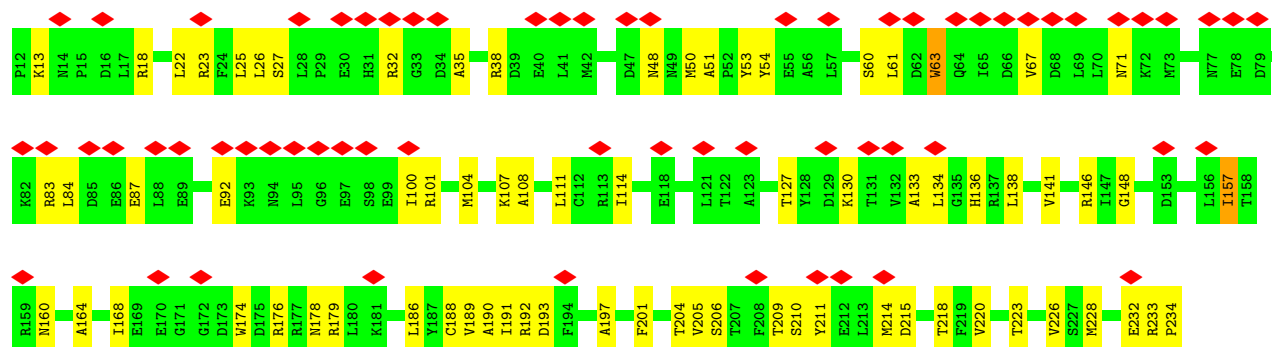


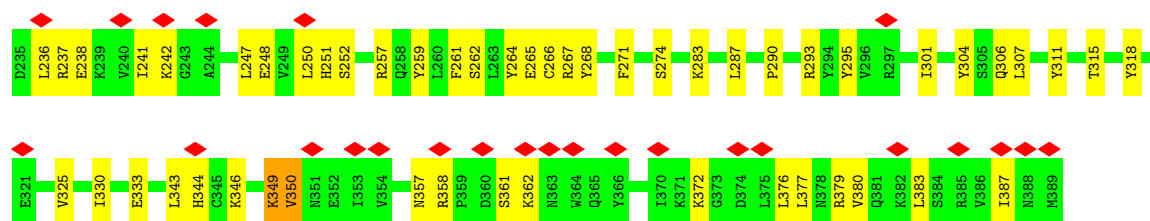


- Molecule 18: 26S proteasome non-ATPase regulatory subunit 11

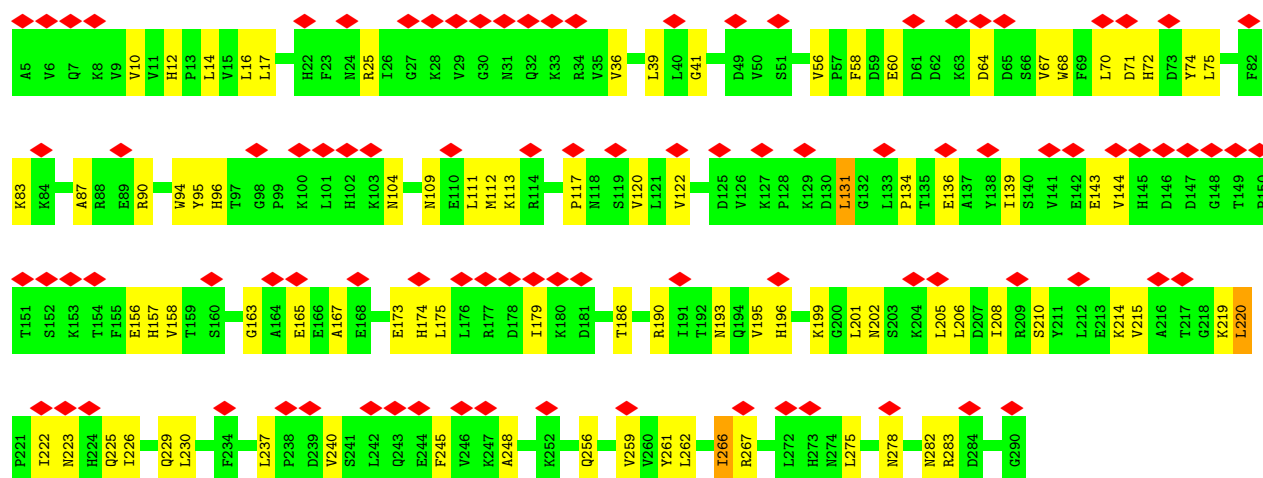


- Molecule 19: 26S proteasome non-ATPase regulatory subunit 6

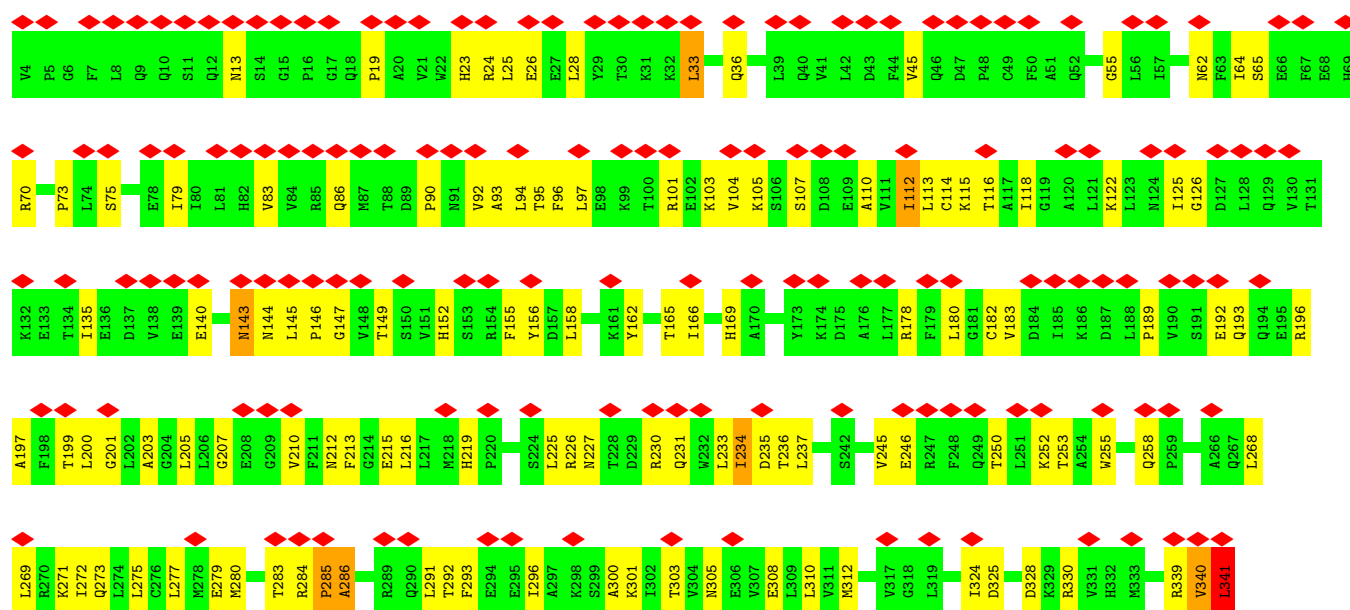


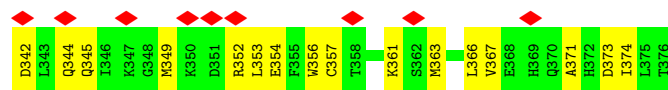


• Molecule 20: 26S proteasome non-ATPase regulatory subunit 7

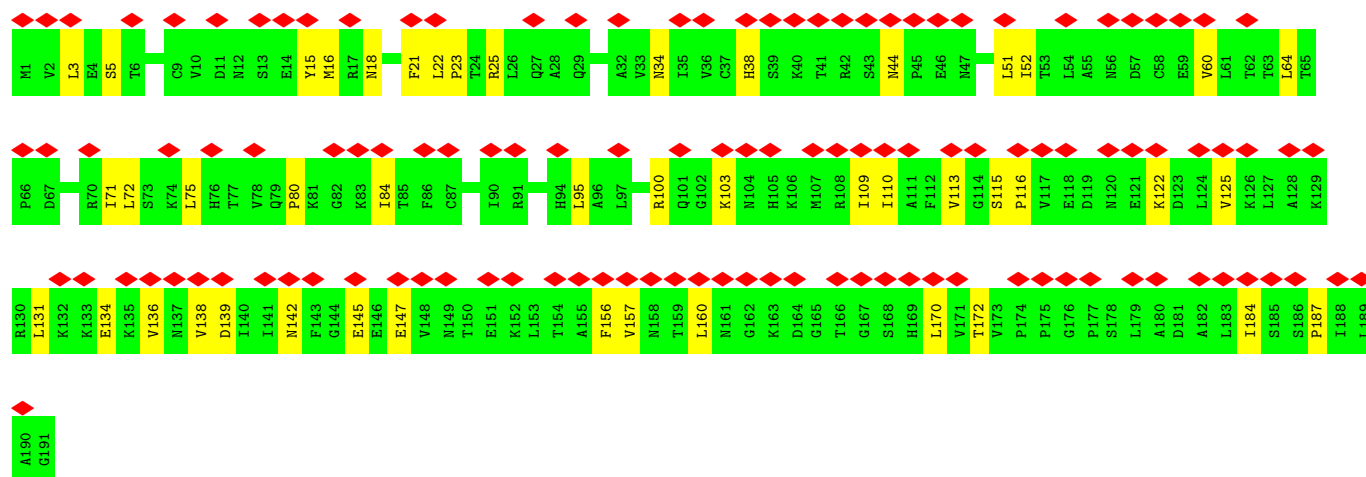
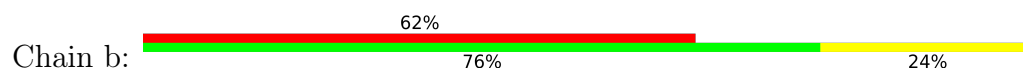


• Molecule 21: 26S proteasome non-ATPase regulatory subunit 13

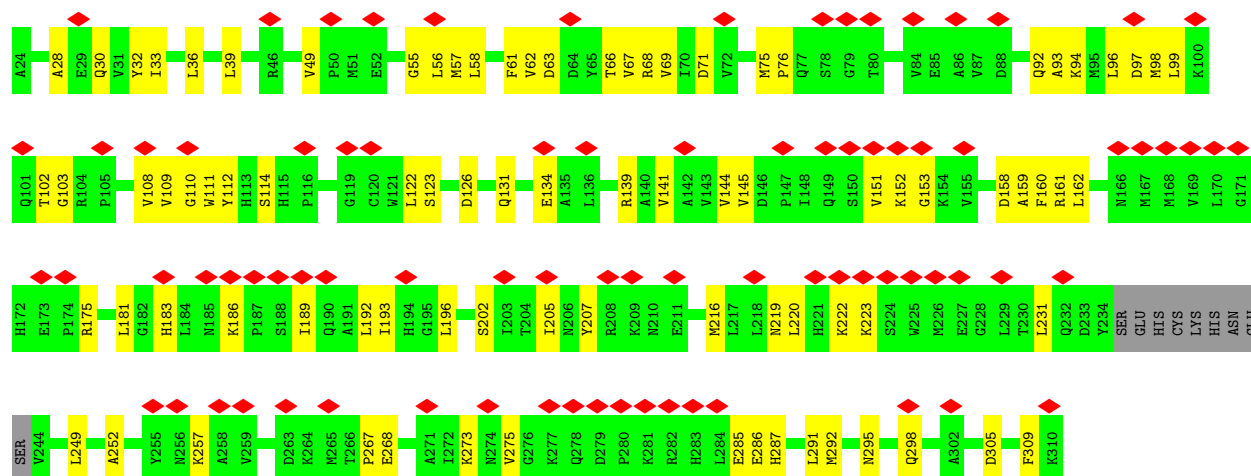




• Molecule 22: 26S proteasome non-ATPase regulatory subunit 4



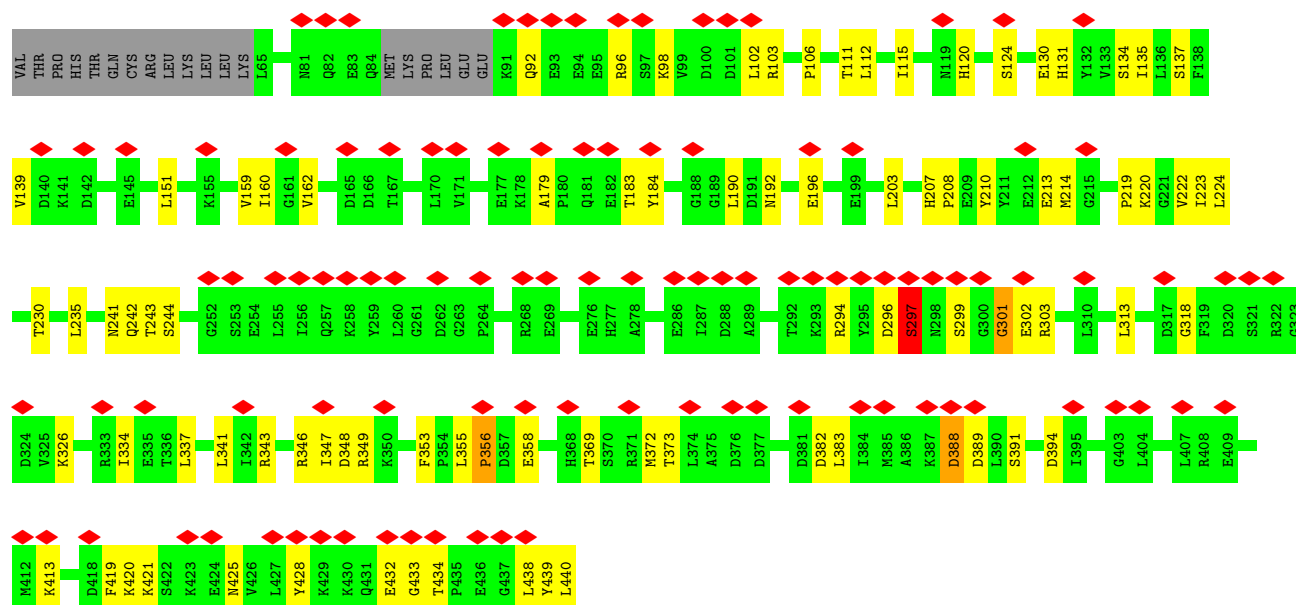
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 14



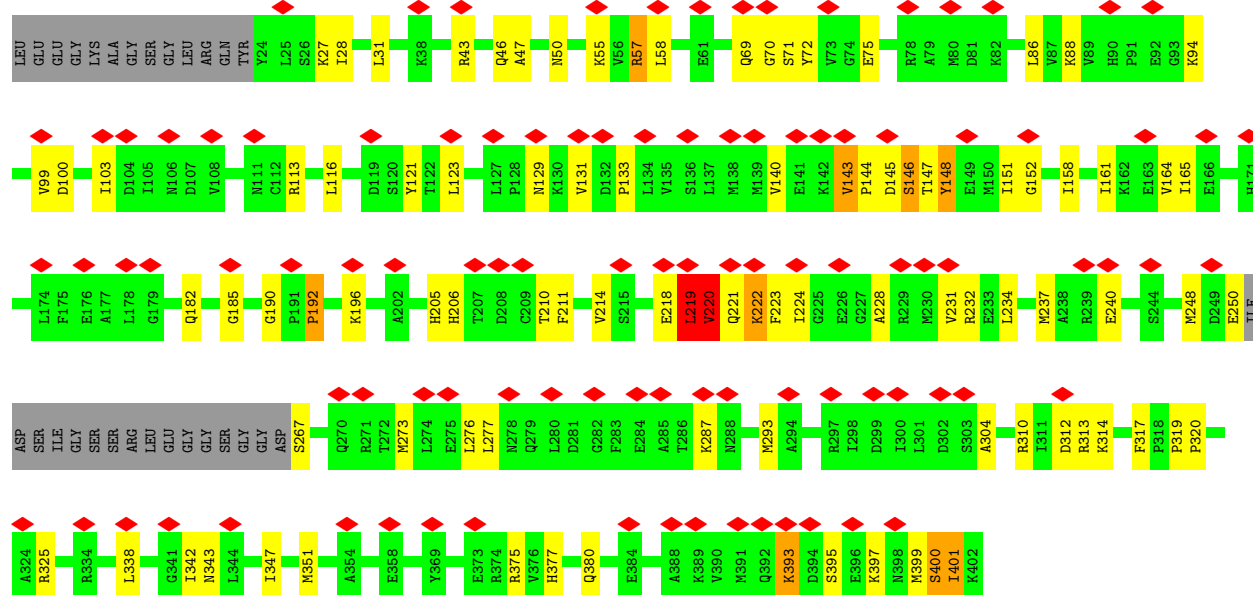
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 8



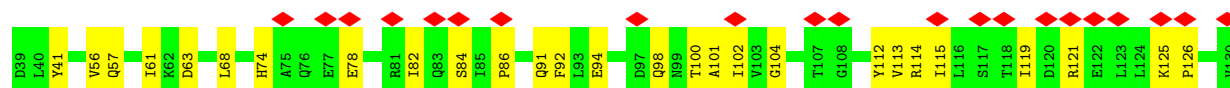


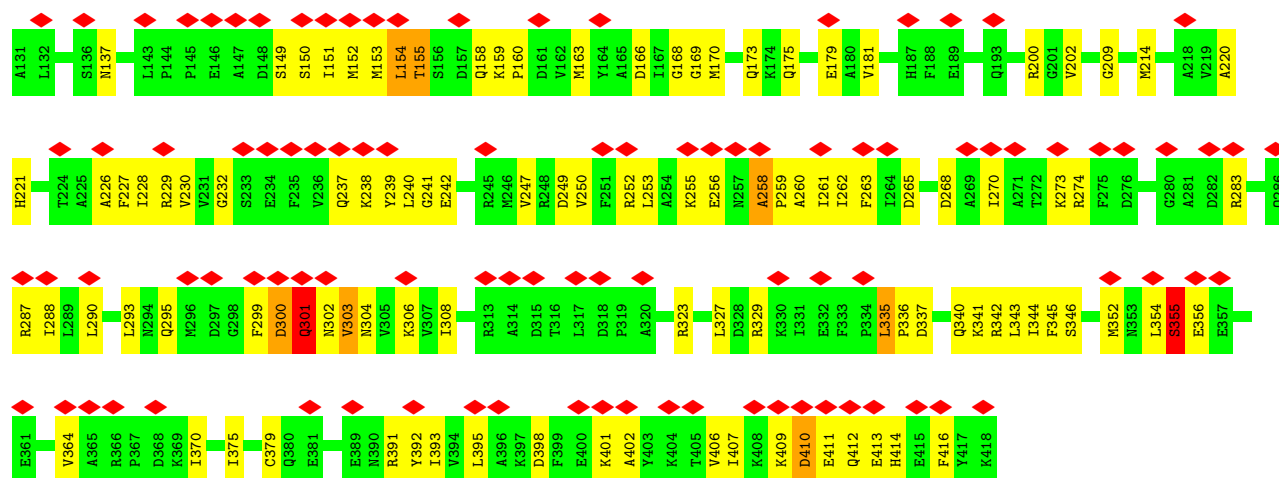


• Molecule 28: 26S proteasome regulatory subunit 8

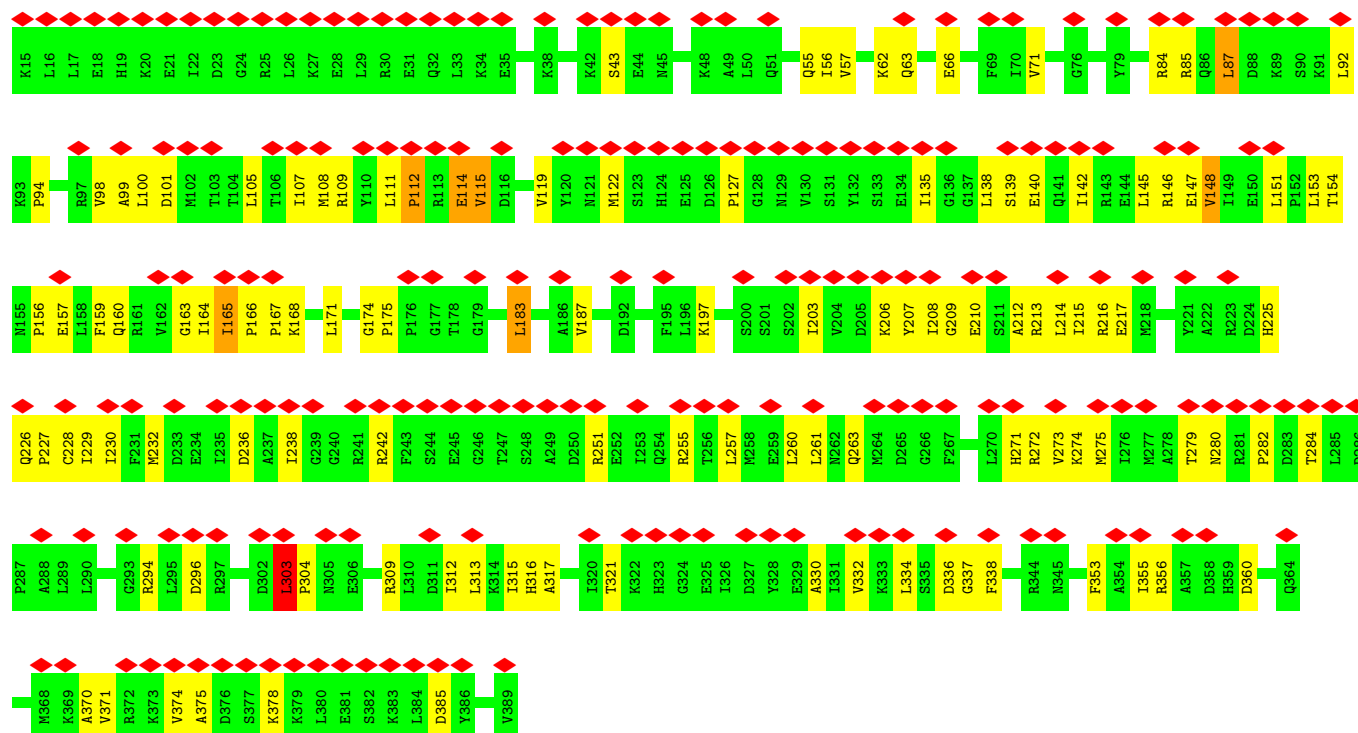


• Molecule 29: 26S proteasome regulatory subunit 6B

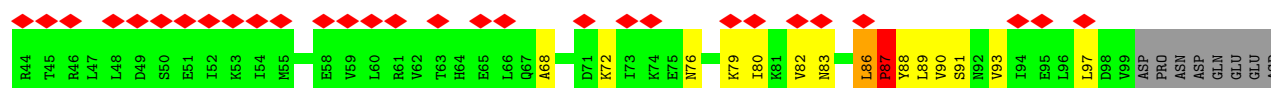


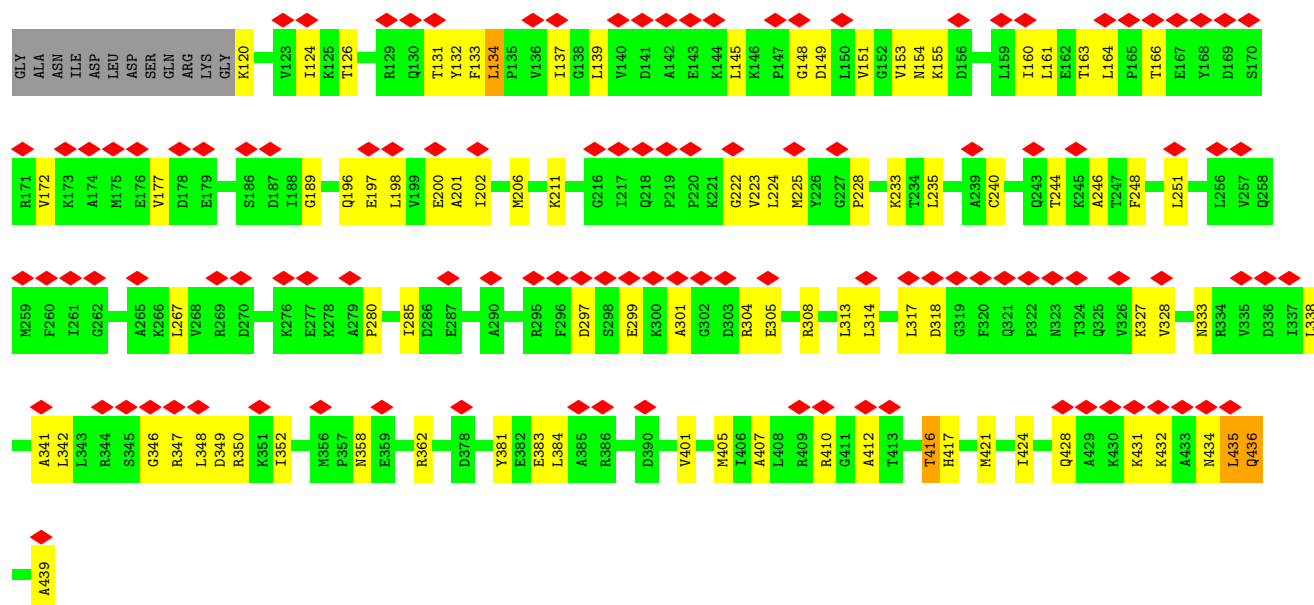


• Molecule 30: 26S proteasome regulatory subunit 10B

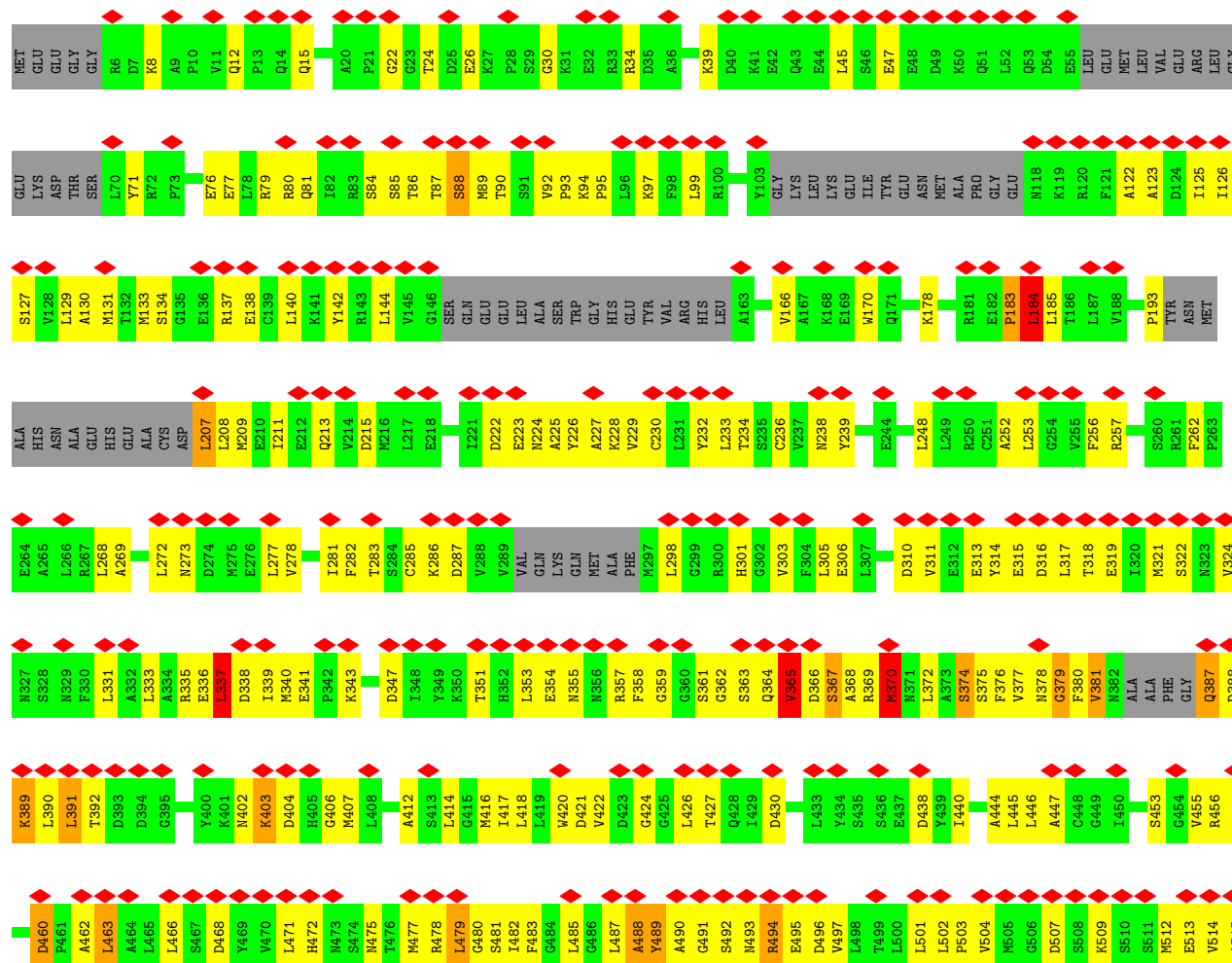


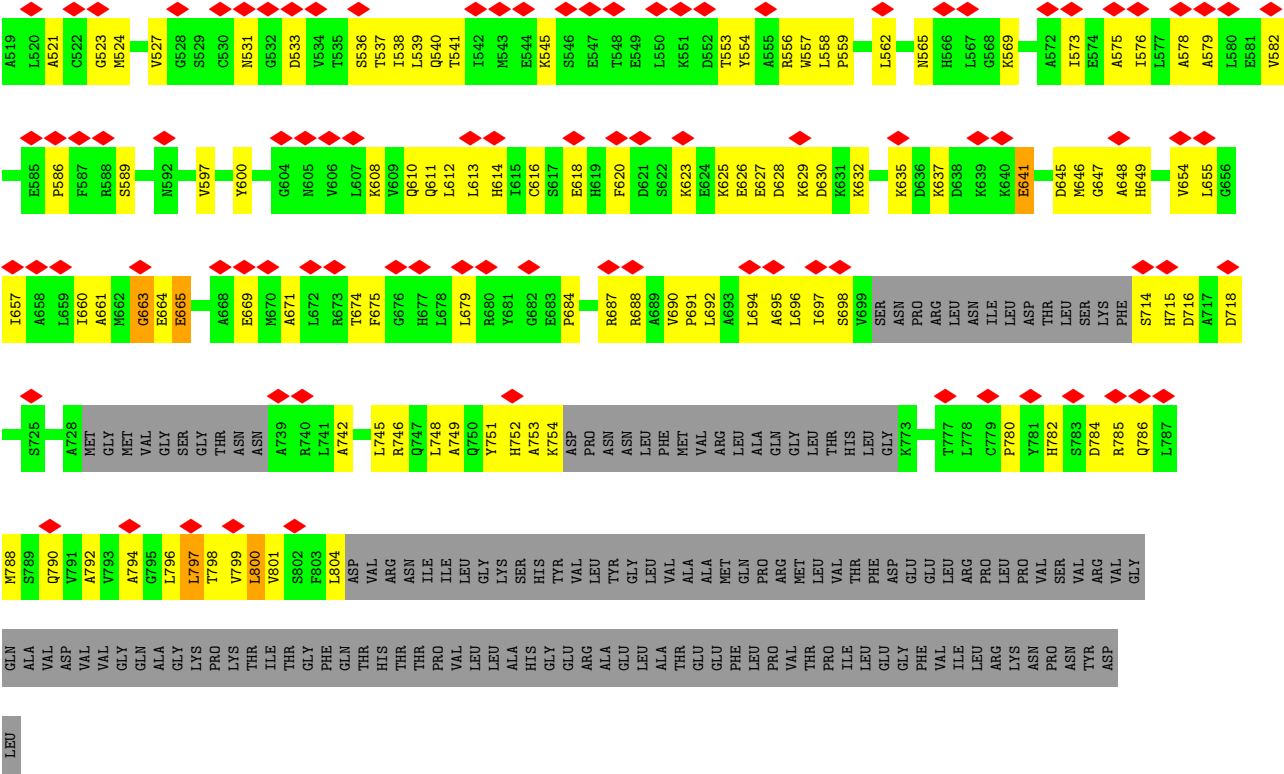
• Molecule 31: 26S proteasome regulatory subunit 6A





• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2





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 ($e^-/\text{\AA}^2$)	30	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	0.020	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00577	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	0.36	0/1853	0.73	0/2515
1	g	0.35	0/1859	0.67	0/2523
2	H	0.36	0/1723	0.72	2/2346 (0.1%)
2	h	0.33	0/1743	0.60	0/2372
3	I	0.37	0/1925	0.81	2/2606 (0.1%)
3	i	0.35	0/1942	0.74	2/2628 (0.1%)
4	J	0.47	0/1728	0.90	7/2358 (0.3%)
4	j	0.42	0/1728	0.90	4/2358 (0.2%)
5	K	0.38	0/1755	0.84	7/2375 (0.3%)
5	k	0.32	0/1747	0.65	0/2364
6	L	0.39	0/1885	0.67	0/2552
6	l	0.37	0/1885	0.67	0/2552
7	M	0.37	0/1891	0.71	4/2552 (0.2%)
7	m	0.37	0/1891	0.67	0/2552
8	N	0.39	0/1454	0.69	1/1967 (0.1%)
8	n	0.40	0/1454	0.73	2/1967 (0.1%)
9	O	0.37	0/1670	0.66	0/2265
9	o	0.39	0/1670	0.74	1/2265 (0.0%)
10	P	0.35	0/1614	0.60	0/2177
10	p	0.39	0/1614	0.62	2/2177 (0.1%)
11	Q	0.43	0/1603	0.76	0/2174
11	q	0.43	0/1603	0.76	1/2174 (0.0%)
12	R	0.37	0/1579	0.59	0/2134
12	r	0.38	0/1579	0.60	0/2134
13	S	0.40	0/1671	0.63	0/2253
13	s	0.39	0/1671	0.63	0/2253
14	T	0.37	0/1700	0.62	0/2305
14	t	0.38	0/1700	0.64	2/2305 (0.1%)
15	U	0.31	0/6396	0.72	4/8646 (0.0%)
16	V	0.39	0/3668	0.87	8/4952 (0.2%)
17	W	0.35	0/3751	0.80	0/5042
18	X	0.34	0/3053	0.77	2/4115 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	0.37	0/3173	0.77	0/4273
20	Z	0.36	0/2324	0.85	4/3150 (0.1%)
21	a	0.34	0/3053	0.89	9/4133 (0.2%)
22	b	0.30	0/1478	0.66	0/2001
23	c	0.35	0/2226	0.80	0/3007
24	d	0.35	0/2162	0.89	8/2919 (0.3%)
25	e	0.31	0/338	0.81	0/450
26	A	0.32	0/2939	0.74	2/3970 (0.1%)
27	B	0.32	0/2844	0.78	6/3846 (0.2%)
28	C	0.36	0/2896	0.94	16/3895 (0.4%)
29	D	0.37	0/3090	0.93	9/4168 (0.2%)
30	E	0.33	0/2904	0.87	9/3924 (0.2%)
31	F	0.33	0/2897	0.77	8/3912 (0.2%)
32	f	0.33	1/5393 (0.0%)	0.87	20/7271 (0.3%)
All	All	0.36	1/102722 (0.0%)	0.77	142/138877 (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
3	i	0	1
4	J	0	1
4	j	0	2
5	K	0	3
5	k	0	1
9	o	0	1
11	q	0	1
16	V	0	3
17	W	0	1
18	X	0	3
19	Y	0	5
20	Z	0	3
21	a	0	4
22	b	0	2
23	c	0	1
24	d	0	3
26	A	0	2
27	B	0	3
28	C	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	D	0	11
30	E	0	6
31	F	0	3
All	All	0	66

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	494	ARG	CA-C	5.21	1.59	1.52

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	488	ALA	N-CA-C	10.59	122.90	111.36
5	K	21	LEU	CA-C-N	10.40	140.42	121.70
5	K	21	LEU	C-N-CA	10.40	140.42	121.70
18	X	393	VAL	N-CA-C	-9.71	103.88	113.20
4	J	2	SER	CA-C-N	9.13	138.98	121.54
4	J	2	SER	C-N-CA	9.13	138.98	121.54
5	K	8	TYR	CA-C-N	8.79	138.33	121.54
5	K	8	TYR	C-N-CA	8.79	138.33	121.54
29	D	412	GLN	CA-C-N	8.76	137.47	121.70
29	D	412	GLN	C-N-CA	8.76	137.47	121.70
7	M	6	GLY	CA-C-N	8.39	136.79	121.70
7	M	6	GLY	C-N-CA	8.39	136.79	121.70
29	D	258	ALA	CA-C-N	-8.28	111.07	119.93
29	D	258	ALA	C-N-CA	-8.28	111.07	119.93
31	F	86	LEU	CA-CB-CG	8.10	144.64	116.30
27	B	388	ASP	N-CA-C	7.77	122.91	112.88
3	I	15	GLU	N-CA-C	7.76	123.47	114.62
2	H	7	SER	CA-C-N	7.71	135.58	121.70
2	H	7	SER	C-N-CA	7.71	135.58	121.70
28	C	393	LYS	CA-C-N	7.67	135.51	121.70
28	C	393	LYS	C-N-CA	7.67	135.51	121.70
28	C	401	ILE	N-CA-C	7.58	125.09	109.34
28	C	224	ILE	N-CA-C	-7.37	106.12	113.20
5	K	19	GLY	CA-C-N	7.23	134.72	121.70
5	K	19	GLY	C-N-CA	7.23	134.72	121.70
24	d	256	ILE	CA-C-N	7.09	134.46	121.70
24	d	256	ILE	C-N-CA	7.09	134.46	121.70
31	F	434	ASN	CA-C-N	7.03	134.34	121.70
31	F	434	ASN	C-N-CA	7.03	134.34	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	493	ASN	N-CA-C	-6.98	95.93	110.80
32	f	493	ASN	CA-C-N	-6.93	111.05	120.82
32	f	493	ASN	C-N-CA	-6.93	111.05	120.82
32	f	472	HIS	CA-C-N	6.92	130.42	120.79
32	f	472	HIS	C-N-CA	6.92	130.42	120.79
28	C	401	ILE	CA-C-N	6.92	134.16	121.70
28	C	401	ILE	C-N-CA	6.92	134.16	121.70
30	E	165	ILE	CA-C-N	6.79	127.37	120.38
30	E	165	ILE	C-N-CA	6.79	127.37	120.38
15	U	223	LEU	CA-C-N	6.78	132.02	122.46
15	U	223	LEU	C-N-CA	6.78	132.02	122.46
16	V	65	ARG	CA-C-N	6.57	130.68	120.82
16	V	65	ARG	C-N-CA	6.57	130.68	120.82
21	a	341	LEU	N-CA-C	-6.44	99.78	109.96
16	V	195	ILE	CA-C-N	6.38	133.74	121.54
16	V	195	ILE	C-N-CA	6.38	133.74	121.54
32	f	492	SER	N-CA-C	-6.36	104.35	111.28
20	Z	64	ASP	CA-C-N	6.21	133.41	121.54
20	Z	64	ASP	C-N-CA	6.21	133.41	121.54
21	a	342	ASP	CA-C-N	6.21	133.40	121.54
21	a	342	ASP	C-N-CA	6.21	133.40	121.54
32	f	370	MET	N-CA-C	-6.20	104.61	111.36
32	f	663	GLY	N-CA-C	6.13	121.37	110.95
4	J	182	GLU	CA-C-N	6.12	132.71	121.70
4	J	182	GLU	C-N-CA	6.12	132.71	121.70
28	C	145	ASP	CA-C-N	6.11	131.10	121.56
28	C	145	ASP	C-N-CA	6.11	131.10	121.56
27	B	192	ASN	N-CA-C	-6.11	105.74	113.43
4	j	7	ILE	N-CA-C	-6.08	107.33	113.47
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	49	SER	CA-C-N	6.00	129.13	120.98
4	j	49	SER	C-N-CA	6.00	129.13	120.98
30	E	148	VAL	CA-C-N	-5.96	117.13	122.97
30	E	148	VAL	C-N-CA	-5.96	117.13	122.97
31	F	435	LEU	CA-C-N	5.96	132.92	121.54
31	F	435	LEU	C-N-CA	5.96	132.92	121.54
32	f	489	TYR	N-CA-C	5.96	118.46	109.23
21	a	96	PHE	CA-C-N	5.94	128.49	120.65
21	a	96	PHE	C-N-CA	5.94	128.49	120.65
4	J	181	ILE	CA-C-N	5.86	132.25	121.70
4	J	181	ILE	C-N-CA	5.86	132.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	400	SER	CA-C-N	5.86	132.51	121.97
28	C	400	SER	C-N-CA	5.86	132.51	121.97
3	I	10	THR	N-CA-C	-5.84	99.89	109.40
32	f	365	VAL	N-CA-C	5.82	121.44	109.34
27	B	439	TYR	CA-C-N	5.79	132.13	121.70
27	B	439	TYR	C-N-CA	5.79	132.13	121.70
4	j	176	TYR	CB-CA-C	-5.76	104.08	111.22
10	p	30	ILE	CA-C-N	5.74	129.43	120.82
10	p	30	ILE	C-N-CA	5.74	129.43	120.82
15	U	258	GLN	CA-C-N	5.72	132.46	121.54
15	U	258	GLN	C-N-CA	5.72	132.46	121.54
3	i	8	ARG	CA-C-N	5.71	129.39	120.82
3	i	8	ARG	C-N-CA	5.71	129.39	120.82
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
29	D	98	GLN	CA-C-N	5.66	130.85	122.82
29	D	98	GLN	C-N-CA	5.66	130.85	122.82
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
8	N	92	GLU	N-CA-C	5.61	118.93	111.75
31	F	436	GLN	N-CA-C	5.59	122.70	110.80
29	D	407	ILE	CA-C-N	5.59	131.76	121.70
29	D	407	ILE	C-N-CA	5.59	131.76	121.70
29	D	303	VAL	N-CA-C	-5.57	99.03	107.73
5	K	20	ARG	N-CA-CB	5.53	119.91	110.50
21	a	285	PRO	CA-C-N	5.53	132.10	121.54
21	a	285	PRO	C-N-CA	5.53	132.10	121.54
21	a	341	LEU	CA-CB-CG	5.52	135.61	116.30
28	C	146	SER	N-CA-C	5.51	118.46	110.42
32	f	337	LEU	N-CA-C	5.50	122.52	110.80
26	A	233	THR	CA-C-N	5.49	132.02	121.54
26	A	233	THR	C-N-CA	5.49	132.02	121.54
24	d	188	LYS	CA-C-N	5.48	131.84	121.97
24	d	188	LYS	C-N-CA	5.48	131.84	121.97
30	E	112	PRO	CA-C-N	5.48	132.01	121.54
30	E	112	PRO	C-N-CA	5.48	132.01	121.54
4	J	6	ALA	N-CA-C	5.43	118.27	109.79
9	o	200	GLY	N-CA-C	5.41	126.01	113.18
30	E	315	ILE	N-CA-C	-5.39	107.57	112.96
28	C	219	LEU	CA-C-N	5.38	131.66	121.97
28	C	219	LEU	C-N-CA	5.38	131.66	121.97
18	X	363	ARG	N-CA-C	-5.35	106.06	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	432	LYS	CA-C-N	5.34	131.31	121.70
31	F	432	LYS	C-N-CA	5.34	131.31	121.70
11	q	1	MET	CG-SD-CE	5.33	112.63	100.90
28	C	218	GLU	CA-C-N	5.33	131.71	121.54
28	C	218	GLU	C-N-CA	5.33	131.71	121.54
8	n	188	VAL	CA-C-N	-5.30	113.09	122.74
8	n	188	VAL	C-N-CA	-5.30	113.09	122.74
16	V	101	LEU	CA-CB-CG	5.18	134.42	116.30
24	d	32	GLU	CA-C-N	-5.17	115.39	121.90
24	d	32	GLU	C-N-CA	-5.17	115.39	121.90
14	t	178	TYR	CA-C-N	-5.16	111.81	121.81
14	t	178	TYR	C-N-CA	-5.16	111.81	121.81
7	M	231	ILE	CA-C-N	5.13	131.33	121.54
7	M	231	ILE	C-N-CA	5.13	131.33	121.54
21	a	340	VAL	N-CA-C	5.12	120.00	109.34
30	E	203	ILE	N-CA-C	-5.12	107.84	112.96
16	V	262	SER	CA-C-N	-5.08	113.36	121.44
16	V	262	SER	C-N-CA	-5.08	113.36	121.44
24	d	227	SER	CA-C-N	5.08	131.24	121.54
24	d	227	SER	C-N-CA	5.08	131.24	121.54
20	Z	131	LEU	CA-C-N	5.07	130.82	121.70
20	Z	131	LEU	C-N-CA	5.07	130.82	121.70
30	E	271	HIS	N-CA-C	5.06	116.83	110.91
28	C	220	VAL	N-CA-C	5.04	119.83	109.34
16	V	160	LEU	N-CA-C	5.03	120.93	109.81
27	B	297	SER	CA-C-N	5.01	131.10	121.54
27	B	297	SER	C-N-CA	5.01	131.10	121.54
32	f	404	ASP	N-CA-C	5.01	117.13	111.02
32	f	493	ASN	CA-C-O	-5.01	113.35	120.51

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A	159	PRO	Peptide
26	A	422	LYS	Peptide
27	B	296	ASP	Peptide
27	B	297	SER	Peptide
27	B	301	GLY	Peptide
28	C	143	VAL	Peptide
28	C	220	VAL	Peptide
28	C	397	LYS	Peptide

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Mol	Chain	Res	Type	Group
28	C	399	MET	Peptide
28	C	400	SER	Peptide
29	D	125	LYS	Peptide
29	D	150	SER	Peptide
29	D	155	THR	Peptide
29	D	240	LEU	Peptide
29	D	299	PHE	Peptide
29	D	300	ASP	Peptide
29	D	301	GLN	Mainchain
29	D	335	LEU	Peptide
29	D	355	SER	Peptide
29	D	410	ASP	Peptide
29	D	84	SER	Peptide
30	E	111	LEU	Peptide
30	E	112	PRO	Peptide
30	E	114	GLU	Peptide
30	E	115	VAL	Peptide
30	E	225	HIS	Peptide
30	E	303	LEU	Peptide
31	F	435	LEU	Peptide
31	F	86	LEU	Peptide
31	F	87	PRO	Peptide
4	J	5	ARG	Peptide
5	K	121	LEU	Peptide
5	K	19	GLY	Peptide
5	K	22	PHE	Peptide
16	V	100	MET	Peptide
16	V	56	ALA	Peptide
16	V	64	GLN	Peptide
17	W	258	ALA	Peptide
18	X	203	PRO	Peptide
18	X	346	GLN	Peptide
18	X	362	GLU	Peptide
19	Y	157	ILE	Peptide
19	Y	311	TYR	Peptide
19	Y	349	LYS	Peptide
19	Y	361	SER	Peptide
19	Y	63	TRP	Peptide
20	Z	143	GLU	Peptide
20	Z	220	LEU	Peptide
20	Z	223	ASN	Peptide
21	a	285	PRO	Peptide

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Mol	Chain	Res	Type	Group
21	a	286	ALA	Mainchain
21	a	339	ARG	Peptide
21	a	341	LEU	Peptide
22	b	21	PHE	Peptide
22	b	22	LEU	Peptide
23	c	189	ILE	Peptide
24	d	185	ALA	Peptide
24	d	186	TYR	Peptide
24	d	215	TRP	Peptide
1	g	222	VAL	Peptide
3	i	8	ARG	Peptide
4	j	180	ALA	Peptide
4	j	4	ASP	Mainchain
5	k	11	GLY	Peptide
9	o	200	GLY	Peptide
11	q	2	GLU	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1820	0	1791	29	0
1	g	1826	0	1796	24	0
2	H	1688	0	1575	24	0
2	h	1708	0	1594	24	0
3	I	1895	0	1833	37	0
3	i	1912	0	1851	29	0
4	J	1704	0	1517	32	0
4	j	1704	0	1517	32	0
5	K	1729	0	1680	41	0
5	k	1722	0	1673	32	0
6	L	1850	0	1822	26	0
6	l	1850	0	1822	32	0
7	M	1856	0	1814	43	0
7	m	1856	0	1814	38	0
8	N	1430	0	1398	14	0
8	n	1430	0	1398	21	0
9	O	1643	0	1644	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	o	1643	0	1644	20	0
10	P	1585	0	1598	25	0
10	p	1585	0	1598	18	0
11	Q	1570	0	1547	29	0
11	q	1570	0	1547	21	0
12	R	1548	0	1499	21	0
12	r	1548	0	1499	22	0
13	S	1641	0	1618	11	0
13	s	1641	0	1618	15	0
14	T	1667	0	1628	25	0
14	t	1667	0	1628	26	0
15	U	6287	0	6336	170	0
16	V	3600	0	3655	128	0
17	W	3703	0	3822	102	0
18	X	3009	0	3113	63	0
19	Y	3115	0	3120	81	0
20	Z	2281	0	2312	71	0
21	a	2995	0	3012	102	0
22	b	1458	0	1505	28	0
23	c	2187	0	2215	61	0
24	d	2116	0	2146	43	0
25	e	334	0	294	10	0
26	A	2893	0	2843	67	0
27	B	2806	0	2770	67	0
28	C	2859	0	2971	64	0
29	D	3040	0	3076	116	0
30	E	2860	0	2828	97	0
31	F	2859	0	2853	71	0
32	f	5319	0	5329	475	0
33	c	1	0	0	0	0
34	A	31	0	12	5	0
34	C	31	0	12	3	0
34	D	31	0	12	9	0
34	F	31	0	12	3	0
All	All	101134	0	100211	2332	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 12.

All (2332) 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)
32:f:753:ALA:O	32:f:754:LYS:HE2	1.27	1.34
32:f:494:ARG:HD3	32:f:496:ASP:OD1	1.26	1.30
32:f:796:LEU:O	32:f:799:VAL:HG22	1.30	1.27
32:f:742:ALA:HA	32:f:745:LEU:CD2	1.66	1.25
32:f:376:PHE:CE1	32:f:798:THR:CG2	2.23	1.22
27:B:208:PRO:HD2	32:f:715:HIS:HB2	1.22	1.18
32:f:471:LEU:CG	32:f:509:LYS:HE3	1.73	1.18
32:f:610:GLN:O	32:f:613:LEU:HG	1.40	1.17
29:D:168:GLY:CA	29:D:344:ILE:HD11	1.74	1.16
32:f:692:LEU:HD12	32:f:748:LEU:HD21	1.19	1.16
32:f:696:LEU:HD13	32:f:752:HIS:CD2	1.80	1.16
32:f:494:ARG:HH21	32:f:495:GLU:HG2	1.02	1.16
32:f:494:ARG:HE	32:f:495:GLU:N	1.44	1.14
32:f:494:ARG:NH2	32:f:495:GLU:HG2	1.64	1.12
32:f:479:LEU:HD21	32:f:513:GLU:CB	1.80	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	1.10
32:f:389:LYS:HG2	32:f:418:LEU:HD21	1.29	1.09
32:f:692:LEU:HD12	32:f:748:LEU:CD2	1.82	1.09
32:f:376:PHE:CE1	32:f:798:THR:HG21	1.85	1.09
32:f:471:LEU:HG	32:f:509:LYS:CE	1.83	1.09
32:f:311:VAL:HB	32:f:490:ALA:HB1	1.17	1.09
30:E:165:ILE:HG22	30:E:166:PRO:CD	1.81	1.09
32:f:483:PHE:CE2	32:f:799:VAL:HB	1.88	1.07
32:f:742:ALA:O	32:f:745:LEU:HG	1.54	1.05
32:f:471:LEU:HD12	32:f:509:LYS:CG	1.87	1.05
32:f:780:PRO:HB3	32:f:800:LEU:HA	1.37	1.03
29:D:168:GLY:HA3	29:D:344:ILE:CD1	1.88	1.03
29:D:261:ILE:HG23	29:D:306:LYS:HB2	1.41	1.02
32:f:494:ARG:CD	32:f:496:ASP:OD1	2.06	1.02
32:f:337:LEU:HD13	32:f:420:TRP:HZ3	1.26	1.01
30:E:165:ILE:HB	30:E:168:LYS:NZ	1.75	1.01
32:f:753:ALA:O	32:f:754:LYS:CE	2.08	1.01
29:D:168:GLY:HA3	29:D:344:ILE:HD11	1.03	1.00
30:E:165:ILE:HG22	30:E:166:PRO:HD2	1.04	1.00
32:f:359:GLY:O	32:f:363:SER:HB3	1.63	0.99
17:W:182:ARG:O	17:W:186:ILE:HB	1.61	0.99
30:E:148:VAL:HG23	30:E:167:PRO:HB2	1.46	0.98
32:f:494:ARG:HG3	32:f:497:VAL:HG12	1.44	0.98
32:f:479:LEU:HD21	32:f:513:GLU:HB2	0.99	0.98
29:D:259:PRO:HB3	29:D:304:ASN:HB2	1.46	0.97
30:E:166:PRO:O	30:E:168:LYS:HE2	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:692:LEU:CD1	32:f:748:LEU:HD21	1.93	0.97
32:f:696:LEU:HD13	32:f:752:HIS:HD2	1.14	0.97
32:f:742:ALA:HA	32:f:745:LEU:HD23	1.46	0.96
32:f:376:PHE:CD1	32:f:416:MET:HE1	2.01	0.96
32:f:780:PRO:CB	32:f:800:LEU:HA	1.96	0.95
32:f:471:LEU:HG	32:f:509:LYS:HE3	0.96	0.95
32:f:95:PRO:O	32:f:99:LEU:HB2	1.67	0.95
32:f:456:ARG:HB3	32:f:489:TYR:CE2	2.00	0.95
32:f:311:VAL:HB	32:f:490:ALA:CB	1.97	0.95
29:D:300:ASP:HB2	29:D:303:VAL:HG23	1.49	0.94
27:B:358:GLU:OE2	27:B:388:ASP:HB3	1.67	0.94
32:f:372:LEU:HD11	32:f:406:GLY:HA3	1.47	0.94
32:f:376:PHE:CE1	32:f:416:MET:HE1	2.03	0.94
32:f:224:ASN:O	32:f:228:LYS:HB3	1.66	0.93
32:f:358:PHE:CZ	32:f:381:VAL:HG21	2.03	0.93
32:f:388:ASP:OD2	32:f:390:LEU:HB2	1.67	0.93
32:f:494:ARG:HE	32:f:495:GLU:H	1.16	0.93
15:U:167:ILE:HG22	15:U:176:MET:HE2	1.52	0.91
32:f:691:PRO:CB	32:f:749:ALA:HB2	1.99	0.91
32:f:376:PHE:CE1	32:f:798:THR:HB	2.06	0.90
32:f:483:PHE:CZ	32:f:799:VAL:HB	2.06	0.90
32:f:376:PHE:CE1	32:f:798:THR:CB	2.55	0.90
32:f:315:GLU:HG2	32:f:491:GLY:HA2	1.51	0.90
32:f:363:SER:O	32:f:365:VAL:N	2.04	0.90
29:D:252:ARG:O	29:D:256:GLU:HB2	1.71	0.90
29:D:344:ILE:HD12	34:D:501:AGS:N1	1.86	0.90
32:f:742:ALA:HA	32:f:745:LEU:HD21	1.53	0.89
32:f:366:ASP:OD1	32:f:367:SER:N	2.04	0.89
32:f:389:LYS:HG2	32:f:418:LEU:CD2	2.02	0.89
30:E:165:ILE:CG2	30:E:166:PRO:HD2	1.97	0.89
32:f:369:ARG:HB3	32:f:370:MET:SD	2.13	0.89
32:f:318:THR:O	32:f:322:SER:HB3	1.73	0.88
32:f:223:GLU:O	32:f:227:ALA:HB3	1.73	0.88
32:f:311:VAL:CB	32:f:490:ALA:HB1	2.03	0.88
32:f:122:ALA:O	32:f:126:ILE:HB	1.72	0.87
32:f:378:ASN:HB3	32:f:391:LEU:HG	1.56	0.87
32:f:378:ASN:HB3	32:f:391:LEU:CG	2.05	0.87
32:f:129:LEU:O	32:f:133:MET:HB3	1.75	0.87
32:f:494:ARG:HH21	32:f:495:GLU:CG	1.88	0.86
32:f:126:ILE:O	32:f:130:ALA:HB3	1.77	0.85
32:f:123:ALA:O	32:f:127:SER:HB2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:441:LYS:O	17:W:445:LEU:HB2	1.75	0.85
32:f:337:LEU:HD13	32:f:420:TRP:CZ3	2.10	0.85
32:f:88:SER:CB	32:f:92:VAL:HG23	2.06	0.85
32:f:796:LEU:O	32:f:799:VAL:CG2	2.22	0.84
32:f:471:LEU:HD12	32:f:509:LYS:HG2	1.58	0.84
32:f:336:GLU:HG3	32:f:337:LEU:HD22	1.60	0.84
30:E:166:PRO:HB3	30:E:274:LYS:HE3	1.58	0.84
32:f:494:ARG:NE	32:f:495:GLU:N	2.26	0.83
32:f:691:PRO:HB2	32:f:749:ALA:HB2	1.58	0.83
32:f:695:ALA:HB3	32:f:752:HIS:HB2	1.59	0.83
32:f:301:HIS:O	32:f:305:LEU:HB2	1.77	0.83
32:f:610:GLN:C	32:f:613:LEU:HG	2.04	0.83
32:f:225:ALA:O	32:f:229:VAL:HB	1.79	0.83
32:f:376:PHE:HE1	32:f:798:THR:CB	1.91	0.82
32:f:696:LEU:CD1	32:f:752:HIS:HD2	1.90	0.82
32:f:714:SER:O	32:f:718:ASP:HB2	1.78	0.81
30:E:165:ILE:HB	30:E:168:LYS:HZ2	1.43	0.81
15:U:27:LEU:O	15:U:31:VAL:HB	1.81	0.81
32:f:479:LEU:CD2	32:f:513:GLU:CB	2.50	0.81
32:f:635:LYS:HZ2	32:f:641:GLU:HG3	1.42	0.81
23:c:305:ASP:O	23:c:309:PHE:HB3	1.80	0.81
32:f:376:PHE:CE1	32:f:416:MET:CE	2.64	0.81
32:f:376:PHE:CZ	32:f:416:MET:SD	2.73	0.81
15:U:173:VAL:HG13	15:U:176:MET:HB3	1.64	0.81
32:f:471:LEU:HD12	32:f:509:LYS:HG3	1.62	0.81
29:D:402:ALA:O	29:D:406:VAL:HB	1.80	0.80
32:f:378:ASN:O	32:f:381:VAL:HG12	1.81	0.80
32:f:88:SER:HB2	32:f:92:VAL:HG23	1.63	0.80
32:f:610:GLN:HB2	32:f:613:LEU:HD21	1.63	0.80
32:f:742:ALA:C	32:f:745:LEU:HG	2.06	0.80
4:J:51:ALA:H	4:J:54:GLN:HE22	1.28	0.79
27:B:92:GLN:CB	27:B:96:ARG:H	1.95	0.79
32:f:232:TYR:O	32:f:236:CYS:HB2	1.82	0.79
32:f:503:PRO:O	32:f:507:ASP:HB2	1.82	0.79
15:U:167:ILE:HG22	15:U:176:MET:CE	2.13	0.79
32:f:376:PHE:HE1	32:f:798:THR:CG2	1.89	0.79
27:B:208:PRO:CD	32:f:715:HIS:HB2	2.10	0.79
29:D:344:ILE:CD1	34:D:501:AGS:N1	2.45	0.79
32:f:612:LEU:O	32:f:616:CYS:HB2	1.83	0.79
32:f:494:ARG:NE	32:f:495:GLU:H	1.80	0.78
3:I:119:GLN:HE21	3:I:123:GLN:HE22	1.27	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:165:ILE:CG2	30:E:166:PRO:CD	2.58	0.78
32:f:796:LEU:HG	32:f:799:VAL:HG21	1.66	0.78
32:f:370:MET:SD	32:f:370:MET:N	2.57	0.78
32:f:392:THR:HG22	32:f:417:ILE:CD1	2.14	0.78
32:f:494:ARG:HE	32:f:494:ARG:C	1.92	0.78
29:D:300:ASP:CB	29:D:303:VAL:HG23	2.14	0.78
32:f:456:ARG:HB3	32:f:489:TYR:HE2	1.47	0.78
32:f:695:ALA:C	32:f:752:HIS:HB3	2.09	0.77
22:b:156:PHE:O	22:b:160:LEU:HB2	1.84	0.77
32:f:745:LEU:HD12	32:f:746:ARG:N	1.99	0.77
30:E:166:PRO:O	30:E:168:LYS:CE	2.32	0.77
32:f:184:LEU:HG	32:f:185:LEU:N	1.98	0.77
30:E:330:ALA:O	30:E:334:LEU:HB2	1.84	0.77
20:Z:214:LYS:HB3	20:Z:220:LEU:H	1.50	0.77
27:B:208:PRO:HD2	32:f:715:HIS:CB	2.11	0.77
15:U:182:LYS:HE3	15:U:214:ILE:HD13	1.67	0.77
17:W:432:LEU:O	17:W:436:MET:HB2	1.85	0.76
32:f:478:ARG:HD3	32:f:504:VAL:HG13	1.68	0.76
20:Z:195:VAL:O	20:Z:199:LYS:HB2	1.86	0.76
27:B:244:SER:HB3	32:f:669:GLU:HB2	1.68	0.76
32:f:635:LYS:HZ2	32:f:641:GLU:CG	1.98	0.76
32:f:675:PHE:O	32:f:679:LEU:HB2	1.85	0.76
32:f:376:PHE:CE1	32:f:798:THR:HG22	2.20	0.75
32:f:691:PRO:HB3	32:f:749:ALA:HB2	1.66	0.75
17:W:60:MET:O	17:W:64:SER:HB2	1.84	0.75
32:f:784:ASP:HB2	32:f:800:LEU:HD21	1.67	0.75
32:f:358:PHE:O	32:f:362:GLY:HA3	1.87	0.75
32:f:635:LYS:NZ	32:f:641:GLU:CG	2.50	0.75
32:f:357:ARG:O	32:f:361:SER:HB2	1.87	0.75
32:f:376:PHE:CZ	32:f:798:THR:HB	2.22	0.74
32:f:664:GLU:HB3	32:f:696:LEU:HG	1.69	0.74
32:f:684:PRO:O	32:f:688:ARG:HB2	1.87	0.74
28:C:375:ARG:HH21	28:C:377:HIS:HB2	1.52	0.74
32:f:392:THR:CG2	32:f:417:ILE:HG21	2.18	0.74
32:f:471:LEU:CD1	32:f:509:LYS:CE	2.65	0.74
32:f:610:GLN:HA	32:f:613:LEU:HD23	1.68	0.74
32:f:613:LEU:HD12	32:f:614:HIS:N	2.03	0.74
17:W:8:ARG:O	17:W:12:ARG:HB2	1.88	0.73
32:f:691:PRO:HG2	32:f:745:LEU:HD13	1.70	0.73
21:a:93:ALA:O	21:a:97:LEU:HB2	1.88	0.73
32:f:211:ILE:O	32:f:215:ASP:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:341:LYS:O	29:D:345:PHE:HB2	1.88	0.73
29:D:258:ALA:O	29:D:259:PRO:C	2.31	0.73
20:Z:214:LYS:HD2	20:Z:219:LYS:H	1.54	0.73
32:f:610:GLN:O	32:f:613:LEU:CG	2.30	0.73
32:f:742:ALA:HA	32:f:745:LEU:CG	2.18	0.73
32:f:494:ARG:CG	32:f:497:VAL:HG12	2.16	0.72
30:E:163:GLY:C	30:E:164:ILE:HD13	2.13	0.72
23:c:93:ALA:O	23:c:97:ASP:HB2	1.89	0.72
30:E:165:ILE:CB	30:E:168:LYS:NZ	2.51	0.72
32:f:88:SER:HB3	32:f:92:VAL:HG23	1.72	0.72
32:f:389:LYS:CG	32:f:418:LEU:CD2	2.63	0.72
15:U:182:LYS:CE	15:U:214:ILE:HD13	2.19	0.72
18:X:163:LYS:HG3	18:X:196:THR:HG23	1.72	0.72
30:E:148:VAL:CG2	30:E:167:PRO:HB2	2.19	0.71
15:U:493:VAL:O	15:U:497:LEU:HB2	1.91	0.71
18:X:141:LYS:HE3	18:X:179:ALA:HB1	1.72	0.71
32:f:610:GLN:HA	32:f:613:LEU:CD2	2.20	0.71
11:Q:21:ALA:HB3	11:Q:29:LYS:HB3	1.73	0.71
32:f:494:ARG:NH2	32:f:495:GLU:CG	2.48	0.71
32:f:389:LYS:HG2	32:f:418:LEU:HD11	1.72	0.71
32:f:797:LEU:O	32:f:800:LEU:HD13	1.91	0.71
32:f:222:ASP:O	32:f:226:TYR:HB3	1.91	0.71
20:Z:267:ARG:NH2	23:c:292:MET:SD	2.64	0.71
15:U:80:TYR:O	15:U:84:ALA:HB3	1.91	0.70
30:E:165:ILE:HB	30:E:168:LYS:HZ1	1.54	0.70
32:f:311:VAL:O	32:f:490:ALA:O	2.09	0.70
17:W:190:MET:HB2	17:W:233:LEU:HD13	1.71	0.70
32:f:389:LYS:CD	32:f:418:LEU:HD21	2.20	0.70
32:f:376:PHE:CD1	32:f:798:THR:HG21	2.26	0.70
32:f:625:LYS:O	32:f:629:LYS:HB2	1.91	0.70
7:M:76:ALA:HB3	7:M:136:MET:HB2	1.73	0.70
32:f:311:VAL:CG2	32:f:527:VAL:O	2.39	0.70
32:f:315:GLU:CG	32:f:491:GLY:HA2	2.20	0.70
4:J:172:LEU:O	4:J:176:TYR:HB2	1.90	0.70
17:W:408:ARG:HD2	18:X:345:VAL:HG13	1.72	0.70
32:f:337:LEU:CD1	32:f:420:TRP:HZ3	2.04	0.70
16:V:474:LEU:HD23	24:d:242:LEU:HD11	1.74	0.70
30:E:165:ILE:CG2	30:E:168:LYS:HZ1	2.05	0.70
32:f:130:ALA:O	32:f:134:SER:HB3	1.92	0.70
32:f:635:LYS:HZ3	32:f:641:GLU:CD	1.99	0.70
32:f:337:LEU:CD1	32:f:420:TRP:CZ3	2.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:117:TYR:HB3	11:Q:125:ALA:HB3	1.74	0.69
32:f:664:GLU:O	32:f:665:GLU:O	2.10	0.69
16:V:199:ASN:HA	16:V:203:LEU:HB2	1.75	0.69
29:D:344:ILE:HG23	34:D:501:AGS:H2	1.73	0.69
32:f:353:LEU:HG	32:f:387:GLN:HG3	1.75	0.69
15:U:599:ILE:O	15:U:603:LEU:HB2	1.92	0.69
4:j:72:ALA:HB3	4:j:132:LEU:HB2	1.74	0.69
20:Z:262:LEU:O	20:Z:266:ILE:HB	1.93	0.69
3:i:106:PRO:HD2	3:i:109:GLN:HE21	1.57	0.69
32:f:392:THR:HG22	32:f:417:ILE:HD12	1.74	0.69
32:f:372:LEU:O	32:f:372:LEU:HD23	1.93	0.69
16:V:493:ALA:O	20:Z:282:ASN:ND2	2.26	0.69
15:U:95:GLU:HA	15:U:98:GLU:HG2	1.76	0.68
21:a:193:GLN:HG2	21:a:196:ARG:HD3	1.75	0.68
30:E:148:VAL:HG23	30:E:167:PRO:CB	2.22	0.68
14:t:27:LEU:HD22	14:t:184:TYR:HB2	1.75	0.68
32:f:695:ALA:HB3	32:f:752:HIS:CB	2.22	0.68
29:D:228:ILE:HB	29:D:262:ILE:HG12	1.74	0.68
16:V:470:ARG:HH12	20:Z:256:GLN:HG2	1.59	0.68
32:f:376:PHE:HE1	32:f:798:THR:HB	1.53	0.68
15:U:226:PRO:HB3	15:U:263:SER:HB2	1.74	0.68
5:k:91:LYS:HE2	5:k:119:LEU:HD11	1.75	0.68
13:S:27:THR:HB	13:S:40:SER:H	1.59	0.68
17:W:82:LEU:O	17:W:93:ARG:NH2	2.26	0.68
21:a:349:MET:O	21:a:353:LEU:HB3	1.93	0.68
32:f:367:SER:HB3	32:f:370:MET:SD	2.34	0.68
32:f:471:LEU:CG	32:f:509:LYS:CE	2.56	0.68
32:f:688:ARG:HA	32:f:745:LEU:HD22	1.75	0.68
27:B:92:GLN:CB	27:B:96:ARG:N	2.57	0.68
7:M:47:PHE:HB2	7:M:214:SER:HB3	1.76	0.68
4:J:109:ARG:NH2	12:R:70:ASN:OD1	2.27	0.68
32:f:494:ARG:HD3	32:f:496:ASP:CG	2.16	0.67
18:X:319:ILE:HA	18:X:322:HIS:HD2	1.60	0.67
21:a:199:THR:O	21:a:203:ALA:HB3	1.95	0.67
21:a:140:GLU:O	21:a:143:ASN:ND2	2.28	0.67
13:s:169:ASP:OD2	13:s:173:ARG:NH2	2.27	0.67
30:E:166:PRO:CB	30:E:274:LYS:HE3	2.24	0.67
32:f:315:GLU:HG2	32:f:491:GLY:CA	2.24	0.67
32:f:625:LYS:HA	32:f:657:ILE:HD11	1.75	0.67
19:Y:387:ILE:HD11	20:Z:283:ARG:HD3	1.75	0.67
30:E:159:PHE:HE2	30:E:167:PRO:HD3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:742:ALA:O	32:f:745:LEU:CG	2.38	0.67
1:g:41:ALA:HB3	1:g:166:THR:HB	1.76	0.67
14:t:1:THR:N	14:t:105:PRO:O	2.28	0.67
32:f:311:VAL:HG21	32:f:527:VAL:O	1.94	0.67
32:f:578:ALA:O	32:f:582:VAL:HB	1.95	0.67
19:Y:344:HIS:ND1	19:Y:357:ASN:OD1	2.28	0.67
11:q:117:TYR:HB3	11:q:125:ALA:HB3	1.75	0.67
32:f:478:ARG:O	32:f:482:ILE:HB	1.94	0.67
15:U:600:ARG:HE	29:D:56:VAL:HG22	1.59	0.67
3:I:38:LEU:HG	3:I:160:LYS:HB3	1.77	0.67
30:E:135:ILE:HD11	30:E:183:LEU:HB2	1.75	0.67
31:F:383:GLU:OE1	31:F:417:HIS:NE2	2.28	0.67
15:U:792:ASN:HB3	15:U:914:LEU:HB3	1.77	0.67
3:i:143:TYR:HB2	3:i:146:GLN:HE21	1.58	0.67
32:f:376:PHE:CE1	32:f:416:MET:SD	2.88	0.67
32:f:804:LEU:H	32:f:804:LEU:HD12	1.60	0.67
3:I:143:TYR:HB2	3:I:146:GLN:HE21	1.60	0.66
24:d:179:ALA:HA	24:d:183:GLU:HB2	1.78	0.66
32:f:337:LEU:HD11	32:f:422:VAL:HG21	1.77	0.66
16:V:345:ARG:HH12	16:V:349:ARG:HD3	1.60	0.66
21:a:162:TYR:O	21:a:165:THR:OG1	2.13	0.66
5:K:125:GLU:HG3	5:K:134:SER:HB2	1.78	0.66
32:f:628:ASP:HB2	32:f:657:ILE:HD13	1.77	0.66
16:V:148:ARG:NH1	16:V:196:SER:O	2.28	0.66
13:s:28:ARG:NH2	13:s:213:ASP:O	2.29	0.66
29:D:168:GLY:CA	29:D:344:ILE:CD1	2.61	0.66
30:E:163:GLY:O	30:E:164:ILE:HD13	1.94	0.66
32:f:372:LEU:HD23	32:f:372:LEU:C	2.20	0.66
24:d:173:THR:O	24:d:175:ARG:NH2	2.27	0.66
11:Q:57:ALA:O	11:Q:61:GLN:HB3	1.96	0.66
15:U:9:ILE:HG13	15:U:12:LEU:HD12	1.78	0.66
16:V:419:LEU:H	16:V:457:TYR:HB3	1.61	0.66
17:W:362:ASN:O	17:W:366:MET:HB2	1.96	0.66
19:Y:247:LEU:O	19:Y:251:HIS:HB2	1.94	0.66
11:Q:169:LYS:HD3	11:Q:170:ARG:HG3	1.77	0.65
16:V:32:PRO:O	16:V:36:GLU:HB3	1.96	0.65
28:C:231:VAL:H	28:C:276:LEU:HD13	1.60	0.65
15:U:361:ARG:NH1	15:U:363:SER:OG	2.29	0.65
32:f:80:ARG:HB3	32:f:95:PRO:HB2	1.78	0.65
16:V:231:LEU:HB2	16:V:250:LEU:HD12	1.78	0.65
3:I:15:GLU:H	3:I:16:GLY:HA2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:177:ALA:O	5:K:181:LEU:HB2	1.97	0.65
32:f:800:LEU:HD12	32:f:800:LEU:N	2.10	0.65
32:f:804:LEU:HD12	32:f:804:LEU:N	2.12	0.65
4:j:131:ALA:H	4:j:147:THR:HG1	1.44	0.65
32:f:692:LEU:HG	32:f:752:HIS:CE1	2.32	0.65
7:m:8:ASP:O	7:m:22:GLN:NE2	2.30	0.65
31:F:82:VAL:HG12	31:F:161:LEU:HD11	1.78	0.65
16:V:416:ARG:NH2	16:V:456:GLY:O	2.30	0.65
18:X:324:ALA:O	18:X:328:ASP:HB2	1.97	0.65
32:f:379:GLY:O	32:f:417:ILE:HG12	1.97	0.65
32:f:389:LYS:HG2	32:f:418:LEU:CG	2.27	0.65
11:q:21:ALA:HB3	11:q:29:LYS:HB3	1.79	0.64
13:S:157:ASN:O	10:p:169:GLN:NE2	2.29	0.64
16:V:337:LEU:O	16:V:401:ASN:ND2	2.30	0.64
14:t:27:LEU:HD11	14:t:34:ALA:HB1	1.79	0.64
14:T:27:LEU:HD22	14:T:184:TYR:HB2	1.78	0.64
21:a:64:ILE:HB	21:a:70:ARG:HH21	1.62	0.64
19:Y:192:ARG:HH21	25:e:42:ASN:HA	1.62	0.64
15:U:625:ILE:HG13	15:U:626:LEU:HG	1.79	0.64
6:l:73:SER:HB3	6:l:133:LEU: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
15:U:182:LYS:HE2	15:U:214:ILE:CD1	2.28	0.64
8:n:91:ARG:HG3	8:n:92:GLU:HG2	1.80	0.64
26:A:302:LEU:O	26:A:306:LEU:HB2	1.97	0.64
32:f:460:ASP:N	32:f:460:ASP:OD1	2.29	0.64
17:W:348:GLU:HA	17:W:351:TRP:HD1	1.63	0.63
20:Z:240:VAL:HA	21:a:352:ARG:HH12	1.64	0.63
9:o:198:ARG:NH1	10:p:152:SER:O	2.31	0.63
13:s:27:THR:HB	13:s:40:SER:H	1.63	0.63
27:B:383:LEU:HD11	27:B:419:PHE:HB3	1.80	0.63
2:H:81:PRO:HG2	29:D:416:PHE:HE1	1.63	0.63
7:M:141:SER:HB3	7:M:144:ASP:HB2	1.80	0.63
7:M:214:SER:OG	7:M:224:HIS:NE2	2.31	0.63
15:U:155:LEU:O	15:U:158:ARG:NH1	2.31	0.63
32:f:664:GLU:HA	32:f:697:ILE:HA	1.80	0.63
32:f:804:LEU:H	32:f:804:LEU:CD1	2.10	0.63
1:g:53:GLN:HA	1:g:215:ILE:HA	1.80	0.63
31:F:189:GLY:H	34:F:501:AGS:HN62	1.45	0.63
32:f:313:GLU:O	32:f:317:LEU:HB2	1.98	0.63
15:U:188:MET:HG2	15:U:194:ARG:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:580:ARG:HD2	15:U:613:ASP:HB3	1.80	0.63
17:W:1:MET:N	17:W:37:GLU:OE1	2.31	0.63
32:f:93:PRO:HB2	32:f:137:ARG:HE	1.63	0.63
10:P:203:ARG:HH12	12:r:191:ASN:HD21	1.46	0.63
11:Q:118:MET:HE1	11:Q:124:LEU:HD23	1.80	0.63
2:h:39:LYS:HE2	2:h:144:PRO:HG2	1.79	0.63
7:m:99:ARG:NH2	7:m:105:ASN:OD1	2.30	0.63
21:a:135:ILE:HG23	21:a:158:LEU:HD13	1.78	0.63
30:E:119:VAL:HA	30:E:122:MET:HE2	1.81	0.63
15:U:549:ALA:HB1	15:U:581:SER:HB2	1.80	0.63
16:V:98:LEU:HG	16:V:144:ASP:HA	1.81	0.63
17:W:23:THR:HA	17:W:26:GLN:HB2	1.81	0.63
27:B:106:PRO:HB3	28:C:121:TYR:HB2	1.80	0.63
31:F:228:PRO:O	31:F:233:LYS:NZ	2.31	0.63
4:J:115:LYS:HE2	4:J:149:PRO:HA	1.81	0.62
6:L:186:GLU:HA	6:L:189:LYS:HG2	1.79	0.62
10:P:101:GLY:O	11:Q:93:ARG:NH1	2.31	0.62
16:V:182:LYS:NZ	16:V:210:CYS:SG	2.70	0.62
16:V:349:ARG:HB3	25:e:43:TRP:HZ2	1.64	0.62
3:i:119:GLN:HE21	3:i:123:GLN:HE22	1.45	0.62
2:H:12:THR:OG1	3:I:20:GLN:NE2	2.32	0.62
5:K:21:LEU:HB3	5:K:23:GLN:H	1.64	0.62
5:K:99:HIS:HB2	5:K:107:MET:HE3	1.79	0.62
18:X:347:ILE:HD11	18:X:352:SER:HB2	1.81	0.62
13:S:209:SER:OG	13:S:212:LYS:NZ	2.31	0.62
14:T:27:LEU:HD11	14:T:34:ALA:HB1	1.81	0.62
4:j:88:ARG:NH1	11:q:69:MET:O	2.32	0.62
9:O:163:ILE:HG12	9:O:169:SER:H	1.63	0.62
17:W:431:LYS:O	17:W:435:LEU:HB2	1.99	0.62
20:Z:25:ARG:HH11	23:c:103:GLY:HA3	1.65	0.62
10:p:107:PRO:HG2	10:p:124:LEU:HB2	1.81	0.62
28:C:113:ARG:NH2	28:C:129:ASN:O	2.32	0.62
30:E:165:ILE:CB	30:E:168:LYS:HZ1	2.11	0.62
23:c:61:PHE:HA	23:c:139:ARG:HH22	1.64	0.62
2:h:34:PRO:HA	2:h:164:GLY:HA3	1.82	0.62
22:b:110:ILE:HG22	22:b:139:ASP:HB2	1.81	0.62
32:f:494:ARG:HH21	32:f:495:GLU:H	1.46	0.62
10:P:169:GLN:NE2	13:s:157:ASN:O	2.29	0.62
24:d:86:LYS:HD2	24:d:88:GLN:HB2	1.82	0.62
5:k:76:CYS:SG	5:k:77:ALA:N	2.73	0.62
32:f:339:ILE:HG23	32:f:340:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.81	0.62
15:U:590:TYR:HD2	15:U:598:ALA:HB2	1.64	0.61
19:Y:101:ARG:NH2	19:Y:127:THR:O	2.33	0.61
22:b:113:VAL:HB	22:b:142:ASN:HD22	1.65	0.61
16:V:203:LEU:O	16:V:207:ALA:HB2	2.00	0.61
15:U:481:LEU:O	15:U:485:ALA:HB3	1.99	0.61
17:W:389:SER:HA	17:W:392:PHE:HB2	1.82	0.61
32:f:234:THR:O	32:f:238:ASN:HB2	2.00	0.61
5:K:173:ALA:HB2	26:A:375:ARG:HG3	1.82	0.61
16:V:483:CYS:HA	16:V:486:ILE:HD12	1.82	0.61
32:f:392:THR:HG23	32:f:417:ILE:HG21	1.81	0.61
32:f:471:LEU:CD1	32:f:509:LYS:HE2	2.30	0.61
2:H:50:LYS:NZ	2:H:62:VAL:O	2.33	0.61
16:V:106:ARG:O	16:V:110:HIS:ND1	2.32	0.61
18:X:415:TYR:O	18:X:419:LYS:HB2	1.99	0.61
32:f:389:LYS:HD3	32:f:389:LYS:N	2.15	0.61
32:f:471:LEU:CD1	32:f:509:LYS:HE3	2.26	0.61
20:Z:10:VAL:HG13	20:Z:163:GLY:HA3	1.81	0.61
24:d:149:ASN:HA	24:d:194:ALA:HB3	1.82	0.61
9:o:163:ILE:HG12	9:o:169:SER:H	1.65	0.61
32:f:687:ARG:HH21	32:f:742:ALA:HB2	1.64	0.61
3:I:25:MET:HA	3:I:28:ILE:HD12	1.81	0.61
9:O:30:ASN:OD1	9:O:187:ARG:NH2	2.33	0.61
3:i:90:LEU:HD12	3:i:114:LEU:HD22	1.82	0.61
32:f:494:ARG:NE	32:f:496:ASP:H	1.99	0.61
32:f:801:VAL:HG13	32:f:801:VAL:O	2.01	0.61
16:V:100:MET:O	16:V:146:GLN:NE2	2.34	0.61
32:f:471:LEU:O	32:f:471:LEU:HD23	2.01	0.61
1:G:11:ARG:O	1:G:24:GLN:NE2	2.33	0.61
9:O:174:ASP:OD2	9:O:187:ARG:NH1	2.34	0.61
9:O:96:ALA:H	9:O:115:PRO:HB3	1.66	0.61
5:k:48:LEU:HD21	5:k:77:ALA:HB2	1.83	0.60
11:q:118:MET:HE1	11:q:124:LEU:HD23	1.83	0.60
28:C:304:ALA:O	28:C:310:ARG:NH1	2.34	0.60
28:C:320:PRO:O	28:C:325:ARG:NH1	2.34	0.60
1:G:34:GLN:NE2	7:M:17:ASP:O	2.34	0.60
4:J:179:GLU:HG2	4:J:180:ALA:HB2	1.83	0.60
5:K:203:LYS:HA	5:K:206:MET:HG2	1.82	0.60
29:D:259:PRO:CB	29:D:304:ASN:HB2	2.28	0.60
18:X:407:MET:HE2	19:Y:376:LEU:HD21	1.84	0.60
21:a:105:LYS:HB2	21:a:110:ALA:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:113:ILE:O	26:A:121:PHE:N	2.27	0.60
16:V:309:MET:HB3	16:V:332:LEU:HG	1.82	0.60
27:B:425:ASN:OD1	28:C:313:ARG:NH1	2.34	0.60
31:F:318:ASP:HB3	31:F:347:ARG:HG3	1.83	0.60
31:F:358:ASN:O	31:F:362:ARG:NH1	2.34	0.60
32:f:232:TYR:O	32:f:236:CYS:CB	2.49	0.60
32:f:376:PHE:HE1	32:f:798:THR:HG21	1.49	0.60
10:P:190:ILE:HG22	10:P:195:ILE:HG23	1.83	0.60
16:V:162:GLU:HB3	16:V:175:MET:HE3	1.84	0.60
21:a:296:ILE:O	21:a:300:ALA:HB3	2.02	0.60
8:n:144:ARG:NH2	8:n:151:GLU:OE1	2.33	0.60
32:f:380:PHE:CB	32:f:751:TYR:HE2	2.14	0.60
5:K:76:CYS:SG	5:K:77:ALA:N	2.74	0.60
14:T:43:MET:HE3	14:T:45:VAL:HG22	1.84	0.60
24:d:49:ILE:HD12	24:d:52:ARG:HH11	1.67	0.60
6:l:120:THR:O	7:m:129:ARG:NH1	2.28	0.60
32:f:378:ASN:HB2	32:f:391:LEU:HD11	1.82	0.60
16:V:393:THR:O	16:V:397:ARG:NH2	2.35	0.60
8:n:19:ARG:NH2	8:n:168:GLY:O	2.34	0.60
31:F:97:LEU:O	31:F:120:LYS:N	2.35	0.60
32:f:501:LEU:HD22	32:f:518:THR:HG23	1.84	0.60
15:U:509:GLY:HA3	15:U:544:ILE:HA	1.84	0.60
1:g:165:ALA:HB3	2:h:56:LEU:HD22	1.84	0.60
29:D:259:PRO:HB3	29:D:304:ASN:CB	2.27	0.60
32:f:376:PHE:CG	32:f:416:MET:HE1	2.35	0.60
8:N:29:ARG:NH1	9:O:139:GLU:OE1	2.32	0.60
18:X:130:GLU:HB3	18:X:153:LEU:HD21	1.83	0.60
19:Y:13:LYS:HE2	19:Y:146:ARG:HD2	1.83	0.60
6:l:186:GLU:HA	6:l:189:LYS:HG2	1.84	0.60
7:m:40:ARG:NH1	7:m:146:ALA:O	2.35	0.60
31:F:223:VAL:HA	31:F:350:ARG:HB2	1.84	0.60
11:Q:104:LEU:HB2	11:Q:116:TYR:HB2	1.84	0.60
15:U:194:ARG:HE	15:U:198:LEU:HD22	1.64	0.60
18:X:342:PHE:HB3	18:X:384:VAL:HG22	1.83	0.60
19:Y:233:ARG:NH2	19:Y:264:TYR:O	2.35	0.60
21:a:201:GLY:O	21:a:205:LEU:HB2	2.02	0.60
6:l:5:GLN:O	6:l:8:ASN:ND2	2.33	0.60
32:f:483:PHE:CE2	32:f:799:VAL:CB	2.75	0.60
1:g:130:GLU:HG2	2:h:4:ARG:HH11	1.67	0.59
27:B:341:LEU:HA	27:B:346:ARG:HD2	1.83	0.59
29:D:119:ILE:O	29:D:121:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:89:MET:HG2	32:f:90:THR:HG23	1.84	0.59
15:U:167:ILE:CG2	15:U:176:MET:HE2	2.30	0.59
30:E:206:LYS:NZ	31:F:301:ALA:O	2.33	0.59
32:f:378:ASN:CB	32:f:391:LEU:HD11	2.33	0.59
32:f:610:GLN:CA	32:f:613:LEU:HG	2.31	0.59
17:W:81:ASP:O	17:W:85:GLU:HB3	2.01	0.59
3:i:171:ALA:HB2	3:i:200:THR:HG21	1.84	0.59
26:A:99:THR:HG22	26:A:115:VAL:HG22	1.83	0.59
26:A:143:ASP:HB3	26:A:147:TYR:H	1.67	0.59
11:Q:181:ARG:NH1	11:Q:190:ASP:OD1	2.35	0.59
16:V:98:LEU:HD12	16:V:142:GLU:HB3	1.84	0.59
23:c:56:LEU:HA	23:c:111:TRP:HA	1.82	0.59
7:m:51:LYS:O	7:m:210:GLU:N	2.33	0.59
32:f:378:ASN:O	32:f:381:VAL:CG1	2.49	0.59
5:K:22:PHE:H	5:K:25:GLU:HB3	1.67	0.59
5:K:37:ALA:HB2	5:K:50:VAL:HG23	1.84	0.59
22:b:16:MET:HA	22:b:25:ARG:HD2	1.84	0.59
27:B:301:GLY:O	27:B:303:ARG:NE	2.35	0.59
32:f:782:HIS:HA	32:f:785:ARG:HG2	1.83	0.59
6:L:44:ALA:HB1	6:L:144:ILE:HD11	1.85	0.59
21:a:226:ARG:HB3	21:a:234:ILE:HG12	1.84	0.59
8:n:14:LEU:HB2	8:n:177:ALA:HB3	1.83	0.59
14:t:9:THR:O	14:t:41:ARG:NH2	2.35	0.59
30:E:156:PRO:HG3	30:E:272:ARG:HH21	1.65	0.59
32:f:389:LYS:HG2	32:f:418:LEU:CD1	2.32	0.59
32:f:494:ARG:NH2	32:f:495:GLU:H	2.00	0.59
1:G:53:GLN:HA	1:G:215:ILE:HA	1.83	0.59
1:g:49:VAL:HG22	1:g:219:VAL:HG23	1.84	0.59
1:g:71:LYS:O	1:g:95:ARG:NH2	2.35	0.59
34:A:501:AGS:S1G	27:B:346:ARG:NH2	2.76	0.59
30:E:56:ILE:HB	30:E:100:LEU:HB2	1.84	0.59
30:E:101:ASP:HB2	30:E:108:MET:HE3	1.83	0.59
15:U:524:LYS:HA	15:U:556:MET:HE2	1.85	0.59
21:a:255:TRP:O	21:a:258:GLN:NE2	2.36	0.59
28:C:55:LYS:HG2	28:C:58:LEU:HD12	1.84	0.59
30:E:165:ILE:CG2	30:E:168:LYS:NZ	2.66	0.59
32:f:315:GLU:CB	32:f:491:GLY:HA2	2.32	0.59
32:f:376:PHE:CZ	32:f:416:MET:HE1	2.36	0.59
32:f:477:MET:O	32:f:481:SER:HB2	2.02	0.59
32:f:618:GLU:HG2	32:f:623:LYS:HD2	1.84	0.59
3:i:123:GLN:NE2	4:j:79:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:219:GLU:OE2	3:i:220:ASN:ND2	2.36	0.59
27:B:244:SER:HB3	32:f:669:GLU:CG	2.33	0.59
22:b:116:PRO:HG3	22:b:147:GLU:H	1.67	0.59
5:k:99:HIS:HB2	5:k:107:MET:HE3	1.84	0.59
32:f:337:LEU:HD22	32:f:337:LEU:N	2.17	0.59
32:f:610:GLN:HA	32:f:613:LEU:CG	2.33	0.59
1:g:54:LYS:NZ	1:g:213:SER:O	2.35	0.58
2:h:71:HIS:HA	2:h:218:PHE:H	1.68	0.58
4:j:109:ARG:NH2	12:r:70:ASN:OD1	2.35	0.58
5:k:77:ALA:HB3	5:k:142:LEU:HB2	1.84	0.58
27:B:244:SER:N	32:f:669:GLU:OE1	2.36	0.58
8:N:19:ARG:HH22	14:t:181:ALA:HA	1.68	0.58
19:Y:192:ARG:NH1	19:Y:290:PRO:O	2.35	0.58
21:a:158:LEU:O	21:a:162:TYR:HB3	2.03	0.58
5:k:37:ALA:HB2	5:k:50:VAL:HG23	1.84	0.58
10:p:189:ILE:HG23	10:p:196:THR:HB	1.85	0.58
29:D:168:GLY:N	29:D:344:ILE:HD11	2.16	0.58
17:W:49:SER:HB3	17:W:96:GLN:HB2	1.84	0.58
21:a:97:LEU:O	21:a:101:ARG:HB3	2.03	0.58
21:a:236:THR:HG21	21:a:253:THR:HB	1.85	0.58
5:k:209:LYS:O	5:k:214:ASN:ND2	2.36	0.58
27:B:135:ILE:HA	27:B:159:VAL:HB	1.85	0.58
16:V:370:GLY:O	16:V:427:GLN:NE2	2.36	0.58
7:m:141:SER:HB3	7:m:144:ASP:HB2	1.85	0.58
8:n:29:ARG:NH1	9:o:139:GLU:OE1	2.36	0.58
28:C:140:VAL:HG11	28:C:211:PHE:HB3	1.86	0.58
32:f:129:LEU:O	32:f:133:MET:CB	2.50	0.58
32:f:541:THR:O	32:f:545:LYS:HB2	2.02	0.58
7:m:163:CYS:SG	7:m:164:ALA:N	2.76	0.58
7:m:173:LYS:HA	7:m:176:ILE:HB	1.85	0.58
7:m:214:SER:OG	7:m:224:HIS:NE2	2.35	0.58
29:D:273:LYS:NZ	31:F:297:ASP:OD2	2.36	0.58
32:f:22:GLY:O	32:f:26:GLU:HB2	2.04	0.58
32:f:127:SER:O	32:f:131:MET:CB	2.52	0.58
1:G:11:ARG:HH11	7:M:16:PRO:HG3	1.68	0.58
7:M:163:CYS:SG	7:M:164:ALA:N	2.76	0.58
16:V:40:GLU:HG3	16:V:108:LEU:HD13	1.85	0.58
18:X:301:ASP:HA	18:X:304:LYS:HE3	1.84	0.58
19:Y:197:ALA:O	19:Y:201:PHE:HB2	2.04	0.58
28:C:99:VAL:HG12	28:C:123:LEU:HD12	1.85	0.58
32:f:378:ASN:HB3	32:f:391:LEU:CD2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:60:GLN:HG2	31:F:439:ALA:HB1	1.86	0.58
29:D:239:TYR:HB3	29:D:242:GLU:HB2	1.86	0.58
29:D:300:ASP:C	29:D:302:ASN:H	2.11	0.58
32:f:438:ASP:N	32:f:438:ASP:OD1	2.36	0.58
3:I:29:GLY:HA2	3:I:165:GLY:HA3	1.85	0.58
6:L:107:ARG:NH2	14:T:79:ASP:OD2	2.37	0.58
15:U:684:ARG:NH2	15:U:723:ASP:OD2	2.36	0.58
9:o:198:ARG:HD2	9:o:201:ARG:HG3	1.86	0.58
32:f:695:ALA:CB	32:f:752:HIS:CB	2.82	0.58
32:f:780:PRO:O	32:f:800:LEU:HG	2.03	0.58
16:V:295:ILE:O	16:V:299:GLN:N	2.35	0.58
17:W:304:ASP:HA	17:W:307:LYS:HE3	1.86	0.58
17:W:417:ARG:NH2	17:W:422:ASN:O	2.37	0.58
24:d:2:TYR:O	24:d:25:ARG:NH2	2.37	0.58
5:k:70:ILE:HD11	5:k:89:ILE:HD12	1.86	0.58
11:q:19:ARG:HH21	11:q:31:ASP:HB2	1.67	0.58
30:E:165:ILE:CB	30:E:168:LYS:HZ2	2.16	0.58
32:f:353:LEU:H	32:f:387:GLN:HG2	1.68	0.58
32:f:487:LEU:HD23	32:f:524:MET:HE1	1.85	0.58
7:M:8:ASP:O	7:M:22:GLN:NE2	2.35	0.58
16:V:66:GLU:O	16:V:70:VAL:HB	2.03	0.58
16:V:137:GLU:HA	16:V:140:ASP:HB2	1.85	0.58
16:V:263:LEU:HD11	24:d:120:GLU:HG3	1.86	0.58
16:V:378:VAL:HA	16:V:382:PHE:HD2	1.68	0.58
17:W:187:LEU:HB3	17:W:226:TYR:HE1	1.69	0.58
24:d:150:LYS:HA	24:d:153:LEU:HB2	1.84	0.58
14:t:54:SER:HB2	14:t:109:THR:HB	1.86	0.58
3:I:106:PRO:HD2	3:I:109:GLN:HE21	1.67	0.57
6:L:73:SER:HB3	6:L:133:LEU:HB2	1.86	0.57
31:F:91:SER:HA	31:F:126:THR:HA	1.86	0.57
32:f:88:SER:HB2	32:f:92:VAL:CG2	2.33	0.57
8:N:127:ILE:HD13	8:N:136:TYR:HB2	1.86	0.57
21:a:227:ASN:O	21:a:231:GLN:NE2	2.37	0.57
32:f:269:ALA:HB2	32:f:277:LEU:HD22	1.86	0.57
6:L:215:VAL:HB	6:L:221:PHE:HD1	1.69	0.57
9:O:18:THR:HB	9:O:31:CYS:H	1.69	0.57
18:X:222:GLU:HA	18:X:225:TRP:HE1	1.69	0.57
4:j:74:ALA:HB2	4:j:161:ILE:HD13	1.86	0.57
30:E:236:ASP:O	30:E:242:ARG:NH2	2.36	0.57
3:I:10:THR:HG22	3:I:11:ILE:HG13	1.87	0.57
8:N:7:GLN:HA	8:N:12:VAL:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:268:LYS:HA	17:W:271:VAL:HG12	1.86	0.57
21:a:45:VAL:HG22	21:a:79:ILE:HD12	1.85	0.57
8:n:21:THR:HG22	8:n:26:ILE:HG13	1.86	0.57
31:F:341:ALA:O	31:F:347:ARG:NH1	2.37	0.57
32:f:140:LEU:O	32:f:144:LEU:HB2	2.04	0.57
15:U:788:VAL:HG12	15:U:909:GLY:HA2	1.85	0.57
24:d:151:VAL:HG21	24:d:174:ILE:HD13	1.86	0.57
10:p:26:ARG:HH21	10:p:38:ASP:HA	1.69	0.57
30:E:236:ASP:HB2	30:E:282:PRO:HB3	1.86	0.57
16:V:231:LEU:HD22	16:V:250:LEU:HB2	1.87	0.57
2:h:222:THR:OG1	2:h:225:GLU:OE1	2.22	0.57
32:f:226:TYR:O	32:f:230:CYS:CB	2.53	0.57
32:f:456:ARG:HD3	32:f:489:TYR:OH	2.03	0.57
1:G:165:ALA:HB3	2:H:56:LEU:HD22	1.86	0.57
17:W:12:ARG:HA	17:W:15:LYS:HD3	1.86	0.57
30:E:371:VAL:O	30:E:375:ALA:HB3	2.05	0.57
32:f:456:ARG:HB3	32:f:489:TYR:CZ	2.39	0.57
32:f:494:ARG:CZ	32:f:496:ASP:H	2.16	0.57
7:M:235:ALA:O	7:M:239:ALA:N	2.33	0.57
20:Z:167:ALA:H	23:c:151:VAL:HG23	1.70	0.57
21:a:231:GLN:O	21:a:235:ASP:N	2.38	0.57
22:b:3:LEU:HD23	22:b:44:ASN:HD21	1.70	0.57
24:d:204:LYS:O	24:d:208:ASP:HB2	2.05	0.57
4:j:131:ALA:N	4:j:147:THR:HG1	2.02	0.57
8:n:7:GLN:HA	8:n:12:VAL:HA	1.87	0.57
11:q:181:ARG:NH1	11:q:190:ASP:OD1	2.38	0.57
31:F:401:VAL:HG12	31:F:405:MET:HE2	1.85	0.57
2:H:222:THR:OG1	2:H:225:GLU:OE1	2.19	0.57
32:f:742:ALA:CA	32:f:745:LEU:HD21	2.31	0.57
3:i:16:GLY:N	4:j:21:TYR:OH	2.38	0.57
32:f:780:PRO:HB2	32:f:800:LEU:HB3	1.86	0.57
3:I:219:GLU:OE2	3:I:220:ASN:ND2	2.38	0.56
15:U:265:ILE:HG13	15:U:268:LEU:HD22	1.86	0.56
16:V:163:VAL:HG23	16:V:175:MET:HE1	1.87	0.56
17:W:72:LYS:HA	17:W:75:TYR:HB2	1.87	0.56
17:W:405:LYS:HD2	17:W:416:GLN:HE22	1.69	0.56
28:C:152:GLY:H	34:C:501:AGS:HN62	1.51	0.56
32:f:494:ARG:CZ	32:f:495:GLU:H	2.17	0.56
3:I:48:GLU:OE2	3:I:50:ARG:NH2	2.38	0.56
5:K:210:LEU:HD11	5:K:215:ILE:HG12	1.86	0.56
16:V:337:LEU:HD22	16:V:367:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:451:ILE:HA	16:V:458:VAL:HA	1.86	0.56
17:W:429:SER:O	17:W:433:ASN:HB3	2.05	0.56
3:i:161:ALA:HB3	4:j:54:GLN:HE22	1.70	0.56
30:E:135:ILE:HB	30:E:312:ILE:HG12	1.87	0.56
6:L:50:LYS:HB3	6:L:59:HIS:HB3	1.86	0.56
11:Q:38:MET:O	11:Q:65:GLN:NE2	2.38	0.56
15:U:520:MET:HB3	15:U:523:SER:HB3	1.87	0.56
16:V:422:ILE:HA	16:V:425:LYS:HG2	1.87	0.56
18:X:114:ILE:HD11	18:X:133:LEU:HD22	1.87	0.56
27:B:244:SER:HB3	32:f:669:GLU:CB	2.33	0.56
30:E:159:PHE:CE2	30:E:167:PRO:HD3	2.39	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:695:ALA:CB	32:f:752:HIS:HB2	2.31	0.56
32:f:780:PRO:HB2	32:f:800:LEU:CB	2.36	0.56
15:U:173:VAL:N	15:U:174:PRO:CD	2.69	0.56
17:W:169:LEU:HD11	17:W:189:GLN:HG3	1.87	0.56
18:X:167:VAL:HA	18:X:170:GLN:HB2	1.86	0.56
32:f:742:ALA:CA	32:f:745:LEU:HG	2.35	0.56
4:J:72:ALA:HB3	4:J:132:LEU:HB2	1.86	0.56
8:n:91:ARG:O	8:n:93:ASP:N	2.28	0.56
9:o:1:THR:HG23	9:o:33:LYS:HE3	1.86	0.56
27:B:210:TYR:HA	27:B:213:GLU:HB2	1.88	0.56
29:D:175:GLN:NE2	29:D:179:GLU:OE2	2.39	0.56
29:D:273:LYS:HZ1	30:E:208:ILE:HG21	1.71	0.56
15:U:374:SER:O	15:U:378:CYS:N	2.39	0.56
17:W:72:LYS:NZ	17:W:119:PRO:O	2.38	0.56
17:W:259:GLU:HG2	17:W:262:LYS:HB3	1.86	0.56
19:Y:179:ARG:NH1	19:Y:209:THR:O	2.38	0.56
4:j:32:ALA:HB2	4:j:45:VAL:HG23	1.88	0.56
14:t:43:MET:HE3	14:t:45:VAL:HG22	1.87	0.56
27:B:382:ASP:OD2	27:B:420:LYS:NZ	2.35	0.56
5:K:117:SER:HB3	6:L:82:ARG:HH22	1.71	0.56
15:U:643:SER:O	15:U:649:ARG:NH1	2.38	0.56
15:U:793:LYS:HE3	15:U:796:LYS:HB2	1.88	0.56
16:V:296:LYS:HA	16:V:299:GLN:HB2	1.87	0.56
26:A:112:ILE:HG12	26:A:122:VAL:HG22	1.86	0.56
32:f:380:PHE:CG	32:f:751:TYR:HE2	2.24	0.56
15:U:98:GLU:HA	15:U:101:ILE:HG12	1.87	0.56
17:W:453:HIS:HA	17:W:456:GLN:HB2	1.88	0.56
21:a:196:ARG:HA	21:a:199:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:36:THR:OG1	10:P:38:ASP:OD1	2.22	0.56
15:U:697:GLN:NE2	15:U:746:ILE:O	2.34	0.56
31:F:410:ARG:NH2	31:F:416:THR:OG1	2.39	0.56
32:f:229:VAL:O	32:f:233:LEU:HB2	2.06	0.56
2:H:46:LEU:HD13	2:H:75:VAL:HG13	1.87	0.56
10:P:15:LYS:HE3	10:P:121:ILE:HG12	1.87	0.56
17:W:243:ILE:HD12	17:W:273:TYR:HB2	1.87	0.56
19:Y:197:ALA:HB3	19:Y:226:VAL:HG21	1.87	0.56
21:a:24:ARG:O	21:a:28:LEU:HB2	2.06	0.56
22:b:72:LEU:HD23	22:b:75:LEU:HD12	1.87	0.56
26:A:95:VAL:O	27:B:131:HIS:ND1	2.39	0.56
29:D:304:ASN:HD22	29:D:304:ASN:N	2.04	0.56
32:f:358:PHE:CE1	32:f:381:VAL:HG21	2.40	0.56
32:f:742:ALA:HA	32:f:745:LEU:HG	1.88	0.56
18:X:336:ILE:HD12	18:X:337:ARG:HG3	1.87	0.55
19:Y:148:GLY:HA3	19:Y:157:ILE:HG21	1.88	0.55
19:Y:228:MET:SD	19:Y:295:TYR:OH	2.59	0.55
13:s:148:LEU:HD23	13:s:178:VAL:HG12	1.88	0.55
26:A:224:LEU:HG	34:A:501:AGS:H3'	1.87	0.55
26:A:308:GLY:H	26:A:311:PRO:HG3	1.71	0.55
28:C:46:GLN:HE22	29:D:61:ILE:HB	1.71	0.55
29:D:100:THR:HA	29:D:114:ARG:HA	1.88	0.55
32:f:317:LEU:O	32:f:321:MET:HB2	2.05	0.55
5:K:221:GLN:HB2	5:K:224:GLN:HB3	1.88	0.55
7:M:192:GLU:HA	7:M:195:LYS:HE3	1.88	0.55
21:a:201:GLY:O	21:a:205:LEU:CB	2.54	0.55
21:a:279:GLU:O	21:a:283:THR:CB	2.54	0.55
24:d:106:LEU:HD12	24:d:109:GLN:HE21	1.70	0.55
1:g:141:ILE:HG22	1:g:151:VAL:HG22	1.89	0.55
4:J:77:THR:HG23	27:B:440:LEU:H	1.71	0.55
18:X:126:ARG:NH2	18:X:130:GLU:OE2	2.39	0.55
22:b:84:ILE:HD13	22:b:115:SER:HB2	1.88	0.55
27:B:244:SER:CB	32:f:669:GLU:HB2	2.34	0.55
29:D:249:ASP:O	29:D:253:LEU:HB3	2.06	0.55
29:D:344:ILE:HD12	34:D:501:AGS:C2	2.34	0.55
32:f:377:VAL:HG22	32:f:751:TYR:HB2	1.88	0.55
5:K:175:GLU:HB3	26:A:348:LEU:HD12	1.88	0.55
6:L:5:GLN:O	6:L:8:ASN:ND2	2.37	0.55
17:W:407:ASP:H	17:W:413:ILE:HG22	1.70	0.55
19:Y:67:VAL:O	19:Y:71:ASN:N	2.39	0.55
5:k:203:LYS:HA	5:k:206:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:37:ILE:HD11	7:m:193:VAL:HG13	1.89	0.55
32:f:575:ALA:O	32:f:579:ALA:HB2	2.07	0.55
32:f:688:ARG:HH12	32:f:788:MET:HA	1.71	0.55
10:P:58:THR:OG1	11:Q:121:LEU:O	2.19	0.55
15:U:157:THR:OG1	15:U:159:ARG:NH2	2.39	0.55
19:Y:193:ASP:OD2	19:Y:197:ALA:N	2.38	0.55
20:Z:267:ARG:HH22	23:c:292:MET:HA	1.69	0.55
23:c:30:GLN:HB3	23:c:66:THR:HG22	1.89	0.55
24:d:52:ARG:HG2	24:d:81:TYR:HB3	1.88	0.55
3:i:155:ASN:HA	4:j:81:ARG:HH22	1.71	0.55
14:t:145:LEU:HB3	14:t:179:ARG:HH21	1.72	0.55
31:F:93:VAL:HB	31:F:149:ASP:HB2	1.88	0.55
32:f:353:LEU:HG	32:f:387:GLN:CG	2.36	0.55
8:N:96:ALA:HB1	8:N:98:ILE:HG12	1.87	0.55
13:S:123:SER:HB3	13:S:136:LYS:HG3	1.88	0.55
20:Z:70:LEU:H	22:b:60:VAL:HG21	1.70	0.55
21:a:73:PRO:HB3	21:a:113:LEU:HD11	1.89	0.55
23:c:57:MET:HE1	23:c:141:VAL:HB	1.87	0.55
3:i:239:LYS:NZ	3:i:243:GLU:OE2	2.39	0.55
32:f:80:ARG:O	32:f:84:SER:HB3	2.07	0.55
32:f:684:PRO:O	32:f:688:ARG:CB	2.54	0.55
22:b:138:VAL:HB	22:b:160:LEU:HD11	1.89	0.55
14:T:9:THR:O	14:T:41:ARG:NH2	2.39	0.55
17:W:224:LEU:O	17:W:253:THR:OG1	2.24	0.55
26:A:113:ILE:HG22	26:A:121:PHE:HB2	1.89	0.55
34:C:501:AGS:O1A	34:C:501:AGS:O1B	2.25	0.55
15:U:446:LEU:HB3	15:U:461:LEU:HD21	1.89	0.55
29:D:200:ARG:NH2	29:D:301:GLN:OE1	2.39	0.55
32:f:301:HIS:O	32:f:305:LEU:CB	2.53	0.55
15:U:341:PHE:O	15:U:345:ASN:HB2	2.07	0.55
10:p:36:THR:OG1	10:p:38:ASP:OD1	2.23	0.55
34:A:501:AGS:S1G	34:A:501:AGS:O1B	2.65	0.55
27:B:92:GLN:H	27:B:96:ARG:CB	2.19	0.55
31:F:134:LEU:HD13	31:F:137:ILE:HA	1.89	0.55
32:f:403:LYS:O	32:f:407:MET:N	2.40	0.55
32:f:610:GLN:HA	32:f:613:LEU:HG	1.87	0.55
1:G:120:ASP:OD1	2:H:84:ARG:NH1	2.40	0.54
10:P:29:GLY:HA3	10:P:34:MET:HA	1.87	0.54
10:p:190:ILE:HG22	10:p:195:ILE:HG23	1.89	0.54
32:f:623:LYS:O	32:f:627:GLU:CB	2.54	0.54
32:f:663:GLY:O	32:f:697:ILE:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:293:ARG:HG2	25:e:59:GLU:HG3	1.89	0.54
23:c:285:GLU:HG2	23:c:286:GLU:H	1.72	0.54
26:A:120:LYS:HD2	31:F:90:VAL:HG11	1.90	0.54
32:f:229:VAL:O	32:f:233:LEU:CB	2.56	0.54
32:f:586:PRO:HA	32:f:589:SER:HB2	1.89	0.54
18:X:177:TYR:O	18:X:182:ASN:N	2.36	0.54
18:X:415:TYR:O	18:X:419:LYS:CB	2.55	0.54
21:a:279:GLU:O	21:a:283:THR:HB	2.07	0.54
11:q:164:LEU:O	11:q:168:GLN:NE2	2.41	0.54
32:f:138:GLU:O	32:f:142:TYR:CB	2.55	0.54
32:f:281:ILE:O	32:f:285:CYS:CB	2.56	0.54
32:f:426:LEU:O	32:f:430:ASP:HB3	2.07	0.54
3:I:7:SER:OG	3:I:8:ARG:N	2.39	0.54
7:M:35:THR:HA	7:M:166:GLY:HA3	1.90	0.54
11:Q:4:LEU:HD22	11:Q:17:SER:HB2	1.90	0.54
15:U:219:CYS:O	15:U:223:LEU:HB3	2.07	0.54
15:U:787:CYS:HB2	15:U:881:PRO:HB2	1.88	0.54
19:Y:111:LEU:HA	19:Y:114:ILE:HD12	1.88	0.54
19:Y:238:GLU:HA	19:Y:242:LYS:HB2	1.88	0.54
20:Z:226:ILE:HA	20:Z:229:GLN:HB3	1.89	0.54
23:c:57:MET:HE3	23:c:109:VAL:HG23	1.89	0.54
26:A:277:ILE:HG22	26:A:280:ILE:HD12	1.88	0.54
30:E:370:ALA:O	30:E:374:VAL:HB	2.07	0.54
32:f:278:VAL:HA	32:f:281:ILE:HG22	1.89	0.54
1:G:141:ILE:HG22	1:G:151:VAL:HG22	1.90	0.54
15:U:678:ASP:O	15:U:684:ARG:NH1	2.35	0.54
15:U:717:ILE:HA	15:U:727:LYS:HD3	1.89	0.54
21:a:23:HIS:HA	21:a:26:GLU:HG2	1.89	0.54
2:h:118:MET:HE2	2:h:151:PRO:HA	1.88	0.54
7:m:47:PHE:HB2	7:m:214:SER:HB3	1.89	0.54
28:C:113:ARG:NH2	29:D:94:GLU:OE2	2.40	0.54
28:C:190:GLY:HA3	28:C:317:PHE:HB2	1.88	0.54
30:E:309:ARG:NH2	30:E:336:ASP:OD1	2.40	0.54
32:f:8:LYS:O	32:f:12:GLN:CB	2.56	0.54
14:T:99:ARG:HG2	14:T:106:LEU:HG	1.88	0.54
4:j:11:SER:OG	4:j:14:GLY:N	2.41	0.54
26:A:274:PHE:HB2	26:A:319:MET:HG2	1.89	0.54
30:E:261:LEU:HD22	30:E:294:ARG:HD3	1.89	0.54
4:J:154:HIS:HE1	5:K:59:MET:HG3	1.73	0.54
17:W:139:GLU:O	17:W:143:ALA:N	2.37	0.54
21:a:230:ARG:HE	21:a:233:LEU:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:161:ARG:NH1	23:c:162:LEU:O	2.40	0.54
8:n:35:THR:OG1	8:n:45:ARG:NH2	2.41	0.54
32:f:253:LEU:O	32:f:257:ARG:HB2	2.07	0.54
32:f:311:VAL:CB	32:f:490:ALA:CB	2.77	0.54
2:H:93:LEU:HD11	2:H:113:ARG:HB3	1.90	0.54
12:R:35:ILE:N	12:R:43:GLY:O	2.41	0.54
15:U:38:ILE:HA	15:U:41:SER:HB3	1.90	0.54
16:V:359:PRO:HB3	16:V:382:PHE:HB3	1.89	0.54
17:W:363:ILE:HG13	17:W:396:LEU:HD13	1.89	0.54
11:q:47:VAL:O	11:q:101:ASN:N	2.38	0.54
32:f:76:GLU:OE1	32:f:79:ARG:NH2	2.41	0.54
32:f:688:ARG:HA	32:f:745:LEU:CD2	2.38	0.54
14:T:136:SER:HB2	14:T:150:LEU:HD13	1.90	0.54
15:U:493:VAL:HG11	15:U:519:VAL:HG11	1.89	0.54
17:W:353:ASP:OD1	17:W:357:ARG:NH2	2.41	0.54
17:W:425:LEU:HA	17:W:428:TRP:HB2	1.90	0.54
18:X:252:LYS:HA	18:X:287:LEU:HD11	1.89	0.54
21:a:45:VAL:HG21	21:a:75:SER:HB2	1.90	0.54
21:a:90:PRO:HA	21:a:93:ALA:HB3	1.89	0.54
21:a:107:SER:HB2	21:a:110:ALA:HB2	1.90	0.54
21:a:152:HIS:HA	21:a:155:PHE:HB3	1.90	0.54
24:d:102:ASN:O	24:d:106:LEU:HB2	2.08	0.54
2:h:50:LYS:NZ	2:h:62:VAL:O	2.41	0.54
28:C:28:ILE:HG23	28:C:31:LEU:HD12	1.89	0.54
29:D:268:ASP:OD2	30:E:255:ARG:NH2	2.40	0.54
31:F:222:GLY:HA3	31:F:348:LEU:HA	1.89	0.54
32:f:211:ILE:O	32:f:215:ASP:CB	2.56	0.54
1:G:70:PHE:HD2	1:G:91:VAL:HG21	1.72	0.53
10:P:107:PRO:HG2	10:P:124:LEU:HB2	1.90	0.53
18:X:292:GLN:OE1	18:X:296:ASN:ND2	2.41	0.53
7:m:40:ARG:HA	7:m:45:VAL:HA	1.90	0.53
7:m:235:ALA:O	7:m:239:ALA:N	2.34	0.53
28:C:196:LYS:N	34:C:501:AGS:O1A	2.41	0.53
29:D:163:MET:HB2	29:D:166:ASP:HB2	1.89	0.53
29:D:181:VAL:HG13	29:D:261:ILE:HD13	1.90	0.53
30:E:321:THR:OG1	30:E:360:ASP:O	2.26	0.53
16:V:258:TYR:O	16:V:262:SER:N	2.30	0.53
17:W:144:ARG:HG3	17:W:147:LYS:HE2	1.89	0.53
17:W:182:ARG:HG2	17:W:186:ILE:HD12	1.89	0.53
24:d:62:SER:HA	24:d:65:ARG:HE	1.72	0.53
4:j:11:SER:OG	4:j:15:HIS:N	2.38	0.53

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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	0.53
32:f:262:PHE:HB3	32:f:281:ILE:HD11	1.91	0.53
32:f:273:ASN:ND2	32:f:310:ASP:OD2	2.41	0.53
17:W:95:SER:HB3	17:W:98:LYS:HE2	1.89	0.53
17:W:136:ILE:HA	17:W:141:GLU:HG3	1.88	0.53
17:W:200:ILE:HD12	17:W:203:GLN:HB2	1.91	0.53
18:X:348:GLU:HG3	18:X:350:ILE:HG22	1.90	0.53
18:X:409:LYS:HD3	23:c:268:GLU:HA	1.90	0.53
3:i:62:SER:OG	3:i:65:ILE:O	2.26	0.53
3:i:140:ASP:OD1	3:i:144:GLY:N	2.36	0.53
26:A:339:ARG:NH2	31:F:405:MET:SD	2.81	0.53
28:C:228:ALA:HB1	28:C:232:ARG:HG2	1.90	0.53
29:D:355:SER:HB3	29:D:393:ILE:HB	1.90	0.53
32:f:477:MET:O	32:f:481:SER:CB	2.56	0.53
16:V:99:ARG:H	16:V:99:ARG:HD3	1.72	0.53
16:V:159:LEU:HD13	16:V:178:SER:HB2	1.90	0.53
21:a:103:LYS:HG3	21:a:104:VAL:HG23	1.91	0.53
23:c:57:MET:HE2	23:c:110:GLY:HA3	1.91	0.53
3:i:154:GLY:O	4:j:81:ARG:NH1	2.42	0.53
26:A:223:THR:HB	34:A:501:AGS:H5'1	1.90	0.53
26:A:237:PHE:HA	26:A:271:LEU:HB2	1.90	0.53
28:C:99:VAL:HA	28:C:123:LEU:HB2	1.90	0.53
31:F:124:ILE:HB	31:F:132:TYR:HB2	1.90	0.53
15:U:377:HIS:ND1	15:U:382:SER:OG	2.41	0.53
15:U:599:ILE:HG23	29:D:56:VAL:HG11	1.90	0.53
16:V:484:LEU:HA	16:V:487:HIS:HD1	1.74	0.53
20:Z:72:HIS:HA	20:Z:75:LEU:HB3	1.90	0.53
22:b:16:MET:HB2	22:b:80:PRO:HB2	1.90	0.53
31:F:83:ASN:OD1	31:F:88:TYR:OH	2.26	0.53
32:f:8:LYS:O	32:f:12:GLN:HB2	2.08	0.53
32:f:80:ARG:O	32:f:84:SER:CB	2.57	0.53
32:f:610:GLN:CB	32:f:613:LEU:HD21	2.35	0.53
15:U:19:LEU:HD13	24:d:31:LEU:HD12	1.91	0.53
15:U:173:VAL:N	15:U:174:PRO:HD3	2.24	0.53
15:U:526:ALA:O	15:U:530:GLU:N	2.36	0.53
15:U:744:VAL:HB	15:U:783:TYR:HB3	1.90	0.53
16:V:33:GLN:HB3	16:V:112:VAL:HG13	1.91	0.53
20:Z:201:LEU:HD13	21:a:357:CYS:HA	1.90	0.53
29:D:237:GLN:HE22	30:E:209:GLY:H	1.56	0.53
30:E:355:ILE:HG12	31:F:211:LYS:HG2	1.90	0.53
9:O:13:VAL:HG22	9:O:177:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:293:ARG:NH2	25:e:52:PHE:O	2.42	0.53
23:c:28:ALA:HB2	23:c:175:ARG:HD2	1.90	0.53
28:C:277:LEU:HD22	28:C:310:ARG:HD3	1.90	0.53
30:E:43:SER:OG	31:F:72:LYS:NZ	2.38	0.53
32:f:313:GLU:O	32:f:317:LEU:CB	2.55	0.53
32:f:376:PHE:CD1	32:f:416:MET:CE	2.83	0.53
8:N:21:THR:HG22	8:N:26:ILE:HG13	1.91	0.53
15:U:520:MET:HE3	15:U:523:SER:HB2	1.90	0.53
21:a:213:PHE:CG	21:a:275:LEU:HD21	2.43	0.53
32:f:366:ASP:O	32:f:367:SER:CB	2.57	0.53
32:f:537:THR:OG1	32:f:538:ILE:N	2.42	0.53
7:M:99:ARG:NH2	7:M:105:ASN:OD1	2.41	0.53
14:T:1:THR:N	14:T:105:PRO:O	2.38	0.53
18:X:82:LYS:HB3	18:X:122:ARG:HH12	1.73	0.53
19:Y:18:ARG:HB2	19:Y:214:MET:HE1	1.91	0.53
20:Z:17:LEU:HD22	23:c:36:LEU:HB3	1.91	0.53
21:a:363:MET:HG2	21:a:366:LEU:HD12	1.90	0.53
15:U:355:ASN:O	15:U:718:ASN:ND2	2.41	0.53
16:V:219:GLU:OE2	16:V:256:ARG:NH2	2.41	0.53
16:V:228:ARG:O	16:V:232:HIS:ND1	2.32	0.53
16:V:483:CYS:O	16:V:487:HIS:ND1	2.42	0.53
19:Y:138:LEU:HD23	19:Y:176:ARG:HD3	1.91	0.53
19:Y:315:THR:HG23	19:Y:318:TYR:H	1.74	0.53
11:q:140:LEU:O	11:q:144:ASP:HB2	2.08	0.53
32:f:314:TYR:CE1	32:f:490:ALA:HB3	2.43	0.53
32:f:358:PHE:HZ	32:f:381:VAL:HG21	1.66	0.53
32:f:378:ASN:HB3	32:f:391:LEU:CD1	2.39	0.53
32:f:610:GLN:CB	32:f:613:LEU:CD2	2.86	0.53
32:f:780:PRO:CB	32:f:800:LEU:CA	2.79	0.53
17:W:436:MET:HA	17:W:439:VAL:HG22	1.91	0.52
20:Z:68:TRP:HH2	20:Z:111:LEU:HD13	1.73	0.52
27:B:244:SER:HB3	32:f:669:GLU:CD	2.34	0.52
32:f:600:TYR:HB3	32:f:608:LYS:HE2	1.91	0.52
32:f:610:GLN:CA	32:f:613:LEU:CD2	2.87	0.52
32:f:714:SER:C	32:f:718:ASP:HB2	2.33	0.52
4:J:74:ALA:HB2	4:J:161:ILE:HD13	1.90	0.52
13:S:148:LEU:HD23	13:S:178:VAL:HG12	1.91	0.52
15:U:510:GLU:O	15:U:514:LEU:HB2	2.09	0.52
19:Y:344:HIS:CE1	19:Y:346:LYS:HE2	2.44	0.52
20:Z:16:LEU:HD11	23:c:216:MET:HE2	1.92	0.52
20:Z:245:PHE:HB3	20:Z:248:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:41:LYS:NZ	6:l:180:MET:O	2.37	0.52
30:E:313:LEU:O	30:E:317:ALA:N	2.39	0.52
20:Z:134:PRO:HB3	23:c:220:LEU:HD21	1.91	0.52
6:l:45:VAL:HG11	6:l:188:VAL:HG22	1.91	0.52
7:m:152:ASP:OD1	7:m:156:VAL:N	2.40	0.52
8:n:127:ILE:HD13	8:n:136:TYR:HB2	1.90	0.52
28:C:146:SER:HB3	28:C:205:HIS:HD2	1.74	0.52
17:W:159:VAL:O	17:W:163:ALA:N	2.41	0.52
20:Z:39:LEU:H	20:Z:94:TRP:HA	1.74	0.52
20:Z:190:ARG:NH2	21:a:371:ALA:O	2.40	0.52
26:A:103:ASN:ND2	31:F:166:THR:O	2.42	0.52
26:A:364:VAL:HA	26:A:404:ALA:H	1.74	0.52
4:J:40:ILE:HA	4:J:212:ARG:HA	1.92	0.52
14:T:96:MET:HE1	14:T:106:LEU:HB2	1.92	0.52
15:U:596:ASN:HA	15:U:599:ILE:HG22	1.91	0.52
17:W:414:ASN:N	17:W:414:ASN:OD1	2.41	0.52
22:b:157:VAL:HG21	22:b:170:LEU:HB2	1.91	0.52
1:g:161:CYS:SG	1:g:162:GLY:N	2.83	0.52
32:f:515:ALA:HB1	32:f:558:LEU:HD21	1.91	0.52
2:H:66:GLU:OE2	2:H:91:ARG:NH2	2.43	0.52
5:K:12:VAL:HB	5:K:123:PHE:HE2	1.75	0.52
6:L:26:MET:HE1	6:L:148:CYS:HB2	1.92	0.52
6:L:146:GLN:HE22	6:L:159:MET:HE2	1.75	0.52
15:U:12:LEU:HA	15:U:20:LYS:HE3	1.91	0.52
15:U:182:LYS:CE	15:U:214:ILE:CD1	2.84	0.52
15:U:708:GLN:O	15:U:712:LEU:HB2	2.10	0.52
17:W:408:ARG:HH22	17:W:409:LEU:HD23	1.74	0.52
18:X:77:LEU:HD12	18:X:88:LEU:HD22	1.92	0.52
19:Y:101:ARG:NH2	19:Y:130:LYS:O	2.43	0.52
27:B:124:SER:HA	27:B:130:GLU:HG2	1.91	0.52
27:B:183:THR:HG23	27:B:242:GLN:HB2	1.90	0.52
29:D:153:MET:HA	29:D:228:ILE:HG12	1.91	0.52
31:F:68:ALA:O	31:F:72:LYS:HB2	2.09	0.52
31:F:172:VAL:HG22	31:F:267:LEU:HD13	1.92	0.52
1:G:41:ALA:HB3	1:G:166:THR:HB	1.92	0.52
2:H:148:GLN:OE1	2:H:158:TRP:NE1	2.43	0.52
9:O:163:ILE:HA	9:O:168:GLY:HA3	1.91	0.52
15:U:719:ASP:O	15:U:727:LYS:NZ	2.42	0.52
16:V:404:LYS:HA	16:V:407:VAL:HG12	1.92	0.52
18:X:348:GLU:OE2	18:X:380:GLN:NE2	2.42	0.52
6:l:109:VAL:HG21	6:l:145:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:306:GLU:HB3	32:f:339:ILE:HD12	1.91	0.52
32:f:468:ASP:OD2	32:f:475:ASN:N	2.42	0.52
32:f:612:LEU:O	32:f:616:CYS:CB	2.56	0.52
2:H:59:GLU:HG2	2:H:206:ASP:HB3	1.92	0.52
15:U:541:HIS:NE2	23:c:63:ASP:OD2	2.42	0.52
15:U:559:ARG:HB3	15:U:562:GLU:HB2	1.91	0.52
10:p:58:THR:O	11:q:85:ARG:NH2	2.43	0.52
32:f:610:GLN:HB2	32:f:613:LEU:CD2	2.37	0.52
17:W:138:VAL:HG12	17:W:139:GLU:H	1.74	0.52
22:b:131:LEU:HA	22:b:134:GLU:HB2	1.92	0.52
5:k:221:GLN:HB2	5:k:224:GLN:HB3	1.91	0.52
13:s:125:ASP:OD1	13:s:129:SER:N	2.39	0.52
26:A:396:ALA:HA	26:A:401:ARG:HH11	1.75	0.52
28:C:71:SER:HB3	29:D:112:TYR:HB3	1.91	0.52
29:D:202:VAL:HA	29:D:329:ARG:HB2	1.92	0.52
32:f:127:SER:O	32:f:131:MET:HB3	2.10	0.52
32:f:463:LEU:HD22	32:f:466:LEU:CD1	2.40	0.52
32:f:502:LEU:HG	32:f:540:GLN:HE22	1.75	0.52
3:I:90:LEU:HD12	3:I:114:LEU:HD22	1.91	0.52
10:P:62:THR:OG1	11:Q:85:ARG:NH2	2.40	0.52
14:T:145:LEU:HB3	14:T:179:ARG:HH21	1.75	0.52
15:U:69:TYR:O	16:V:236:ARG:NH2	2.31	0.52
17:W:39:ARG:H	17:W:44:ILE:HD12	1.76	0.52
19:Y:283:LYS:NZ	25:e:61:GLU:OE2	2.42	0.52
24:d:244:LYS:HD3	24:d:247:ILE:HD12	1.91	0.52
25:e:60:LEU:HA	25:e:63:HIS:HB2	1.92	0.52
5:k:228:MET:N	5:k:228:MET:SD	2.83	0.52
27:B:203:LEU:HD12	27:B:207:HIS:HB3	1.92	0.52
28:C:71:SER:OG	28:C:116:LEU:N	2.43	0.52
15:U:376:MET:HA	15:U:740:GLY:H	1.74	0.51
16:V:196:SER:OG	16:V:197:THR:N	2.39	0.51
16:V:224:LEU:HD13	16:V:227:VAL:HB	1.91	0.51
17:W:187:LEU:HD22	17:W:229:LEU:HD13	1.92	0.51
18:X:409:LYS:HZ2	23:c:267:PRO:HG2	1.74	0.51
9:o:106:THR:OG1	9:o:109:HIS:NE2	2.35	0.51
14:t:136:SER:HB2	14:t:150:LEU:HD13	1.92	0.51
32:f:336:GLU:CG	32:f:337:LEU:HD22	2.36	0.51
7:M:37:ILE:HD11	7:M:193:VAL:HG13	1.91	0.51
11:Q:44:LEU:HD11	11:Q:102:LEU:HD22	1.92	0.51
15:U:98:GLU:O	15:U:102:ALA:HB2	2.10	0.51
18:X:367:GLN:HA	18:X:370:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:o:46:ALA:HB3	9:o:97:ALA:HB3	1.90	0.51
12:r:12:VAL:HB	12:r:179:VAL:HB	1.92	0.51
30:E:99:ALA:N	30:E:109:ARG:O	2.40	0.51
32:f:337:LEU:N	32:f:337:LEU:CD2	2.73	0.51
7:M:40:ARG:HE	7:M:161:TRP:CD1	2.27	0.51
12:R:196:HIS:O	12:R:200:SER:HB3	2.11	0.51
15:U:236:LEU:HB3	15:U:245:ALA:HB2	1.92	0.51
19:Y:259:TYR:HB2	19:Y:274:SER:HB2	1.92	0.51
20:Z:220:LEU:O	20:Z:222:ILE:N	2.44	0.51
21:a:196:ARG:O	21:a:200:LEU:HB2	2.09	0.51
23:c:36:LEU:HD11	23:c:71:ASP:HA	1.91	0.51
13:s:123:SER:HB3	13:s:136:LYS:HG3	1.93	0.51
31:F:93:VAL:HG11	31:F:145:LEU:HD22	1.90	0.51
31:F:251:LEU:HB3	31:F:285:ILE:HG12	1.92	0.51
31:F:381:TYR:HA	31:F:384:LEU:HD12	1.91	0.51
32:f:337:LEU:HD22	32:f:337:LEU:H	1.75	0.51
32:f:800:LEU:N	32:f:800:LEU:CD1	2.73	0.51
4:J:11:SER:OG	4:J:15:HIS:N	2.37	0.51
16:V:47:SER:O	16:V:51:ALA:HB2	2.10	0.51
16:V:436:PHE:HE2	24:d:145:GLU:HG2	1.75	0.51
17:W:451:MET:HE1	20:Z:156:GLU:HA	1.93	0.51
21:a:101:ARG:NH1	21:a:114:CYS:SG	2.84	0.51
27:B:111:THR:O	27:B:124:SER:N	2.44	0.51
28:C:75:GLU:HB3	28:C:88:LYS:HB3	1.92	0.51
30:E:87:LEU:HD22	30:E:92:LEU:HD11	1.93	0.51
32:f:440:ILE:O	32:f:444:ALA:HB2	2.10	0.51
3:I:105:ILE:HG12	3:I:110:LEU:HB2	1.91	0.51
12:R:97:MET:HB3	12:R:116:SER:HB3	1.93	0.51
17:W:244:CYS:HA	17:W:273:TYR:HE2	1.75	0.51
4:j:38:ARG:NH1	4:j:182:GLU:O	2.34	0.51
8:n:127:ILE:HB	8:n:132:SER:HB2	1.91	0.51
32:f:24:THR:HG22	32:f:71:TYR:HB2	1.91	0.51
32:f:376:PHE:CZ	32:f:798:THR:CG2	2.91	0.51
32:f:380:PHE:CG	32:f:751:TYR:CE2	2.99	0.51
11:q:135:GLY:O	11:q:139:THR:OG1	2.22	0.51
26:A:398:ARG:NH2	27:B:196:GLU:OE2	2.44	0.51
28:C:214:VAL:HB	28:C:248:MET:HG3	1.93	0.51
29:D:214:MET:HB2	34:D:501:AGS:H3'	1.91	0.51
32:f:635:LYS:NZ	32:f:641:GLU:CD	2.66	0.51
32:f:742:ALA:CA	32:f:745:LEU:CD2	2.61	0.51
12:R:164:THR:HG22	12:R:170:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:449:GLU:O	17:W:453:HIS:ND1	2.40	0.51
21:a:292:THR:OG1	21:a:293:PHE:N	2.43	0.51
6:l:44:ALA:HB1	6:l:144:ILE:HD11	1.92	0.51
10:p:29:GLY:HA3	10:p:34:MET:HA	1.93	0.51
26:A:329:PRO:HA	26:A:332:MET:HB2	1.91	0.51
30:E:138:LEU:HB3	30:E:142:ILE:HG13	1.93	0.51
31:F:421:MET:HA	31:F:424:ILE:HD12	1.92	0.51
32:f:455:VAL:HG12	32:f:457:ASN:H	1.76	0.51
4:J:114:LEU:O	4:J:118:TYR:HB2	2.11	0.51
17:W:76:GLU:O	17:W:80:TRP:HB2	2.11	0.51
18:X:178:HIS:HE1	18:X:220:ALA:HB2	1.74	0.51
23:c:94:LYS:HG2	23:c:98:MET:HE3	1.93	0.51
28:C:47:ALA:HA	29:D:61:ILE:HG21	1.92	0.51
31:F:90:VAL:HG12	31:F:164:LEU:HD21	1.91	0.51
32:f:691:PRO:HG2	32:f:745:LEU:CD1	2.41	0.51
15:U:80:TYR:O	15:U:84:ALA:CB	2.58	0.51
20:Z:113:LYS:NZ	20:Z:117:PRO:O	2.41	0.51
7:m:170:GLN:HA	7:m:173:LYS:HE2	1.93	0.51
30:E:56:ILE:O	30:E:100:LEU:N	2.37	0.51
30:E:147:GLU:HG3	30:E:151:LEU:HD12	1.92	0.51
32:f:268:LEU:O	32:f:272:LEU:HB2	2.10	0.51
32:f:343:LYS:NZ	32:f:804:LEU:HD23	2.26	0.51
32:f:389:LYS:HD2	32:f:418:LEU:HD21	1.92	0.51
32:f:623:LYS:O	32:f:627:GLU:HB2	2.11	0.51
3:I:178:ASP:OD2	3:I:195:LYS:NZ	2.38	0.51
17:W:405:LYS:HA	18:X:342:PHE:HB2	1.93	0.51
3:i:3:ARG:HH11	4:j:5:ARG:HH12	1.59	0.51
26:A:260:LEU:HA	26:A:263:MET:HE2	1.91	0.51
27:B:151:LEU:HB2	27:B:160:ILE:HB	1.92	0.51
32:f:336:GLU:HG3	32:f:337:LEU:H	1.76	0.51
32:f:347:ASP:O	32:f:351:THR:OG1	2.25	0.51
32:f:485:LEU:HD12	32:f:488:ALA:HB3	1.92	0.51
3:I:47:ALA:HB3	3:I:212:GLU:HB3	1.94	0.50
3:I:171:ALA:HB2	3:I:200:THR:HG21	1.91	0.50
5:K:236:GLU:HA	5:K:239:LYS:HE3	1.93	0.50
30:E:210:GLU:HG3	30:E:213:ARG:HE	1.75	0.50
30:E:257:LEU:HA	30:E:260:LEU:HD12	1.93	0.50
31:F:224:LEU:O	31:F:352:ILE:N	2.41	0.50
32:f:343:LYS:HZ2	32:f:804:LEU:HD23	1.76	0.50
32:f:691:PRO:HA	32:f:694:LEU:HB3	1.93	0.50
1:G:17:SER:OG	1:G:21:ARG:O	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:26:LEU:HD11	19:Y:35:ALA:HB3	1.93	0.50
19:Y:92:GLU:HB3	19:Y:100:ILE:HD11	1.93	0.50
20:Z:199:LYS:HD3	20:Z:202:ASN:HD21	1.76	0.50
1:G:161:CYS:SG	1:G:162:GLY:N	2.83	0.50
10:P:2:SER:OG	10:P:3:ILE:N	2.44	0.50
16:V:197:THR:O	16:V:199:ASN:N	2.44	0.50
29:D:306:LYS:N	29:D:306:LYS:HD2	2.26	0.50
30:E:71:VAL:HG11	30:E:100:LEU:HD21	1.93	0.50
31:F:313:LEU:O	31:F:317:LEU:HB2	2.11	0.50
32:f:556:ARG:NH1	32:f:786:GLN:OE1	2.44	0.50
32:f:745:LEU:HD12	32:f:745:LEU:C	2.36	0.50
16:V:179:LYS:HZ1	16:V:217:VAL:HG21	1.76	0.50
18:X:236:PHE:HB2	18:X:250:SER:HB3	1.92	0.50
7:m:40:ARG:HE	7:m:161:TRP:CD1	2.29	0.50
28:C:267:SER:N	28:C:273:MET:SD	2.84	0.50
32:f:226:TYR:O	32:f:230:CYS:HB2	2.11	0.50
32:f:523:GLY:O	32:f:527:VAL:N	2.43	0.50
32:f:536:SER:HA	32:f:539:LEU:HB3	1.93	0.50
32:f:647:GLY:HA2	32:f:655:LEU:HG	1.92	0.50
10:P:189:ILE:HG23	10:P:196:THR:HB	1.94	0.50
12:R:125:THR:OG1	11:q:170:ARG:NH2	2.45	0.50
15:U:682:TYR:OH	23:c:183:HIS:NE2	2.37	0.50
24:d:80:CYS:HA	24:d:83:PHE:HB3	1.94	0.50
26:A:359:ALA:HA	26:A:362:MET:HG2	1.93	0.50
29:D:391:ARG:HH22	29:D:395:LEU:H	1.60	0.50
32:f:343:LYS:O	32:f:347:ASP:N	2.40	0.50
32:f:392:THR:HG22	32:f:417:ILE:HD13	1.92	0.50
32:f:463:LEU:HD22	32:f:466:LEU:HD11	1.93	0.50
5:K:228:MET:N	5:K:228:MET:SD	2.84	0.50
15:U:205:TYR:HB3	15:U:215:ASN:HD22	1.76	0.50
15:U:481:LEU:O	15:U:485:ALA:CB	2.60	0.50
17:W:184:GLU:HG3	17:W:223:LYS:HE3	1.92	0.50
23:c:144:VAL:O	23:c:158:ASP:N	2.40	0.50
29:D:352:MET:HE1	29:D:379:CYS:HB3	1.94	0.50
30:E:62:LYS:HA	30:E:94:PRO:HB3	1.94	0.50
30:E:228:CYS:HB3	30:E:273:VAL:HG22	1.92	0.50
15:U:79:ASN:HA	15:U:82:LEU:HD12	1.93	0.50
16:V:171:VAL:HA	16:V:174:PHE:HB2	1.94	0.50
16:V:235:LEU:O	16:V:239:THR:N	2.44	0.50
21:a:146:PRO:O	21:a:149:THR:OG1	2.30	0.50
5:k:206:MET:HE1	5:k:210:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:168:ALA:HB1	7:m:171:ALA:HB3	1.93	0.50
31:F:240:CYS:O	31:F:244:THR:OG1	2.23	0.50
32:f:392:THR:CG2	32:f:417:ILE:HD13	2.42	0.50
32:f:479:LEU:HA	32:f:517:VAL:HG21	1.93	0.50
32:f:790:GLN:HG3	32:f:792:ALA:H	1.76	0.50
10:P:9:GLY:N	10:P:181:SER:OG	2.38	0.50
15:U:214:ILE:HA	15:U:217:CYS:HB3	1.94	0.50
15:U:378:CYS:HA	15:U:411:ILE:HA	1.92	0.50
15:U:609:ASP:O	15:U:615:ARG:NH1	2.43	0.50
21:a:367:VAL:O	21:a:371:ALA:HB3	2.12	0.50
3:i:136:TYR:HB2	3:i:148:TYR:HB2	1.93	0.50
28:C:50:ASN:HD22	29:D:61:ILE:HG23	1.77	0.50
29:D:392:TYR:HD2	29:D:393:ILE:HD12	1.76	0.50
32:f:657:ILE:HA	32:f:660:ILE:HD12	1.94	0.50
15:U:163:PHE:O	15:U:166:THR:OG1	2.29	0.50
16:V:490:SER:HB2	20:Z:278:ASN:HD22	1.77	0.50
3:i:162:THR:OG1	3:i:163:CYS:N	2.44	0.50
6:l:39:LYS:HA	6:l:44:ALA:HA	1.94	0.50
27:B:137:SER:OG	27:B:139:VAL:O	2.29	0.50
29:D:100:THR:OG1	29:D:114:ARG:NH1	2.45	0.50
29:D:249:ASP:O	29:D:253:LEU:CB	2.60	0.50
29:D:252:ARG:O	29:D:256:GLU:CB	2.54	0.50
32:f:234:THR:HG23	32:f:637:LYS:HE2	1.94	0.50
7:M:144:ASP:O	7:M:147:GLN:NE2	2.41	0.49
9:O:46:ALA:HB3	9:O:97:ALA:HB3	1.93	0.49
11:Q:3:TYR:CZ	11:Q:131:ALA:HA	2.47	0.49
16:V:386:PHE:O	16:V:390:GLY:N	2.41	0.49
16:V:406:GLY:HA3	16:V:426:LEU:HD11	1.94	0.49
20:Z:193:ASN:HA	20:Z:196:HIS:CE1	2.46	0.49
21:a:252:LYS:HA	21:a:255:TRP:HD1	1.77	0.49
24:d:114:GLU:HA	24:d:117:THR:HG22	1.93	0.49
4:j:7:ILE:HG13	4:j:123:GLY:HA2	1.92	0.49
6:l:16:GLN:OE1	6:l:18:ARG:NH2	2.31	0.49
32:f:140:LEU:O	32:f:144:LEU:CB	2.60	0.49
32:f:178:LYS:NZ	32:f:215:ASP:O	2.42	0.49
32:f:336:GLU:HG3	32:f:337:LEU:CD2	2.38	0.49
32:f:692:LEU:HG	32:f:752:HIS:HE1	1.77	0.49
7:M:51:LYS:O	7:M:210:GLU:N	2.39	0.49
10:P:205:ASP:HB3	12:r:192:VAL:HG11	1.93	0.49
16:V:440:LYS:HG3	24:d:146:GLY:HA3	1.93	0.49
21:a:296:ILE:O	21:a:300:ALA:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:p:2:SER:OG	10:p:3:ILE:N	2.45	0.49
31:F:134:LEU:HD21	31:F:160:ILE:HG13	1.94	0.49
32:f:632:LYS:HD2	32:f:661:ALA:HA	1.92	0.49
15:U:94:SER:HB3	15:U:97:VAL:HG12	1.93	0.49
17:W:356:ASN:O	17:W:360:GLU:HB2	2.12	0.49
21:a:122:LYS:HG2	21:a:126:GLY:HA3	1.94	0.49
21:a:212:ASN:HB2	21:a:215:GLU:HB3	1.95	0.49
32:f:94:LYS:HA	32:f:97:LYS:HG2	1.94	0.49
4:J:159:ASN:OD1	4:J:160:ALA:N	2.46	0.49
6:L:109:VAL:HG21	6:L:145:PHE:HD2	1.76	0.49
12:R:22:ALA:N	12:R:25:TYR:O	2.40	0.49
15:U:10:SER:HB2	24:d:73:ARG:HG3	1.93	0.49
19:Y:304:TYR:HA	19:Y:307:LEU:HB3	1.94	0.49
21:a:158:LEU:O	21:a:162:TYR:CB	2.59	0.49
30:E:251:ARG:O	30:E:255:ARG:NE	2.40	0.49
9:O:113:ILE:HG12	9:O:119:THR:HG22	1.95	0.49
16:V:469:THR:O	16:V:473:GLN:NE2	2.45	0.49
17:W:371:THR:O	17:W:372:ARG:NE	2.40	0.49
14:t:180:ASP:HB3	14:t:183:SER:HB3	1.94	0.49
30:E:174:GLY:O	30:E:280:ASN:ND2	2.42	0.49
32:f:691:PRO:HB3	32:f:749:ALA:CB	2.38	0.49
2:H:107:THR:HA	2:H:110:LEU:HD13	1.94	0.49
7:M:152:ASP:OD1	7:M:156:VAL:N	2.44	0.49
15:U:353:LEU:O	15:U:357:LYS:HB2	2.13	0.49
16:V:188:SER:O	16:V:193:GLN:NE2	2.46	0.49
16:V:412:LEU:O	19:Y:346:LYS:NZ	2.34	0.49
19:Y:190:ALA:HA	19:Y:287:LEU:HB2	1.93	0.49
9:o:216:ILE:HG23	10:p:194:LYS:HE3	1.94	0.49
26:A:212:VAL:HG22	26:A:339:ARG:HB2	1.93	0.49
27:B:139:VAL:HG21	27:B:162:VAL:HB	1.94	0.49
5:K:117:SER:O	6:L:82:ARG:NH2	2.46	0.49
7:M:136:MET:HE3	7:M:148:LEU:HD11	1.95	0.49
7:M:173:LYS:HA	7:M:176:ILE:HB	1.95	0.49
12:R:97:MET:O	12:R:116:SER:N	2.43	0.49
15:U:249:CYS:HB3	15:U:328:ILE:HG21	1.94	0.49
15:U:265:ILE:HA	15:U:268:LEU:HD13	1.94	0.49
19:Y:261:PHE:O	19:Y:265:GLU:HB2	2.12	0.49
6:l:50:LYS:HB3	6:l:59:HIS:HB3	1.94	0.49
12:r:35:ILE:N	12:r:43:GLY:O	2.45	0.49
28:C:164:VAL:HG13	28:C:165:ILE:HG13	1.95	0.49
32:f:714:SER:O	32:f:718:ASP:CB	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:144:ARG:NH2	8:N:151:GLU:OE1	2.46	0.49
12:R:4:LEU:HA	12:R:127:SER:HA	1.94	0.49
16:V:490:SER:O	20:Z:278:ASN:ND2	2.45	0.49
17:W:19:ASP:OD2	17:W:23:THR:N	2.37	0.49
20:Z:131:LEU:HG	20:Z:195:VAL:HG13	1.94	0.49
20:Z:208:ILE:HD13	21:a:354:GLU:HB2	1.94	0.49
26:A:161:VAL:HA	26:A:164:MET:HE3	1.95	0.49
26:A:415:LYS:HA	26:A:419:SER:HB2	1.93	0.49
27:B:222:VAL:HG22	27:B:349:ARG:HB2	1.94	0.49
31:F:124:ILE:O	31:F:132:TYR:N	2.45	0.49
32:f:333:LEU:HA	32:f:338:ASP:HB2	1.95	0.49
32:f:531:ASN:HA	32:f:569:LYS:HA	1.93	0.49
10:P:159:ASP:N	10:P:159:ASP:OD1	2.43	0.49
15:U:327:LYS:O	15:U:330:SER:OG	2.29	0.49
16:V:179:LYS:HD2	16:V:214:HIS:CD2	2.47	0.49
17:W:343:SER:HB2	17:W:347:GLY:HA3	1.95	0.49
1:g:120:ASP:OD1	2:h:84:ARG:NH1	2.46	0.49
12:r:105:ASP:N	12:r:108:GLY:O	2.45	0.49
29:D:169:GLY:O	29:D:340:GLN:NE2	2.46	0.49
29:D:237:GLN:N	29:D:242:GLU:OE1	2.37	0.49
30:E:98:VAL:HG21	30:E:107:ILE:HG12	1.95	0.49
30:E:157:GLU:HA	30:E:160:GLN:HB2	1.94	0.49
6:L:50:LYS:HE2	6:L:61:LYS:HA	1.95	0.49
10:P:26:ARG:HH21	10:P:38:ASP:HA	1.78	0.49
11:Q:170:ARG:NH2	12:r:125:THR:OG1	2.46	0.49
15:U:84:ALA:HB3	15:U:88:PHE:HB2	1.95	0.49
20:Z:41:GLY:N	20:Z:90:ARG:O	2.37	0.49
21:a:325:ASP:HB3	21:a:330:ARG:HB2	1.95	0.49
2:h:107:THR:HA	2:h:110:LEU:HD13	1.95	0.49
6:l:59:HIS:ND1	6:l:208:LYS:O	2.44	0.49
26:A:102:ILE:HD12	26:A:112:ILE:HG22	1.95	0.49
30:E:337:GLY:HA2	30:E:378:LYS:HD3	1.95	0.49
31:F:333:ASN:OD1	34:F:501:AGS:O2G	2.31	0.49
31:F:346:GLY:HA2	31:F:349:ASP:HB2	1.93	0.49
32:f:336:GLU:HB3	32:f:337:LEU:HD23	1.95	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:CB	2.60	0.49
15:U:185:MET:SD	15:U:194:ARG:NH1	2.79	0.48
15:U:234:GLU:O	15:U:238:LYS:HB2	2.13	0.48
15:U:616:ARG:HE	15:U:647:HIS:HA	1.78	0.48
16:V:200:ARG:HA	16:V:204:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:379:ARG:HD3	19:Y:383:LEU:HD13	1.95	0.48
5:k:182:GLN:NE2	6:l:55:GLU:OE1	2.46	0.48
14:t:153:VAL:O	14:t:157:GLN:N	2.44	0.48
29:D:238:LYS:HD3	29:D:274:ARG:HD3	1.95	0.48
30:E:207:TYR:HE2	31:F:304:ARG:HH22	1.59	0.48
31:F:338:LEU:HB3	31:F:342:LEU:HD12	1.95	0.48
32:f:445:LEU:HG	32:f:462:ALA:HB2	1.95	0.48
32:f:517:VAL:O	32:f:521:ALA:HB3	2.12	0.48
32:f:671:ALA:O	32:f:674:THR:OG1	2.26	0.48
7:M:37:ILE:HA	7:M:164:ALA:HA	1.95	0.48
12:R:105:ASP:N	12:R:108:GLY:O	2.43	0.48
12:R:196:HIS:O	12:R:200:SER:CB	2.61	0.48
17:W:308:LEU:HD12	17:W:320:LEU:HD11	1.94	0.48
21:a:33:LEU:HA	22:b:18:ASN:HB2	1.95	0.48
21:a:272:ILE:HA	21:a:275:LEU:HB3	1.95	0.48
4:j:4:ASP:HB3	5:k:126:GLU:HB3	1.95	0.48
29:D:151:ILE:HD12	29:D:155:THR:HB	1.95	0.48
29:D:159:LYS:HD2	29:D:221:HIS:HD2	1.77	0.48
32:f:389:LYS:HB3	32:f:392:THR:HG21	1.95	0.48
1:G:127:GLN:NE2	2:H:128:ARG:O	2.46	0.48
15:U:356:THR:HG21	15:U:731:ILE:HD13	1.94	0.48
16:V:247:GLN:O	16:V:251:LEU:HB2	2.13	0.48
18:X:164:ALA:HB2	18:X:200:ILE:HD11	1.95	0.48
18:X:337:ARG:HH11	18:X:354:ILE:HD12	1.78	0.48
19:Y:372:LYS:O	19:Y:376:LEU:HB3	2.12	0.48
2:h:118:MET:HE3	2:h:130:PHE:HB2	1.95	0.48
5:k:196:LYS:HA	5:k:199:LEU:HG	1.95	0.48
28:C:43:ARG:HH21	29:D:57:GLN:HB3	1.78	0.48
29:D:154:LEU:HD23	29:D:227:PHE:HD2	1.78	0.48
29:D:181:VAL:CG1	29:D:261:ILE:HD13	2.43	0.48
29:D:209:GLY:HA2	34:D:501:AGS:H5'2	1.95	0.48
32:f:376:PHE:CZ	32:f:798:THR:CB	2.91	0.48
1:G:123:GLN:NE2	2:H:82:ASP:OD1	2.46	0.48
14:T:115:TYR:HE2	14:T:194:GLU:HB3	1.78	0.48
15:U:479:LEU:O	15:U:483:LEU:HB2	2.14	0.48
21:a:116:THR:HG22	21:a:158:LEU:HD23	1.93	0.48
25:e:63:HIS:HA	25:e:66:LYS:HG3	1.94	0.48
7:m:192:GLU:HA	7:m:195:LYS:HE3	1.94	0.48
12:r:4:LEU:HA	12:r:127:SER:HA	1.95	0.48
26:A:217:PRO:O	26:A:220:THR:OG1	2.24	0.48
26:A:257:VAL:HG11	26:A:302:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:398:ASP:HA	29:D:401:LYS:HB2	1.95	0.48
31:F:225:MET:HG3	31:F:352:ILE:HB	1.95	0.48
31:F:246:ALA:HB1	31:F:280:PRO:HB2	1.95	0.48
32:f:387:GLN:N	32:f:387:GLN:NE2	2.60	0.48
32:f:392:THR:HA	32:f:414:LEU:CD2	2.44	0.48
32:f:456:ARG:HD3	32:f:489:TYR:CZ	2.49	0.48
1:G:49:VAL:HG22	1:G:219:VAL:HG23	1.94	0.48
13:S:125:ASP:OD1	13:S:129:SER:N	2.42	0.48
18:X:334:ASN:O	18:X:338:VAL:HB	2.12	0.48
19:Y:237:ARG:O	19:Y:241:ILE:HB	2.13	0.48
24:d:253:LEU:O	24:d:257:VAL:N	2.45	0.48
28:C:146:SER:HB2	28:C:206:HIS:CE1	2.48	0.48
32:f:559:PRO:HA	32:f:562:LEU:HB2	1.96	0.48
32:f:695:ALA:CB	32:f:752:HIS:HB3	2.44	0.48
4:J:154:HIS:CE1	5:K:59:MET:HG3	2.49	0.48
6:L:42:THR:O	6:L:137:TYR:OH	2.32	0.48
8:N:18:SER:OG	8:N:19:ARG:N	2.39	0.48
20:Z:12:HIS:CE1	20:Z:165:GLU:HB2	2.48	0.48
23:c:123:SER:N	23:c:126:ASP:OD2	2.46	0.48
2:h:9:SER:OG	2:h:123:GLN:O	2.25	0.48
7:m:228:PRO:HB2	7:m:231:ILE:HB	1.96	0.48
11:q:13:VAL:HB	11:q:183:ILE:HD12	1.94	0.48
28:C:182:GLN:HE21	28:C:287:LYS:HB2	1.79	0.48
3:I:245:ALA:HA	3:I:248:GLU:HG2	1.95	0.48
5:K:200:ILE:HA	5:K:203:LYS:HZ3	1.79	0.48
15:U:899:ARG:O	15:U:917:THR:OG1	2.24	0.48
16:V:309:MET:HE3	16:V:332:LEU:HG	1.95	0.48
19:Y:84:LEU:HD21	19:Y:107:LYS:HB2	1.95	0.48
19:Y:232:GLU:O	19:Y:236:LEU:N	2.43	0.48
1:g:34:GLN:NE2	7:m:17:ASP:O	2.47	0.48
7:m:230:ASP:OD1	7:m:230:ASP:N	2.46	0.48
10:p:58:THR:OG1	11:q:121:LEU:O	2.18	0.48
13:s:68:ILE:HD11	13:s:92:LEU:HD13	1.95	0.48
30:E:304:PRO:HD2	30:E:338:PHE:CD1	2.49	0.48
31:F:222:GLY:HA2	31:F:328:VAL:HB	1.96	0.48
32:f:479:LEU:HD23	32:f:513:GLU:CB	2.42	0.48
32:f:597:VAL:HG22	32:f:630:ASP:HB2	1.95	0.48
22:b:51:LEU:HD23	22:b:71:ILE:HG23	1.95	0.48
6:l:189:LYS:HZ3	6:l:193:ARG:HH22	1.61	0.48
12:r:59:LEU:HD22	12:r:83:LEU:HB2	1.96	0.48
12:r:153:TYR:HB3	12:r:157:ARG:HH22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:91:GLN:NE2	29:D:92:PHE:O	2.47	0.48
29:D:343:LEU:O	29:D:346:SER:OG	2.26	0.48
30:E:57:VAL:N	31:F:131:THR:O	2.43	0.48
32:f:331:LEU:O	32:f:335:ARG:NH1	2.47	0.48
32:f:376:PHE:CZ	32:f:416:MET:CE	2.95	0.48
16:V:354:LYS:HA	16:V:357:LEU:HG	1.95	0.48
17:W:47:LEU:HD23	17:W:50:LEU:HD12	1.96	0.48
17:W:142:ARG:HH21	17:W:178:GLU:HB2	1.79	0.48
2:h:6:TYR:HE2	2:h:126:GLY:HA3	1.79	0.48
28:C:161:ILE:HA	28:C:164:VAL:HG12	1.96	0.48
31:F:79:LYS:HD3	31:F:139:LEU:HD11	1.95	0.48
31:F:235:LEU:HD11	34:F:501:AGS:H2'	1.96	0.48
32:f:127:SER:O	32:f:131:MET:HB2	2.13	0.48
32:f:209:MET:SD	32:f:213:GLN:NE2	2.87	0.48
32:f:626:GLU:OE1	32:f:782:HIS:NE2	2.47	0.48
7:M:9:LEU:O	7:M:22:GLN:NE2	2.46	0.48
16:V:72:LEU:O	16:V:76:LYS:N	2.35	0.48
16:V:269:LYS:HA	16:V:272:SER:HB2	1.95	0.48
20:Z:67:VAL:HG12	22:b:95:LEU:HD23	1.96	0.48
1:g:116:LYS:HG2	1:g:160:TYR:CZ	2.49	0.48
6:l:26:MET:HE1	6:l:148:CYS:HB2	1.94	0.48
6:l:125:ARG:NH2	6:l:128:TYR:OH	2.47	0.48
9:o:18:THR:HB	9:o:31:CYS:H	1.77	0.48
13:s:35:ILE:HB	14:t:151:ARG:HH12	1.78	0.48
27:B:98:LYS:O	27:B:102:LEU:N	2.46	0.48
29:D:344:ILE:CG2	34:D:501:AGS:C2	2.92	0.48
31:F:196:GLN:O	31:F:200:GLU:HB2	2.14	0.48
32:f:30:GLY:O	32:f:34:ARG:HB2	2.14	0.48
32:f:675:PHE:O	32:f:679:LEU:CB	2.59	0.48
2:H:39:LYS:HE2	2:H:144:PRO:HG2	1.96	0.47
6:L:158:ALA:HB1	6:L:172:LEU:HD22	1.96	0.47
12:R:1:THR:N	12:R:169:TYR:O	2.47	0.47
15:U:705:LYS:HD3	15:U:708:GLN:HG3	1.96	0.47
17:W:397:VAL:HB	18:X:343:SER:HB2	1.95	0.47
18:X:337:ARG:HH12	18:X:355:LYS:HB3	1.77	0.47
19:Y:232:GLU:HG3	19:Y:234:PRO:HD2	1.96	0.47
20:Z:94:TRP:NE1	20:Z:112:MET:SD	2.85	0.47
20:Z:190:ARG:HA	20:Z:193:ASN:HD22	1.79	0.47
22:b:122:LYS:HA	22:b:125:VAL:HG12	1.95	0.47
34:D:501:AGS:O1B	34:D:501:AGS:O3G	2.30	0.47
30:E:63:GLN:HE21	30:E:66:GLU:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:453:SER:O	32:f:488:ALA:O	2.31	0.47
32:f:479:LEU:CD2	32:f:513:GLU:HB3	2.39	0.47
1:G:32:ILE:HA	1:G:82:GLY:HA2	1.96	0.47
5:K:55:THR:HG21	26:A:430:MET:HE2	1.96	0.47
7:M:30:VAL:HG11	7:M:134:SER:HB3	1.95	0.47
15:U:500:ASN:OD1	15:U:508:THR:OG1	2.24	0.47
16:V:258:TYR:O	16:V:261:TYR:N	2.46	0.47
16:V:419:LEU:HD11	16:V:435:GLU:HG3	1.96	0.47
18:X:74:ARG:HH22	18:X:116:TRP:HB2	1.79	0.47
24:d:170:LEU:HA	24:d:173:THR:HG22	1.96	0.47
2:h:66:GLU:OE2	2:h:91:ARG:NH2	2.45	0.47
4:j:131:ALA:N	4:j:147:THR:OG1	2.34	0.47
10:p:159:ASP:N	10:p:159:ASP:OD1	2.45	0.47
14:t:114:GLY:O	14:t:121:PHE:N	2.47	0.47
28:C:231:VAL:HA	28:C:234:LEU:HB3	1.96	0.47
32:f:166:VAL:O	32:f:170:TRP:HB2	2.14	0.47
32:f:252:ALA:O	32:f:256:PHE:HB2	2.14	0.47
32:f:372:LEU:C	32:f:372:LEU:CD2	2.86	0.47
32:f:483:PHE:HE2	32:f:799:VAL:HB	1.70	0.47
4:J:88:ARG:NH1	11:Q:69:MET:O	2.47	0.47
10:P:61:GLN:HE22	11:Q:124:LEU:HB2	1.80	0.47
15:U:34:PHE:HB3	15:U:37:GLU:HB2	1.96	0.47
21:a:92:VAL:O	21:a:95:THR:OG1	2.29	0.47
22:b:15:TYR:O	22:b:25:ARG:NH1	2.46	0.47
5:k:195:ILE:O	5:k:198:SER:OG	2.32	0.47
29:D:170:MET:HB3	29:D:173:GLN:HB2	1.96	0.47
32:f:424:GLY:HA2	32:f:427:THR:HG22	1.96	0.47
32:f:796:LEU:HG	32:f:799:VAL:CG2	2.42	0.47
6:L:52:ALA:HB2	6:L:59:HIS:CD2	2.49	0.47
14:T:15:LYS:HG2	14:T:20:VAL:HG22	1.96	0.47
16:V:338:LEU:HD22	16:V:397:ARG:HD2	1.96	0.47
18:X:251:LEU:HA	18:X:254:MET:HG2	1.96	0.47
20:Z:14:LEU:HG	23:c:39:LEU:HD13	1.96	0.47
8:n:96:ALA:HB1	8:n:98:ILE:HG12	1.96	0.47
12:r:97:MET:O	12:r:116:SER:N	2.39	0.47
31:F:93:VAL:O	31:F:148:GLY:N	2.41	0.47
32:f:538:ILE:HA	32:f:541:THR:HG22	1.97	0.47
4:J:158:ALA:HB1	4:J:172:LEU:HD13	1.96	0.47
14:T:180:ASP:HB3	14:T:183:SER:HB3	1.95	0.47
19:Y:101:ARG:HD3	19:Y:130:LYS:HE3	1.95	0.47
14:t:178:TYR:OH	14:t:208:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:315:GLU:HA	32:f:318:THR:HG22	1.95	0.47
32:f:336:GLU:CG	32:f:337:LEU:CD2	2.92	0.47
5:K:211:ASN:OD1	5:K:214:ASN:ND2	2.48	0.47
15:U:637:VAL:HA	15:U:640:LEU:HD12	1.95	0.47
17:W:165:ILE:HA	17:W:168:GLU:HB2	1.97	0.47
1:g:109:ILE:HD13	1:g:114:LEU:HD12	1.95	0.47
6:l:107:ARG:NH2	14:t:79:ASP:OD2	2.35	0.47
7:m:144:ASP:O	7:m:147:GLN:NE2	2.47	0.47
28:C:100:ASP:H	28:C:103:ILE:HD11	1.80	0.47
29:D:290:LEU:HD23	29:D:293:LEU:HD12	1.95	0.47
32:f:376:PHE:CZ	32:f:798:THR:HG22	2.50	0.47
5:K:85:ALA:HB2	5:K:139:VAL:HG21	1.97	0.47
5:K:196:LYS:HA	5:K:199:LEU:HG	1.97	0.47
9:O:106:THR:OG1	9:O:109:HIS:NE2	2.31	0.47
13:S:73:LYS:O	13:S:77:HIS:ND1	2.37	0.47
15:U:161:ASP:OD1	15:U:162:VAL:N	2.47	0.47
15:U:731:ILE:HD12	15:U:734:GLN:HB2	1.96	0.47
16:V:255:LEU:HD22	16:V:291:TYR:HB3	1.96	0.47
17:W:112:VAL:HG23	17:W:120:ILE:HG21	1.97	0.47
17:W:452:ILE:HD12	20:Z:214:LYS:HE2	1.97	0.47
19:Y:134:LEU:HB2	19:Y:168:ILE:HG23	1.95	0.47
20:Z:56:VAL:HG13	20:Z:58:PHE:HB2	1.96	0.47
4:j:159:ASN:OD1	4:j:160:ALA:N	2.48	0.47
10:p:62:THR:OG1	11:q:85:ARG:NH2	2.47	0.47
12:r:97:MET:HB3	12:r:116:SER:HB3	1.97	0.47
14:t:4:PRO:HG3	14:t:107:TRP:CE2	2.50	0.47
26:A:55:LEU:CB	32:f:239:TYR:HD1	2.27	0.47
28:C:71:SER:OG	28:C:72:TYR:N	2.47	0.47
29:D:263:PHE:HD1	29:D:308:ILE:HB	1.80	0.47
30:E:156:PRO:HG3	30:E:272:ARG:NH2	2.29	0.47
32:f:248:LEU:O	32:f:252:ALA:CB	2.62	0.47
32:f:253:LEU:O	32:f:257:ARG:CB	2.61	0.47
32:f:487:LEU:HD22	32:f:801:VAL:HG11	1.95	0.47
32:f:645:ASP:HB3	32:f:648:ALA:HB3	1.95	0.47
1:G:212:PRO:HB3	1:G:235:ILE:HG22	1.95	0.47
2:H:6:TYR:HE2	2:H:14:SER:HA	1.79	0.47
3:I:136:TYR:HB2	3:I:148:TYR:HB2	1.97	0.47
4:J:180:ALA:HA	4:J:181:ILE:HA	1.76	0.47
5:K:167:ALA:HB3	5:K:181:LEU:HD21	1.96	0.47
7:M:36:ALA:O	7:M:165:ILE:N	2.41	0.47
8:N:144:ARG:H	8:N:147:MET:HE3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:337:ALA:O	17:W:342:GLY:N	2.34	0.47
18:X:258:LYS:HE3	18:X:270:LEU:HD12	1.96	0.47
18:X:362:GLU:HG2	18:X:365:LEU:HD13	1.96	0.47
21:a:328:ASP:HB2	21:a:330:ARG:HG3	1.96	0.47
12:r:161:TYR:HH	12:r:196:HIS:HD1	1.60	0.47
26:A:101:ILE:HA	26:A:113:ILE:HG12	1.96	0.47
29:D:237:GLN:NE2	31:F:299:GLU:OE2	2.48	0.47
14:T:46:ASN:OD1	14:T:46:ASN:N	2.47	0.47
15:U:633:CYS:HA	15:U:636:VAL:HG22	1.97	0.47
19:Y:104:MET:O	19:Y:108:ALA:CB	2.63	0.47
19:Y:204:THR:OG1	19:Y:205:VAL:N	2.46	0.47
29:D:261:ILE:HG12	29:D:306:LYS:HD3	1.97	0.47
15:U:521:LEU:HD13	15:U:554:LEU:HD23	1.96	0.47
16:V:171:VAL:O	16:V:175:MET:N	2.35	0.47
17:W:143:ALA:HA	17:W:146:THR:HG22	1.96	0.47
29:D:270:ILE:HG23	29:D:288:ILE:HB	1.95	0.47
29:D:283:ARG:O	29:D:287:ARG:HB3	2.15	0.47
31:F:80:ILE:HA	31:F:83:ASN:HB2	1.97	0.47
7:M:168:ALA:HB1	7:M:171:ALA:HB3	1.96	0.46
7:M:170:GLN:HA	7:M:173:LYS:HE2	1.96	0.46
12:R:9:ARG:NH2	12:R:146:ASP:OD1	2.33	0.46
15:U:497:LEU:HD23	15:U:516:LEU:HB2	1.96	0.46
15:U:644:TYR:HB3	28:C:57:ARG:NH2	2.30	0.46
16:V:47:SER:O	16:V:51:ALA:CB	2.63	0.46
19:Y:22:LEU:HA	19:Y:25:LEU:HB3	1.97	0.46
19:Y:186:LEU:HD12	19:Y:201:PHE:HZ	1.80	0.46
20:Z:36:VAL:HG22	20:Z:96:HIS:HB2	1.97	0.46
9:o:11:GLY:HA2	9:o:108:PRO:HB3	1.96	0.46
27:B:179:ALA:HB1	27:B:241:ASN:HA	1.97	0.46
32:f:688:ARG:CA	32:f:745:LEU:HD22	2.44	0.46
6:L:72:ILE:HG22	6:L:134:ILE:HG12	1.96	0.46
11:Q:177:THR:HG22	11:Q:195:SER:HB3	1.97	0.46
14:t:115:TYR:HE2	14:t:194:GLU:HB3	1.80	0.46
27:B:334:ILE:HA	27:B:337:LEU:HD23	1.97	0.46
30:E:175:PRO:HG2	30:E:303:LEU:HA	1.97	0.46
31:F:206:MET:HB2	31:F:327:LYS:HE2	1.97	0.46
31:F:314:LEU:HD21	31:F:342:LEU:HD23	1.96	0.46
7:M:6:GLY:HA3	7:M:7:TYR:HB2	1.96	0.46
12:R:38:ASN:HD22	12:R:41:LEU:HD12	1.79	0.46
16:V:150:ARG:HA	16:V:153:LYS:HE3	1.97	0.46
16:V:252:ASN:ND2	16:V:284:GLU:OE2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:252:LYS:HE2	18:X:315:ASP:HB2	1.97	0.46
20:Z:173:GLU:HB2	23:c:152:LYS:HB2	1.97	0.46
23:c:99:LEU:HA	23:c:102:THR:HB	1.98	0.46
23:c:219:ASN:O	23:c:223:LYS:HB2	2.16	0.46
4:j:172:LEU:HA	4:j:175:ASN:HB3	1.98	0.46
9:o:112:SER:HB3	9:o:125:VAL:HG11	1.97	0.46
26:A:422:LYS:HZ1	26:A:427:PRO:HG3	1.80	0.46
27:B:243:THR:C	32:f:669:GLU:OE2	2.59	0.46
29:D:232:GLY:N	29:D:265:ASP:O	2.39	0.46
32:f:695:ALA:O	32:f:752:HIS:HB3	2.15	0.46
2:H:10:LEU:O	3:I:128:ARG:NH2	2.48	0.46
11:Q:52:ASP:OD1	12:R:88:TYR:OH	2.31	0.46
14:T:28:GLY:HA3	14:T:36:PHE:HB2	1.96	0.46
15:U:177:LEU:HD23	15:U:208:LEU:HG	1.97	0.46
17:W:439:VAL:HB	23:c:231:LEU:HD23	1.96	0.46
19:Y:138:LEU:HD22	19:Y:168:ILE:HG21	1.98	0.46
7:m:27:MET:HA	7:m:153:PRO:HG2	1.97	0.46
29:D:370:ILE:HG22	29:D:375:ILE:HG13	1.97	0.46
30:E:309:ARG:HE	30:E:338:PHE:HE1	1.61	0.46
32:f:281:ILE:O	32:f:285:CYS:HB3	2.16	0.46
32:f:475:ASN:O	32:f:478:ARG:HB3	2.15	0.46
9:O:50:ALA:HB2	10:P:129:CYS:HB2	1.98	0.46
15:U:666:LYS:HA	15:U:669:ILE:HD12	1.98	0.46
16:V:490:SER:HB3	20:Z:275:LEU:HD23	1.96	0.46
20:Z:60:GLU:HG2	20:Z:104:ASN:HD22	1.81	0.46
1:g:132:ARG:HA	1:g:133:PRO:HD3	1.78	0.46
13:s:28:ARG:O	13:s:42:LYS:NZ	2.49	0.46
27:B:120:HIS:HA	27:B:134:SER:HA	1.97	0.46
29:D:149:SER:H	29:D:152:MET:HA	1.80	0.46
32:f:392:THR:HB	32:f:414:LEU:HD22	1.98	0.46
1:G:114:LEU:HD22	1:G:140:LEU:HD21	1.97	0.46
5:K:33:LEU:HD13	26:A:432:TYR:CG	2.50	0.46
11:Q:4:LEU:HD12	11:Q:45:LEU:HB3	1.98	0.46
15:U:724:VAL:HA	15:U:727:LYS:HG2	1.98	0.46
16:V:436:PHE:HE1	24:d:148:TYR:H	1.62	0.46
19:Y:358:ARG:NH1	19:Y:362:LYS:HB3	2.31	0.46
21:a:169:HIS:CD2	21:a:207:GLY:HA3	2.50	0.46
5:k:99:HIS:CG	5:k:107:MET:HB2	2.50	0.46
6:l:146:GLN:HE21	6:l:154:PHE:HD2	1.63	0.46
31:F:407:ALA:HB1	31:F:412:ALA:HB3	1.98	0.46
32:f:359:GLY:O	32:f:363:SER:CB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:28:ASN:ND2	8:N:31:THR:OG1	2.48	0.46
11:Q:101:ASN:HB3	11:Q:132:HIS:CD2	2.51	0.46
15:U:24:LEU:HA	15:U:27:LEU:HD12	1.98	0.46
15:U:650:TYR:HE2	15:U:768:GLN:HE22	1.63	0.46
19:Y:48:ASN:HB3	19:Y:114:ILE:HG12	1.97	0.46
20:Z:179:ILE:HD11	23:c:222:LYS:HE3	1.98	0.46
23:c:114:SER:HA	23:c:145:VAL:HG12	1.98	0.46
5:k:100:TRP:O	12:r:57:ARG:NH2	2.48	0.46
14:t:141:TYR:HA	14:t:144:TYR:HD2	1.81	0.46
26:A:389:CYS:HA	26:A:409:PHE:HE1	1.81	0.46
27:B:343:ARG:HD3	27:B:346:ARG:HE	1.80	0.46
29:D:238:LYS:NZ	31:F:297:ASP:O	2.44	0.46
30:E:55:GLN:N	31:F:133:PHE:O	2.48	0.46
32:f:378:ASN:HB3	32:f:391:LEU:HD21	1.97	0.46
1:G:61:LEU:HG	7:M:160:TYR:HE1	1.81	0.46
1:G:88:ARG:NH1	7:M:157:SER:O	2.45	0.46
2:H:42:ASN:ND2	2:H:183:GLU:OE1	2.48	0.46
5:K:32:LYS:HZ1	5:K:173:ALA:H	1.64	0.46
11:Q:88:LEU:HB3	11:Q:122:ALA:HB2	1.98	0.46
13:S:172:MET:HE1	13:S:195:ILE:HG21	1.97	0.46
15:U:559:ARG:HD2	15:U:562:GLU:HB2	1.97	0.46
16:V:197:THR:HA	28:C:31:LEU:HD13	1.96	0.46
16:V:393:THR:HB	16:V:397:ARG:HH22	1.80	0.46
21:a:250:THR:HA	21:a:253:THR:HG22	1.98	0.46
21:a:341:LEU:HB2	21:a:345:GLN:HG2	1.97	0.46
10:p:126:LEU:HD12	10:p:127:ILE:HG23	1.98	0.46
13:s:64:LEU:HD21	13:s:92:LEU:HD11	1.97	0.46
27:B:313:LEU:O	27:B:346:ARG:NH1	2.48	0.46
31:F:206:MET:HE3	31:F:246:ALA:HB2	1.98	0.46
32:f:635:LYS:NZ	32:f:641:GLU:HG3	2.16	0.46
32:f:796:LEU:HD12	32:f:799:VAL:HG11	1.98	0.46
12:R:7:LYS:HA	12:R:12:VAL:HA	1.97	0.46
15:U:680:VAL:HA	23:c:186:LYS:HE2	1.97	0.46
16:V:38:LYS:HA	16:V:41:ALA:HB3	1.98	0.46
23:c:131:GLN:HA	23:c:134:GLU:HG2	1.98	0.46
7:m:201:HIS:HE1	7:m:206:ASP:HB2	1.80	0.46
8:n:18:SER:OG	8:n:19:ARG:N	2.48	0.46
32:f:79:ARG:HE	32:f:95:PRO:HG3	1.80	0.46
32:f:226:TYR:O	32:f:230:CYS:HB3	2.16	0.46
32:f:675:PHE:CG	32:f:694:LEU:HD23	2.51	0.46
15:U:216:VAL:O	15:U:220:LEU:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:124:LEU:HA	17:W:127:THR:HG22	1.97	0.46
17:W:366:MET:HB3	17:W:370:TYR:CZ	2.50	0.46
19:Y:266:CYS:SG	19:Y:306:GLN:NE2	2.89	0.46
21:a:25:LEU:HD12	21:a:28:LEU:HD22	1.98	0.46
6:l:148:CYS:SG	6:l:152:ASN:N	2.83	0.46
13:s:13:LEU:HD11	13:s:149:LEU:HD11	1.96	0.46
26:A:172:VAL:HG11	26:A:224:LEU:HD22	1.98	0.46
32:f:193:PRO:C	32:f:208:LEU:HD12	2.40	0.46
16:V:326:GLN:HB3	16:V:353:LEU:HD22	1.98	0.45
16:V:340:GLY:HA2	16:V:401:ASN:HA	1.97	0.45
19:Y:174:TRP:HZ2	19:Y:206:SER:HB2	1.81	0.45
19:Y:188:CYS:C	19:Y:193:ASP:HB2	2.40	0.45
20:Z:226:ILE:O	20:Z:230:LEU:HB2	2.16	0.45
21:a:273:GLN:HE21	21:a:310:LEU:HD12	1.81	0.45
21:a:284:ARG:HH22	21:a:291:LEU:HD13	1.81	0.45
10:p:45:MET:HE3	10:p:71:LEU:HD22	1.97	0.45
32:f:353:LEU:H	32:f:387:GLN:CG	2.29	0.45
32:f:641:GLU:HG3	32:f:641:GLU:O	2.09	0.45
5:K:91:LYS:HD2	5:K:119:LEU:HD21	1.98	0.45
5:K:108:THR:O	5:K:111:SER:OG	2.30	0.45
7:M:201:HIS:CE1	7:M:206:ASP:H	2.34	0.45
15:U:237:VAL:HG13	15:U:321:GLN:HG3	1.98	0.45
16:V:101:LEU:HD22	16:V:102:PRO:HD2	1.97	0.45
20:Z:74:TYR:HD1	23:c:98:MET:HB3	1.81	0.45
23:c:96:LEU:HD23	23:c:99:LEU:HD12	1.97	0.45
24:d:111:ARG:HB3	24:d:114:GLU:HB2	1.99	0.45
29:D:74:HIS:O	29:D:78:GLU:HB2	2.16	0.45
30:E:98:VAL:HB	30:E:107:ILE:HG23	1.98	0.45
32:f:696:LEU:HD12	32:f:696:LEU:HA	1.78	0.45
4:J:211:MET:HG2	4:J:213:ARG:H	1.81	0.45
6:L:225:ASP:OD1	6:L:225:ASP:N	2.49	0.45
9:O:41:ILE:HG12	9:O:76:VAL:HG22	1.98	0.45
15:U:45:ILE:HG21	15:U:64:ALA:HB2	1.98	0.45
15:U:126:ILE:HG23	15:U:130:LEU:HD11	1.98	0.45
15:U:250:PHE:O	15:U:254:GLU:HB2	2.17	0.45
17:W:139:GLU:HG2	17:W:142:ARG:HB2	1.97	0.45
17:W:294:LYS:HG2	17:W:295:LYS:HE3	1.99	0.45
19:Y:215:ASP:O	19:Y:218:THR:OG1	2.30	0.45
22:b:138:VAL:H	22:b:160:LEU:HD21	1.80	0.45
23:c:58:LEU:HA	23:c:108:VAL:HA	1.98	0.45
24:d:215:TRP:NE1	24:d:221:ASN:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:46:LEU:HD13	2:h:75:VAL:HG13	1.97	0.45
4:J:170:GLU:HA	4:J:173:GLU:OE1	2.16	0.45
9:O:67:SER:HB3	9:O:74:PRO:HG3	1.97	0.45
15:U:341:PHE:O	15:U:345:ASN:CB	2.64	0.45
15:U:692:ALA:HB2	15:U:733:ALA:HB1	1.99	0.45
16:V:286:ALA:HA	16:V:315:LYS:HD2	1.98	0.45
19:Y:23:ARG:O	19:Y:27:SER:HB2	2.16	0.45
19:Y:164:ALA:HA	19:Y:168:ILE:HD12	1.99	0.45
21:a:112:ILE:H	21:a:112:ILE:HG13	1.66	0.45
32:f:125:ILE:HA	32:f:129:LEU:HD12	1.98	0.45
14:T:192:VAL:HG12	14:T:197:VAL:HG22	1.98	0.45
15:U:216:VAL:O	15:U:220:LEU:HB2	2.16	0.45
15:U:898:CYS:SG	15:U:899:ARG:N	2.89	0.45
16:V:249:THR:OG1	16:V:250:LEU:N	2.48	0.45
19:Y:83:ARG:O	19:Y:87:GLU:HB2	2.16	0.45
4:j:134:VAL:HG22	4:j:144:LEU:HB2	1.98	0.45
6:l:51:ARG:O	6:l:60:GLN:N	2.38	0.45
29:D:337:ASP:OD1	29:D:337:ASP:N	2.49	0.45
32:f:541:THR:O	32:f:545:LYS:CB	2.64	0.45
7:M:230:ASP:OD1	7:M:230:ASP:N	2.49	0.45
16:V:65:ARG:HG3	16:V:69:THR:HB	1.99	0.45
17:W:4:GLY:HA3	17:W:34:LEU:HD21	1.98	0.45
18:X:46:LYS:HD3	18:X:49:SER:HB3	1.98	0.45
20:Z:139:ILE:N	20:Z:156:GLU:O	2.37	0.45
7:m:52:LEU:HA	7:m:209:PHE:HA	1.97	0.45
29:D:301:GLN:C	29:D:302:ASN:OD1	2.60	0.45
29:D:301:GLN:O	29:D:302:ASN:OD1	2.35	0.45
30:E:165:ILE:HG22	30:E:168:LYS:HZ1	1.81	0.45
32:f:379:GLY:O	32:f:417:ILE:CG1	2.65	0.45
32:f:533:ASP:OD1	32:f:565:ASN:ND2	2.50	0.45
3:I:62:SER:OG	3:I:65:ILE:O	2.35	0.45
7:M:180:GLN:HB3	7:M:184:MET:HE3	1.98	0.45
15:U:177:LEU:HB3	15:U:208:LEU:HD11	1.99	0.45
15:U:751:ARG:HH11	15:U:908:ILE:HG22	1.81	0.45
19:Y:330:ILE:HA	19:Y:333:GLU:HB3	1.98	0.45
2:h:93:LEU:HD11	2:h:113:ARG:HB3	1.98	0.45
27:B:433:GLY:HA2	27:B:434:THR:HA	1.75	0.45
30:E:242:ARG:HD3	30:E:284:THR:HG22	1.98	0.45
32:f:316:ASP:HA	32:f:319:GLU:HG2	1.99	0.45
32:f:608:LYS:HA	32:f:611:GLN:HB3	1.99	0.45
32:f:664:GLU:C	32:f:665:GLU:O	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:797:LEU:HD22	32:f:797:LEU:HA	1.76	0.45
10:P:138:VAL:HB	10:P:146:MET:HE3	1.98	0.45
16:V:99:ARG:CZ	16:V:104:THR:HG23	2.47	0.45
18:X:346:GLN:NE2	18:X:353:LEU:HG	2.31	0.45
19:Y:210:SER:OG	19:Y:211:TYR:N	2.49	0.45
20:Z:174:HIS:HB2	23:c:153:GLY:HA2	1.98	0.45
21:a:90:PRO:O	21:a:94:LEU:N	2.40	0.45
21:a:101:ARG:HH12	21:a:114:CYS:HA	1.81	0.45
21:a:245:VAL:HG13	21:a:246:GLU:H	1.82	0.45
22:b:184:ILE:HA	22:b:187:PRO:HD2	1.98	0.45
23:c:291:LEU:O	23:c:295:ASN:ND2	2.49	0.45
26:A:113:ILE:HD12	26:A:123:VAL:HG21	1.98	0.45
30:E:309:ARG:NH1	30:E:332:VAL:O	2.50	0.45
32:f:45:LEU:HD22	32:f:86:THR:HG21	1.99	0.45
3:I:162:THR:OG1	3:I:163:CYS:N	2.47	0.45
15:U:158:ARG:NH1	29:D:41:TYR:OH	2.50	0.45
15:U:465:LEU:HD11	15:U:477:GLY:HA3	1.98	0.45
16:V:175:MET:HB3	16:V:179:LYS:HZ1	1.81	0.45
16:V:194:LYS:HE2	28:C:27:LYS:HG3	1.99	0.45
16:V:231:LEU:HD11	16:V:247:GLN:HA	1.98	0.45
16:V:423:ALA:HB2	16:V:434:ALA:HB2	1.99	0.45
16:V:470:ARG:O	16:V:474:LEU:N	2.50	0.45
17:W:79:GLU:O	17:W:83:LEU:HB2	2.16	0.45
19:Y:301:ILE:HG13	19:Y:343:LEU:HD12	1.97	0.45
21:a:101:ARG:HA	21:a:104:VAL:HB	1.99	0.45
21:a:182:CYS:SG	21:a:183:VAL:N	2.90	0.45
5:k:85:ALA:HB2	5:k:139:VAL:HG21	1.99	0.45
6:l:189:LYS:HG3	6:l:193:ARG:HH12	1.81	0.45
26:A:245:LEU:HD12	26:A:280:ILE:HG12	1.99	0.45
29:D:247:VAL:HA	29:D:250:VAL:HB	1.99	0.45
1:G:196:GLU:HA	1:G:242:LEU:HD22	1.99	0.45
13:S:68:ILE:HD11	13:S:92:LEU:HD13	1.98	0.45
15:U:348:THR:HG21	15:U:376:MET:HB2	1.98	0.45
19:Y:191:ILE:HD11	25:e:41:ASP:HA	1.99	0.45
21:a:189:PRO:HB2	21:a:192:GLU:HB3	1.99	0.45
4:j:156:TRP:CD1	5:k:59:MET:HA	2.51	0.45
11:q:88:LEU:HB3	11:q:122:ALA:HB2	1.97	0.45
27:B:224:LEU:HD21	27:B:235:LEU:HD12	1.98	0.45
21:a:178:ARG:O	21:a:182:CYS:HB3	2.17	0.44
2:h:9:SER:HA	2:h:126:GLY:H	1.81	0.44
2:h:181:ASP:OD1	2:h:181:ASP:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:175:ARG:HG2	8:n:188:VAL:HG22	1.99	0.44
32:f:130:ALA:O	32:f:134:SER:CB	2.64	0.44
32:f:420:TRP:CG	32:f:421:ASP:H	2.34	0.44
32:f:664:GLU:HA	32:f:697:ILE:CA	2.46	0.44
2:H:80:GLY:HA2	2:H:83:TYR:HB3	1.99	0.44
3:I:105:ILE:HA	3:I:106:PRO:HD3	1.80	0.44
7:M:40:ARG:NH1	7:M:146:ALA:O	2.50	0.44
15:U:559:ARG:HG3	15:U:563:ALA:HB2	2.00	0.44
16:V:33:GLN:HE21	16:V:115:LYS:HB2	1.82	0.44
17:W:375:MET:SD	17:W:413:ILE:HD13	2.57	0.44
18:X:143:TYR:CZ	19:Y:252:SER:HB2	2.51	0.44
23:c:55:GLY:HA3	23:c:112:TYR:CZ	2.53	0.44
24:d:171:LEU:HD13	24:d:196:ARG:HD3	1.99	0.44
4:j:169:ARG:HA	4:j:172:LEU:HB2	1.99	0.44
26:A:423:PHE:HA	26:A:424:SER:HA	1.72	0.44
6:L:104:PRO:HD2	6:L:107:ARG:HD2	1.99	0.44
15:U:167:ILE:CG2	15:U:176:MET:CE	2.92	0.44
15:U:261:LEU:HA	15:U:264:VAL:HG12	1.99	0.44
15:U:446:LEU:HA	15:U:449:ILE:HD12	1.98	0.44
17:W:379:ALA:HB1	17:W:386:VAL:HA	2.00	0.44
19:Y:349:LYS:HG3	19:Y:350:VAL:H	1.82	0.44
21:a:279:GLU:O	21:a:283:THR:OG1	2.32	0.44
9:o:163:ILE:HA	9:o:168:GLY:HA3	1.99	0.44
11:q:145:ARG:NH1	11:q:146:TYR:OH	2.51	0.44
12:r:115:ASP:HB2	12:r:119:ASN:H	1.83	0.44
26:A:121:PHE:HA	31:F:87:PRO:HA	1.99	0.44
28:C:393:LYS:HG3	28:C:395:SER:HB2	1.98	0.44
32:f:692:LEU:HD12	32:f:748:LEU:HD23	1.84	0.44
1:G:84:THR:HB	7:M:156:VAL:HG22	1.99	0.44
16:V:203:LEU:HA	16:V:206:VAL:HB	2.00	0.44
19:Y:133:ALA:HB3	19:Y:136:HIS:HD2	1.83	0.44
21:a:55:GLY:HA3	21:a:86:GLN:HB2	1.99	0.44
24:d:54:ILE:HA	24:d:57:ILE:HG22	2.00	0.44
32:f:22:GLY:O	32:f:26:GLU:CB	2.66	0.44
32:f:286:LYS:HD3	32:f:326:LEU:HD23	2.00	0.44
32:f:378:ASN:CB	32:f:391:LEU:CD1	2.94	0.44
32:f:646:MET:HA	32:f:649:HIS:HD1	1.82	0.44
14:T:171:ARG:NH2	9:o:140:ASP:OD1	2.48	0.44
15:U:691:SER:HA	15:U:694:ILE:HG22	1.99	0.44
16:V:480:ILE:HA	16:V:483:CYS:HB2	2.00	0.44
17:W:389:SER:HB3	17:W:393:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:268:TYR:HA	19:Y:271:PHE:CD2	2.53	0.44
21:a:156:TYR:OH	21:a:196:ARG:NH1	2.51	0.44
23:c:32:TYR:HB2	23:c:68:ARG:HA	1.99	0.44
23:c:75:MET:SD	23:c:92:GLN:NE2	2.90	0.44
2:h:14:SER:OG	2:h:17:GLY:N	2.50	0.44
3:i:126:GLY:HA3	4:j:3:TYR:HE2	1.83	0.44
8:n:88:TYR:OH	14:t:59:ASP:OD1	2.33	0.44
30:E:272:ARG:O	30:E:274:LYS:NZ	2.45	0.44
31:F:89:LEU:HD11	31:F:126:THR:HB	1.99	0.44
32:f:354:GLU:HG3	32:f:355:ASN:H	1.82	0.44
32:f:357:ARG:NH2	32:f:754:LYS:HG3	2.33	0.44
32:f:688:ARG:HG3	32:f:745:LEU:HB3	1.99	0.44
3:I:174:MET:O	3:I:178:ASP:HB2	2.17	0.44
4:J:2:SER:HB3	4:J:11:SER:HA	2.00	0.44
15:U:474:ARG:NH2	15:U:496:LEU:HD13	2.32	0.44
16:V:296:LYS:HB3	16:V:301:GLU:HB3	1.99	0.44
17:W:244:CYS:HA	17:W:273:TYR:CE2	2.53	0.44
18:X:177:TYR:HB3	18:X:182:ASN:HB3	2.00	0.44
19:Y:60:SER:HB3	19:Y:63:TRP:HE1	1.83	0.44
24:d:171:LEU:HB3	24:d:196:ARG:HG2	2.00	0.44
6:l:225:ASP:OD1	6:l:225:ASP:N	2.51	0.44
26:A:339:ARG:HB3	26:A:341:ILE:HG13	2.00	0.44
28:C:219:LEU:HD21	29:D:241:GLY:HA3	1.98	0.44
30:E:212:ALA:HA	30:E:215:ILE:HD12	1.99	0.44
32:f:281:ILE:O	32:f:285:CYS:HB2	2.18	0.44
32:f:536:SER:O	32:f:540:GLN:CB	2.66	0.44
5:K:104:ASN:OD1	12:R:57:ARG:NH2	2.47	0.44
18:X:134:VAL:HG13	18:X:172:LEU:HD23	1.99	0.44
24:d:204:LYS:HA	24:d:207:THR:HB	2.00	0.44
12:r:19:ARG:NH1	12:r:170:SER:O	2.51	0.44
12:r:196:HIS:O	12:r:200:SER:HB3	2.18	0.44
32:f:412:ALA:HA	32:f:447:ALA:HB2	2.00	0.44
1:G:39:SER:OG	1:G:168:ALA:O	2.28	0.44
5:K:70:ILE:HD11	5:K:89:ILE:HD12	1.99	0.44
9:O:11:GLY:HA2	9:O:108:PRO:HB3	2.00	0.44
13:S:13:LEU:HD11	13:S:149:LEU:HD11	1.98	0.44
15:U:602:LEU:HG	15:U:618:ALA:HB1	2.00	0.44
16:V:227:VAL:HA	16:V:230:PHE:HB3	2.00	0.44
20:Z:175:LEU:HD21	23:c:207:TYR:HB2	1.99	0.44
2:h:80:GLY:HA2	2:h:83:TYR:HB3	1.98	0.44
26:A:227:ARG:NH2	27:B:318:GLY:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:365:GLU:HG2	26:A:367:ASP:H	1.83	0.44
26:A:375:ARG:HD3	26:A:376:LEU:HG	1.99	0.44
28:C:219:LEU:HD11	29:D:241:GLY:HA3	1.99	0.44
32:f:380:PHE:CD2	32:f:380:PHE:O	2.70	0.44
32:f:509:LYS:HB3	32:f:514:VAL:HG21	1.99	0.44
32:f:664:GLU:HB3	32:f:696:LEU:CG	2.43	0.44
32:f:664:GLU:CB	32:f:696:LEU:HG	2.45	0.44
21:a:169:HIS:NE2	21:a:203:ALA:O	2.51	0.44
21:a:199:THR:O	21:a:203:ALA:CB	2.63	0.44
26:A:125:LEU:HA	26:A:149:ILE:H	1.83	0.44
26:A:347:ASP:OD1	26:A:347:ASP:N	2.51	0.44
27:B:220:LYS:N	27:B:348:ASP:OD2	2.45	0.44
28:C:192:PRO:C	29:D:323:ARG:HH22	2.24	0.44
29:D:336:PRO:HG3	29:D:370:ILE:H	1.82	0.44
29:D:410:ASP:OD1	29:D:410:ASP:N	2.51	0.44
30:E:165:ILE:CG2	30:E:166:PRO:HD3	2.47	0.44
32:f:311:VAL:CA	32:f:490:ALA:HB1	2.48	0.44
32:f:380:PHE:CB	32:f:751:TYR:CE2	2.99	0.44
1:G:243:ALA:HB1	17:W:85:GLU:HB2	2.00	0.43
7:M:228:PRO:HB2	7:M:231:ILE:HB	1.98	0.43
8:N:135:ILE:O	8:N:139:VAL:HB	2.18	0.43
15:U:885:MET:HG2	15:U:887:ALA:H	1.83	0.43
16:V:331:LEU:HD22	16:V:389:ASP:HB3	2.00	0.43
20:Z:205:LEU:HA	20:Z:208:ILE:HG22	2.00	0.43
1:g:83:MET:SD	1:g:132:ARG:NH1	2.92	0.43
8:n:135:ILE:O	8:n:139:VAL:HB	2.18	0.43
28:C:219:LEU:HB3	28:C:220:VAL:H	1.47	0.43
28:C:237:MET:HA	28:C:240:GLU:HB2	2.00	0.43
31:F:89:LEU:N	31:F:153:VAL:O	2.44	0.43
7:M:201:HIS:HE1	7:M:206:ASP:HB2	1.84	0.43
15:U:140:ARG:O	15:U:144:ASP:HB2	2.18	0.43
15:U:241:ASN:HD22	15:U:244:MET:HE3	1.84	0.43
16:V:68:ASP:O	16:V:72:LEU:HB2	2.18	0.43
16:V:357:LEU:O	16:V:360:TYR:N	2.51	0.43
18:X:394:ASP:OD1	18:X:394:ASP:N	2.51	0.43
19:Y:247:LEU:HD12	19:Y:250:LEU:HD11	2.00	0.43
22:b:5:SER:HB3	22:b:64:LEU:HD21	2.00	0.43
23:c:30:GLN:O	23:c:67:VAL:N	2.47	0.43
1:g:130:GLU:HG2	2:h:4:ARG:NH1	2.33	0.43
3:i:232:GLU:HA	3:i:235:GLN:HG2	2.00	0.43
7:m:106:ILE:HG12	7:m:111:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:432:GLU:HA	27:B:433:GLY:HA3	1.77	0.43
30:E:84:ARG:O	30:E:85:ARG:NE	2.39	0.43
32:f:645:ASP:O	32:f:649:HIS:ND1	2.51	0.43
15:U:106:ASP:HA	15:U:109:THR:HG22	2.00	0.43
17:W:262:LYS:HA	17:W:265:GLN:HG2	2.00	0.43
18:X:170:GLN:NE2	18:X:173:GLU:OE1	2.51	0.43
20:Z:71:ASP:HB3	20:Z:74:TYR:HB3	1.99	0.43
20:Z:95:TYR:HB3	20:Z:122:VAL:HB	2.00	0.43
20:Z:259:VAL:HA	20:Z:262:LEU:HD12	2.01	0.43
21:a:373:ASP:H	24:d:251:ARG:HH12	1.66	0.43
23:c:160:PHE:HD1	23:c:202:SER:HA	1.83	0.43
24:d:69:PRO:HA	24:d:72:GLU:HG2	1.99	0.43
1:g:6:SER:HB2	1:g:11:ARG:HE	1.84	0.43
3:i:135:LEU:HD23	3:i:135:LEU:HA	1.80	0.43
4:j:211:MET:HG2	4:j:213:ARG:H	1.83	0.43
12:r:37:ILE:HG23	12:r:60:ALA:HB2	2.00	0.43
28:C:219:LEU:O	28:C:221:GLN:N	2.45	0.43
32:f:471:LEU:HD11	32:f:509:LYS:HE2	2.00	0.43
32:f:690:VAL:O	32:f:694:LEU:HB2	2.18	0.43
3:I:232:GLU:HA	3:I:235:GLN:HG2	2.00	0.43
4:J:32:ALA:HB2	4:J:45:VAL:HG23	2.00	0.43
4:J:134:VAL:HG22	4:J:144:LEU:HB2	2.00	0.43
15:U:163:PHE:HZ	15:U:201:LEU:HD11	1.83	0.43
15:U:179:TYR:CD1	15:U:182:LYS:HD2	2.53	0.43
15:U:542:GLU:HG3	15:U:546:ARG:HH12	1.83	0.43
3:i:25:MET:HA	3:i:28:ILE:HD12	2.00	0.43
26:A:189:GLU:O	26:A:193:THR:OG1	2.36	0.43
29:D:304:ASN:N	29:D:304:ASN:ND2	2.66	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
32:f:283:THR:O	32:f:287:ASP:HB2	2.18	0.43
18:X:178:HIS:CE1	18:X:220:ALA:HB2	2.52	0.43
19:Y:220:VAL:HA	19:Y:223:THR:HG22	2.00	0.43
20:Z:94:TRP:HZ3	20:Z:96:HIS:HB3	1.83	0.43
20:Z:225:GLN:NE2	20:Z:229:GLN:OE1	2.52	0.43
21:a:357:CYS:O	21:a:361:LYS:CB	2.66	0.43
4:j:169:ARG:HA	4:j:172:LEU:HD12	2.01	0.43
6:l:130:VAL:HG22	6:l:132:LEU:HG	1.99	0.43
7:m:100:SER:HA	14:t:65:GLN:HE21	1.82	0.43
26:A:323:ARG:HD2	27:B:294:ARG:HG2	2.00	0.43
30:E:171:LEU:HD11	30:E:279:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:197:GLU:O	31:F:201:ALA:HB3	2.18	0.43
32:f:794:ALA:HA	32:f:797:LEU:HB2	2.01	0.43
15:U:252:LEU:HD21	15:U:264:VAL:HG11	1.99	0.43
15:U:446:LEU:HD23	15:U:461:LEU:HD11	2.01	0.43
15:U:450:HIS:NE2	15:U:457:ILE:HB	2.34	0.43
20:Z:71:ASP:O	20:Z:75:LEU:N	2.52	0.43
21:a:210:VAL:O	21:a:271:LYS:NZ	2.48	0.43
23:c:144:VAL:HB	23:c:158:ASP:HB3	2.00	0.43
3:i:164:ILE:HG22	3:i:165:GLY:H	1.83	0.43
6:l:174:ARG:HG3	6:l:175:HIS:ND1	2.34	0.43
26:A:277:ILE:H	26:A:277:ILE:HG13	1.56	0.43
28:C:69:GLN:HE22	29:D:137:ASN:HD22	1.66	0.43
32:f:303:VAL:HG22	32:f:339:ILE:HA	2.00	0.43
32:f:446:LEU:HD13	32:f:480:GLY:HA2	2.00	0.43
32:f:623:LYS:O	32:f:627:GLU:HB3	2.18	0.43
14:T:25:ASP:HA	14:T:187:PHE:HA	2.01	0.43
15:U:559:ARG:HB2	15:U:589:ALA:HB1	2.00	0.43
16:V:228:ARG:HH12	16:V:254:LEU:HA	1.84	0.43
17:W:41:GLN:HE22	17:W:92:LYS:HD2	1.83	0.43
1:g:84:THR:HB	7:m:156:VAL:HG22	2.00	0.43
2:h:65:VAL:HA	2:h:75:VAL:HG12	2.01	0.43
28:C:147:THR:O	28:C:147:THR:OG1	2.37	0.43
30:E:142:ILE:O	30:E:146:ARG:HB2	2.18	0.43
30:E:168:LYS:HB2	30:E:296:ASP:H	1.83	0.43
31:F:317:LEU:HG	31:F:318:ASP:HB2	2.01	0.43
32:f:355:ASN:HA	32:f:358:PHE:HD2	1.83	0.43
1:G:7:ALA:HA	1:G:8:GLY:HA3	1.75	0.43
4:J:68:ASN:HA	4:J:211:MET:HE1	2.00	0.43
14:T:144:TYR:HB3	9:o:132:LEU:HD13	2.00	0.43
15:U:325:MET:HA	15:U:328:ILE:HG12	2.01	0.43
16:V:327:THR:HG21	25:e:9:ASP:HB3	2.00	0.43
17:W:311:THR:HA	17:W:365:ILE:HG21	2.00	0.43
20:Z:215:VAL:HG13	21:a:344:GLN:HG3	2.01	0.43
26:A:365:GLU:HB3	26:A:368:ILE:HG23	2.01	0.43
29:D:158:GLN:OE1	29:D:229:ARG:NH2	2.51	0.43
29:D:247:VAL:HG11	29:D:295:GLN:HB3	2.01	0.43
29:D:413:GLU:HA	29:D:414:HIS:HA	1.77	0.43
4:J:51:ALA:N	4:J:54:GLN:HE22	2.07	0.43
16:V:434:ALA:HA	16:V:437:ILE:HG22	2.00	0.43
18:X:327:TYR:HD1	18:X:364:LYS:HE3	1.84	0.43
21:a:97:LEU:O	21:a:101:ARG:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:157:ASP:OD2	5:k:159:SER:OG	2.32	0.43
5:k:167:ALA:HB3	5:k:181:LEU:HD21	2.00	0.43
6:l:189:LYS:HA	6:l:192:LEU:HG	2.01	0.43
8:n:134:TYR:O	8:n:137:GLY:N	2.51	0.43
14:t:192:VAL:HG12	14:t:197:VAL:HG22	2.00	0.43
28:C:343:ASN:O	28:C:380:GLN:NE2	2.52	0.43
29:D:228:ILE:HG22	29:D:230:VAL:HG23	2.00	0.43
29:D:261:ILE:HG23	29:D:306:LYS:CB	2.30	0.43
30:E:57:VAL:HB	31:F:131:THR:HB	2.00	0.43
30:E:166:PRO:HG2	30:E:272:ARG:HA	2.00	0.43
32:f:358:PHE:O	32:f:362:GLY:CA	2.63	0.43
32:f:494:ARG:NE	32:f:494:ARG:CA	2.82	0.43
32:f:632:LYS:NZ	32:f:660:ILE:O	2.46	0.43
3:I:164:ILE:HG22	3:I:165:GLY:H	1.83	0.43
15:U:445:ALA:HA	15:U:448:LEU:HD12	2.01	0.43
15:U:503:GLN:HG3	15:U:508:THR:HG21	2.01	0.43
16:V:211:TYR:HA	16:V:214:HIS:HD1	1.84	0.43
19:Y:50:MET:SD	19:Y:53:TYR:OH	2.74	0.43
23:c:159:ALA:HB3	23:c:205:ILE:HD11	1.99	0.43
23:c:249:LEU:HA	23:c:252:ALA:HB3	2.00	0.43
3:i:13:SER:O	4:j:21:TYR:OH	2.26	0.43
11:q:19:ARG:HE	11:q:31:ASP:HA	1.84	0.43
26:A:302:LEU:O	26:A:306:LEU:CB	2.66	0.43
29:D:160:PRO:HG2	29:D:220:ALA:HB3	2.01	0.43
30:E:153:LEU:HD13	30:E:227:PRO:HG2	2.01	0.43
30:E:312:ILE:O	30:E:316:HIS:HB2	2.18	0.43
31:F:76:ASN:HA	31:F:79:LYS:HB2	2.00	0.43
32:f:494:ARG:HE	32:f:494:ARG:CA	2.31	0.43
2:H:48:THR:OG1	2:H:49:GLU:N	2.52	0.42
3:I:161:ALA:HB1	3:I:175:LEU:HD13	2.01	0.42
4:J:97:THR:OG1	4:J:98:VAL:N	2.52	0.42
9:O:122:LEU:HD23	9:O:122:LEU:HA	1.90	0.42
9:O:172:ASN:HB3	9:O:191:VAL:HG22	2.01	0.42
11:Q:19:ARG:HB3	11:Q:31:ASP:HA	2.00	0.42
15:U:12:LEU:HD23	15:U:20:LYS:HE3	2.01	0.42
15:U:520:MET:HE2	15:U:525:ASN:HD22	1.83	0.42
16:V:95:LEU:O	16:V:111:TYR:OH	2.32	0.42
16:V:245:ASP:O	16:V:247:GLN:N	2.52	0.42
20:Z:206:LEU:O	20:Z:210:SER:OG	2.33	0.42
24:d:209:TYR:HA	24:d:212:LYS:HB2	2.00	0.42
3:i:105:ILE:HD11	3:i:109:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:149:GLN:NE2	3:i:162:THR:OG1	2.52	0.42
5:k:16:SER:HB3	5:k:19:GLY:H	1.83	0.42
13:s:29:LEU:HB3	13:s:37:THR:HG22	2.01	0.42
14:t:46:ASN:OD1	14:t:46:ASN:N	2.51	0.42
14:t:63:LEU:HD23	14:t:63:LEU:HA	1.87	0.42
27:B:112:LEU:HD13	27:B:115:ILE:HD11	2.01	0.42
27:B:373:THR:HB	27:B:413:LYS:HG2	2.00	0.42
27:B:421:LYS:O	27:B:425:ASN:HB2	2.18	0.42
32:f:207:LEU:HD13	32:f:207:LEU:HA	1.86	0.42
32:f:513:GLU:HG3	32:f:557:TRP:HZ3	1.84	0.42
3:l:14:PRO:HB3	4:j:21:TYR:CE2	2.54	0.42
5:K:44:GLU:OE1	5:K:191:LEU:N	2.51	0.42
11:Q:158:GLU:HG3	11:Q:162:LYS:HE3	2.02	0.42
15:U:258:GLN:HB3	15:U:486:MET:HE2	2.01	0.42
15:U:723:ASP:HB2	15:U:726:ALA:HB3	2.00	0.42
16:V:296:LYS:O	16:V:301:GLU:N	2.46	0.42
16:V:442:ILE:HA	16:V:446:VAL:HG12	2.01	0.42
17:W:16:MET:HE3	17:W:54:THR:HB	2.01	0.42
17:W:276:LEU:HD11	17:W:340:VAL:HG13	2.00	0.42
18:X:236:PHE:HE1	18:X:247:ALA:HB1	1.84	0.42
18:X:302:PHE:O	18:X:306:LEU:HB2	2.18	0.42
6:l:155:ASP:HB3	7:m:62:SER:HB2	2.00	0.42
10:p:34:MET:HE3	10:p:34:MET:HB2	1.91	0.42
27:B:391:SER:N	27:B:394:ASP:OD2	2.41	0.42
29:D:101:ALA:N	29:D:113:VAL:O	2.51	0.42
32:f:122:ALA:HB1	32:f:126:ILE:HD12	2.01	0.42
32:f:368:ALA:O	32:f:372:LEU:HB2	2.18	0.42
11:Q:19:ARG:HH21	11:Q:31:ASP:HB2	1.84	0.42
17:W:339:ASP:O	17:W:350:ARG:NH1	2.52	0.42
18:X:173:GLU:HA	18:X:176:THR:HG22	2.00	0.42
22:b:109:ILE:HD12	22:b:136:VAL:HG11	2.02	0.42
26:A:194:PRO:HB3	26:A:201:PHE:CE2	2.54	0.42
28:C:347:ILE:HG22	28:C:351:MET:HE3	1.99	0.42
30:E:232:MET:HE1	30:E:260:LEU:HD22	2.00	0.42
32:f:228:LYS:O	32:f:232:TYR:HB3	2.19	0.42
32:f:389:LYS:HD3	32:f:389:LYS:H	1.81	0.42
1:G:70:PHE:CD2	1:G:91:VAL:HG21	2.54	0.42
18:X:325:LYS:O	18:X:329:ASN:HB2	2.19	0.42
21:a:212:ASN:HD21	21:a:216:LEU:HD23	1.84	0.42
24:d:99:LEU:HB3	24:d:133:ILE:HD11	2.01	0.42
1:g:51:VAL:HG23	1:g:217:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:110:GLU:HG3	5:k:162:PHE:HE2	1.84	0.42
7:m:15:SER:OG	7:m:18:GLY:N	2.48	0.42
10:p:2:SER:N	10:p:5:SER:HB2	2.34	0.42
28:C:86:LEU:HD11	28:C:94:LYS:HD2	2.01	0.42
29:D:91:GLN:N	29:D:104:GLY:O	2.46	0.42
30:E:127:PRO:HD2	30:E:197:LYS:HE3	2.02	0.42
32:f:77:GLU:O	32:f:81:GLN:HB2	2.19	0.42
2:H:8:PHE:HA	2:H:9:SER:HA	1.75	0.42
2:H:82:ASP:HB3	2:H:130:PHE:HD1	1.84	0.42
3:I:125:GLY:HA2	3:I:126:GLY:HA2	1.59	0.42
12:R:178:HIS:CE1	12:R:180:ARG:HG2	2.53	0.42
17:W:251:TYR:HE1	17:W:263:TRP:HE1	1.67	0.42
18:X:373:LYS:HE3	18:X:373:LYS:HB3	1.87	0.42
20:Z:186:THR:OG1	21:a:374:ILE:O	2.37	0.42
6:l:72:ILE:HG22	6:l:134:ILE:HG12	2.00	0.42
11:q:177:THR:HG22	11:q:195:SER:HB3	2.01	0.42
28:C:276:LEU:HD23	28:C:276:LEU:HA	1.76	0.42
32:f:80:ARG:HE	32:f:99:LEU:HD13	1.85	0.42
32:f:629:LYS:HE2	32:f:660:ILE:HG21	2.02	0.42
6:L:201:ALA:O	6:L:239:ARG:NH1	2.50	0.42
7:M:37:ILE:HG12	7:M:197:ILE:HD11	2.02	0.42
15:U:474:ARG:HH22	15:U:496:LEU:HD13	1.85	0.42
15:U:620:GLU:OE2	15:U:768:GLN:NE2	2.46	0.42
16:V:470:ARG:HA	16:V:473:GLN:HE21	1.85	0.42
21:a:197:ALA:HB2	21:a:225:LEU:HB3	2.02	0.42
23:c:273:LYS:HE2	23:c:275:VAL:HB	2.01	0.42
5:k:103:TYR:HB3	5:k:105:GLU:HG2	2.02	0.42
32:f:183:PRO:HB2	32:f:184:LEU:H	1.63	0.42
32:f:573:ILE:HG22	32:f:576:ILE:HB	2.01	0.42
3:I:34:CYS:H	3:I:164:ILE:HG13	1.85	0.42
6:L:189:LYS:HA	6:L:192:LEU:HG	2.00	0.42
8:N:18:SER:HB2	8:N:31:THR:H	1.85	0.42
14:T:41:ARG:HH21	14:T:54:SER:HA	1.85	0.42
15:U:685:GLN:HB2	15:U:726:ALA:HA	1.99	0.42
15:U:803:LYS:HB2	15:U:838:LYS:HB2	2.01	0.42
16:V:183:GLU:HA	16:V:186:LYS:HB3	2.01	0.42
17:W:135:LYS:HB2	17:W:137:TYR:HD1	1.85	0.42
17:W:144:ARG:HA	17:W:147:LYS:HG2	2.02	0.42
18:X:409:LYS:NZ	23:c:267:PRO:HG2	2.32	0.42
19:Y:262:SER:O	19:Y:266:CYS:N	2.53	0.42
23:c:122:LEU:H	23:c:192:LEU:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:39:SER:OG	1:g:168:ALA:O	2.23	0.42
9:o:17:ASP:O	9:o:33:LYS:NZ	2.38	0.42
12:r:104:TRP:NE1	12:r:181:GLU:HG3	2.35	0.42
12:r:158:ARG:HH12	12:r:199:TYR:HB3	1.85	0.42
26:A:285:PHE:CD2	27:B:302:GLU:HG2	2.54	0.42
27:B:219:PRO:O	27:B:326:LYS:NZ	2.51	0.42
27:B:428:TYR:O	28:C:314:LYS:NZ	2.32	0.42
28:C:338:LEU:HB3	28:C:342:ILE:HD13	2.02	0.42
30:E:228:CYS:SG	30:E:229:ILE:N	2.92	0.42
6:L:122:ARG:HG2	7:M:128:VAL:HG12	2.02	0.42
16:V:269:LYS:O	16:V:273:LYS:N	2.52	0.42
18:X:337:ARG:NH1	18:X:354:ILE:HD12	2.35	0.42
19:Y:251:HIS:HA	19:Y:257:ARG:HD3	2.00	0.42
21:a:374:ILE:HG22	24:d:251:ARG:HG3	2.01	0.42
22:b:34:ASN:O	22:b:38:HIS:ND1	2.35	0.42
9:o:98:LEU:HB2	9:o:113:ILE:HB	2.02	0.42
26:A:355:PHE:HD2	26:A:370:PHE:HB3	1.85	0.42
29:D:181:VAL:HG22	29:D:306:LYS:CG	2.50	0.42
30:E:385:ASP:OD1	30:E:385:ASP:N	2.53	0.42
32:f:402:ASN:OD1	32:f:403:LYS:N	2.52	0.42
5:K:101:PHE:O	12:R:57:ARG:NH2	2.45	0.42
7:M:67:PHE:HB2	7:M:75:MET:HB2	2.01	0.42
15:U:147:TYR:OH	15:U:172:ASP:OD2	2.25	0.42
16:V:131:LEU:HD23	16:V:134:PHE:HD2	1.85	0.42
17:W:395:ASN:HA	17:W:398:VAL:HG22	2.01	0.42
20:Z:136:GLU:HG2	20:Z:157:HIS:HE1	1.84	0.42
21:a:62:ASN:HA	21:a:65:SER:HB3	2.02	0.42
21:a:308:GLU:HB3	21:a:312:MET:HE2	2.01	0.42
11:q:7:ILE:HG12	11:q:143:LEU:HD21	2.01	0.42
26:A:194:PRO:HB3	26:A:201:PHE:HE2	1.85	0.42
28:C:231:VAL:HG23	28:C:276:LEU:HD22	2.02	0.42
30:E:216:ARG:HD2	30:E:263:GLN:HE22	1.85	0.42
32:f:613:LEU:HD12	32:f:613:LEU:C	2.44	0.42
32:f:688:ARG:HA	32:f:745:LEU:CB	2.49	0.42
3:I:105:ILE:HD11	3:I:109:GLN:HG3	2.01	0.42
3:I:159:TRP:CE3	4:J:54:GLN:HB3	2.54	0.42
10:P:126:LEU:HD12	10:P:127:ILE:HG23	2.00	0.42
15:U:599:ILE:HD12	15:U:599:ILE:HA	1.93	0.42
15:U:650:TYR:HA	15:U:683:VAL:HG23	2.02	0.42
16:V:442:ILE:O	16:V:444:ASP:N	2.53	0.42
19:Y:51:ALA:HA	19:Y:54:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:247:LEU:O	19:Y:251:HIS:CB	2.63	0.42
23:c:33:ILE:HA	23:c:69:VAL:HG12	2.00	0.42
1:g:122:SER:O	1:g:126:THR:OG1	2.35	0.42
26:A:224:LEU:O	26:A:228:ALA:HB2	2.20	0.42
27:B:369:THR:HA	27:B:372:MET:HG2	2.01	0.42
28:C:250:GLU:HB2	28:C:293:MET:HE3	2.01	0.42
29:D:155:THR:OG1	29:D:158:GLN:OE1	2.37	0.42
29:D:300:ASP:C	29:D:302:ASN:N	2.77	0.42
31:F:134:LEU:HD11	31:F:160:ILE:HD12	2.01	0.42
1:G:123:GLN:O	1:G:127:GLN:N	2.41	0.41
5:K:21:LEU:HA	5:K:22:PHE:HB2	2.02	0.41
13:S:29:LEU:HB3	13:S:37:THR:HG22	2.01	0.41
16:V:246:GLY:O	16:V:249:THR:OG1	2.26	0.41
2:h:119:GLN:O	2:h:122:THR:OG1	2.26	0.41
6:l:104:PRO:HD2	6:l:107:ARG:HD2	2.02	0.41
13:s:186:ASP:OD2	13:s:189:THR:OG1	2.30	0.41
26:A:97:ARG:HG2	27:B:131:HIS:CE1	2.55	0.41
29:D:255:LYS:HE2	29:D:303:VAL:HG13	2.02	0.41
31:F:177:VAL:HG11	31:F:248:PHE:HD2	1.84	0.41
4:J:131:ALA:N	4:J:147:THR:OG1	2.43	0.41
6:L:189:LYS:NZ	6:L:193:ARG:HH12	2.19	0.41
9:O:132:LEU:HB3	14:t:145:LEU:HD23	2.03	0.41
15:U:607:VAL:HG11	29:D:63:ASP:HB3	2.02	0.41
15:U:640:LEU:HA	15:U:640:LEU:HD23	1.90	0.41
17:W:189:GLN:HA	17:W:192:LEU:HD12	2.02	0.41
17:W:243:ILE:HA	17:W:246:HIS:HB3	2.02	0.41
17:W:438:LEU:HD23	17:W:441:LYS:HG3	2.01	0.41
21:a:13:ASN:HB3	21:a:19:PRO:HG3	2.02	0.41
5:k:89:ILE:HD13	5:k:89:ILE:HA	1.91	0.41
26:A:190:VAL:HG21	26:A:212:VAL:HG21	2.02	0.41
28:C:70:GLY:HA3	29:D:113:VAL:HG12	2.03	0.41
29:D:327:LEU:HD23	29:D:327:LEU:HA	1.95	0.41
30:E:114:GLU:HG3	30:E:115:VAL:HG22	2.02	0.41
32:f:333:LEU:HD23	32:f:338:ASP:HB3	2.02	0.41
32:f:338:ASP:HA	32:f:341:GLU:HG3	2.02	0.41
12:R:122:SER:OG	12:R:123:GLY:N	2.54	0.41
17:W:136:ILE:HB	17:W:175:GLY:HA3	2.03	0.41
17:W:273:TYR:HA	17:W:276:LEU:HD13	2.01	0.41
20:Z:68:TRP:CD1	20:Z:104:ASN:HD21	2.38	0.41
21:a:115:LYS:HD3	21:a:118:ILE:HD12	2.02	0.41
21:a:122:LYS:HA	21:a:125:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:277:LEU:HA	21:a:280:MET:HG2	2.01	0.41
5:k:210:LEU:HA	5:k:214:ASN:HD22	1.84	0.41
27:B:223:ILE:HG13	27:B:347:ILE:HG21	2.02	0.41
27:B:389:ASP:OD1	27:B:389:ASP:N	2.53	0.41
29:D:200:ARG:HH22	29:D:301:GLN:HA	1.84	0.41
29:D:255:LYS:NZ	29:D:303:VAL:HA	2.36	0.41
30:E:230:ILE:HB	30:E:275:MET:HA	2.02	0.41
32:f:86:THR:HG23	32:f:87:THR:H	1.85	0.41
32:f:389:LYS:CD	32:f:389:LYS:N	2.83	0.41
1:G:58:ASP:HB3	1:G:61:LEU:HB2	2.01	0.41
2:H:181:ASP:OD1	2:H:181:ASP:N	2.49	0.41
3:I:140:ASP:OD1	3:I:144:GLY:N	2.51	0.41
10:P:45:MET:HE3	10:P:71:LEU:HD22	2.03	0.41
11:Q:7:ILE:N	11:Q:14:LEU:O	2.53	0.41
15:U:146:LYS:HB3	15:U:149:GLN:HG2	2.02	0.41
15:U:250:PHE:O	15:U:254:GLU:CB	2.67	0.41
16:V:101:LEU:O	16:V:103:SER:N	2.54	0.41
16:V:400:HIS:HA	16:V:403:ILE:HG22	2.02	0.41
19:Y:189:VAL:HG13	19:Y:287:LEU:HD13	2.02	0.41
21:a:268:LEU:HD23	21:a:271:LYS:HD3	2.01	0.41
21:a:269:LEU:HD22	21:a:301:LYS:HD2	2.03	0.41
21:a:356:TRP:HH2	23:c:309:PHE:HA	1.85	0.41
22:b:34:ASN:HD22	22:b:38:HIS:HE1	1.68	0.41
4:j:55:ASP:OD1	4:j:56:GLU:N	2.53	0.41
5:k:99:HIS:O	5:k:103:TYR:HB2	2.20	0.41
7:m:136:MET:HE3	7:m:148:LEU:HD11	2.01	0.41
12:r:182:ASP:OD1	12:r:182:ASP:N	2.52	0.41
26:A:255:ARG:O	26:A:259:GLU:HG2	2.20	0.41
26:A:414:ASN:O	26:A:419:SER:N	2.41	0.41
27:B:183:THR:HG22	27:B:184:TYR:H	1.85	0.41
29:D:226:ALA:O	29:D:260:ALA:HA	2.20	0.41
30:E:139:SER:OG	30:E:140:GLU:N	2.54	0.41
32:f:479:LEU:HD11	32:f:514:VAL:HG23	2.03	0.41
32:f:533:ASP:OD1	32:f:533:ASP:N	2.53	0.41
1:G:31:ALA:HB1	1:G:83:MET:HE3	2.02	0.41
7:M:216:VAL:HB	7:M:224:HIS:CD2	2.56	0.41
9:O:136:ALA:HB2	14:t:179:ARG:HH22	1.85	0.41
14:T:145:LEU:HD23	9:o:132:LEU:HB3	2.02	0.41
16:V:210:CYS:HA	16:V:213:TYR:HD2	1.85	0.41
17:W:259:GLU:HG3	17:W:262:LYS:H	1.85	0.41
18:X:172:LEU:HD12	18:X:175:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:139:ILE:HB	20:Z:158:VAL:HG23	2.01	0.41
23:c:249:LEU:HD11	23:c:298:GLN:HB2	2.02	0.41
6:l:153:TYR:OH	7:m:85:ARG:NH1	2.54	0.41
27:B:297:SER:HB2	27:B:301:GLY:HA3	2.02	0.41
27:B:355:LEU:HA	27:B:356:PRO:HD3	1.93	0.41
28:C:72:TYR:HB2	28:C:116:LEU:HB3	2.01	0.41
28:C:185:GLY:O	28:C:312:ASP:N	2.41	0.41
29:D:253:LEU:HA	29:D:256:GLU:HB3	2.03	0.41
31:F:151:VAL:HG12	31:F:163:THR:HA	2.01	0.41
32:f:8:LYS:HD3	32:f:39:LYS:HD2	2.02	0.41
32:f:512:MET:HE1	32:f:554:TYR:HA	2.02	0.41
32:f:635:LYS:HD3	32:f:641:GLU:HG2	2.01	0.41
8:N:35:THR:OG1	8:N:45:ARG:NH2	2.53	0.41
10:P:22:ILE:HG23	10:P:188:HIS:HB2	2.03	0.41
17:W:444:HIS:HD2	17:W:448:LYS:HZ1	1.67	0.41
18:X:394:ASP:OD1	23:c:257:LYS:NZ	2.34	0.41
21:a:180:LEU:HD11	21:a:219:HIS:CD2	2.56	0.41
1:g:58:ASP:HB3	1:g:61:LEU:HB2	2.02	0.41
6:l:50:LYS:HE2	6:l:61:LYS:HA	2.03	0.41
8:n:144:ARG:H	8:n:147:MET:HE3	1.86	0.41
29:D:181:VAL:HG22	29:D:306:LYS:HG2	2.02	0.41
32:f:298:LEU:HA	32:f:301:HIS:CD2	2.55	0.41
3:I:229:LYS:N	3:I:232:GLU:OE2	2.54	0.41
15:U:257:SER:HB2	15:U:486:MET:HE1	2.02	0.41
15:U:493:VAL:HG22	15:U:497:LEU:HD22	2.03	0.41
16:V:32:PRO:O	16:V:36:GLU:CB	2.68	0.41
16:V:255:LEU:HD13	16:V:291:TYR:HB3	2.03	0.41
16:V:468:SER:O	20:Z:261:TYR:OH	2.27	0.41
18:X:325:LYS:HD3	18:X:325:LYS:HA	1.82	0.41
19:Y:32:ARG:HD3	19:Y:38:ARG:HH22	1.86	0.41
21:a:293:PHE:HA	21:a:296:ILE:HD13	2.03	0.41
23:c:175:ARG:HG2	23:c:181:LEU:HD13	2.03	0.41
1:g:212:PRO:HB3	1:g:235:ILE:HG22	2.02	0.41
2:h:105:ILE:HG12	2:h:110:LEU:HD12	2.03	0.41
4:j:221:ASN:HA	4:j:222:PRO:HD3	1.90	0.41
5:k:104:ASN:OD1	12:r:57:ARG:NH1	2.50	0.41
7:m:201:HIS:CE1	7:m:206:ASP:H	2.38	0.41
8:n:18:SER:HB2	8:n:31:THR:H	1.86	0.41
26:A:395:PHE:HA	26:A:398:ARG:HD2	2.02	0.41
27:B:111:THR:N	27:B:124:SER:O	2.53	0.41
27:B:210:TYR:O	27:B:214:MET:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:55:LYS:HA	28:C:58:LEU:HB2	2.01	0.41
7:M:58:TYR:OH	7:M:62:SER:O	2.39	0.41
16:V:255:LEU:HD12	16:V:269:LYS:HE2	2.03	0.41
18:X:275:LEU:HD12	18:X:278:ARG:HB3	2.02	0.41
19:Y:60:SER:OG	19:Y:61:LEU:N	2.49	0.41
21:a:145:LEU:O	21:a:147:GLY:N	2.52	0.41
21:a:280:MET:HE1	21:a:296:ILE:HG13	2.03	0.41
4:j:175:ASN:HD21	4:j:190:LEU:HG	1.86	0.41
26:A:238:ILE:N	26:A:271:LEU:O	2.54	0.41
30:E:145:LEU:HD23	30:E:187:VAL:HB	2.03	0.41
30:E:151:LEU:O	30:E:154:THR:OG1	2.28	0.41
32:f:170:TRP:CZ3	32:f:208:LEU:HB3	2.56	0.41
32:f:392:THR:CG2	32:f:417:ILE:CG2	2.94	0.41
3:I:180:LYS:HD3	3:I:192:LEU:HD13	2.03	0.41
3:I:245:ALA:O	3:I:249:ARG:NH2	2.54	0.41
4:J:90:GLU:HG2	4:J:110:TYR:CG	2.56	0.41
5:K:167:ALA:H	6:L:56:LEU:HD13	1.86	0.41
5:K:241:ILE:HD12	5:K:241:ILE:HA	1.97	0.41
12:R:40:TYR:HB3	12:R:73:ARG:HH21	1.85	0.41
14:T:141:TYR:HA	14:T:144:TYR:HD2	1.86	0.41
15:U:43:ASP:OD1	15:U:43:ASP:N	2.52	0.41
15:U:619:VAL:HG23	15:U:651:GLY:HA3	2.02	0.41
17:W:231:ILE:HD13	17:W:250:ILE:HG22	2.03	0.41
17:W:444:HIS:HD2	17:W:448:LYS:NZ	2.19	0.41
20:Z:83:LYS:HD2	20:Z:87:ALA:HA	2.03	0.41
21:a:36:GLN:HE22	22:b:145:GLU:HG3	1.85	0.41
21:a:252:LYS:HA	21:a:252:LYS:HD2	1.95	0.41
21:a:303:THR:HG23	21:a:305:ASN:H	1.86	0.41
22:b:142:ASN:HB2	22:b:172:THR:HA	2.02	0.41
24:d:51:ALA:HA	24:d:54:ILE:HG12	2.03	0.41
3:i:114:LEU:HD12	3:i:114:LEU:HA	1.93	0.41
3:i:118:LYS:HE2	3:i:152:PRO:HA	2.03	0.41
5:k:44:GLU:OE1	5:k:191:LEU:N	2.54	0.41
7:m:58:TYR:OH	7:m:62:SER:O	2.39	0.41
7:m:216:VAL:HB	7:m:224:HIS:CD2	2.56	0.41
13:s:49:LYS:HD2	13:s:113:LEU:HB2	2.03	0.41
14:t:25:ASP:HA	14:t:187:PHE:HA	2.03	0.41
27:B:103:ARG:HA	27:B:160:ILE:HG12	2.02	0.41
28:C:192:PRO:HG2	28:C:319:PRO:HG3	2.02	0.41
28:C:220:VAL:O	28:C:223:PHE:N	2.40	0.41
29:D:94:GLU:O	29:D:102:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:238:ILE:HD12	30:E:238:ILE:HA	1.97	0.41
31:F:198:LEU:HD22	31:F:202:ILE:HD12	2.02	0.41
31:F:305:GLU:HA	31:F:308:ARG:HB2	2.03	0.41
31:F:431:LYS:HA	31:F:431:LYS:HD3	1.91	0.41
32:f:374:SER:O	32:f:375:SER:C	2.59	0.41
32:f:620:PHE:HD2	32:f:623:LYS:HG2	1.85	0.41
32:f:687:ARG:O	32:f:745:LEU:HD22	2.21	0.41
32:f:698:SER:OG	32:f:716:ASP:OD1	2.36	0.41
7:M:52:LEU:HA	7:M:209:PHE:HA	2.02	0.41
7:M:66:LEU:HD13	7:M:214:SER:HB2	2.02	0.41
10:P:17:LYS:HB2	10:P:158:MET:H	1.86	0.41
10:P:158:MET:HE2	10:P:163:LEU:HA	2.02	0.41
15:U:895:PRO:HB2	15:U:898:CYS:HB2	2.03	0.41
16:V:56:ALA:HB2	16:V:201:ARG:HH11	1.86	0.41
17:W:118:LEU:HA	17:W:121:LYS:HE3	2.02	0.41
17:W:317:TRP:CD1	17:W:358:VAL:HG11	2.56	0.41
20:Z:109:ASN:HA	20:Z:112:MET:HG2	2.04	0.41
20:Z:240:VAL:HG13	21:a:352:ARG:HH22	1.86	0.41
23:c:193:ILE:O	23:c:196:LEU:C	2.64	0.41
6:l:201:ALA:O	6:l:239:ARG:NH1	2.53	0.41
7:m:36:ALA:O	7:m:165:ILE:N	2.50	0.41
7:m:69:VAL:H	7:m:74:GLY:HA2	1.86	0.41
8:n:166:ARG:HA	8:n:166:ARG:HD3	1.91	0.41
9:o:200:GLY:HA3	9:o:201:ARG:HA	1.76	0.41
26:A:358:HIS:CE1	26:A:386:ARG:HB2	2.55	0.41
27:B:303:ARG:HB3	28:C:222:LYS:HE3	2.02	0.41
29:D:342:ARG:HG3	29:D:364:VAL:HG11	2.03	0.41
32:f:81:GLN:O	32:f:85:SER:HB2	2.21	0.41
1:G:103:TYR:HB2	8:N:61:TYR:CD1	2.56	0.40
15:U:580:ARG:NH2	15:U:768:GLN:HG3	2.36	0.40
15:U:703:CYS:HA	15:U:704:PRO:HD3	1.91	0.40
16:V:357:LEU:HB2	16:V:360:TYR:HB3	2.01	0.40
17:W:356:ASN:O	17:W:360:GLU:CB	2.69	0.40
19:Y:141:VAL:HG13	19:Y:160:ASN:HB2	2.03	0.40
20:Z:58:PHE:CE1	20:Z:68:TRP:HB2	2.56	0.40
24:d:183:GLU:HB3	24:d:184:LYS:H	1.60	0.40
24:d:238:PRO:HA	24:d:241:GLU:HG2	2.03	0.40
3:i:72:MET:HB2	3:i:72:MET:HE3	1.88	0.40
3:i:245:ALA:HA	3:i:248:GLU:HG2	2.02	0.40
4:j:40:ILE:HA	4:j:212:ARG:HA	2.03	0.40
5:k:227:HIS:NE2	5:k:229:PHE:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:o:172:ASN:HB3	9:o:191:VAL:HG22	2.03	0.40
11:q:43:LEU:HA	11:q:43:LEU:HD23	1.89	0.40
27:B:230:THR:HG21	27:B:353:PHE:HB3	2.03	0.40
28:C:148:TYR:HD1	28:C:148:TYR:HA	1.72	0.40
4:J:122:ASN:HD21	5:K:125:GLU:HB3	1.86	0.40
5:K:46:VAL:HG23	5:K:151:PRO:HB2	2.03	0.40
5:K:227:HIS:CE1	5:K:229:PHE:HB3	2.56	0.40
6:L:121:GLN:HE22	7:M:131:PHE:HE1	1.69	0.40
11:Q:37:LYS:O	11:Q:61:GLN:NE2	2.44	0.40
14:T:114:GLY:O	14:T:121:PHE:N	2.52	0.40
15:U:141:CYS:HB3	15:U:149:GLN:HB3	2.01	0.40
15:U:191:LYS:HA	15:U:194:ARG:HB3	2.03	0.40
16:V:203:LEU:O	16:V:207:ALA:CB	2.69	0.40
17:W:86:ASN:O	17:W:88:MET:HG3	2.21	0.40
18:X:227:THR:HA	29:D:343:LEU:HD21	2.03	0.40
19:Y:267:ARG:HD2	19:Y:267:ARG:HA	1.92	0.40
19:Y:325:VAL:HG21	25:e:66:LYS:HB3	2.02	0.40
20:Z:36:VAL:HA	20:Z:96:HIS:HA	2.01	0.40
22:b:52:ILE:HA	22:b:52:ILE:HD12	1.83	0.40
5:k:157:ASP:OD1	5:k:161:THR:N	2.55	0.40
6:l:215:VAL:HB	6:l:221:PHE:HD1	1.86	0.40
7:m:136:MET:HE3	7:m:136:MET:HB3	1.95	0.40
8:n:151:GLU:O	8:n:155:PHE:HB2	2.21	0.40
26:A:407:LYS:HA	26:A:410:LEU:HD12	2.03	0.40
29:D:68:LEU:HD23	29:D:68:LEU:HA	1.89	0.40
30:E:353:PHE:HA	30:E:356:ARG:HB2	2.03	0.40
3:I:164:ILE:HD12	3:I:164:ILE:HG23	1.91	0.40
5:K:193:GLU:O	5:K:197:SER:OG	2.34	0.40
10:P:58:THR:O	11:Q:85:ARG:NH2	2.54	0.40
11:Q:57:ALA:O	11:Q:61:GLN:CB	2.66	0.40
14:T:67:LEU:HA	14:T:67:LEU:HD23	1.82	0.40
15:U:14:GLU:O	15:U:20:LYS:NZ	2.51	0.40
15:U:22:PHE:HE2	24:d:31:LEU:HA	1.86	0.40
15:U:789:ILE:HB	15:U:911:ILE:HA	2.04	0.40
19:Y:372:LYS:HB3	19:Y:376:LEU:HD13	2.03	0.40
19:Y:377:LEU:HA	19:Y:380:VAL:HG22	2.03	0.40
23:c:219:ASN:O	23:c:223:LYS:CB	2.70	0.40
24:d:39:THR:HG23	24:d:45:LYS:HD2	2.02	0.40
24:d:215:TRP:O	24:d:217:LEU:N	2.54	0.40
1:g:165:ALA:HB1	1:g:179:LEU:HD13	2.02	0.40
34:A:501:AGS:O1B	27:B:346:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:344:ILE:CG1	34:D:501:AGS:N1	2.84	0.40
31:F:154:ASN:OD1	31:F:155:LYS:N	2.55	0.40
32:f:553:THR:HA	32:f:556:ARG:HE	1.86	0.40
14:T:63:LEU:HD23	14:T:63:LEU:HA	1.82	0.40
18:X:180:LEU:HB3	19:Y:248:GLU:HG3	2.04	0.40
19:Y:174:TRP:NE1	19:Y:178:ASN:HD21	2.20	0.40
20:Z:14:LEU:HA	23:c:39:LEU:HD13	2.04	0.40
22:b:100:ARG:HH12	22:b:103:LYS:HA	1.87	0.40
24:d:194:ALA:HA	24:d:199:PHE:CZ	2.56	0.40
9:o:67:SER:HB3	9:o:74:PRO:HG3	2.02	0.40
26:A:218:PRO:HB2	27:B:343:ARG:HD2	2.02	0.40
26:A:273:PHE:HD1	26:A:318:LEU:HB2	1.86	0.40
28:C:219:LEU:HA	28:C:219:LEU:HD13	1.74	0.40
29:D:354:LEU:O	29:D:356:GLU:N	2.47	0.40
30:E:242:ARG:NH1	30:E:282:PRO:HA	2.37	0.40
32:f:86:THR:O	32:f:87:THR:HB	2.21	0.40
32:f:88:SER:CB	32:f:92:VAL:CG2	2.90	0.40
32:f:89:MET:SD	32:f:89:MET:N	2.94	0.40
2:H:74:LEU:HD21	2:H:134:LEU:HD22	2.03	0.40
4:J:32:ALA:HB3	4:J:161:ILE:HD11	2.03	0.40
4:J:156:TRP:CD1	5:K:59:MET:HA	2.56	0.40
15:U:358:ASP:OD1	15:U:358:ASP:N	2.51	0.40
15:U:375:PHE:HE1	15:U:780:SER:HB3	1.86	0.40
15:U:559:ARG:NH1	15:U:562:GLU:OE1	2.54	0.40
16:V:148:ARG:NH1	16:V:198:GLN:HB2	2.36	0.40
16:V:293:GLY:HA3	16:V:309:MET:SD	2.61	0.40
17:W:437:SER:O	17:W:441:LYS:HG2	2.22	0.40
18:X:379:ASP:HB3	18:X:385:LEU:HA	2.04	0.40
21:a:79:ILE:O	21:a:83:VAL:HG23	2.21	0.40
21:a:234:ILE:HA	21:a:237:LEU:HB2	2.02	0.40
21:a:252:LYS:HD2	21:a:255:TRP:CD1	2.57	0.40
23:c:75:MET:HE3	23:c:76:PRO:HD2	2.02	0.40
30:E:145:LEU:HA	30:E:148:VAL:HG12	2.02	0.40
30:E:214:LEU:HA	30:E:217:GLU:HB3	2.03	0.40
32:f:380:PHE:CD2	32:f:751:TYR:CE2	3.09	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%)	214 (90%)	23 (10%)	0	100	100
1	g	238/240 (99%)	219 (92%)	19 (8%)	0	100	100
2	H	228/232 (98%)	210 (92%)	18 (8%)	0	100	100
2	h	230/232 (99%)	219 (95%)	11 (5%)	0	100	100
3	I	246/250 (98%)	222 (90%)	22 (9%)	2 (1%)	16	52
3	i	248/250 (99%)	218 (88%)	29 (12%)	1 (0%)	30	66
4	J	237/243 (98%)	221 (93%)	15 (6%)	1 (0%)	30	66
4	j	237/243 (98%)	218 (92%)	15 (6%)	4 (2%)	7	35
5	K	224/234 (96%)	204 (91%)	19 (8%)	1 (0%)	30	66
5	k	224/234 (96%)	204 (91%)	19 (8%)	1 (0%)	30	66
6	L	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
6	l	236/238 (99%)	220 (93%)	16 (7%)	0	100	100
7	M	238/245 (97%)	218 (92%)	20 (8%)	0	100	100
7	m	238/245 (97%)	219 (92%)	19 (8%)	0	100	100
8	N	189/191 (99%)	178 (94%)	10 (5%)	1 (0%)	24	62
8	n	189/191 (99%)	178 (94%)	8 (4%)	3 (2%)	7	37
9	O	218/220 (99%)	206 (94%)	12 (6%)	0	100	100
9	o	218/220 (99%)	208 (95%)	10 (5%)	0	100	100
10	P	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
10	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
11	Q	197/199 (99%)	180 (91%)	16 (8%)	1 (0%)	24	62
11	q	197/199 (99%)	183 (93%)	14 (7%)	0	100	100
12	R	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
12	r	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
13	S	211/213 (99%)	198 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	s	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
14	T	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
14	t	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
15	U	798/911 (88%)	737 (92%)	61 (8%)	0	100	100
16	V	441/480 (92%)	371 (84%)	62 (14%)	8 (2%)	6	33
17	W	454/456 (100%)	396 (87%)	54 (12%)	4 (1%)	14	49
18	X	378/380 (100%)	339 (90%)	38 (10%)	1 (0%)	36	71
19	Y	376/378 (100%)	328 (87%)	47 (12%)	1 (0%)	36	71
20	Z	284/286 (99%)	243 (86%)	40 (14%)	1 (0%)	30	66
21	a	371/373 (100%)	314 (85%)	53 (14%)	4 (1%)	11	45
22	b	189/191 (99%)	167 (88%)	21 (11%)	1 (0%)	24	62
23	c	274/287 (96%)	239 (87%)	34 (12%)	1 (0%)	30	66
24	d	255/257 (99%)	206 (81%)	44 (17%)	5 (2%)	6	32
25	e	36/70 (51%)	28 (78%)	8 (22%)	0	100	100
26	A	376/399 (94%)	320 (85%)	53 (14%)	3 (1%)	16	52
27	B	366/389 (94%)	299 (82%)	65 (18%)	2 (0%)	24	62
28	C	359/392 (92%)	304 (85%)	48 (13%)	7 (2%)	6	32
29	D	378/380 (100%)	307 (81%)	63 (17%)	8 (2%)	5	30
30	E	373/375 (100%)	317 (85%)	54 (14%)	2 (0%)	24	62
31	F	372/396 (94%)	329 (88%)	40 (11%)	3 (1%)	16	52
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	10	42
All	All	12904/13558 (95%)	11544 (90%)	1286 (10%)	74 (1%)	23	58

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	196	SER
16	V	198	GLN
17	W	314	LEU
21	a	286	ALA
21	a	340	VAL
24	d	189	ILE
8	n	91	ARG
8	n	92	GLU
27	B	299	SER

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Mol	Chain	Res	Type
28	C	220	VAL
29	D	411	GLU
30	E	303	LEU
31	F	436	GLN
32	f	337	LEU
32	f	364	GLN
32	f	367	SER
32	f	665	GLU
4	J	176	TYR
5	K	10	ARG
16	V	246	GLY
21	a	144	ASN
23	c	287	HIS
24	d	216	VAL
4	j	181	ILE
28	C	219	LEU
32	f	183	PRO
32	f	365	VAL
16	V	443	ARG
16	V	458	VAL
18	X	355	LYS
19	Y	350	VAL
24	d	232	PRO
5	k	11	GLY
26	A	431	THR
32	f	184	LEU
32	f	326	LEU
3	I	7	SER
8	N	19	ARG
11	Q	72	GLY
16	V	467	TYR
17	W	87	ILE
8	n	19	ARG
26	A	423	PHE
28	C	143	VAL
29	D	409	LYS
31	F	428	GLN
17	W	139	GLU
17	W	313	GLU
21	a	143	ASN
24	d	3	GLU
24	d	183	GLU

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Mol	Chain	Res	Type
4	j	9	VAL
4	j	97	THR
27	B	356	PRO
29	D	301	GLN
29	D	335	LEU
29	D	355	SER
22	b	23	PRO
4	j	98	VAL
26	A	109	PRO
29	D	82	ILE
29	D	86	PRO
28	C	133	PRO
28	C	144	PRO
28	C	192	PRO
28	C	401	ILE
16	V	101	LEU
3	i	221	GLY
29	D	126	PRO
3	I	221	GLY
16	V	442	ILE
31	F	87	PRO
20	Z	144	VAL
30	E	226	GLN

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%)	162 (100%)	0	100	100
2	h	164/190 (86%)	164 (100%)	0	100	100
3	I	191/210 (91%)	191 (100%)	0	100	100
3	i	193/210 (92%)	191 (99%)	2 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	152/207 (73%)	149 (98%)	3 (2%)	48	65
4	j	152/207 (73%)	151 (99%)	1 (1%)	76	78
5	K	187/196 (95%)	187 (100%)	0	100	100
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%)	191 (100%)	1 (0%)	81	81
7	m	192/202 (95%)	191 (100%)	1 (0%)	81	81
8	N	148/148 (100%)	148 (100%)	0	100	100
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%)	162 (99%)	2 (1%)	63	73
11	q	164/170 (96%)	160 (98%)	4 (2%)	43	63
12	R	153/156 (98%)	152 (99%)	1 (1%)	76	78
12	r	153/156 (98%)	152 (99%)	1 (1%)	76	78
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%)	677 (99%)	8 (1%)	63	73
16	V	387/414 (94%)	382 (99%)	5 (1%)	61	71
17	W	416/416 (100%)	415 (100%)	1 (0%)	87	85
18	X	327/327 (100%)	321 (98%)	6 (2%)	51	66
19	Y	334/334 (100%)	334 (100%)	0	100	100
20	Z	257/257 (100%)	254 (99%)	3 (1%)	63	73
21	a	333/333 (100%)	328 (98%)	5 (2%)	57	70
22	b	167/167 (100%)	167 (100%)	0	100	100
23	c	243/252 (96%)	241 (99%)	2 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d	231/231 (100%)	229 (99%)	2 (1%)	70	75
25	e	38/63 (60%)	38 (100%)	0	100	100
26	A	297/343 (87%)	295 (99%)	2 (1%)	76	78
27	B	300/345 (87%)	298 (99%)	2 (1%)	76	78
28	C	315/340 (93%)	308 (98%)	7 (2%)	45	64
29	D	333/333 (100%)	331 (99%)	2 (1%)	78	80
30	E	298/329 (91%)	295 (99%)	3 (1%)	68	75
31	F	296/340 (87%)	294 (99%)	2 (1%)	76	78
32	f	580/763 (76%)	564 (97%)	16 (3%)	38	59
All	All	10715/11562 (93%)	10628 (99%)	87 (1%)	70	77

All (87) 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
4	J	5	ARG
4	J	7	ILE
4	J	161	ILE
7	M	87	LEU
11	Q	25	ILE
11	Q	171	PHE
12	R	128	VAL
15	U	221	ILE
15	U	268	LEU
15	U	364	VAL
15	U	472	ILE
15	U	496	LEU
15	U	554	LEU
15	U	611	ASN
15	U	913	ILE
16	V	104	THR
16	V	145	LEU
16	V	263	LEU
16	V	318	GLN
16	V	458	VAL
17	W	186	ILE
18	X	50	ILE

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Mol	Chain	Res	Type
18	X	200	ILE
18	X	217	ILE
18	X	341	PRO
18	X	369	ILE
18	X	385	LEU
20	Z	120	VAL
20	Z	237	LEU
20	Z	266	ILE
21	a	33	LEU
21	a	112	ILE
21	a	166	ILE
21	a	234	ILE
21	a	324	ILE
23	c	49	VAL
23	c	62	VAL
24	d	158	ILE
24	d	256	ILE
1	g	66	VAL
1	g	215	ILE
3	i	206	LEU
3	i	228	LEU
4	j	161	ILE
7	m	87	LEU
11	q	4	LEU
11	q	25	ILE
11	q	140	LEU
11	q	167	LEU
12	r	128	VAL
26	A	113	ILE
26	A	403	ILE
27	B	190	LEU
27	B	438	LEU
28	C	57	ARG
28	C	131	VAL
28	C	148	TYR
28	C	151	ILE
28	C	158	ILE
28	C	210	THR
28	C	222	LYS
29	D	115	ILE
29	D	154	LEU
30	E	87	LEU

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Mol	Chain	Res	Type
30	E	105	LEU
30	E	183	LEU
31	F	134	LEU
31	F	416	THR
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 (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	68	HIS
1	G	75	ASN
1	G	123	GLN
1	G	150	GLN
1	G	224	ASN
2	H	95	GLN
2	H	102	GLN
2	H	119	GLN
3	I	20	GLN
3	I	30	HIS
3	I	102	GLN
3	I	109	GLN
3	I	119	GLN
3	I	146	GLN
4	J	54	GLN
4	J	85	ASN
4	J	122	ASN
4	J	154	HIS

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Mol	Chain	Res	Type
5	K	99	HIS
5	K	178	GLN
5	K	214	ASN
6	L	68	ASN
6	L	90	GLN
6	L	146	GLN
7	M	180	GLN
8	N	28	ASN
8	N	158	ASN
11	Q	55	GLN
11	Q	63	ASN
11	Q	71	ASN
11	Q	132	HIS
12	R	38	ASN
13	S	152	GLN
14	T	65	GLN
14	T	213	HIS
15	U	18	GLN
15	U	89	ASN
15	U	111	GLN
15	U	192	GLN
15	U	267	ASN
15	U	345	ASN
15	U	366	HIS
15	U	491	GLN
15	U	503	GLN
15	U	596	ASN
15	U	632	GLN
15	U	685	GLN
15	U	768	GLN
16	V	193	GLN
16	V	318	GLN
16	V	319	HIS
16	V	401	ASN
16	V	473	GLN
17	W	53	GLN
17	W	106	GLN
17	W	203	GLN
17	W	264	GLN
18	X	178	HIS
18	X	292	GLN
18	X	296	ASN

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Mol	Chain	Res	Type
19	Y	273	GLN
19	Y	306	GLN
19	Y	351	ASN
20	Z	32	GLN
20	Z	104	ASN
20	Z	225	GLN
20	Z	243	GLN
20	Z	278	ASN
21	a	46	GLN
21	a	194	GLN
21	a	273	GLN
21	a	372	HIS
22	b	34	ASN
23	c	190	GLN
24	d	102	ASN
24	d	109	GLN
24	d	128	GLN
24	d	252	GLN
25	e	55	GLN
1	g	12	HIS
1	g	75	ASN
2	h	71	HIS
2	h	102	GLN
3	i	119	GLN
3	i	146	GLN
3	i	149	GLN
4	j	92	GLN
5	k	178	GLN
5	k	214	ASN
6	l	53	GLN
6	l	90	GLN
6	l	117	GLN
6	l	146	GLN
7	m	180	GLN
8	n	158	ASN
9	o	62	ASN
9	o	116	HIS
11	q	71	ASN
11	q	101	ASN
11	q	132	HIS
12	r	85	ASN
13	s	58	HIS

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Mol	Chain	Res	Type
13	s	146	GLN
14	t	38	ASN
14	t	81	HIS
14	t	213	HIS
26	A	197	HIS
28	C	36	ASN
28	C	171	HIS
28	C	182	GLN
28	C	205	HIS
28	C	278	ASN
28	C	332	HIS
29	D	137	ASN
29	D	237	GLN
29	D	304	ASN
29	D	340	GLN
30	E	63	GLN
30	E	124	HIS
30	E	300	HIS
30	E	359	HIS
31	F	214	ASN
32	f	12	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	501	-	32,33,33	0.81	1 (3%)	45,52,52	1.12	5 (11%)
34	AGS	D	501	-	32,33,33	0.85	3 (9%)	45,52,52	1.09	2 (4%)
34	AGS	F	501	-	32,33,33	0.89	3 (9%)	45,52,52	1.10	4 (8%)
34	AGS	A	501	-	32,33,33	1.08	3 (9%)	45,52,52	1.20	6 (13%)

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	C	501	-	-	9/21/38/38	0/3/3/3
34	AGS	D	501	-	-	7/21/38/38	0/3/3/3
34	AGS	F	501	-	-	4/21/38/38	0/3/3/3
34	AGS	A	501	-	-	7/21/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	501	AGS	PA-O3A	-3.62	1.55	1.59
34	A	501	AGS	PB-O3B	-2.98	1.56	1.59
34	F	501	AGS	PB-O3B	-2.48	1.56	1.59
34	F	501	AGS	PB-O3A	-2.36	1.56	1.59
34	D	501	AGS	PA-O3A	-2.35	1.57	1.59
34	C	501	AGS	PB-O3A	-2.32	1.57	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	501	AGS	PB-O3B	-2.16	1.57	1.59
34	A	501	AGS	PA-O2A	-2.05	1.45	1.55
34	F	501	AGS	PG-S1G	2.02	1.95	1.90
34	D	501	AGS	PG-S1G	2.01	1.95	1.90

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	501	AGS	PB-O3B-PG	-5.47	113.15	133.17
34	F	501	AGS	PB-O3B-PG	-5.00	114.87	133.17
34	A	501	AGS	PB-O3B-PG	-4.22	117.72	133.17
34	C	501	AGS	PB-O3B-PG	-3.68	119.72	133.17
34	A	501	AGS	C4-N9-C1'	2.91	133.43	126.63
34	C	501	AGS	O2B-PB-O3A	2.86	115.01	107.27
34	C	501	AGS	O3A-PB-O1B	-2.80	102.29	110.70
34	F	501	AGS	O2B-PB-O3A	2.78	114.80	107.27
34	A	501	AGS	O3A-PA-O1A	-2.73	102.49	110.70
34	A	501	AGS	C1'-N9-C8	-2.52	121.50	127.09
34	A	501	AGS	O3B-PB-O1B	-2.30	103.80	110.70
34	C	501	AGS	O2B-PB-O3B	2.29	113.45	107.27
34	D	501	AGS	O2G-PG-O3B	2.25	112.16	104.64
34	F	501	AGS	O2B-PB-O3B	2.11	112.98	107.27
34	F	501	AGS	O3B-PB-O1B	-2.05	104.54	110.70
34	C	501	AGS	C3'-C2'-C1'	2.05	105.34	101.46
34	A	501	AGS	O2B-PB-O3B	2.03	112.77	107.27

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	AGS	C5'-O5'-PA-O1A
34	A	501	AGS	C5'-O5'-PA-O3A
34	C	501	AGS	PB-O3B-PG-O2G
34	C	501	AGS	PB-O3B-PG-O3G
34	C	501	AGS	C5'-O5'-PA-O1A
34	C	501	AGS	C5'-O5'-PA-O2A
34	C	501	AGS	C5'-O5'-PA-O3A
34	D	501	AGS	C5'-O5'-PA-O1A
34	D	501	AGS	C5'-O5'-PA-O3A
34	F	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O2A
34	F	501	AGS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
34	C	501	AGS	O4'-C4'-C5'-O5'
34	C	501	AGS	C3'-C4'-C5'-O5'
34	A	501	AGS	C4'-C5'-O5'-PA
34	D	501	AGS	C4'-C5'-O5'-PA
34	D	501	AGS	PG-O3B-PB-O1B
34	C	501	AGS	PB-O3A-PA-O1A
34	A	501	AGS	C5'-O5'-PA-O2A
34	D	501	AGS	C5'-O5'-PA-O2A
34	A	501	AGS	C2'-C1'-N9-C8
34	D	501	AGS	PA-O3A-PB-O2B
34	A	501	AGS	C2'-C1'-N9-C4
34	F	501	AGS	C4'-C5'-O5'-PA
34	D	501	AGS	PA-O3A-PB-O1B
34	A	501	AGS	PA-O3A-PB-O2B
34	C	501	AGS	PB-O3A-PA-O2A

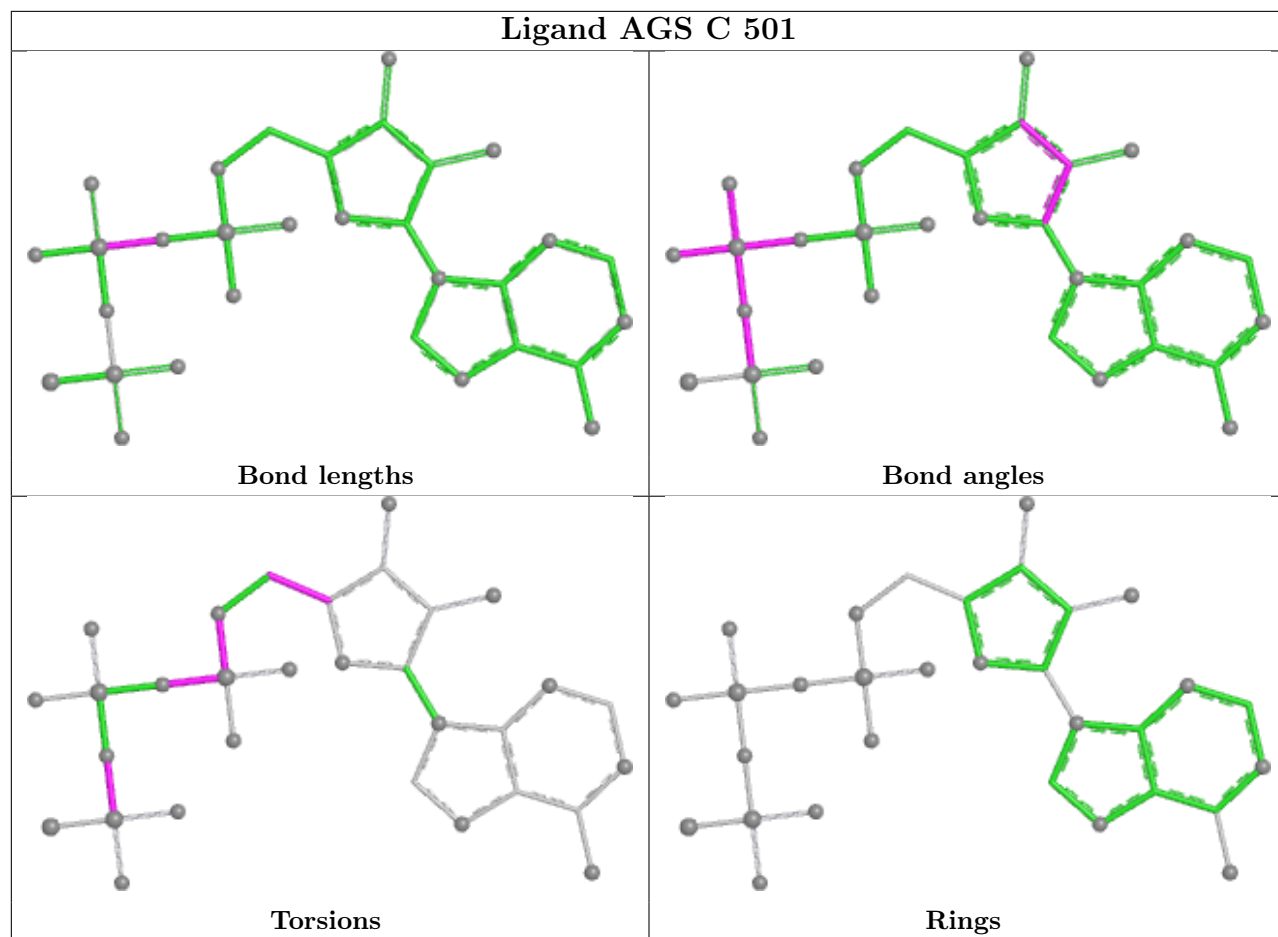
There are no ring outliers.

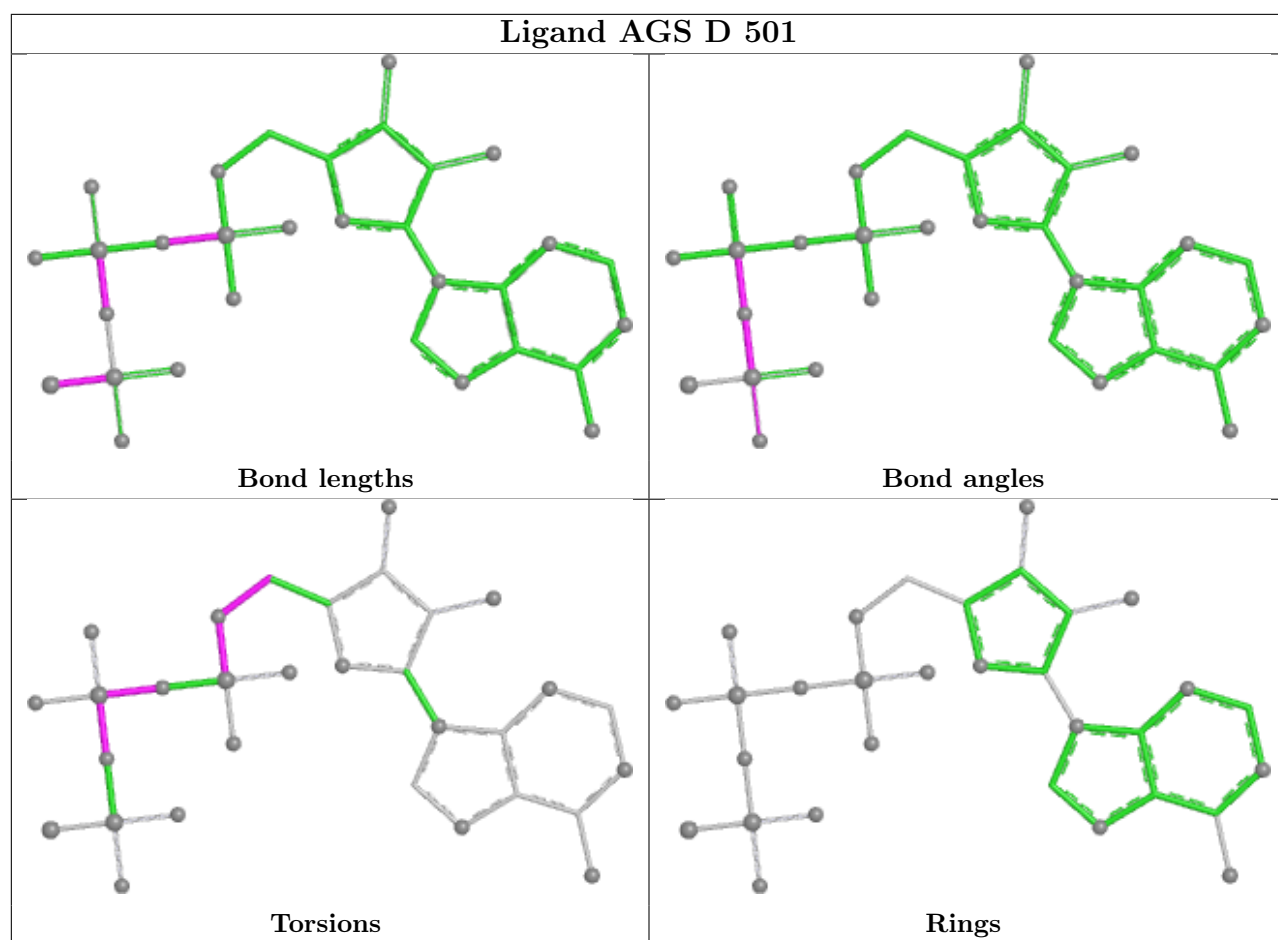
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	501	AGS	3	0
34	D	501	AGS	9	0
34	F	501	AGS	3	0
34	A	501	AGS	5	0

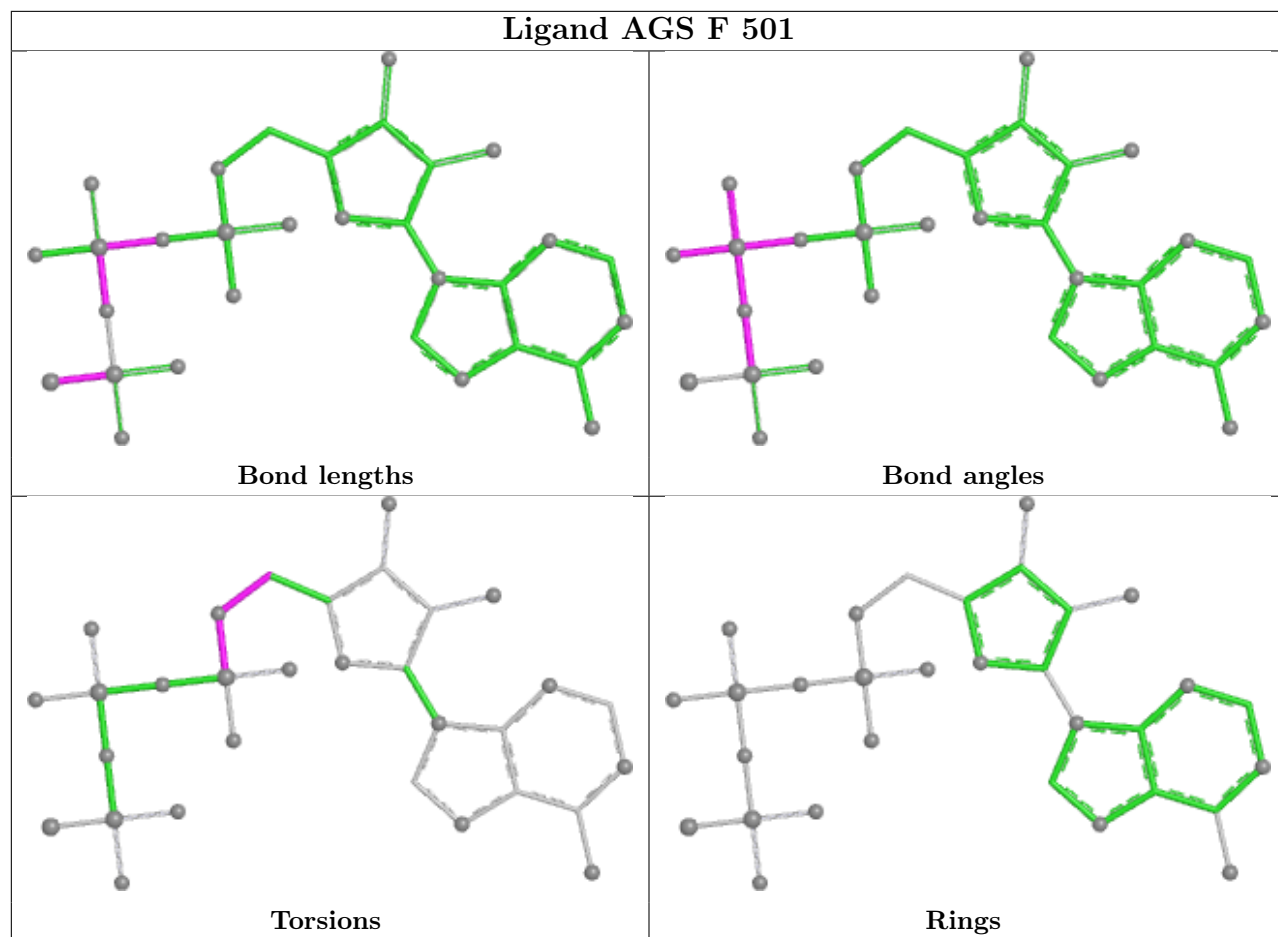
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

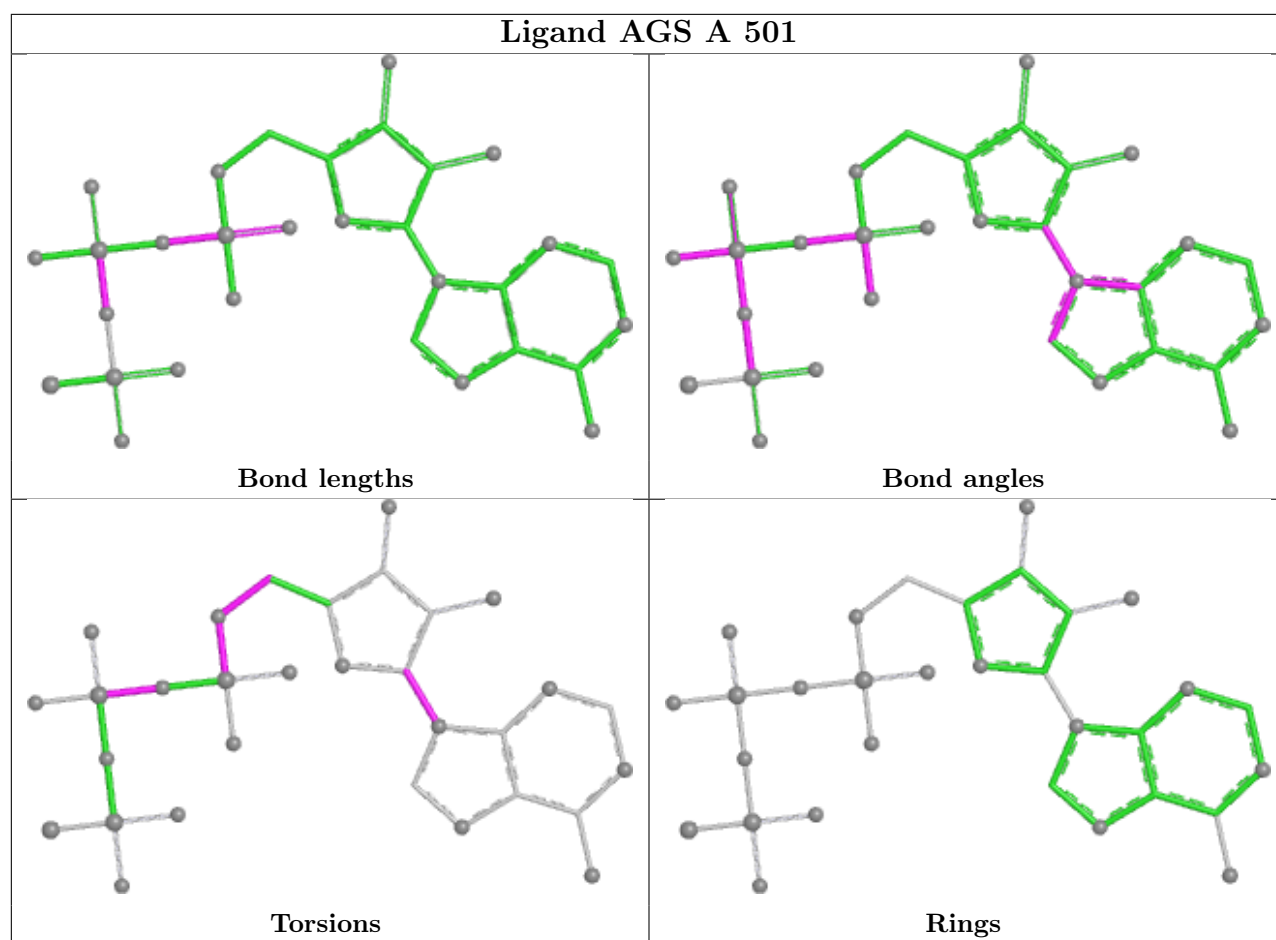
Ligand AGS C 501





Ligand AGS F 501





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.

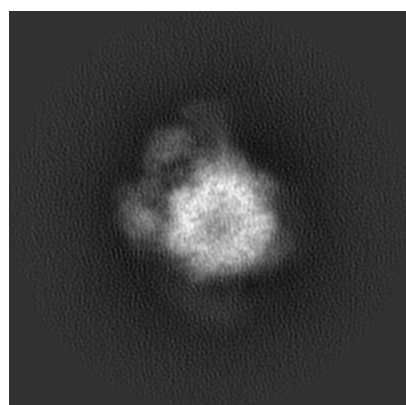
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8664. These allow visual inspection of the internal detail of the map and identification of artifacts.

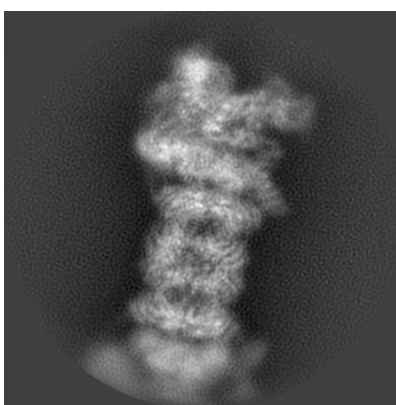
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

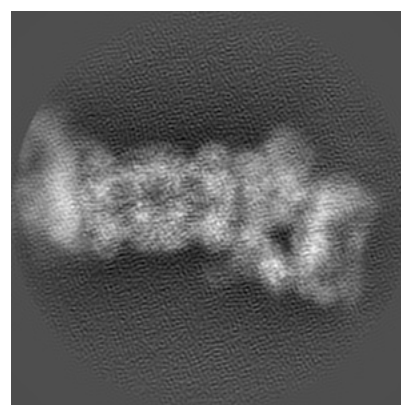
6.1.1 Primary map



X



Y

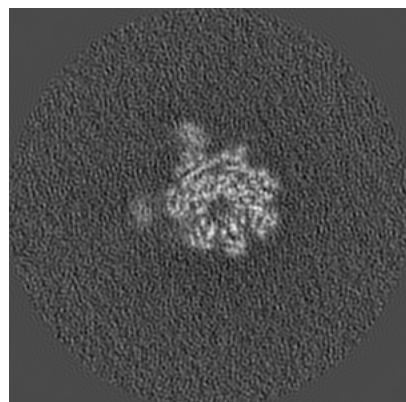


Z

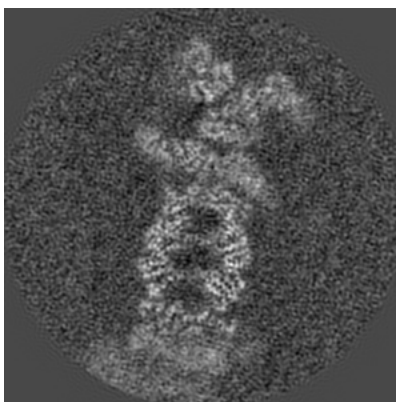
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

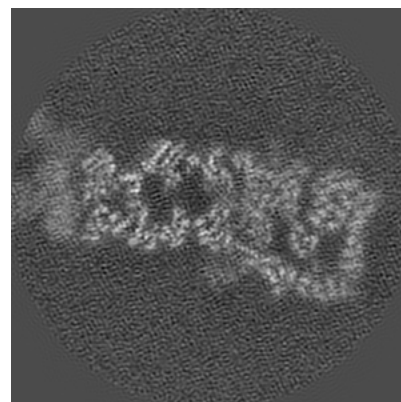
6.2.1 Primary map



X Index: 280



Y Index: 280

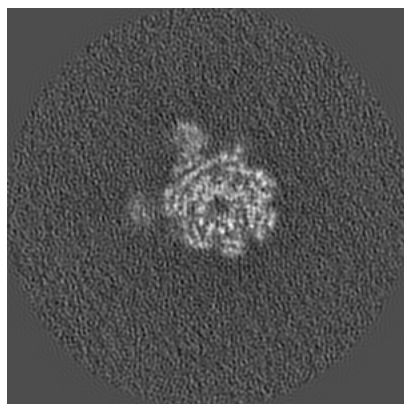


Z Index: 280

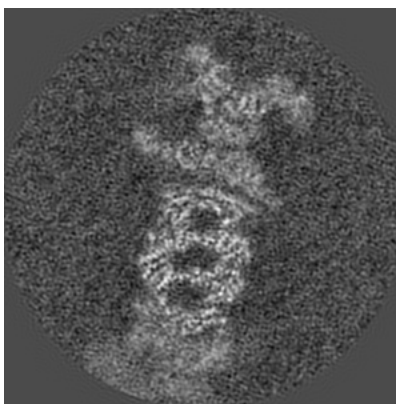
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

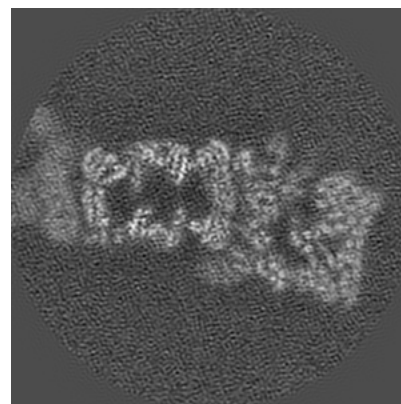
6.3.1 Primary map



X Index: 282



Y Index: 274

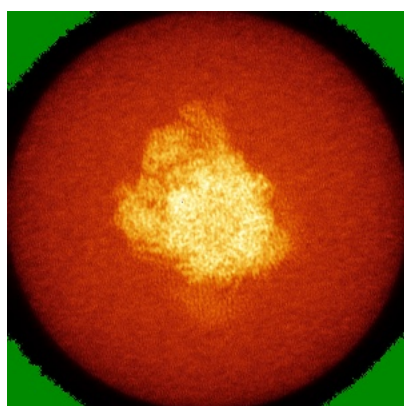


Z Index: 271

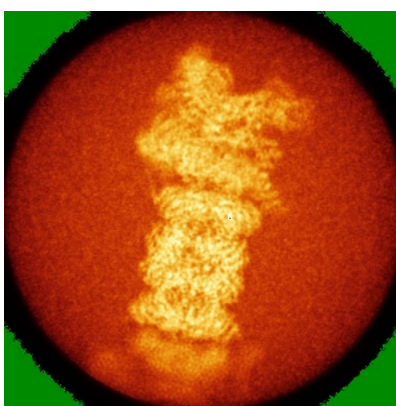
The images above show the largest variance slices of the map in three orthogonal directions.

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

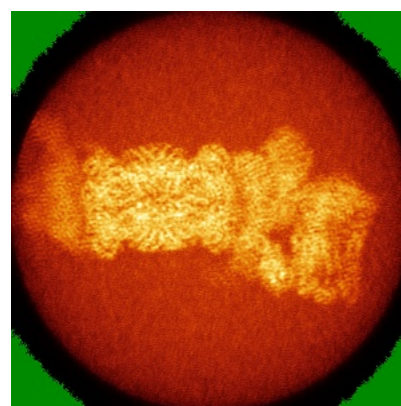
6.4.1 Primary map



X



Y

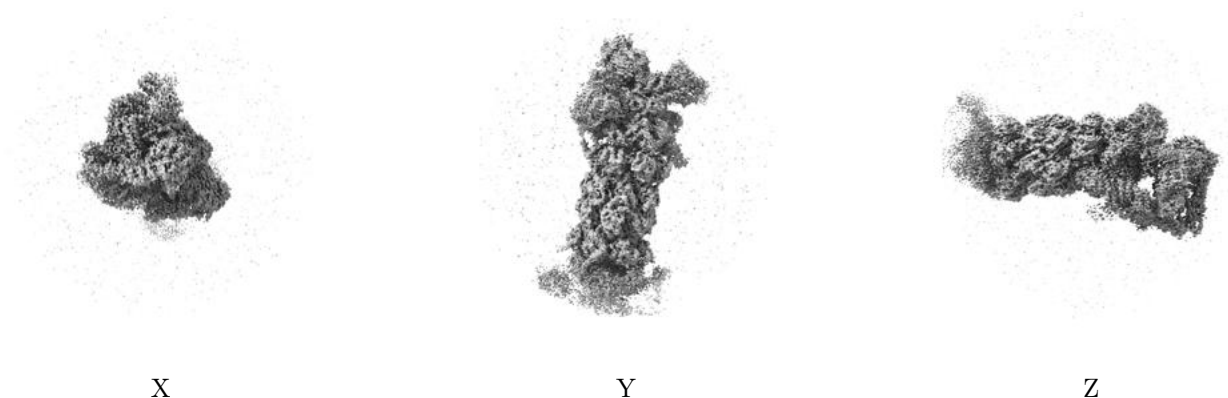


Z

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 0.00577. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

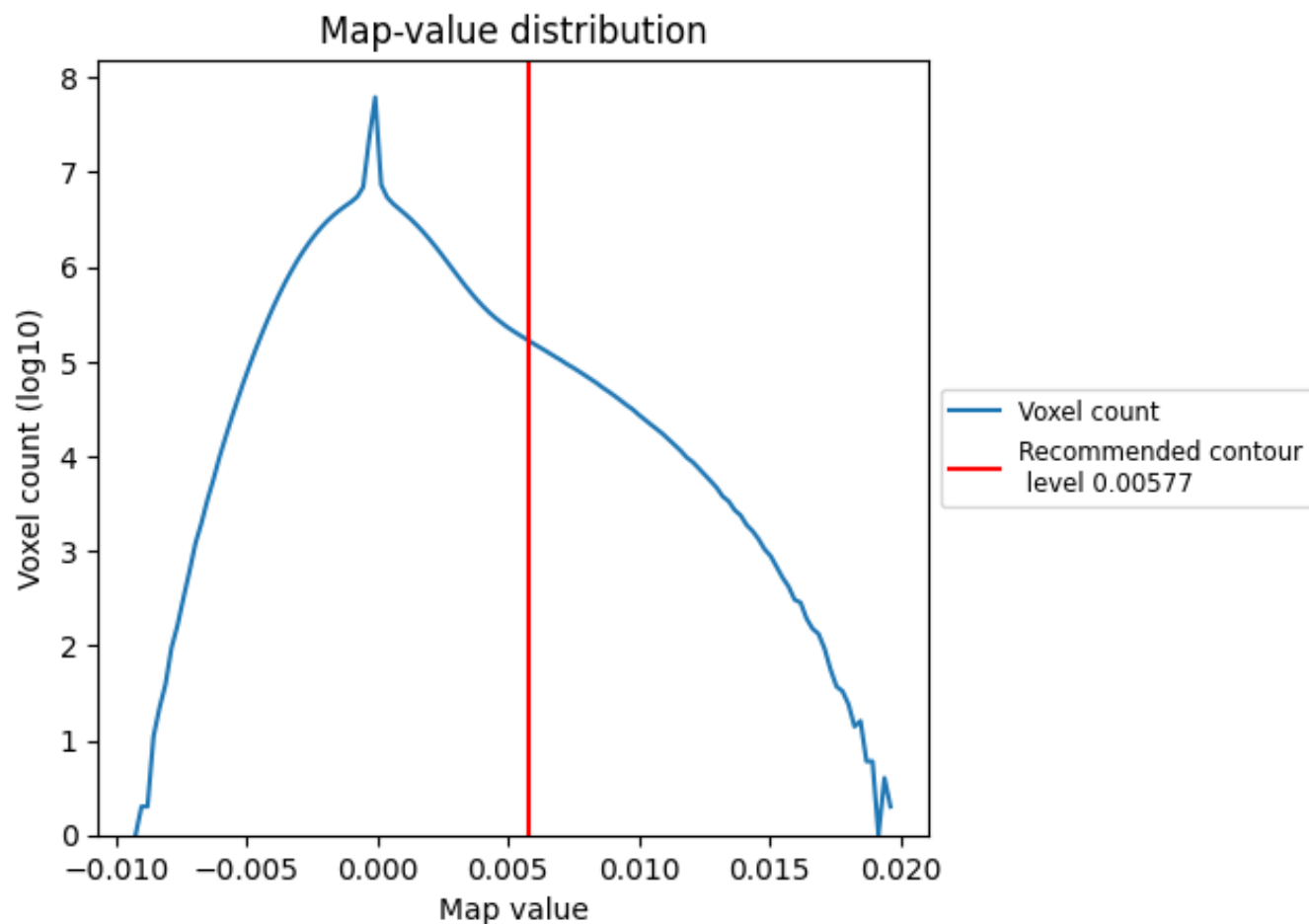
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

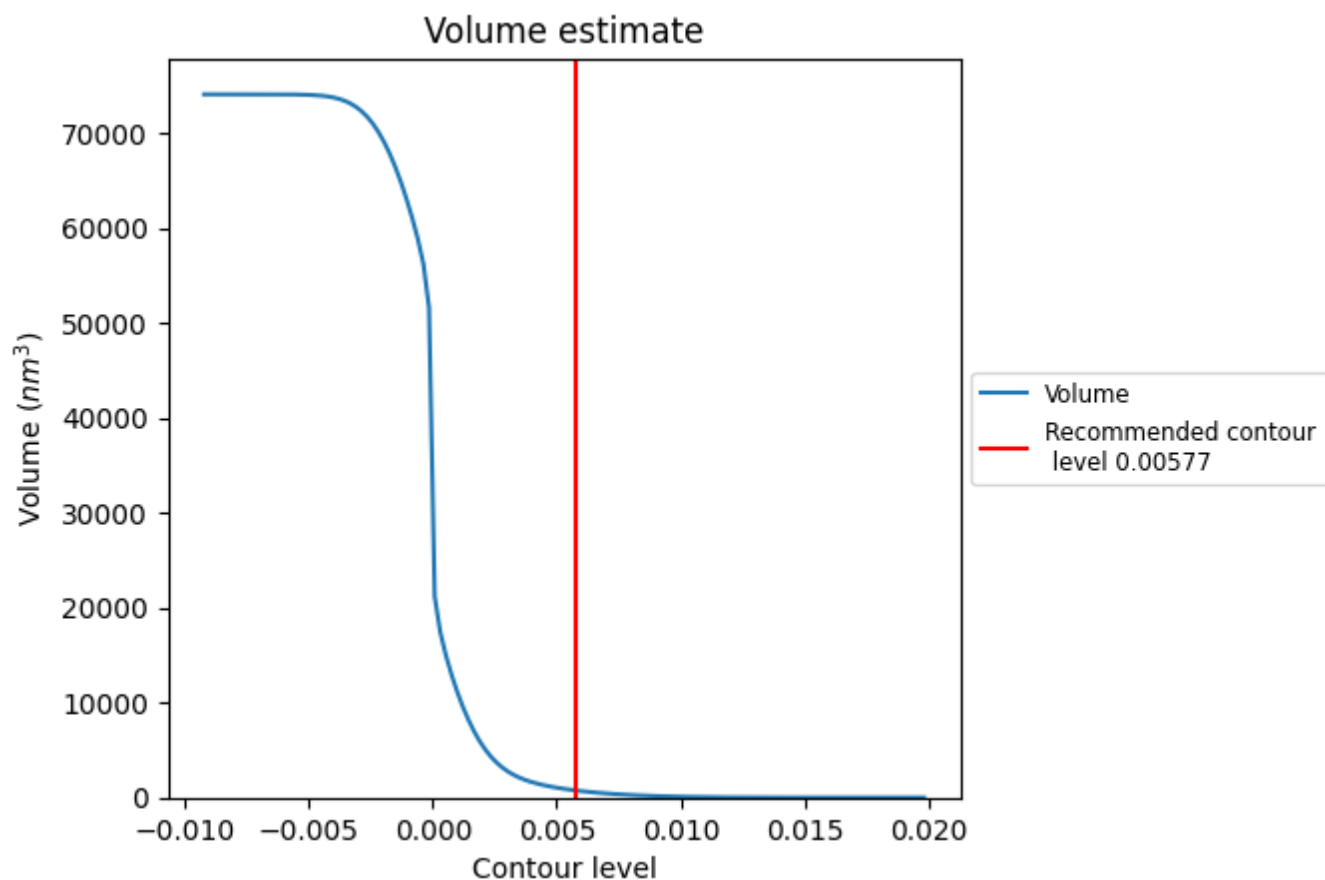
This section contains the results of statistical analysis of the map.

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.

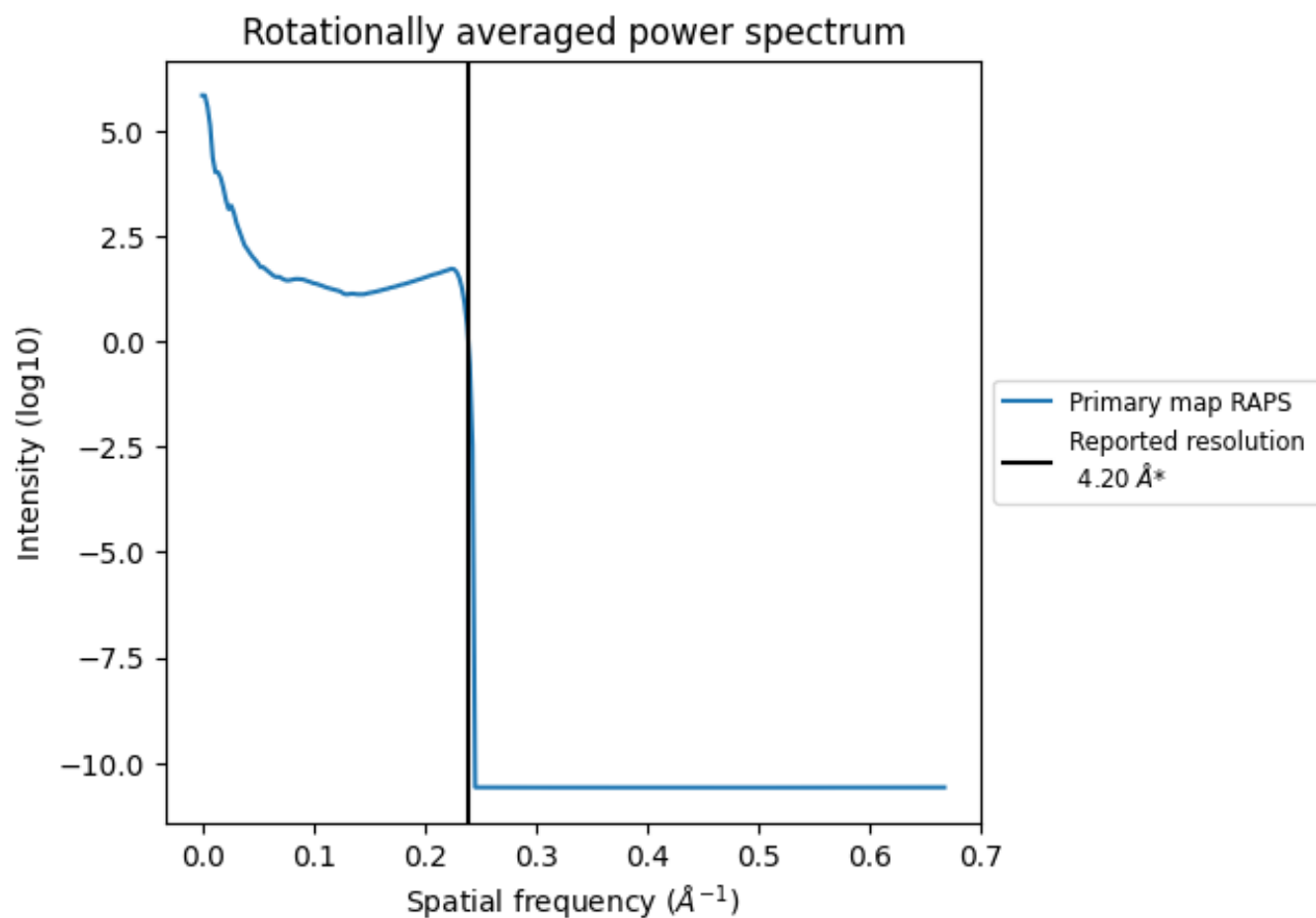
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm³; this corresponds to an approximate mass of 675 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 $\text{\AA}^{-1}$

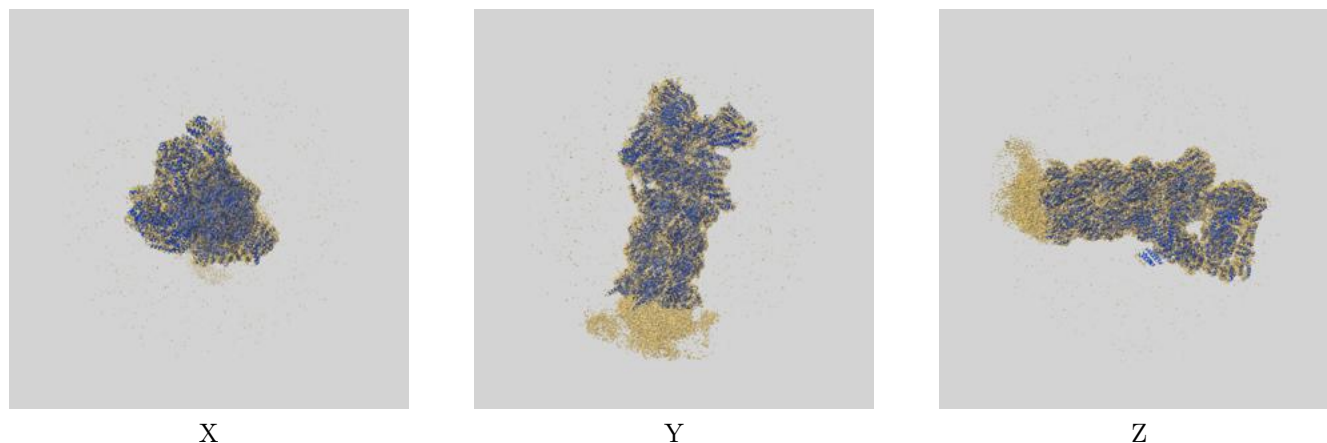
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

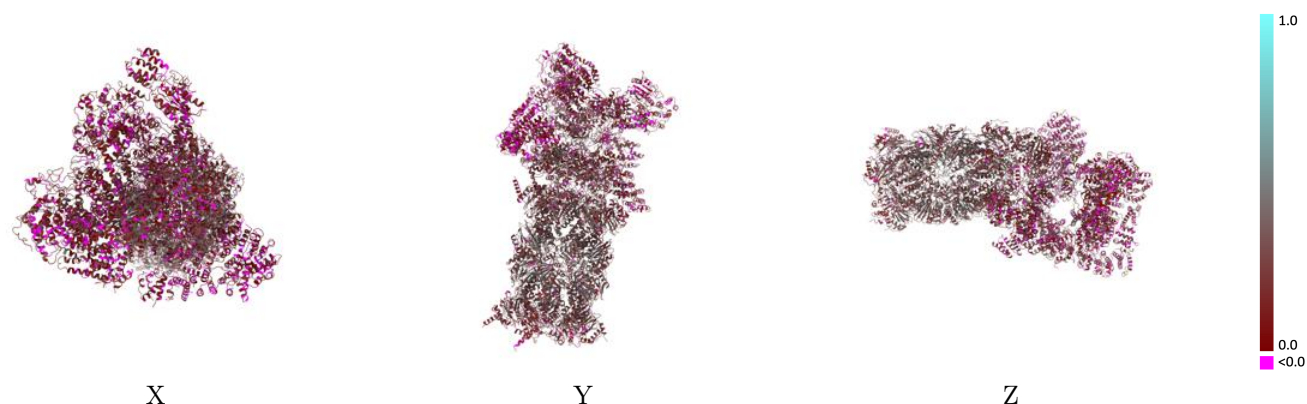
This section contains information regarding the fit between EMDB map EMD-8664 and PDB model 5VFQ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



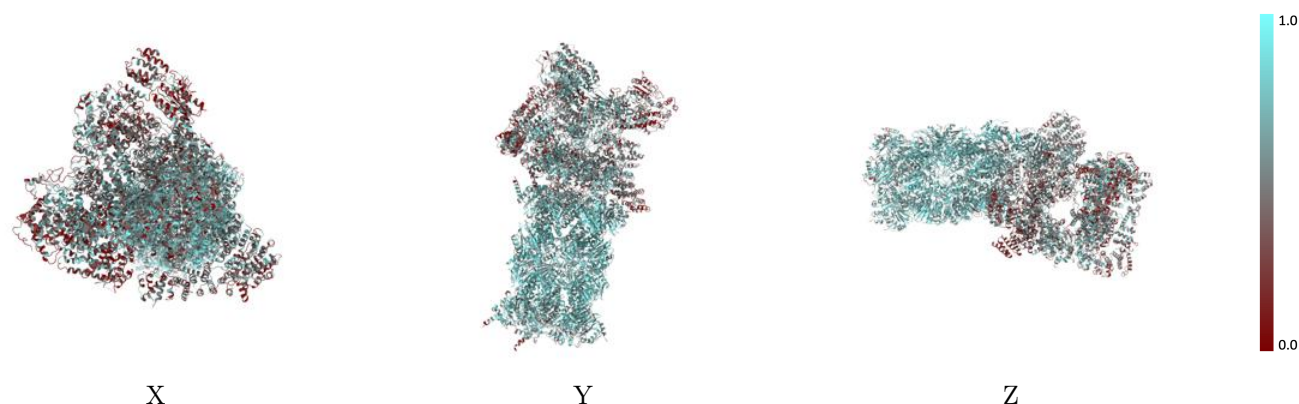
The images above show the 3D surface view of the map at the recommended contour level 0.00577 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



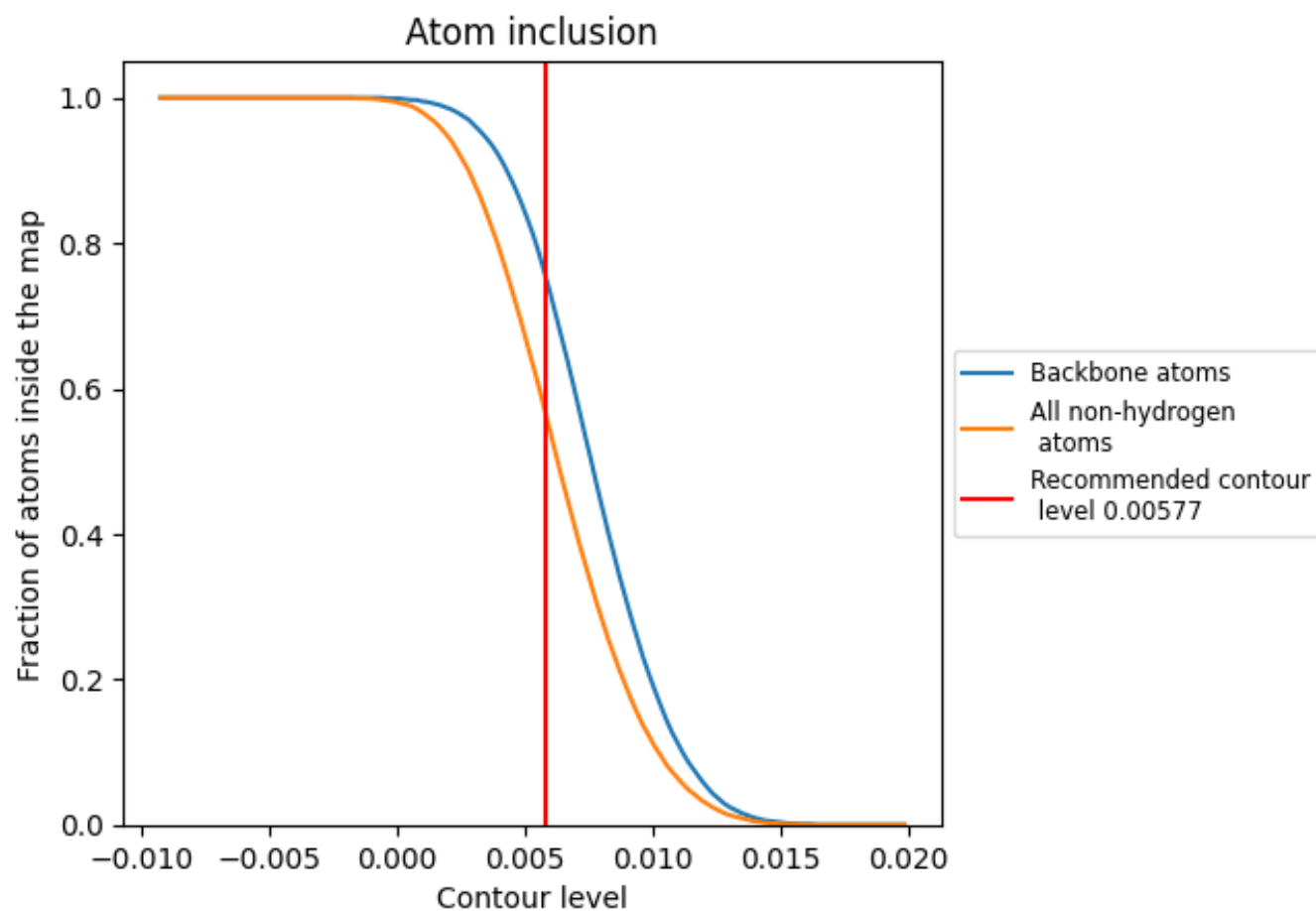
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00577).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00577) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5710	 0.2320
A	 0.5550	 0.2440
B	 0.5410	 0.2530
C	 0.5410	 0.2550
D	 0.5100	 0.2380
E	 0.3740	 0.1640
F	 0.4880	 0.2180
G	 0.6260	 0.2550
H	 0.6820	 0.2870
I	 0.6040	 0.2560
J	 0.6470	 0.2710
K	 0.6430	 0.2680
L	 0.7180	 0.3020
M	 0.6720	 0.2740
N	 0.7410	 0.3140
O	 0.7300	 0.3220
P	 0.7300	 0.3280
Q	 0.7200	 0.3070
R	 0.7730	 0.3440
S	 0.7260	 0.3400
T	 0.7570	 0.3390
U	 0.5270	 0.1670
V	 0.4320	 0.1550
W	 0.3890	 0.1540
X	 0.3430	 0.1720
Y	 0.5730	 0.1910
Z	 0.4950	 0.1860
a	 0.4360	 0.1550
b	 0.3210	 0.1270
c	 0.5350	 0.1960
d	 0.3570	 0.1420
e	 0.4000	 0.1480
f	 0.4210	 0.0820
g	 0.6300	 0.2490
h	 0.6500	 0.2730



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Chain	Atom inclusion	Q-score
i	 0.5990	 0.2280
j	 0.6290	 0.2470
k	 0.6460	 0.2620
l	 0.6950	 0.2700
m	 0.6430	 0.2620
n	 0.7520	 0.3230
o	 0.7230	 0.3260
p	 0.7110	 0.3170
q	 0.7500	 0.3390
r	 0.7830	 0.3330
s	 0.7180	 0.3250
t	 0.7610	 0.3290