



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:19 PM UTC

PDB ID : 5T0J / pdb_00005t0j
EMDB ID : EMD-8337
Title : Structural basis for dynamic regulation of the human 26S proteasome
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : 2016-08-16
Resolution : 8.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

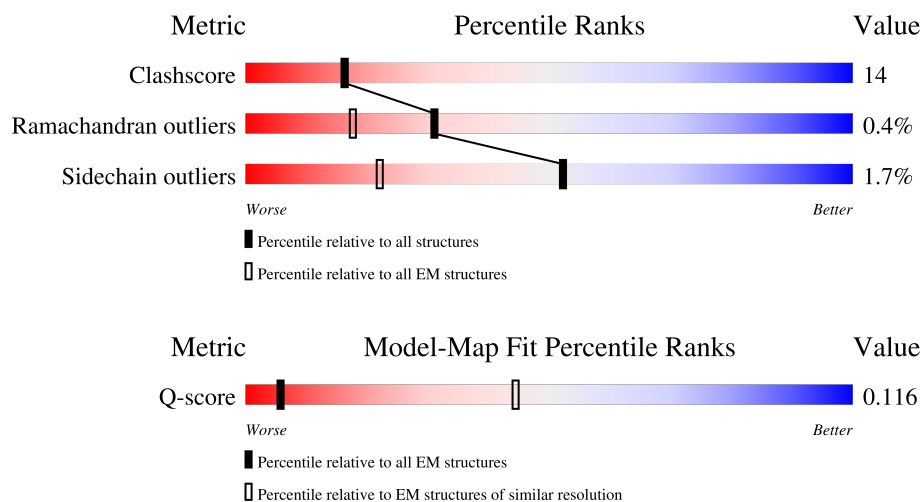
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	f	749	
2	G	245	
3	H	233	
4	I	260	

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Mol	Chain	Length	Quality of chain
5	J	247	
6	K	240	
7	L	268	
8	M	254	
9	N	238	
10	O	276	
11	P	204	
12	Q	201	
13	R	262	
14	S	240	
15	T	263	
16	A	433	
17	B	440	
18	D	418	
19	E	403	
20	F	439	
21	C	398	
22	U	953	
23	V	533	
24	W	456	
25	X	422	
26	Y	389	
27	Z	324	
28	a	376	
29	b	377	

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Mol	Chain	Length	Quality of chain
30	c	309	37%56%32%10%
31	d	349	39%48%25%26%
32	e	70	26%31%24%43%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 76674 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 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 5 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 9 is a protein called Proteasome subunit beta type-6.

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

- Molecule 10 is a protein called Proteasome subunit beta type-7.

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

- Molecule 11 is a protein called Proteasome subunit beta type-3.

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

- Molecule 12 is a protein called Proteasome subunit beta type-2.

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

- Molecule 13 is a protein called Proteasome subunit beta type-5.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is a protein called Proteasome subunit beta type-4.

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

- Molecule 16 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

- Molecule 17 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	348	Total	C	N	O	S	0	0
			2717	1708	460	537	12		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 19 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	392	Total	C	N	O	S	0	0
			3078	1932	551	577	18		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

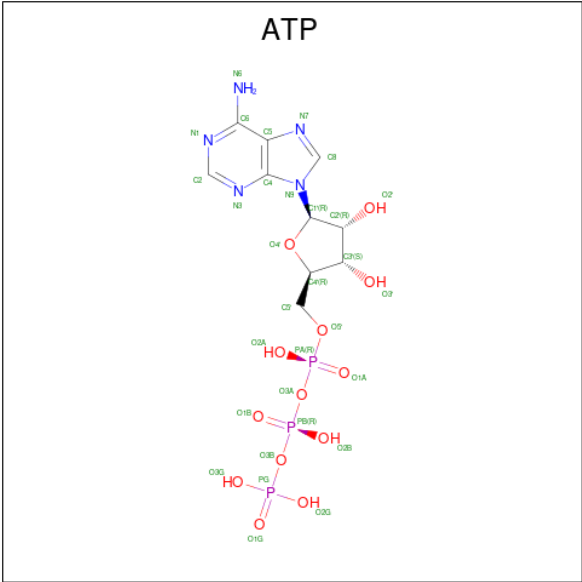
- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 32 is a protein called 26S proteasome complex subunit DSS1.

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

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

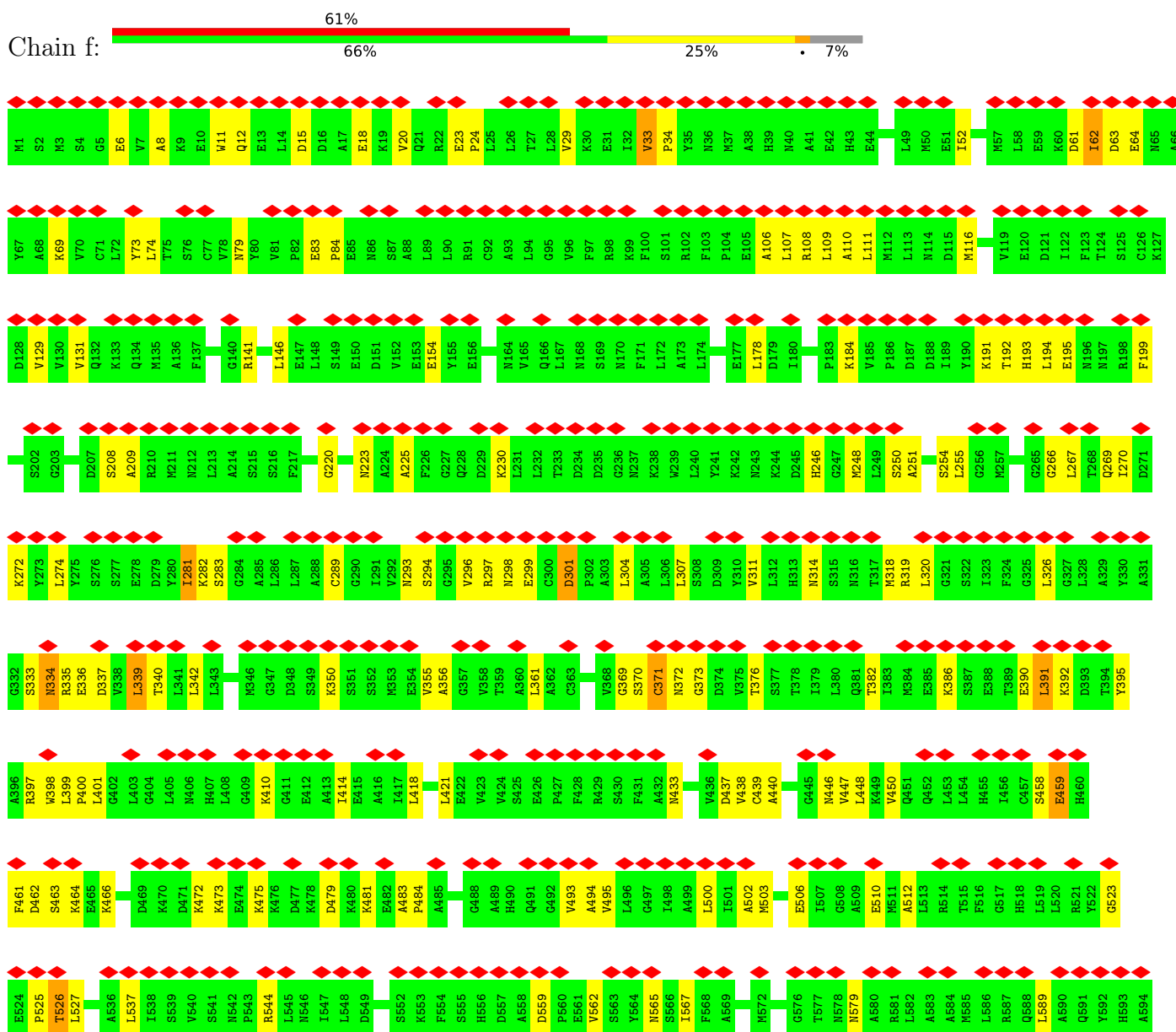
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

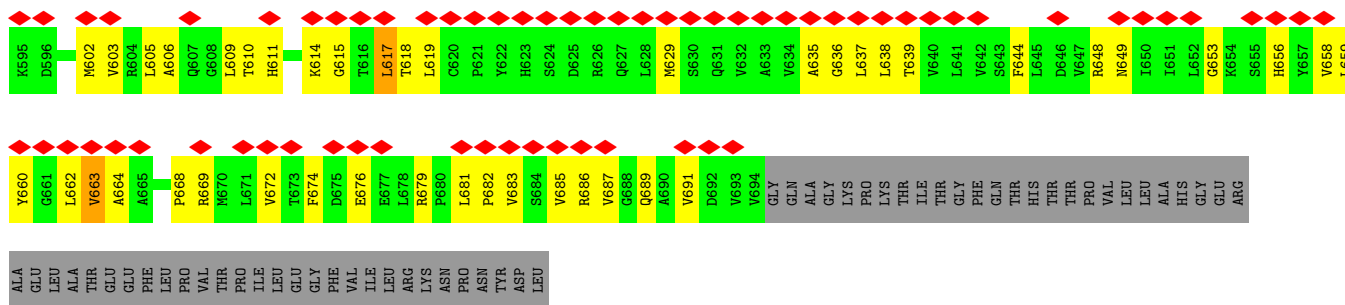
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

3 Residue-property plots

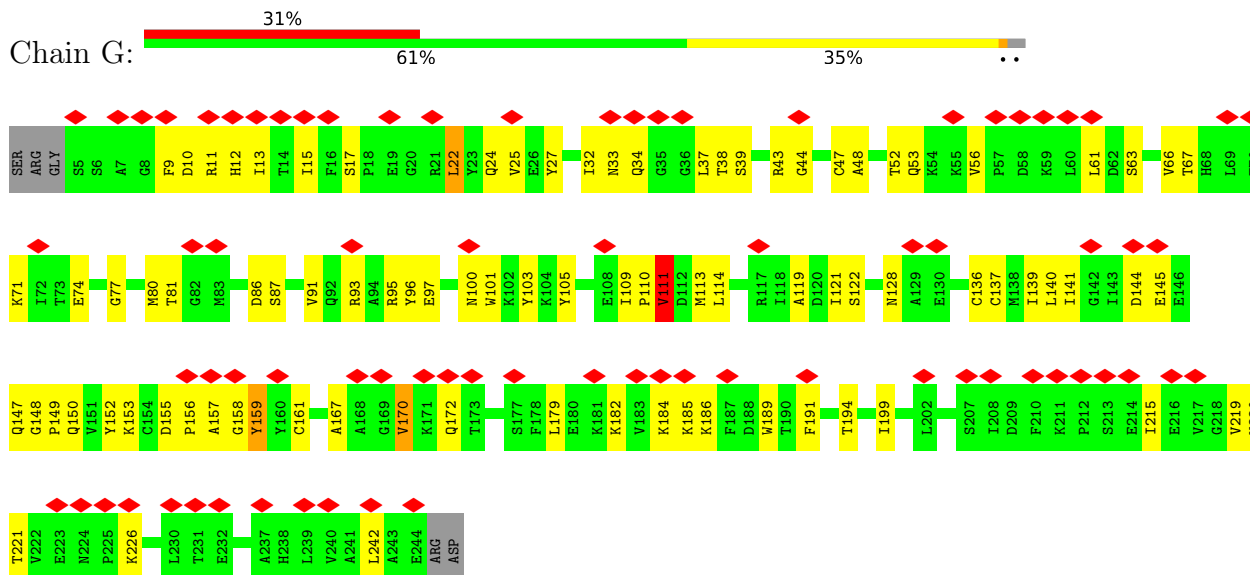
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 2

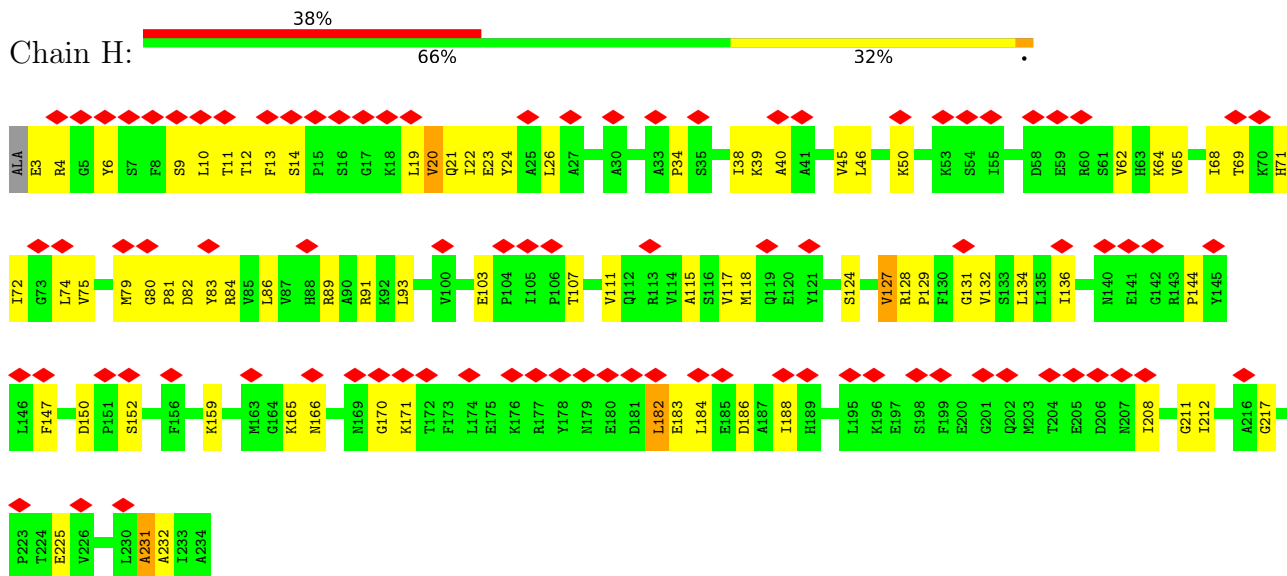




- Molecule 2: Proteasome subunit alpha type-6

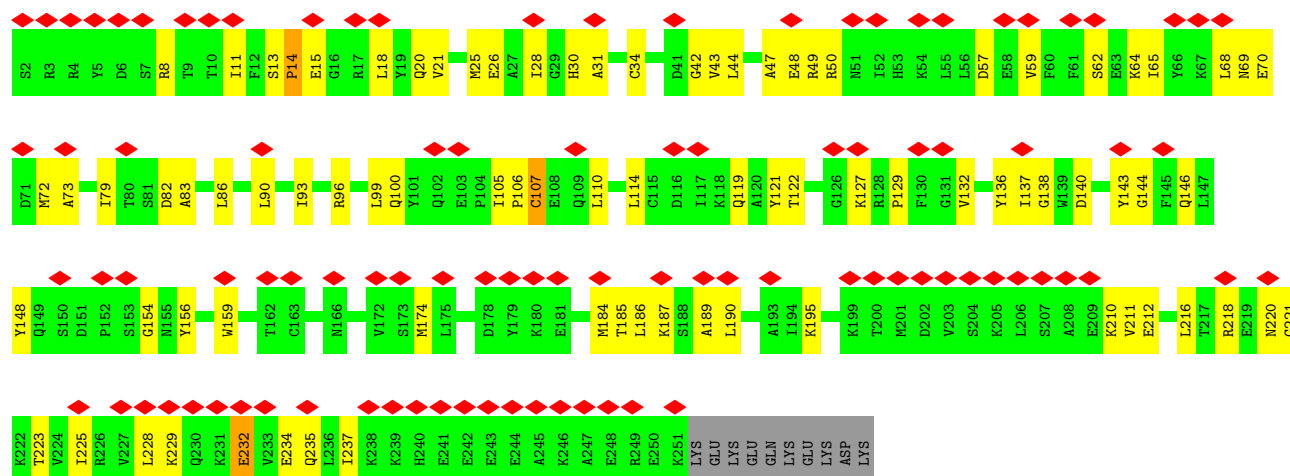


- Molecule 3: Proteasome subunit alpha type-2

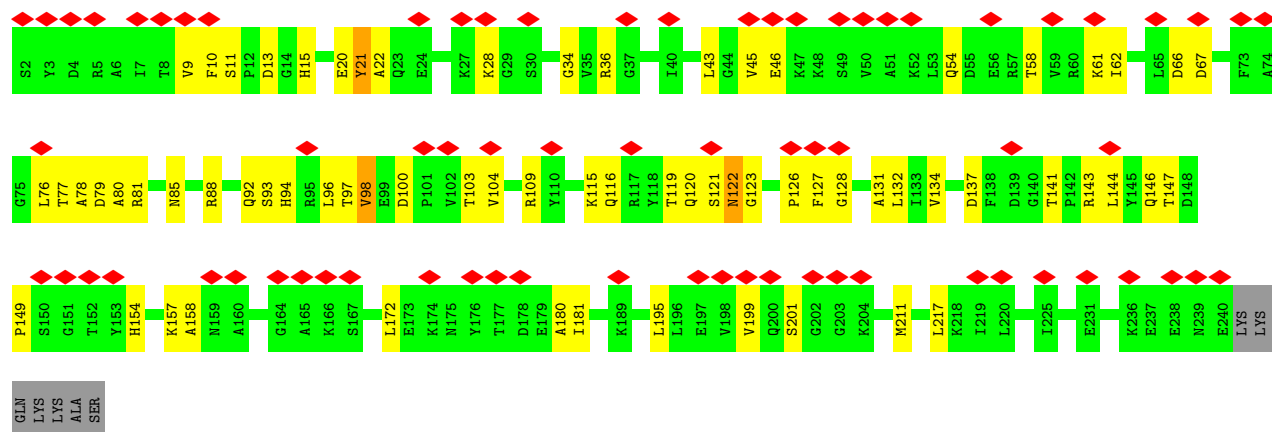


- Molecule 4: Proteasome subunit alpha type-4

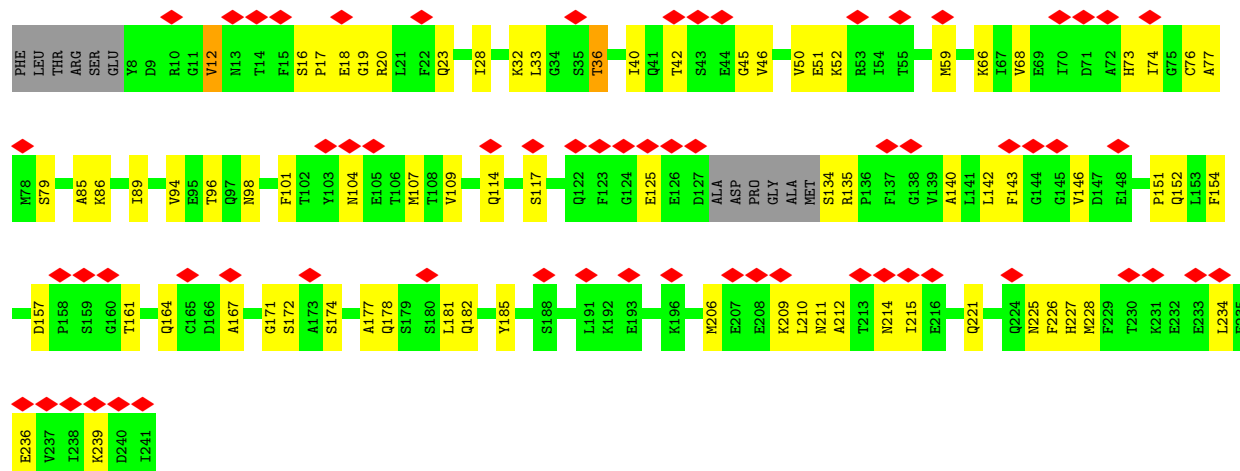


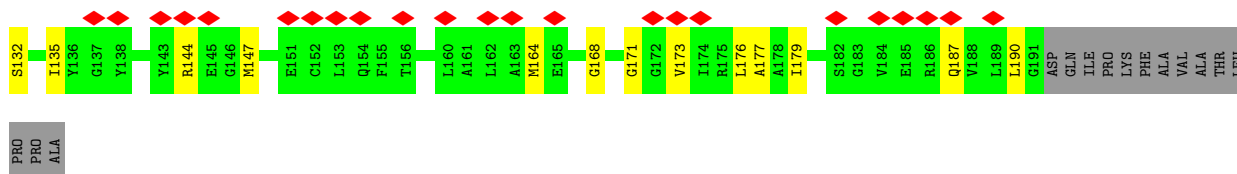


• Molecule 5: Proteasome subunit alpha type-7

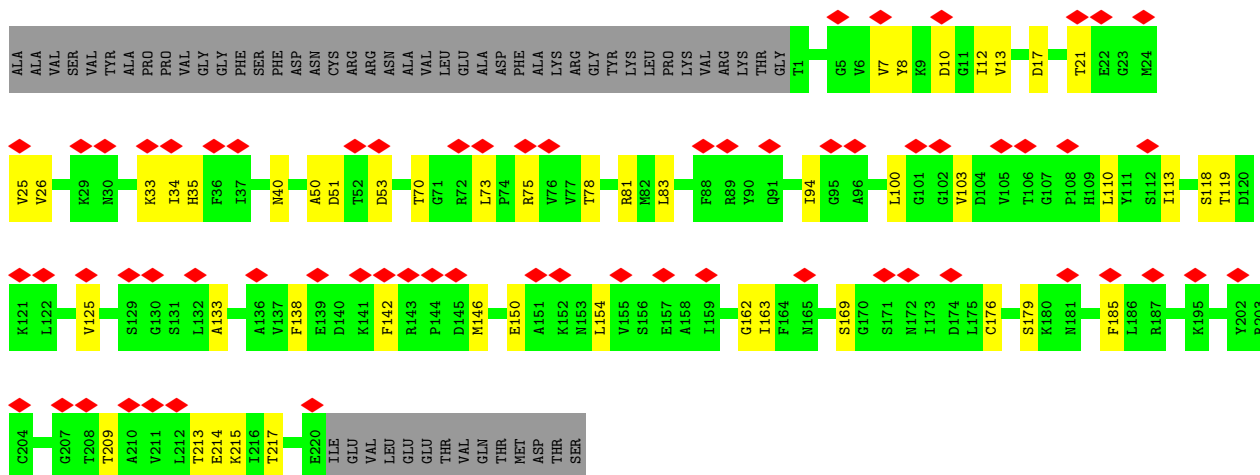


• Molecule 6: Proteasome subunit alpha type-5

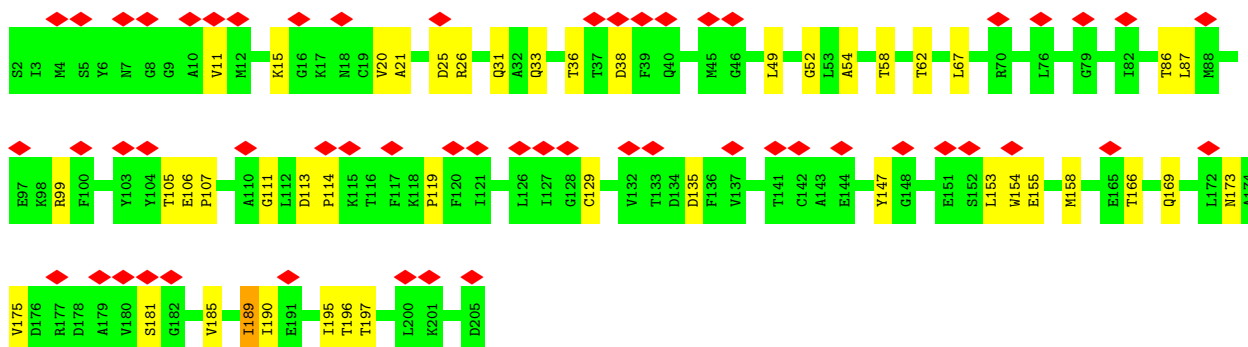
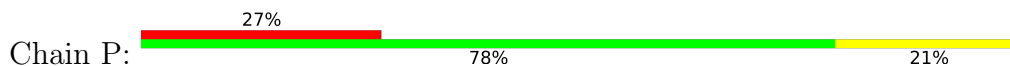




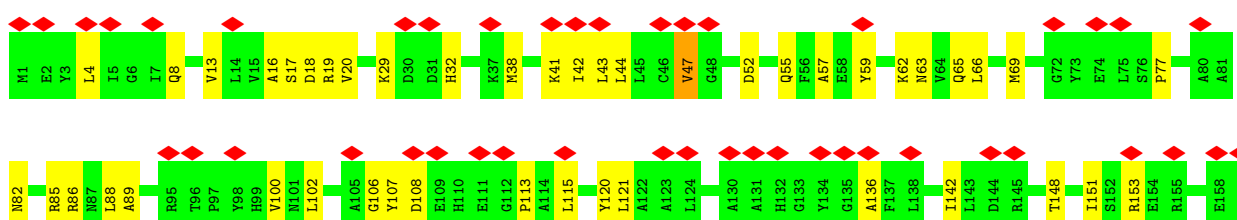
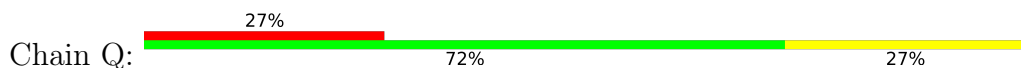
• Molecule 10: Proteasome subunit beta type-7

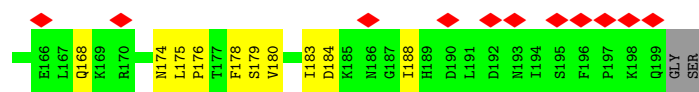


• Molecule 11: Proteasome subunit beta type-3

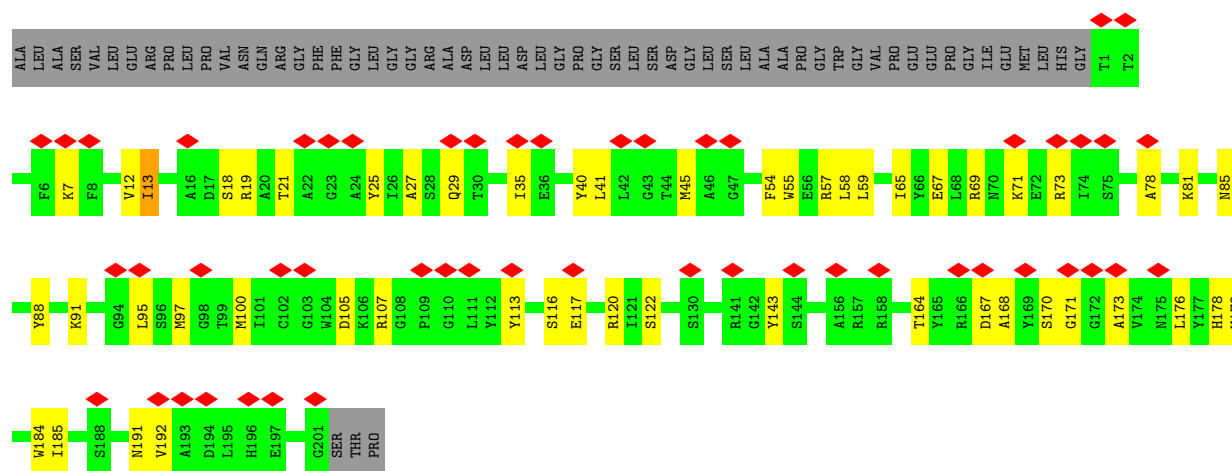


• Molecule 12: Proteasome subunit beta type-2

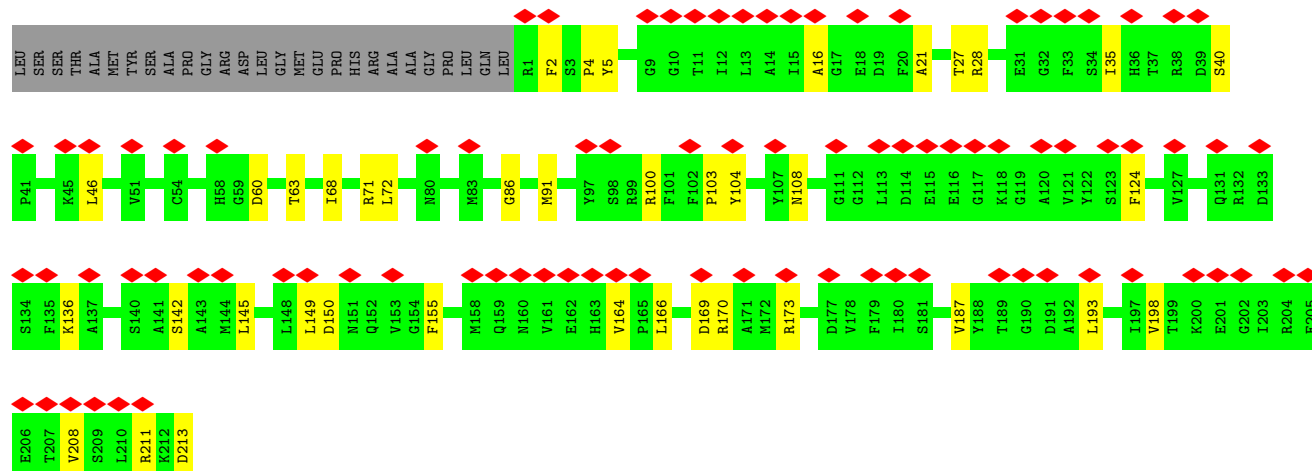
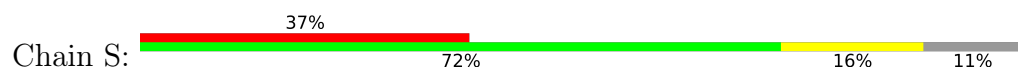




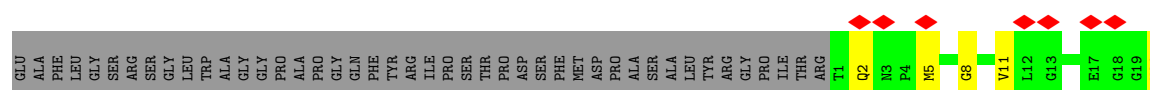
• Molecule 13: Proteasome subunit beta type-5

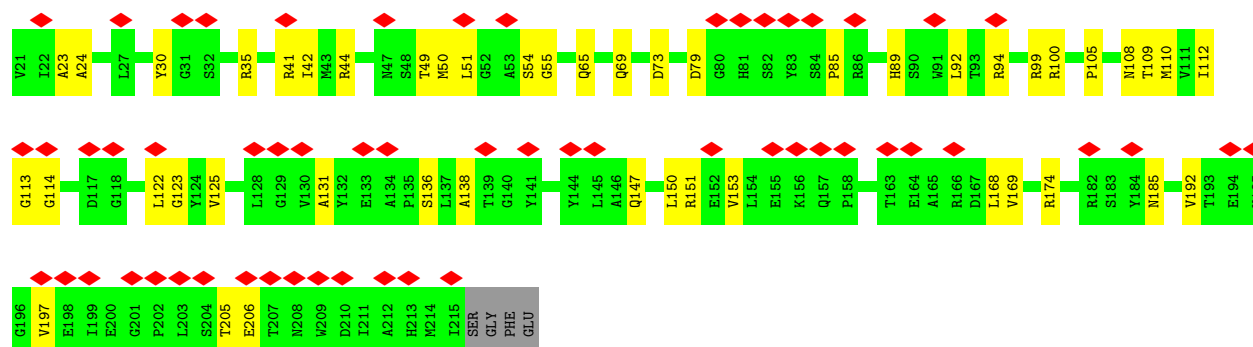


• Molecule 14: Proteasome subunit beta type-1

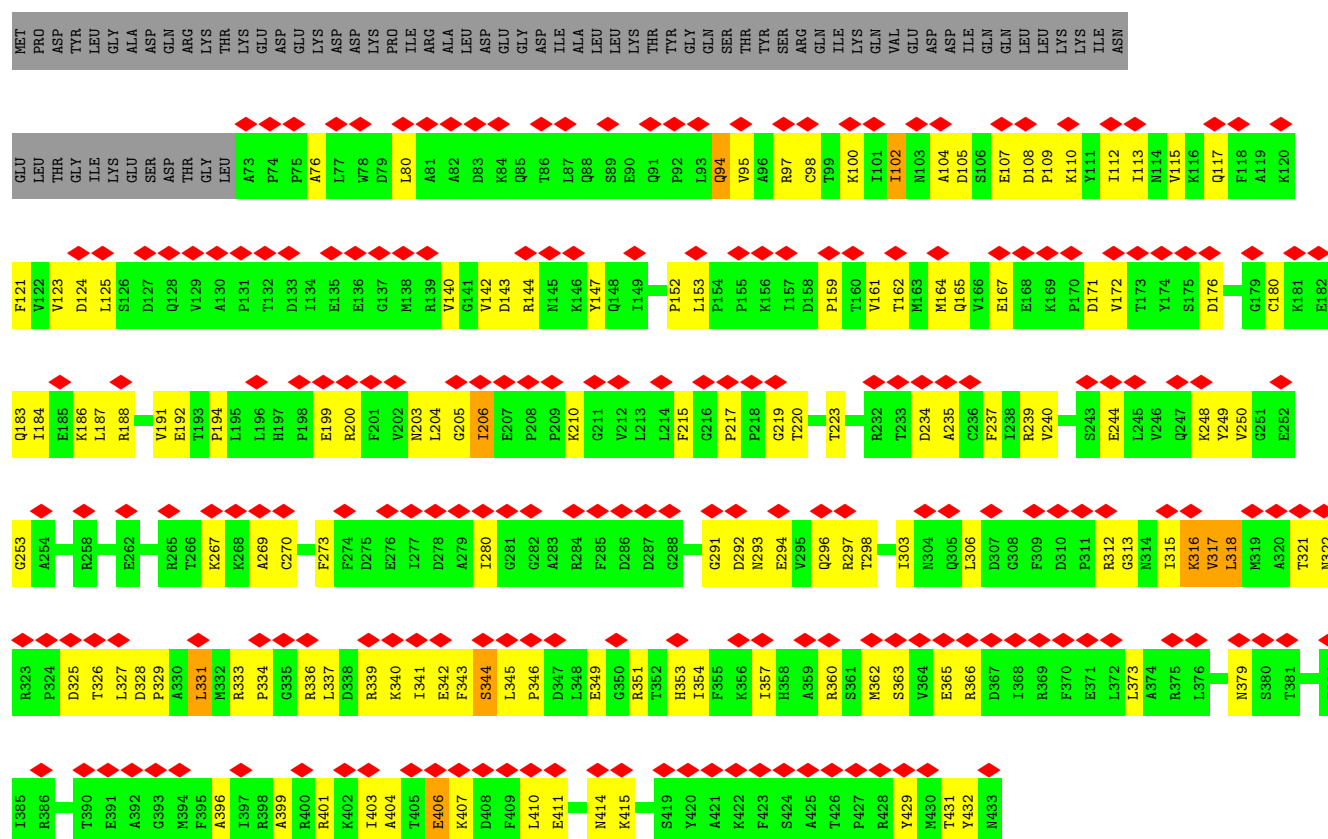


• Molecule 15: Proteasome subunit beta type-4

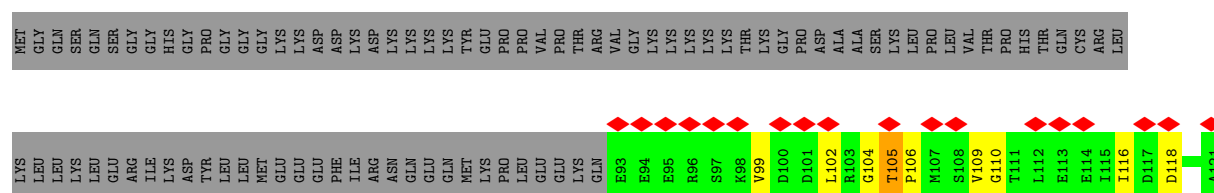


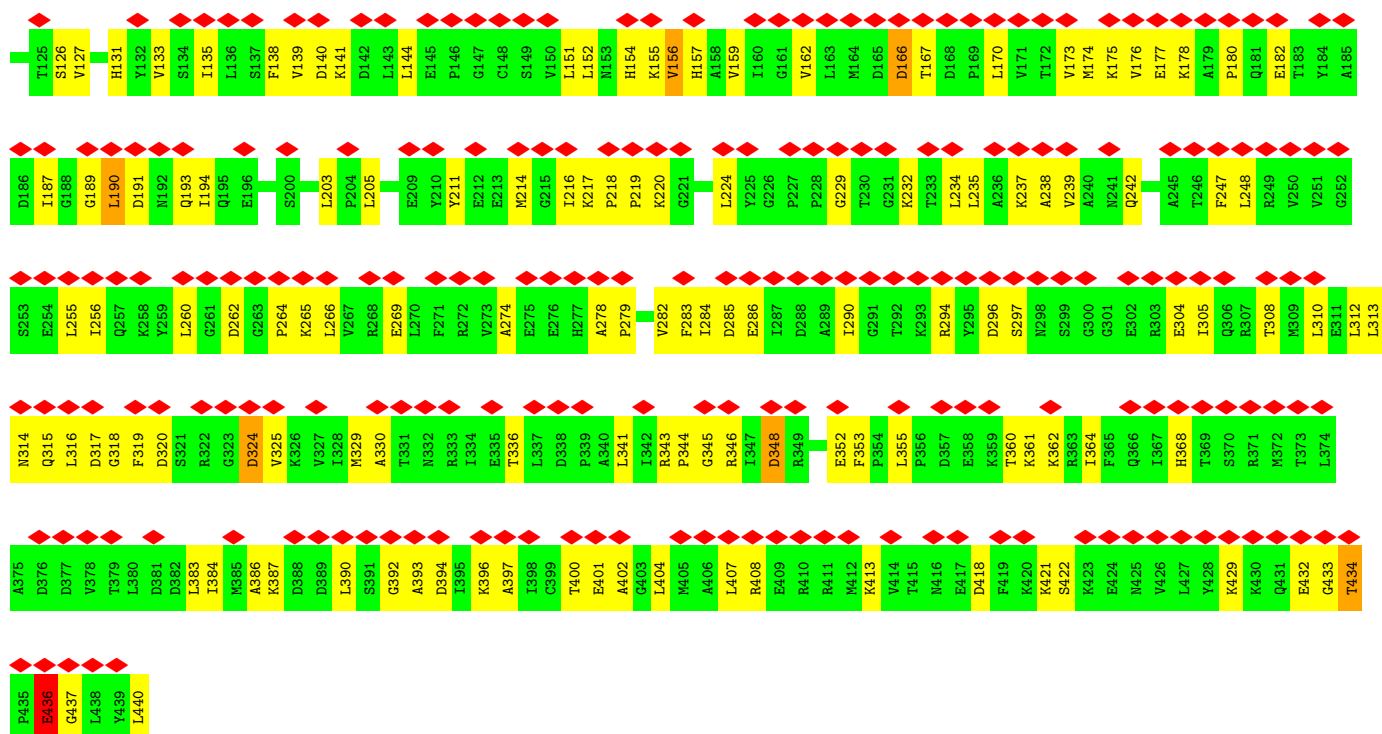


• Molecule 16: 26S protease regulatory subunit 7

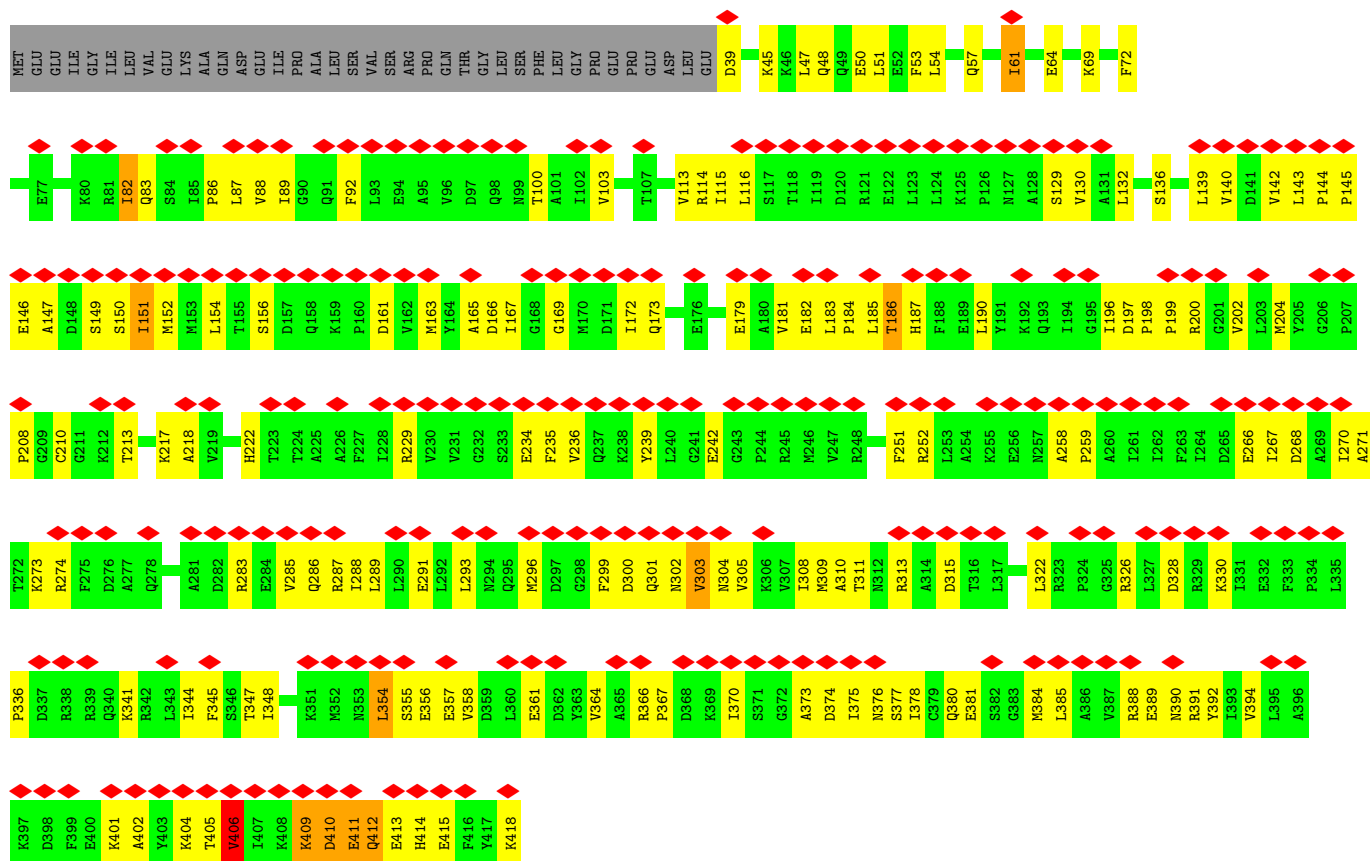


• Molecule 17: 26S protease regulatory subunit 4

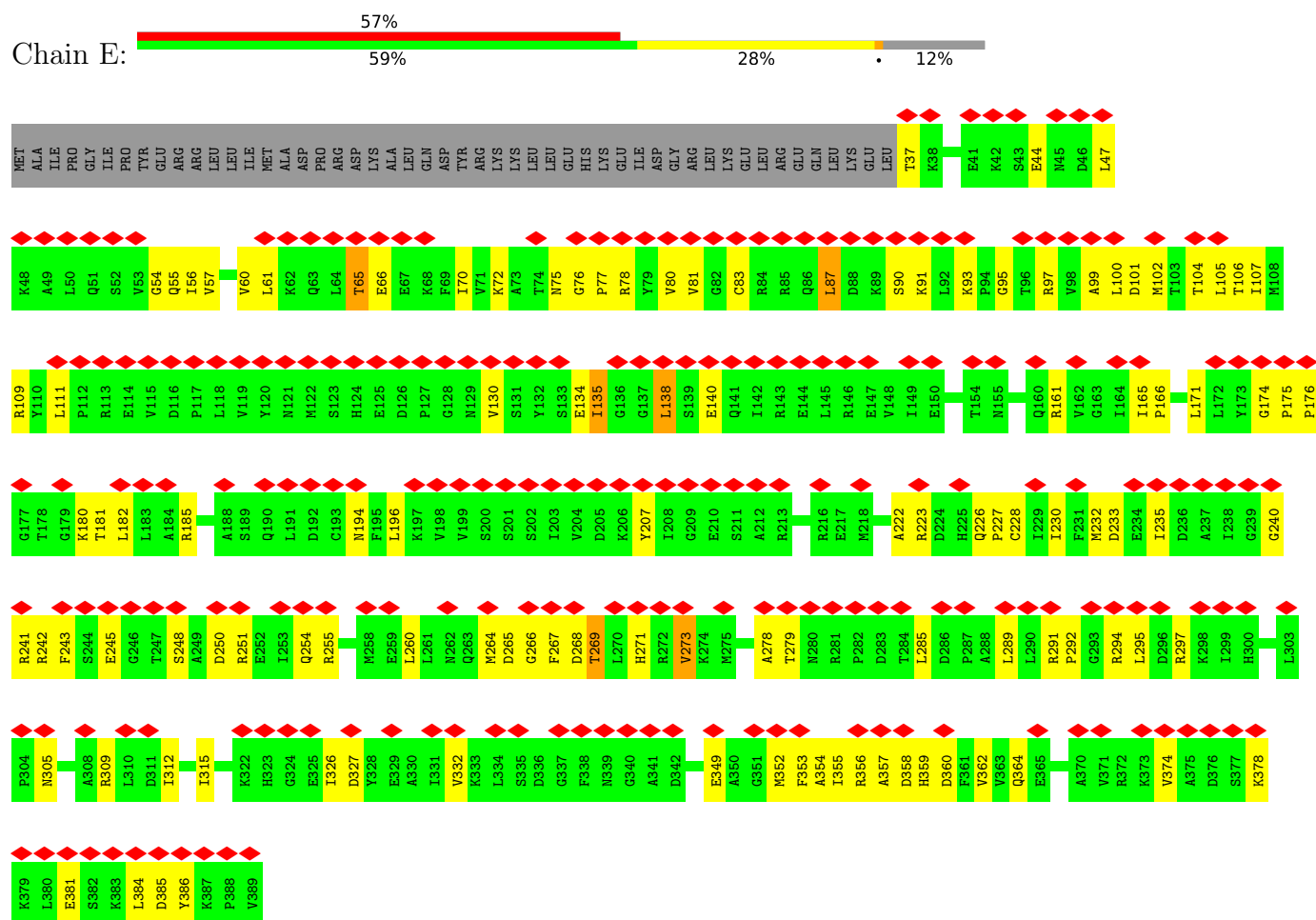




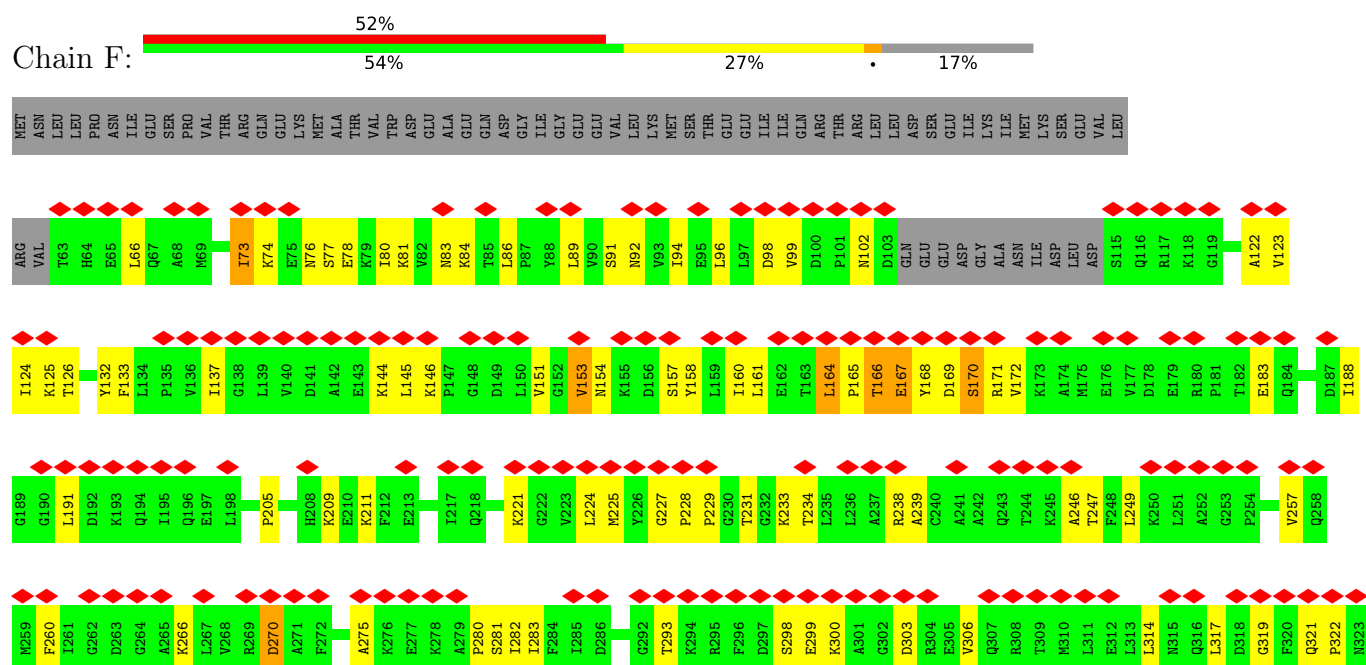
• Molecule 18: 26S protease regulatory subunit 6B

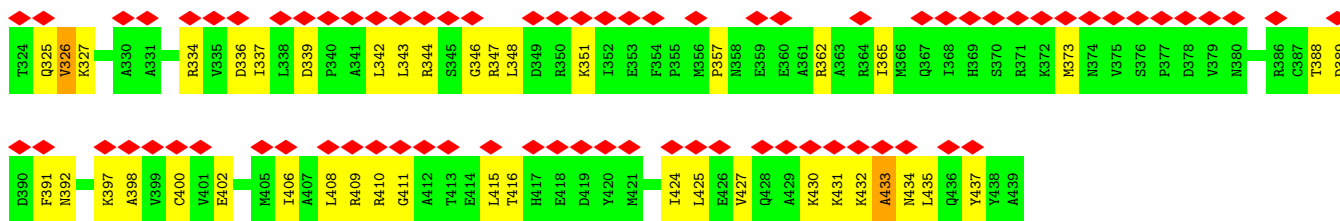


• Molecule 19: 26S protease regulatory subunit 10B

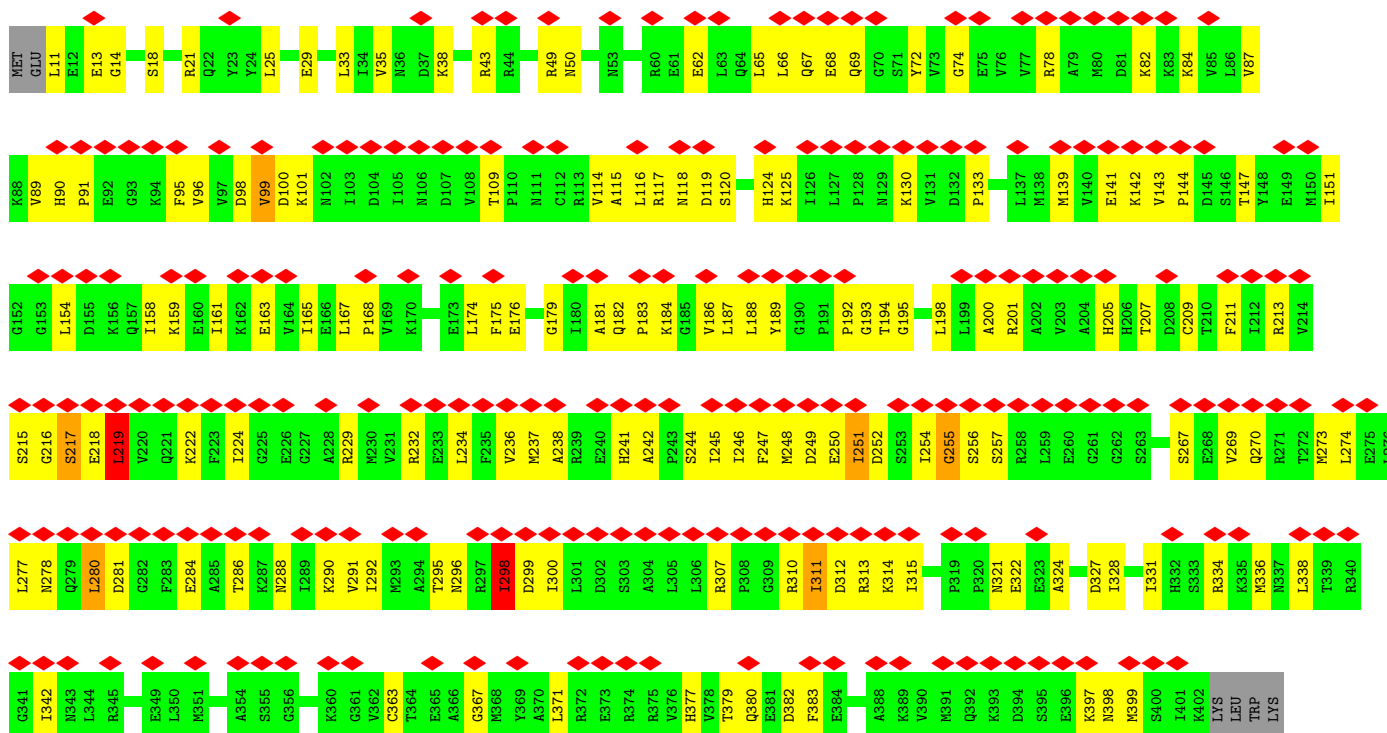


• Molecule 20: 26S protease regulatory subunit 6A

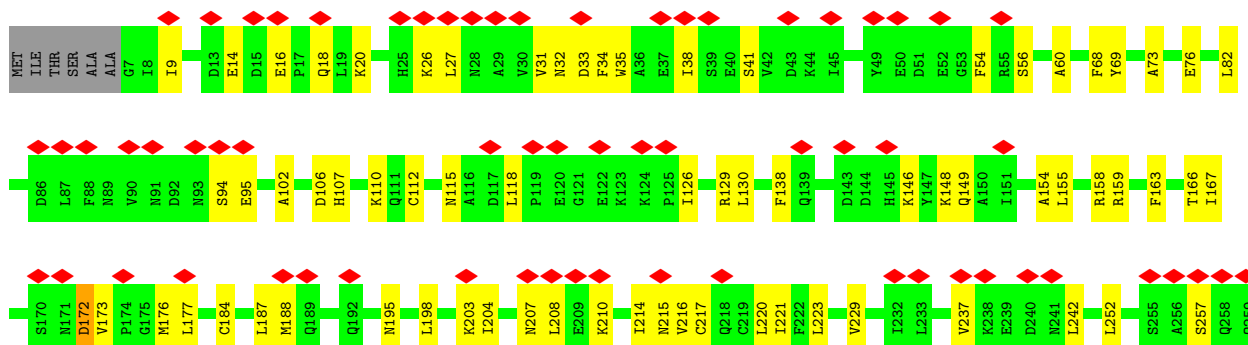


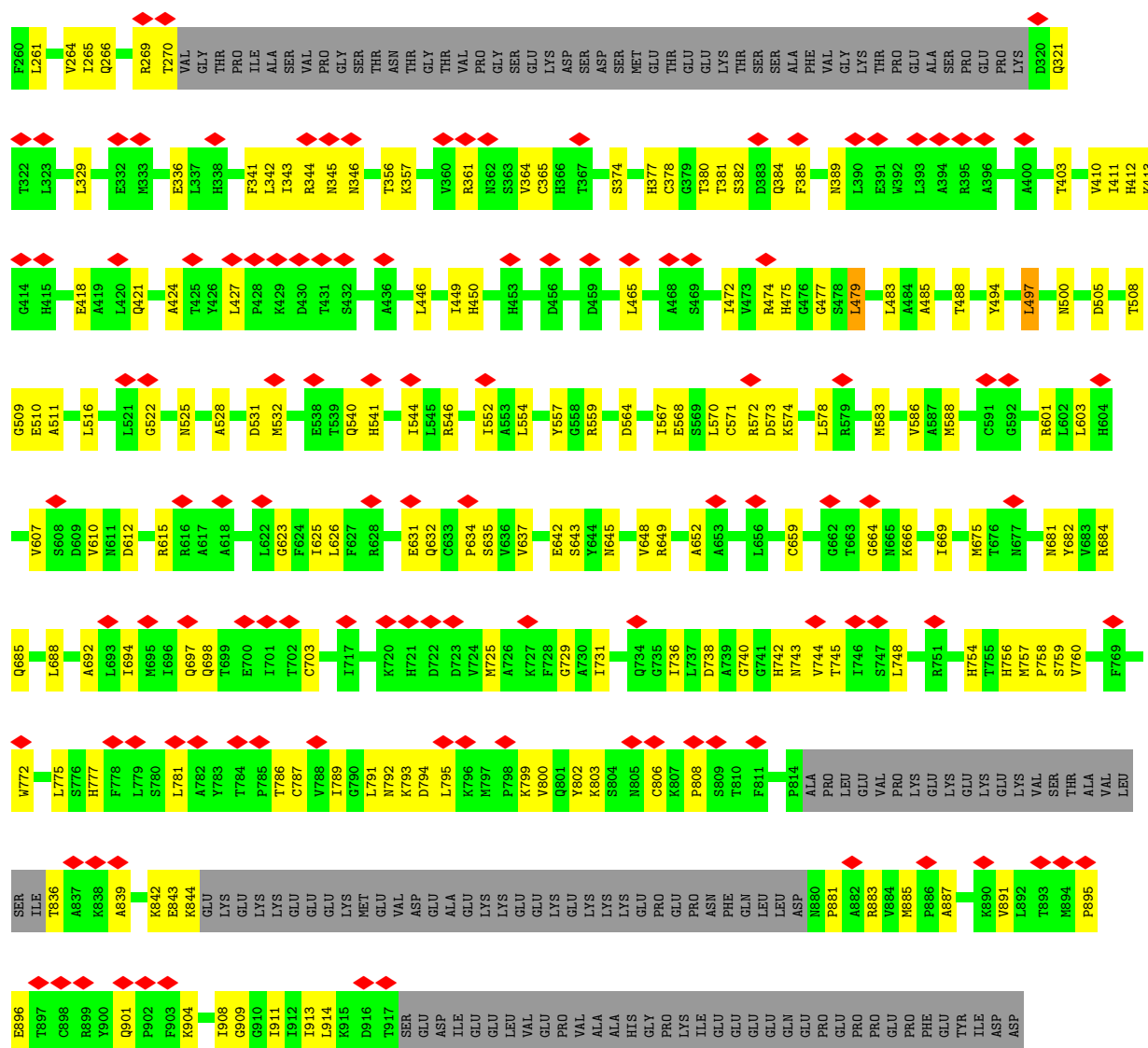


• Molecule 21: 26S protease regulatory subunit 8

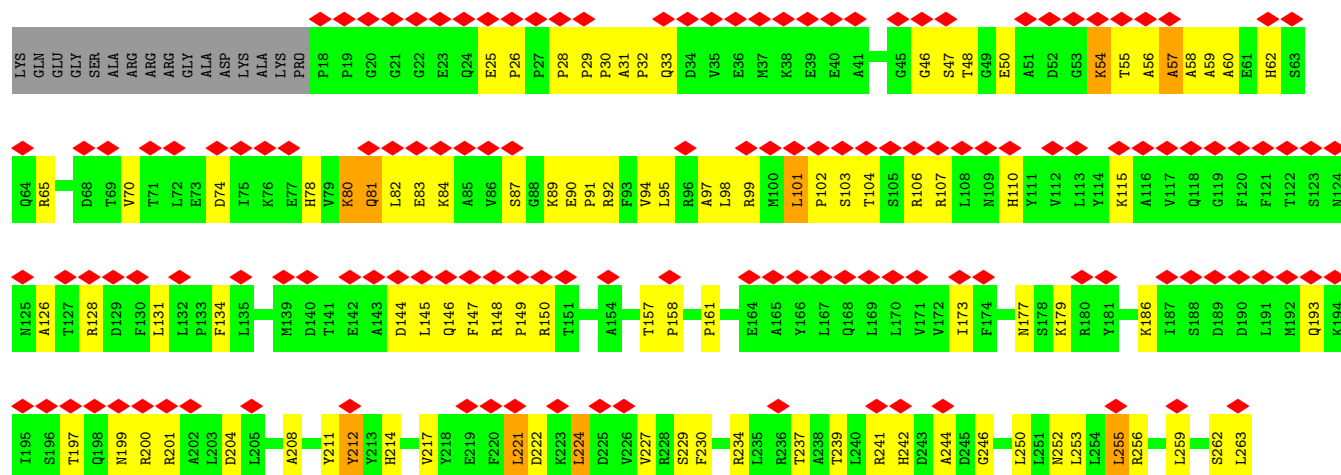


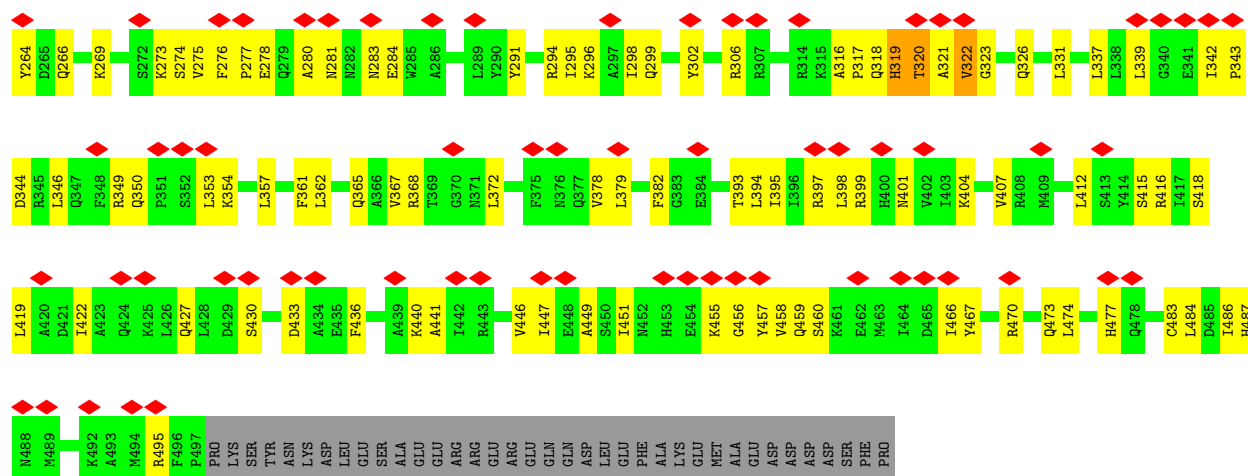
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1



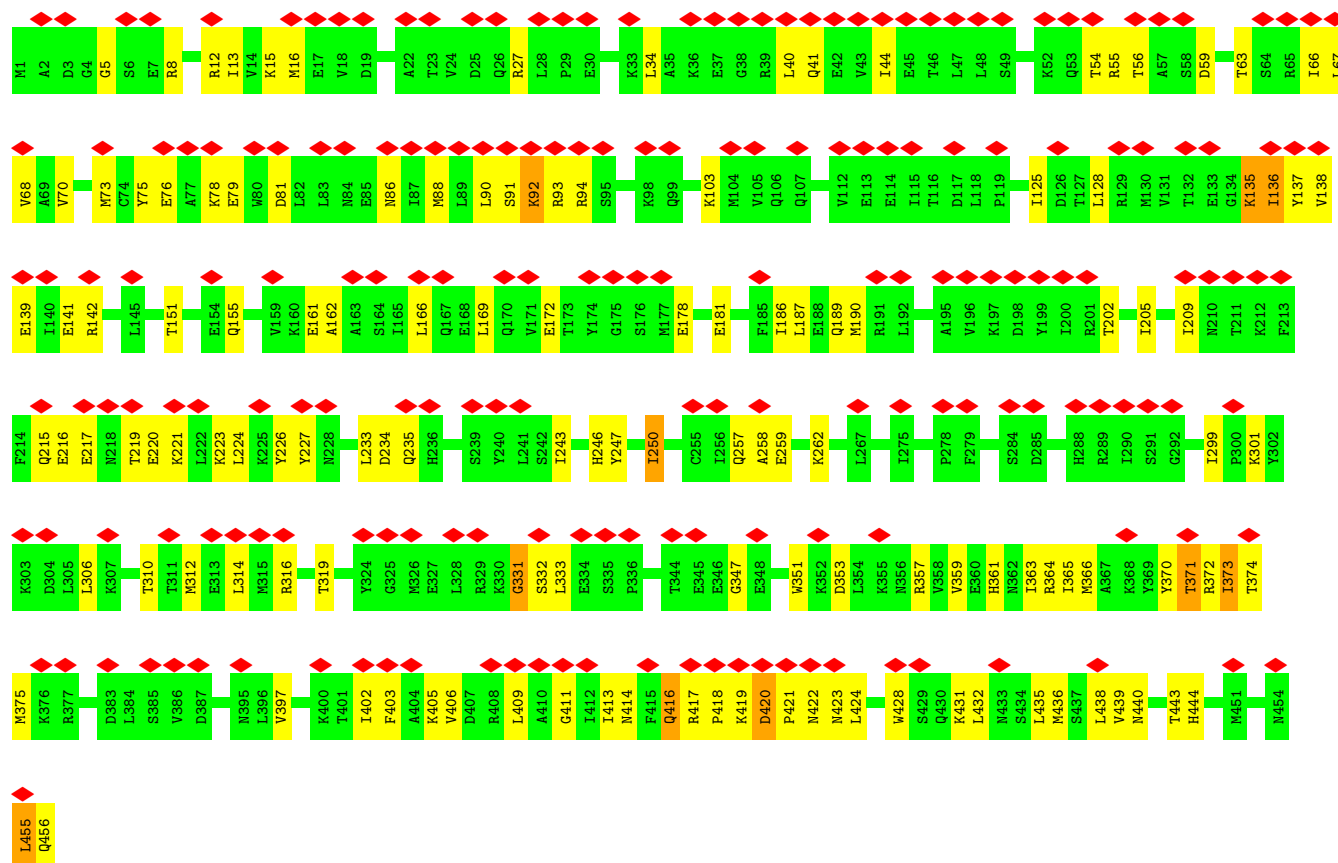
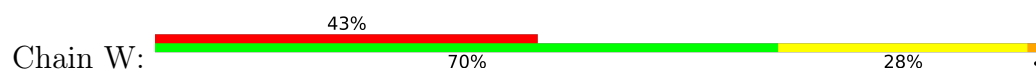


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 3

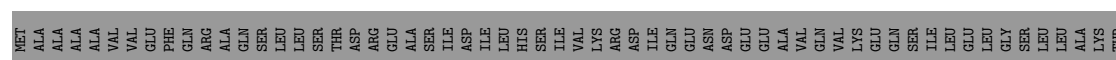
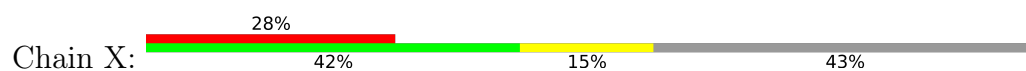




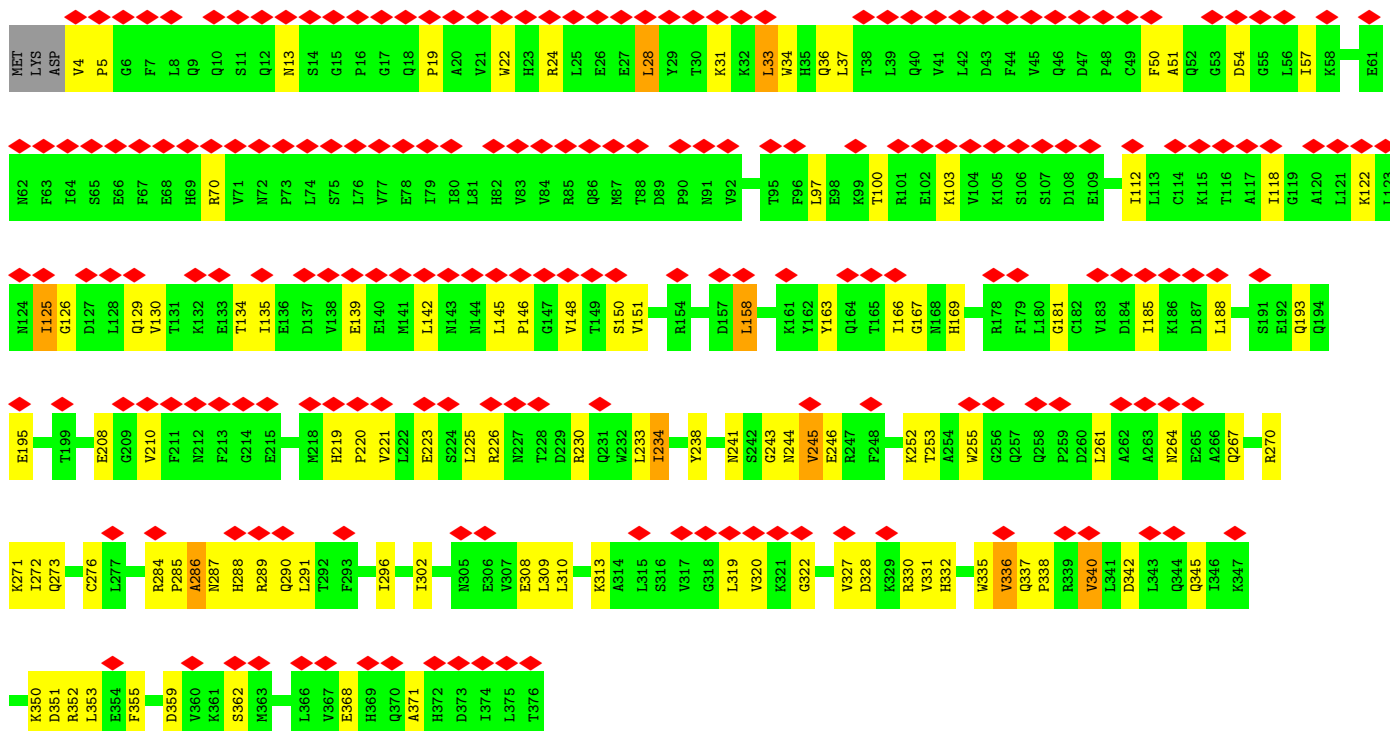
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 12



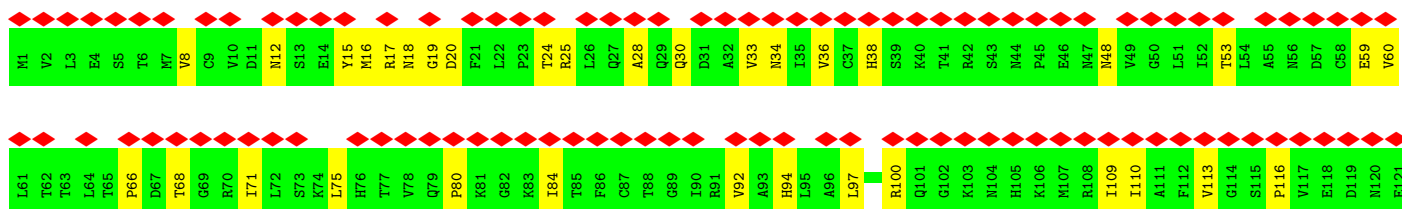
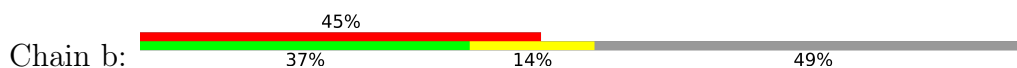
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 11



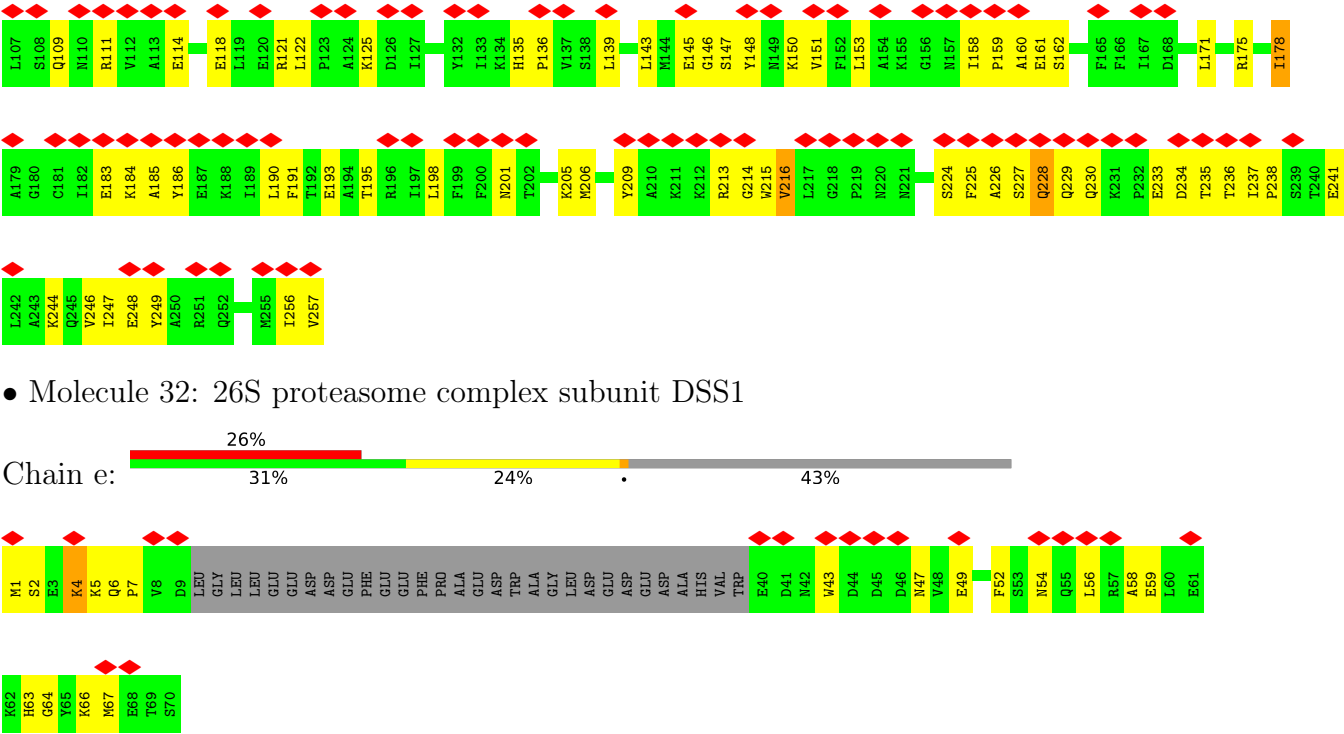
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 13



- Molecule 29: 26S proteasome non-ATPase regulatory subunit 4







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14382	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	0.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	309.6, 309.6, 309.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	f	0.17	0/5413	0.53	10/7317 (0.1%)
2	G	0.12	0/1859	0.39	0/2523
3	H	0.14	0/1743	0.45	3/2372 (0.1%)
4	I	0.79	1/1942 (0.1%)	0.58	4/2628 (0.2%)
5	J	1.63	6/1728 (0.3%)	0.39	1/2358 (0.0%)
6	K	0.12	0/1747	0.37	0/2364
7	L	0.11	0/1885	0.37	0/2552
8	M	0.12	0/1891	0.30	0/2552
9	N	0.09	0/1454	0.27	0/1967
10	O	0.09	0/1670	0.26	0/2265
11	P	0.09	0/1614	0.30	1/2177 (0.0%)
12	Q	0.10	0/1603	0.28	0/2174
13	R	0.09	0/1579	0.29	0/2134
14	S	0.09	0/1671	0.26	0/2253
15	T	0.08	0/1700	0.28	0/2305
16	A	0.17	0/2886	0.52	5/3899 (0.1%)
17	B	0.20	0/2756	0.55	6/3721 (0.2%)
18	D	0.21	0/3090	0.58	5/4168 (0.1%)
19	E	0.29	1/2835 (0.0%)	0.44	0/3821
20	F	0.19	0/2903	0.55	6/3912 (0.2%)
21	C	0.20	1/3117 (0.0%)	0.49	4/4189 (0.1%)
22	U	0.10	0/6396	0.34	2/8646 (0.0%)
23	V	0.69	6/3929 (0.2%)	0.56	11/5309 (0.2%)
24	W	0.17	0/3751	0.50	5/5042 (0.1%)
25	X	0.14	0/1936	0.37	0/2614
26	Y	0.15	0/3173	0.50	5/4273 (0.1%)
27	Z	0.16	0/2324	0.51	4/3150 (0.1%)
28	a	0.14	0/3053	0.42	0/4133
29	b	0.17	0/1478	0.35	0/2001
30	c	0.17	0/2226	0.43	0/3007
31	d	0.19	0/2162	0.53	3/2919 (0.1%)
32	e	3.03	1/338 (0.3%)	0.80	2/450 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.40	16/77852 (0.0%)	0.45	77/105195 (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
17	B	0	1
18	D	0	3
23	V	0	1
24	W	0	1
26	Y	0	1
28	a	0	1
31	d	0	1
All	All	0	9

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	e	4	LYS	CD-CE	55.58	3.19	1.52
5	J	21	TYR	CD2-CE2	33.79	2.40	1.38
4	I	14	PRO	CA-C	33.58	2.00	1.52
5	J	21	TYR	CD1-CE1	33.17	2.38	1.38
5	J	21	TYR	CE1-CZ	26.85	2.02	1.38
5	J	21	TYR	CE2-CZ	24.81	1.97	1.38
5	J	21	TYR	CG-CD2	22.48	1.86	1.39
5	J	21	TYR	CG-CD1	22.10	1.85	1.39
23	V	212	TYR	CD2-CE2	20.52	2.00	1.38
23	V	212	TYR	CD1-CE1	20.43	2.00	1.38
23	V	212	TYR	CE1-CZ	16.11	1.76	1.38
23	V	212	TYR	CE2-CZ	15.79	1.76	1.38
23	V	212	TYR	CG-CD2	14.19	1.69	1.39
23	V	212	TYR	CG-CD1	14.00	1.68	1.39
19	E	175	PRO	C-N	13.69	1.65	1.33
21	C	242	ALA	C-N	5.86	1.47	1.33

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	14	PRO	O-C-N	-18.24	98.01	122.64
32	e	4	LYS	CG-CD-CE	9.69	133.60	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	636	GLY	N-CA-C	9.34	124.72	113.79
1	f	459	GLU	N-CA-C	9.26	127.58	113.51
27	Z	63	LYS	N-CA-C	8.18	121.37	111.40
4	I	14	PRO	N-CA-CB	-8.10	94.75	103.25
21	C	217	SER	CA-C-N	7.97	136.05	121.70
21	C	217	SER	C-N-CA	7.97	136.05	121.70
26	Y	63	TRP	CA-C-N	7.96	136.03	121.70
26	Y	63	TRP	C-N-CA	7.96	136.03	121.70
5	J	122	ASN	N-CA-C	7.90	122.50	113.02
4	I	14	PRO	N-CA-C	7.41	127.73	112.47
24	W	92	LYS	CA-C-N	7.26	134.76	121.70
24	W	92	LYS	C-N-CA	7.26	134.76	121.70
24	W	135	LYS	CA-C-N	7.24	134.72	121.70
24	W	135	LYS	C-N-CA	7.24	134.72	121.70
18	D	409	LYS	CA-C-N	7.21	134.68	121.70
18	D	409	LYS	C-N-CA	7.21	134.68	121.70
4	I	14	PRO	CB-CA-C	6.94	123.01	111.56
1	f	459	GLU	CA-C-N	6.80	133.94	121.70
1	f	459	GLU	C-N-CA	6.80	133.94	121.70
23	V	57	ALA	CA-C-N	6.75	133.85	121.70
23	V	57	ALA	C-N-CA	6.75	133.85	121.70
16	A	406	GLU	CA-C-N	6.66	133.69	121.70
16	A	406	GLU	C-N-CA	6.66	133.69	121.70
18	D	410	ASP	CA-C-N	6.66	133.68	121.70
18	D	410	ASP	C-N-CA	6.66	133.68	121.70
3	H	231	ALA	N-CA-C	6.55	119.75	111.69
26	Y	356	THR	CA-C-N	6.52	133.44	121.70
26	Y	356	THR	C-N-CA	6.52	133.44	121.70
17	B	434	THR	CA-C-N	6.51	126.27	119.76
17	B	434	THR	C-N-CA	6.51	126.27	119.76
3	H	231	ALA	CA-C-N	6.44	133.28	121.70
3	H	231	ALA	C-N-CA	6.44	133.28	121.70
26	Y	170	GLU	N-CA-C	6.38	118.77	111.11
23	V	81	GLN	CA-C-N	6.29	133.01	121.70
23	V	81	GLN	C-N-CA	6.29	133.01	121.70
20	F	433	ALA	CA-C-N	6.22	132.89	121.70
20	F	433	ALA	C-N-CA	6.22	132.89	121.70
31	d	228	GLN	N-CA-C	6.19	123.13	113.72
24	W	331	GLY	CA-C-O	-6.05	118.29	122.22
20	F	167	GLU	CB-CA-C	-6.04	109.63	116.63
1	f	617	LEU	CA-C-N	5.98	132.46	121.70
1	f	617	LEU	C-N-CA	5.98	132.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	63	LYS	CA-C-N	5.96	132.43	121.70
27	Z	63	LYS	C-N-CA	5.96	132.43	121.70
32	e	4	LYS	CD-CE-NZ	5.86	130.65	111.90
1	f	459	GLU	N-CA-CB	-5.82	108.28	114.10
1	f	617	LEU	N-CA-C	5.78	117.44	111.03
16	A	406	GLU	N-CA-C	5.76	118.77	111.69
20	F	164	LEU	CA-C-N	5.69	126.96	119.84
20	F	164	LEU	C-N-CA	5.69	126.96	119.84
23	V	316	ALA	CA-C-N	5.67	126.93	119.84
23	V	316	ALA	C-N-CA	5.67	126.93	119.84
1	f	459	GLU	CB-CA-C	-5.60	104.29	109.83
18	D	144	PRO	N-CA-C	5.57	117.49	110.70
31	d	236	THR	CA-C-N	5.49	123.70	120.24
31	d	236	THR	C-N-CA	5.49	123.70	120.24
16	A	344	SER	CA-C-N	5.37	131.36	121.70
16	A	344	SER	C-N-CA	5.37	131.36	121.70
20	F	170	SER	CB-CA-C	-5.36	110.38	116.54
21	C	255	GLY	CA-C-N	5.30	131.24	121.70
21	C	255	GLY	C-N-CA	5.30	131.24	121.70
27	Z	222	ILE	N-CA-C	5.29	118.52	111.44
17	B	324	ASP	CA-C-N	5.28	131.20	121.70
17	B	324	ASP	C-N-CA	5.28	131.20	121.70
22	U	172	ASP	CA-C-N	5.22	131.10	121.70
22	U	172	ASP	C-N-CA	5.22	131.10	121.70
1	f	459	GLU	CA-C-O	-5.19	114.93	119.18
17	B	166	ASP	CA-C-N	5.16	130.98	121.70
17	B	166	ASP	C-N-CA	5.16	130.98	121.70
23	V	128	ARG	CB-CA-C	-5.15	110.23	117.23
23	V	80	LYS	CA-C-N	5.12	130.92	121.70
23	V	80	LYS	C-N-CA	5.12	130.92	121.70
23	V	54	LYS	CA-C-N	5.10	130.88	121.70
23	V	54	LYS	C-N-CA	5.10	130.88	121.70
11	P	31	GLN	CB-CA-C	-5.00	110.42	117.23

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	B	436	GLU	Peptide
18	D	258	ALA	Peptide
18	D	406	VAL	Peptide
18	D	412	GLN	Peptide

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Mol	Chain	Res	Type	Group
23	V	319	HIS	Peptide
24	W	416	GLN	Peptide
26	Y	357	ASN	Peptide
28	a	286	ALA	Peptide
31	d	3	GLU	Peptide

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	f	5331	0	5344	135	0
2	G	1826	0	1796	73	0
3	H	1708	0	1594	61	0
4	I	1912	0	1851	87	0
5	J	1704	0	1517	89	0
6	K	1722	0	1673	53	0
7	L	1850	0	1822	53	0
8	M	1856	0	1814	49	0
9	N	1430	0	1398	24	0
10	O	1643	0	1644	33	0
11	P	1585	0	1598	30	0
12	Q	1570	0	1547	41	0
13	R	1548	0	1499	36	0
14	S	1641	0	1618	26	0
15	T	1667	0	1628	37	0
16	A	2835	0	2879	116	0
17	B	2717	0	2755	122	0
18	D	3040	0	3076	129	0
19	E	2790	0	2846	90	0
20	F	2863	0	2931	102	0
21	C	3078	0	3193	135	0
22	U	6287	0	6338	148	0
23	V	3852	0	3893	165	0
24	W	3703	0	3822	103	0
25	X	1905	0	1951	49	0
26	Y	3115	0	3120	108	0
27	Z	2281	0	2312	91	0
28	a	2995	0	3012	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	b	1458	0	1505	38	0
30	c	2187	0	2215	82	0
31	d	2116	0	2146	61	0
32	e	334	0	294	42	0
33	A	31	0	12	1	0
33	D	31	0	12	2	0
33	E	31	0	12	3	0
33	F	31	0	12	1	0
34	c	1	0	0	0	0
All	All	76674	0	76679	2178	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 14.

All (2178) 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)
23:V:212:TYR:CE1	23:V:212:TYR:CZ	1.76	1.73
5:J:21:TYR:CG	5:J:21:TYR:CD1	1.85	1.64
5:J:21:TYR:CG	5:J:21:TYR:CD2	1.86	1.64
23:V:212:TYR:CZ	23:V:212:TYR:CE2	1.76	1.63
5:J:21:TYR:CZ	5:J:21:TYR:CE2	1.97	1.51
23:V:212:TYR:CE1	23:V:212:TYR:CD1	2.00	1.49
23:V:212:TYR:CE2	23:V:212:TYR:CD2	2.00	1.49
5:J:21:TYR:CZ	5:J:21:TYR:CE1	2.02	1.47
4:I:14:PRO:CA	4:I:14:PRO:C	2.00	1.35
4:I:14:PRO:HA	5:J:21:TYR:CG	1.63	1.32
4:I:14:PRO:HA	5:J:21:TYR:CD1	1.63	1.31
4:I:15:GLU:N	5:J:21:TYR:CZ	2.02	1.28
4:I:14:PRO:C	5:J:21:TYR:CE2	2.13	1.25
4:I:14:PRO:C	5:J:21:TYR:CE1	2.15	1.24
4:I:14:PRO:C	5:J:21:TYR:CZ	2.19	1.21
4:I:14:PRO:C	5:J:21:TYR:CD1	2.19	1.21
4:I:14:PRO:C	5:J:21:TYR:CD2	2.23	1.17
5:J:21:TYR:CD1	5:J:21:TYR:CE1	2.38	1.11
4:I:14:PRO:O	5:J:21:TYR:CG	2.03	1.11
23:V:212:TYR:CE1	32:e:4:LYS:CE	2.35	1.10
5:J:21:TYR:CD2	5:J:21:TYR:CE2	2.40	1.10
4:I:15:GLU:N	5:J:21:TYR:CE1	2.20	1.09
4:I:14:PRO:CA	5:J:21:TYR:CD1	2.35	1.08
23:V:212:TYR:CZ	32:e:4:LYS:CE	2.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:212:TYR:CD2	32:e:4:LYS:CD	2.37	1.08
4:I:14:PRO:C	5:J:21:TYR:CG	2.34	1.05
23:V:212:TYR:CE2	32:e:4:LYS:CE	2.39	1.05
4:I:14:PRO:O	5:J:21:TYR:CD2	2.11	1.04
23:V:212:TYR:CD1	32:e:4:LYS:CE	2.40	1.04
4:I:14:PRO:HB2	5:J:21:TYR:CE2	1.92	1.04
23:V:212:TYR:CE2	32:e:4:LYS:CD	2.40	1.03
4:I:14:PRO:CA	5:J:21:TYR:CE1	2.42	1.03
23:V:212:TYR:CD1	32:e:4:LYS:CD	2.43	1.02
23:V:212:TYR:CD2	32:e:4:LYS:CE	2.44	1.00
21:C:217:SER:HB3	21:C:218:GLU:HB3	1.40	1.00
4:I:14:PRO:CA	5:J:21:TYR:CG	2.45	0.98
23:V:212:TYR:CG	32:e:4:LYS:CD	2.45	0.98
4:I:14:PRO:CA	5:J:21:TYR:CZ	2.47	0.98
23:V:212:TYR:CZ	32:e:4:LYS:CD	2.46	0.97
23:V:212:TYR:CE1	32:e:4:LYS:CD	2.47	0.97
4:I:14:PRO:CA	5:J:21:TYR:CD2	2.48	0.97
23:V:212:TYR:CG	32:e:4:LYS:CE	2.48	0.95
4:I:14:PRO:CA	5:J:21:TYR:CE2	2.53	0.92
23:V:212:TYR:CZ	32:e:4:LYS:HE2	2.02	0.92
23:V:212:TYR:CG	32:e:4:LYS:HD2	2.05	0.92
17:B:166:ASP:HB3	17:B:167:THR:HA	1.52	0.91
28:a:13:ASN:OD1	28:a:19:PRO:HG2	1.71	0.91
4:I:14:PRO:N	5:J:21:TYR:CE1	2.40	0.89
4:I:14:PRO:CB	5:J:21:TYR:CE2	2.54	0.89
28:a:13:ASN:OD1	28:a:19:PRO:CG	2.21	0.88
23:V:212:TYR:CE1	32:e:4:LYS:HE3	2.08	0.88
30:c:174:PRO:HB2	30:c:175:ARG:HD3	1.57	0.87
23:V:212:TYR:CE2	32:e:4:LYS:HD3	2.09	0.87
24:W:40:LEU:HB2	24:W:41:GLN:HA	1.56	0.84
30:c:272:ILE:HG21	30:c:276:GLY:H	1.43	0.84
6:K:225:ASN:HA	6:K:227:HIS:HB3	1.59	0.84
24:W:416:GLN:HB3	24:W:417:ARG:HA	1.61	0.82
3:H:10:LEU:HB3	3:H:124:SER:HA	1.62	0.82
18:D:389:GLU:HA	18:D:390:ASN:HB2	1.62	0.81
19:E:266:GLY:HA2	19:E:267:PHE:HB3	1.62	0.81
18:D:166:ASP:HB3	33:D:501:ATP:HN61	1.46	0.81
1:f:391:LEU:HD12	1:f:392:LYS:H	1.46	0.81
2:G:159:TYR:HB3	3:H:81:PRO:HG3	1.63	0.81
4:I:14:PRO:CB	5:J:21:TYR:CD2	2.65	0.80
21:C:144:PRO:HD2	21:C:201:ARG:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:14:PRO:C	4:I:14:PRO:HA	2.02	0.80
18:D:303:VAL:HG23	18:D:304:ASN:HB2	1.62	0.80
21:C:158:ILE:HA	21:C:161:ILE:HG22	1.64	0.80
20:F:431:LYS:HD2	20:F:434:ASN:HB3	1.62	0.80
13:R:19:ARG:HE	13:R:29:GLN:HE22	1.29	0.79
23:V:212:TYR:CD1	32:e:4:LYS:HE3	2.15	0.79
26:Y:170:GLU:HG3	26:Y:171:GLY:HA3	1.63	0.79
23:V:212:TYR:CE2	32:e:4:LYS:HE2	2.18	0.79
1:f:617:LEU:HB3	1:f:618:THR:HB	1.63	0.79
1:f:615:GLY:HA2	1:f:619:LEU:H	1.46	0.79
23:V:212:TYR:CD2	32:e:4:LYS:HD3	2.18	0.78
18:D:100:THR:HB	18:D:114:ARG:HD2	1.64	0.78
31:d:3:GLU:HB3	31:d:4:GLN:HA	1.64	0.78
17:B:220:LYS:HB3	17:B:346:ARG:HB3	1.64	0.78
19:E:174:GLY:HA2	19:E:176:PRO:HD2	1.63	0.78
18:D:283:ARG:HA	18:D:286:GLN:HE21	1.49	0.77
23:V:57:ALA:HB3	23:V:58:ALA:HB3	1.64	0.77
1:f:371:CYS:SG	1:f:372:ASN:N	2.54	0.77
16:A:333:ARG:HB2	16:A:337:LEU:HB2	1.66	0.77
16:A:102:ILE:HA	16:A:113:ILE:HA	1.65	0.77
21:C:310:ARG:HG3	21:C:311:ILE:HG23	1.64	0.77
16:A:267:LYS:HB3	16:A:270:CYS:HB3	1.67	0.76
18:D:199:PRO:HG3	18:D:328:ASP:HB2	1.66	0.76
20:F:409:ARG:HB2	20:F:411:GLY:HA2	1.67	0.76
18:D:410:ASP:HB3	18:D:412:GLN:N	1.99	0.76
4:I:15:GLU:N	5:J:21:TYR:CE2	2.53	0.76
21:C:195:GLY:HA2	21:C:198:LEU:HB2	1.66	0.75
28:a:188:LEU:HD11	28:a:193:GLN:HG3	1.65	0.75
23:V:80:LYS:HE2	23:V:87:SER:HA	1.68	0.75
23:V:212:TYR:CD1	32:e:4:LYS:HD2	2.22	0.75
4:I:14:PRO:O	5:J:21:TYR:CD1	2.41	0.74
17:B:177:GLU:H	17:B:178:LYS:HA	1.53	0.74
16:A:401:ARG:HD2	16:A:407:LYS:HE2	1.70	0.74
21:C:254:ILE:HG23	21:C:257:SER:HB3	1.69	0.74
30:c:124:GLY:O	30:c:128:ASN:ND2	2.20	0.74
28:a:286:ALA:HB1	28:a:287:ASN:HA	1.70	0.74
30:c:211:GLU:HA	30:c:214:GLN:HB3	1.70	0.74
24:W:92:LYS:H	24:W:93:ARG:HB3	1.52	0.73
1:f:361:LEU:HD13	1:f:398:TRP:HB3	1.68	0.73
20:F:299:GLU:HB3	20:F:300:LYS:HB3	1.71	0.73
19:E:245:GLU:HG2	19:E:250:ASP:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:E:401:ATP:H4'	20:F:344:ARG:HE	1.53	0.73
20:F:168:TYR:HB2	20:F:169:ASP:HB2	1.71	0.73
3:H:14:SER:HB3	3:H:19:LEU:HA	1.70	0.73
16:A:407:LYS:NZ	16:A:411:GLU:OE1	2.21	0.73
22:U:418:GLU:HG3	22:U:421:GLN:HE21	1.53	0.73
1:f:399:LEU:HD23	1:f:418:LEU:HD21	1.71	0.73
1:f:662:LEU:H	1:f:664:ALA:HA	1.52	0.73
3:H:39:LYS:HE2	3:H:144:PRO:HG2	1.71	0.73
19:E:222:ALA:HB1	19:E:273:VAL:HG21	1.70	0.73
17:B:396:LYS:HD3	21:C:181:ALA:HB3	1.68	0.72
7:L:67:ASP:HB3	7:L:70:ILE:HB	1.69	0.72
23:V:81:GLN:HB3	23:V:82:LEU:C	2.14	0.72
18:D:208:PRO:HB3	19:E:291:ARG:HH12	1.53	0.72
27:Z:176:LEU:HD12	27:Z:177:ARG:H	1.53	0.72
1:f:503:MET:SD	1:f:669:ARG:NH1	2.63	0.72
2:G:33:ASN:HA	2:G:170:VAL:HG22	1.71	0.72
20:F:165:PRO:HB2	20:F:166:THR:HG22	1.72	0.72
28:a:320:VAL:HG22	28:a:322:GLY:H	1.55	0.71
12:Q:4:LEU:HD22	12:Q:17:SER:HA	1.70	0.71
24:W:90:LEU:HA	24:W:94:ARG:HD2	1.72	0.71
24:W:257:GLN:HA	24:W:258:ALA:HB3	1.72	0.71
18:D:210:CYS:SG	18:D:376:ASN:ND2	2.64	0.70
25:X:229:TYR:OH	25:X:258:LYS:NZ	2.23	0.70
20:F:357:PRO:O	20:F:362:ARG:NH1	2.25	0.70
2:G:113:MET:HE3	10:O:70:THR:HA	1.73	0.70
21:C:313:ARG:NH1	21:C:314:LYS:O	2.24	0.70
27:Z:63:LYS:HB2	27:Z:64:ASP:HB2	1.74	0.70
28:a:270:ARG:HH11	28:a:313:LYS:HB3	1.57	0.70
22:U:261:LEU:HD22	22:U:329:LEU:HD22	1.73	0.69
16:A:140:VAL:HA	16:A:152:PRO:HA	1.74	0.69
23:V:255:LEU:HD22	23:V:291:TYR:HB3	1.74	0.69
26:Y:358:ARG:HD2	26:Y:359:PRO:HD2	1.73	0.69
30:c:180:ASN:HB2	30:c:204:THR:HG21	1.74	0.69
9:N:144:ARG:H	9:N:147:MET:HE3	1.57	0.69
21:C:72:TYR:HB2	21:C:116:LEU:HB3	1.74	0.69
6:K:50:VAL:HG11	6:K:66:LYS:HB2	1.74	0.69
16:A:172:VAL:HG13	33:A:501:ATP:H3'	1.74	0.69
26:Y:356:THR:OG1	26:Y:357:ASN:O	2.10	0.69
1:f:663:VAL:HG13	1:f:664:ALA:HB2	1.75	0.69
16:A:80:LEU:HB3	17:B:99:VAL:HG11	1.74	0.69
18:D:204:MET:HE3	18:D:310:ALA:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:440:LYS:NZ	31:d:143:LEU:O	2.26	0.69
1:f:154:GLU:HB3	1:f:184:LYS:HD3	1.75	0.69
16:A:404:ALA:HA	16:A:407:LYS:HD3	1.73	0.69
19:E:44:GLU:OE1	20:F:76:ASN:ND2	2.23	0.69
20:F:137:ILE:HG21	20:F:160:ILE:HB	1.75	0.69
26:Y:101:ARG:NH2	26:Y:126:LYS:O	2.23	0.68
1:f:33:VAL:HG23	1:f:34:PRO:HD3	1.74	0.68
8:M:190:VAL:HG11	8:M:232:ARG:HH11	1.57	0.68
19:E:81:VAL:HG11	19:E:105:LEU:HB2	1.73	0.68
17:B:285:ASP:HA	17:B:330:ALA:HB3	1.76	0.68
11:P:26:ARG:HH21	11:P:38:ASP:HA	1.59	0.68
18:D:375:ILE:H	18:D:378:ILE:HD12	1.59	0.68
23:V:455:LYS:N	23:V:456:GLY:HA2	2.09	0.68
28:a:13:ASN:OD1	28:a:19:PRO:HG3	1.94	0.68
2:G:109:ILE:HG12	2:G:111:VAL:H	1.58	0.68
22:U:842:LYS:HA	22:U:843:GLU:HB3	1.75	0.68
31:d:215:TRP:CD1	31:d:216:VAL:H	2.11	0.68
23:V:80:LYS:HA	23:V:81:GLN:HB2	1.76	0.68
23:V:275:VAL:H	23:V:276:PHE:HA	1.58	0.68
1:f:372:ASN:N	1:f:373:GLY:HA2	2.09	0.67
17:B:317:ASP:HB3	17:B:318:GLY:HA2	1.76	0.67
5:J:122:ASN:N	5:J:123:GLY:HA3	2.09	0.67
19:E:138:LEU:HD22	19:E:140:GLU:HG2	1.76	0.67
1:f:296:VAL:HG12	1:f:297:ARG:HG2	1.75	0.67
5:J:61:LYS:HG3	5:J:62:ILE:HD12	1.76	0.67
15:T:99:ARG:HG3	15:T:105:PRO:HA	1.76	0.67
17:B:407:LEU:HB3	21:C:163:GLU:HG2	1.75	0.67
1:f:294:SER:O	1:f:298:ASN:ND2	2.27	0.67
31:d:49:ILE:HD11	31:d:89:LEU:HD22	1.75	0.67
11:P:105:THR:HG23	11:P:107:PRO:HD3	1.76	0.67
8:M:41:CYS:HB3	8:M:189:ILE:HG13	1.76	0.66
22:U:155:LEU:O	22:U:158:ARG:NH1	2.27	0.66
26:Y:190:ALA:HA	26:Y:287:LEU:HD13	1.77	0.66
4:I:8:ARG:HD3	4:I:11:ILE:HB	1.78	0.66
21:C:38:LYS:HG2	23:V:495:ARG:HB3	1.77	0.66
27:Z:179:ILE:HG12	30:c:222:LYS:HE3	1.77	0.66
18:D:410:ASP:HB3	18:D:411:GLU:C	2.20	0.66
24:W:428:TRP:NE1	30:c:247:GLU:OE1	2.28	0.66
28:a:135:ILE:HG12	28:a:158:LEU:HD13	1.78	0.66
7:L:122:ARG:HG2	8:M:128:VAL:HG12	1.76	0.66
18:D:236:VAL:HG22	18:D:285:VAL:HG11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:416:ARG:HG3	23:V:459:GLN:HA	1.77	0.66
3:H:68:ILE:HA	3:H:91:ARG:HE	1.60	0.65
7:L:85:CYS:SG	7:L:89:ARG:NH1	2.69	0.65
20:F:321:GLN:HG3	20:F:322:PRO:HD3	1.78	0.65
16:A:186:LYS:HB3	16:A:339:ARG:HD2	1.77	0.65
17:B:174:MET:HA	17:B:248:LEU:HD13	1.77	0.65
22:U:904:LYS:H	22:U:913:ILE:HD11	1.60	0.65
24:W:436:MET:O	24:W:440:ASN:ND2	2.27	0.65
28:a:34:TRP:HD1	29:b:19:GLY:H	1.43	0.65
16:A:113:ILE:O	16:A:121:PHE:N	2.28	0.65
16:A:147:TYR:HB3	20:F:86:LEU:HD13	1.78	0.65
18:D:198:PRO:HD2	18:D:302:ASN:HD21	1.62	0.65
20:F:424:ILE:HG22	20:F:425:LEU:HD12	1.77	0.65
29:b:15:TYR:O	29:b:25:ARG:NH1	2.29	0.65
18:D:182:GLU:HA	18:D:185:LEU:HD13	1.78	0.65
19:E:83:CYS:HB3	19:E:87:LEU:HD21	1.78	0.65
23:V:224:LEU:HD13	23:V:227:VAL:HB	1.79	0.65
2:G:159:TYR:H	18:D:418:LYS:HZ1	1.45	0.65
4:I:174:MET:SD	4:I:195:LYS:NZ	2.70	0.65
7:L:52:ALA:HB2	7:L:59:HIS:HA	1.79	0.65
18:D:293:LEU:O	18:D:326:ARG:NH1	2.30	0.65
16:A:95:VAL:HG12	16:A:144:ARG:HG2	1.78	0.65
18:D:405:THR:HA	18:D:406:VAL:C	2.22	0.65
23:V:97:ALA:HB1	23:V:150:ARG:HH22	1.62	0.65
26:Y:349:LYS:HG3	26:Y:350:VAL:HG13	1.79	0.65
4:I:216:LEU:HD12	4:I:225:ILE:HG12	1.77	0.65
7:L:10:VAL:HG22	7:L:21:GLN:HG3	1.79	0.65
31:d:147:SER:HA	31:d:148:TYR:HB2	1.78	0.65
21:C:69:GLN:HB2	21:C:118:ASN:HB2	1.77	0.64
21:C:217:SER:HB3	21:C:218:GLU:CB	2.21	0.64
4:I:136:TYR:HB2	4:I:148:TYR:HB2	1.80	0.64
18:D:89:ILE:HD11	19:E:80:VAL:HG13	1.77	0.64
28:a:286:ALA:HA	28:a:288:HIS:HB2	1.79	0.64
2:G:140:LEU:HB2	2:G:152:TYR:HB2	1.79	0.64
3:H:74:LEU:HD21	3:H:134:LEU:HD22	1.78	0.64
16:A:331:LEU:HD13	20:F:229:PRO:HB2	1.79	0.64
17:B:402:ALA:O	17:B:421:LYS:NZ	2.30	0.64
23:V:451:ILE:HG13	23:V:458:VAL:HG13	1.78	0.64
24:W:331:GLY:HA2	24:W:332:SER:HB3	1.79	0.64
31:d:229:GLN:HG2	31:d:230:GLN:HG3	1.79	0.64
22:U:221:ILE:HB	22:U:754:HIS:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:356:THR:HG21	22:U:731:ILE:HD13	1.80	0.64
32:e:58:ALA:HB3	32:e:59:GLU:HA	1.79	0.64
4:I:14:PRO:HA	5:J:21:TYR:CD2	2.32	0.64
23:V:148:ARG:HG3	23:V:149:PRO:HD3	1.80	0.64
2:G:182:LYS:O	2:G:185:LYS:NZ	2.30	0.64
16:A:171:ASP:OD1	16:A:239:ARG:NH2	2.31	0.64
21:C:209:CYS:HB2	21:C:244:SER:HA	1.79	0.64
1:f:20:VAL:HG12	1:f:24:PRO:HD3	1.80	0.64
2:G:11:ARG:NH1	2:G:27:TYR:OH	2.31	0.64
2:G:139:ILE:HG13	2:G:153:LYS:HG3	1.80	0.64
4:I:121:TYR:HA	4:I:127:LYS:HE2	1.79	0.64
13:R:100:MET:HG2	13:R:113:TYR:HD1	1.63	0.64
16:A:306:LEU:O	16:A:336:ARG:NH2	2.31	0.64
20:F:229:PRO:O	20:F:392:ASN:ND2	2.31	0.64
4:I:228:LEU:HD11	4:I:232:GLU:HG2	1.80	0.63
7:L:48:ALA:HB3	7:L:211:SER:HB2	1.80	0.63
25:X:318:ILE:O	25:X:322:HIS:ND1	2.32	0.63
26:Y:64:GLN:HG2	26:Y:65:ILE:HG22	1.79	0.63
26:Y:101:ARG:HA	26:Y:104:MET:HE3	1.79	0.63
15:T:185:ASN:ND2	15:T:205:THR:OG1	2.31	0.63
18:D:61:ILE:HD12	21:C:43:ARG:HG3	1.80	0.63
26:Y:51:ALA:HA	26:Y:54:TYR:HB2	1.79	0.63
26:Y:77:ASN:O	26:Y:81:LEU:N	2.31	0.63
2:G:148:GLY:O	2:G:150:GLN:NE2	2.32	0.63
10:O:217:THR:HB	11:P:195:ILE:HB	1.81	0.63
22:U:789:ILE:HG23	22:U:844:LYS:HG2	1.81	0.63
28:a:270:ARG:NH1	28:a:310:LEU:O	2.30	0.63
4:I:72:MET:HG2	4:I:138:GLY:HA3	1.80	0.63
23:V:262:SER:HB2	23:V:263:LEU:HB2	1.80	0.63
1:f:311:VAL:HB	1:f:319:ARG:HG2	1.81	0.63
4:I:13:SER:C	5:J:21:TYR:CE1	2.77	0.63
16:A:165:GLN:HG2	16:A:240:VAL:HG13	1.81	0.63
2:G:159:TYR:H	18:D:418:LYS:NZ	1.95	0.63
16:A:280:ILE:HA	17:B:310:LEU:HD11	1.81	0.63
18:D:83:GLN:HG3	18:D:87:LEU:HD11	1.79	0.63
3:H:82:ASP:OD1	3:H:128:ARG:NH2	2.31	0.63
8:M:141:SER:HB3	8:M:144:ASP:HB2	1.81	0.63
26:Y:63:TRP:HB3	26:Y:64:GLN:HB3	1.81	0.63
2:G:105:TYR:HA	10:O:78:THR:HG23	1.80	0.63
4:I:159:TRP:HB3	5:J:54:GLN:HB3	1.81	0.63
9:N:22:THR:HG22	9:N:27:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:434:ASN:OD1	20:F:435:LEU:N	2.32	0.63
24:W:55:ARG:HH22	24:W:79:GLU:HG3	1.64	0.63
4:I:47:ALA:HB3	4:I:212:GLU:HB3	1.80	0.62
29:b:164:ASP:N	29:b:165:GLY:HA2	2.14	0.62
1:f:494:ALA:HB1	1:f:527:LEU:HD13	1.81	0.62
19:E:194:ASN:ND2	19:E:227:PRO:O	2.32	0.62
23:V:91:PRO:HG3	23:V:126:ALA:HB3	1.81	0.62
19:E:222:ALA:O	19:E:226:GLN:NE2	2.31	0.62
21:C:21:ARG:NH2	22:U:102:ALA:O	2.31	0.62
8:M:194:ALA:HB1	8:M:238:TYR:HD1	1.64	0.62
16:A:215:PHE:HB3	16:A:321:THR:HG23	1.80	0.62
16:A:248:LYS:HB3	17:B:260:LEU:HD21	1.80	0.62
20:F:164:LEU:HD12	20:F:165:PRO:HD2	1.82	0.62
23:V:393:THR:O	23:V:397:ARG:NH2	2.31	0.62
26:Y:346:LYS:HB2	26:Y:355:GLU:HB3	1.81	0.62
31:d:228:GLN:N	31:d:229:GLN:HA	2.14	0.62
6:K:225:ASN:HB2	6:K:226:PHE:CG	2.34	0.62
17:B:166:ASP:CB	17:B:167:THR:HA	2.29	0.62
18:D:197:ASP:OD2	18:D:301:GLN:NE2	2.33	0.62
18:D:286:GLN:NE2	21:C:218:GLU:OE2	2.32	0.62
19:E:233:ASP:HA	19:E:278:ALA:HB3	1.81	0.62
23:V:266:GLN:O	23:V:269:LYS:NZ	2.33	0.62
4:I:48:GLU:HA	4:I:211:VAL:HA	1.82	0.62
2:G:145:GLU:OE2	10:O:75:ARG:NH2	2.33	0.62
5:J:116:GLN:OE1	6:K:135:ARG:NH2	2.33	0.62
24:W:259:GLU:HG2	24:W:262:LYS:HB3	1.80	0.62
26:Y:138:LEU:HD12	26:Y:141:VAL:HB	1.81	0.62
30:c:151:VAL:HG13	30:c:152:LYS:HG2	1.82	0.62
3:H:38:ILE:HB	3:H:45:VAL:HB	1.80	0.62
3:H:39:LYS:HB3	3:H:159:LYS:HA	1.82	0.61
22:U:252:LEU:HD21	22:U:264:VAL:HG11	1.81	0.61
5:J:115:LYS:HG3	5:J:127:PHE:HD2	1.65	0.61
1:f:502:ALA:HB1	1:f:537:LEU:HD12	1.81	0.61
7:L:66:VAL:HG13	7:L:89:ARG:HD3	1.81	0.61
16:A:194:PRO:HB3	16:A:200:ARG:HB2	1.82	0.61
17:B:264:PRO:HA	17:B:315:GLN:HG3	1.82	0.61
27:Z:33:LYS:NZ	27:Z:34:ARG:O	2.27	0.61
3:H:20:VAL:HG12	3:H:21:GLN:H	1.65	0.61
22:U:341:PHE:HB2	22:U:881:PRO:HD2	1.81	0.61
23:V:455:LYS:HD2	23:V:457:TYR:HE2	1.66	0.61
7:L:164:ARG:HD2	7:L:199:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:400:THR:HG21	21:C:183:PRO:HD3	1.82	0.61
26:Y:138:LEU:HD23	26:Y:176:ARG:HB2	1.82	0.61
31:d:147:SER:OG	31:d:151:VAL:N	2.30	0.61
1:f:390:GLU:HG3	1:f:395:TYR:HB3	1.83	0.61
10:O:17:ASP:O	10:O:33:LYS:NZ	2.26	0.61
12:Q:29:LYS:NZ	13:R:122:SER:O	2.31	0.61
16:A:206:ILE:HG13	20:F:373:MET:HE2	1.82	0.61
17:B:313:LEU:HG	17:B:341:LEU:HD11	1.81	0.61
19:E:260:LEU:HB3	19:E:264:MET:HE2	1.82	0.61
21:C:284:GLU:HG3	21:C:286:THR:H	1.66	0.61
23:V:321:ALA:HB1	23:V:322:VAL:HB	1.83	0.61
25:X:252:LYS:HD3	25:X:287:LEU:HD21	1.81	0.61
1:f:629:MET:HE2	1:f:649:ASN:HD21	1.64	0.61
18:D:392:TYR:HE1	19:E:161:ARG:HH22	1.49	0.61
30:c:229:LEU:HD22	30:c:231:LEU:HD13	1.81	0.61
5:J:137:ASP:N	5:J:141:THR:O	2.33	0.61
6:K:32:LYS:HD2	6:K:172:SER:HA	1.82	0.61
7:L:151:ALA:O	8:M:85:ARG:NH2	2.33	0.61
26:Y:145:LEU:HG	26:Y:160:ASN:HD21	1.65	0.61
7:L:33:SER:HB2	7:L:49:LEU:HB3	1.82	0.61
18:D:354:LEU:HA	18:D:355:SER:C	2.24	0.61
26:Y:357:ASN:HB2	26:Y:358:ARG:HA	1.83	0.61
28:a:319:LEU:HA	28:a:337:GLN:HE21	1.65	0.61
4:I:14:PRO:HB3	5:J:21:TYR:CD2	2.35	0.60
5:J:119:THR:HG22	5:J:126:PRO:HB3	1.83	0.60
17:B:404:LEU:HD12	21:C:163:GLU:HB2	1.83	0.60
20:F:247:THR:O	20:F:281:SER:OG	2.17	0.60
23:V:379:LEU:HD13	23:V:395:ILE:HG12	1.83	0.60
1:f:589:LEU:HB3	1:f:603:VAL:HG22	1.83	0.60
9:N:19:ARG:NH1	9:N:168:GLY:O	2.33	0.60
10:O:142:PHE:HB2	10:O:154:LEU:HD21	1.83	0.60
13:R:91:LYS:NZ	13:R:117:GLU:OE1	2.31	0.60
18:D:169:GLY:HA3	18:D:173:GLN:HB3	1.82	0.60
24:W:219:THR:HA	24:W:220:GLU:HB2	1.82	0.60
5:J:115:LYS:HE2	5:J:149:PRO:HA	1.84	0.60
17:B:390:LEU:HD13	17:B:432:GLU:HG3	1.83	0.60
21:C:213:ARG:NH2	21:C:249:ASP:OD2	2.34	0.60
2:G:38:THR:H	2:G:53:GLN:HE22	1.47	0.60
19:E:207:TYR:HB3	20:F:260:PHE:HB3	1.82	0.60
21:C:50:ASN:ND2	22:U:642:GLU:O	2.33	0.60
28:a:284:ARG:HH12	28:a:291:LEU:HD21	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:12:LYS:HG2	31:d:57:ILE:HD11	1.83	0.60
11:P:153:LEU:HB3	11:P:166:THR:HG23	1.82	0.60
17:B:361:LYS:HE2	17:B:390:LEU:H	1.67	0.60
24:W:91:SER:HB2	24:W:92:LYS:HD2	1.82	0.60
30:c:226:MET:HB3	30:c:230:THR:HG22	1.82	0.60
17:B:294:ARG:NH1	17:B:297:SER:O	2.35	0.60
28:a:34:TRP:H	29:b:18:ASN:HB2	1.65	0.60
8:M:76:ALA:HB3	8:M:136:MET:HB2	1.83	0.60
19:E:384:LEU:HD12	19:E:385:ASP:HA	1.82	0.60
20:F:362:ARG:NH2	20:F:388:THR:O	2.34	0.60
25:X:203:PRO:HB3	25:X:206:LEU:HB2	1.83	0.60
28:a:226:ARG:HB3	28:a:234:ILE:HG12	1.83	0.60
16:A:123:VAL:HG22	16:A:124:ASP:O	2.02	0.60
17:B:383:LEU:O	17:B:387:LYS:NZ	2.34	0.60
20:F:433:ALA:HA	20:F:434:ASN:OD1	2.01	0.60
30:c:131:GLN:HA	30:c:134:GLU:HG2	1.84	0.60
6:K:77:ALA:HB3	6:K:142:LEU:HB2	1.83	0.60
7:L:120:THR:O	8:M:129:ARG:NH1	2.35	0.60
18:D:136:SER:HB3	21:C:67:GLN:HA	1.82	0.60
20:F:246:ALA:HB1	20:F:281:SER:HA	1.84	0.60
27:Z:97:THR:HA	27:Z:124:ILE:HG13	1.84	0.60
31:d:235:THR:HG22	31:d:237:ILE:H	1.67	0.60
6:K:18:GLU:HB2	6:K:19:GLY:HA2	1.83	0.60
23:V:252:ASN:ND2	23:V:284:GLU:OE2	2.29	0.60
9:N:5:ALA:HB3	9:N:126:ALA:HB3	1.83	0.59
14:S:27:THR:HB	14:S:40:SER:H	1.67	0.59
20:F:257:VAL:HG22	20:F:306:VAL:HG21	1.83	0.59
3:H:231:ALA:H	3:H:232:ALA:HB3	1.67	0.59
6:K:143:PHE:HB2	6:K:154:PHE:HB2	1.82	0.59
20:F:231:THR:OG1	20:F:233:LYS:NZ	2.27	0.59
27:Z:243:GLN:HG3	30:c:309:PHE:HE1	1.67	0.59
7:L:107:ARG:NH2	15:T:79:ASP:OD2	2.35	0.59
19:E:305:ASN:O	19:E:309:ARG:N	2.28	0.59
22:U:742:HIS:HB2	22:U:883:ARG:HH12	1.68	0.59
4:I:25:MET:HA	4:I:28:ILE:HD12	1.83	0.59
13:R:21:THR:HG22	13:R:27:ALA:H	1.68	0.59
13:R:73:ARG:HH22	13:R:107:ARG:HG3	1.67	0.59
21:C:255:GLY:H	21:C:256:SER:HB2	1.67	0.59
25:X:242:ILE:HG22	25:X:243:ASP:H	1.67	0.59
31:d:175:ARG:HA	31:d:178:ILE:HD12	1.83	0.59
2:G:159:TYR:CG	18:D:418:LYS:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:20:GLN:HG2	4:I:129:PRO:HG3	1.84	0.59
16:A:357:ILE:HG13	16:A:360:ARG:HH21	1.68	0.59
20:F:280:PRO:HA	20:F:326:VAL:HG22	1.83	0.59
22:U:237:VAL:HG13	22:U:321:GLN:HG3	1.82	0.59
27:Z:202:ASN:OD1	27:Z:203:SER:N	2.35	0.59
27:Z:245:PHE:O	27:Z:249:PHE:N	2.35	0.59
31:d:145:GLU:N	31:d:146:GLY:HA2	2.17	0.59
31:d:233:GLU:N	31:d:234:ASP:HA	2.18	0.59
16:A:399:ALA:HB3	16:A:401:ARG:HE	1.68	0.59
18:D:163:MET:HG3	18:D:165:ALA:H	1.68	0.59
20:F:96:LEU:HB3	20:F:122:ALA:HA	1.83	0.59
28:a:125:ILE:N	28:a:126:GLY:HA2	2.17	0.59
3:H:166:ASN:O	3:H:170:GLY:N	2.27	0.59
20:F:409:ARG:HG3	20:F:410:ARG:HA	1.83	0.59
22:U:424:ALA:HA	22:U:427:LEU:HD13	1.84	0.59
24:W:66:ILE:HG23	24:W:67:LEU:HB2	1.83	0.59
25:X:223:LYS:NZ	26:Y:242:LYS:O	2.36	0.59
28:a:264:ASN:ND2	28:a:267:GLN:OE1	2.36	0.59
1:f:293:ASN:HB3	1:f:307:LEU:HD11	1.85	0.59
11:P:49:LEU:HG	11:P:111:GLY:HA3	1.85	0.59
23:V:237:THR:OG1	23:V:241:ARG:NH2	2.34	0.59
28:a:287:ASN:HB3	28:a:289:ARG:HB2	1.83	0.59
1:f:109:LEU:HB2	1:f:141:ARG:HH12	1.67	0.59
2:G:22:LEU:HD13	2:G:25:VAL:HB	1.83	0.59
4:I:31:ALA:O	4:I:50:ARG:NH2	2.36	0.59
6:K:104:ASN:ND2	14:S:86:GLY:O	2.36	0.59
13:R:97:MET:H	13:R:116:SER:HB3	1.68	0.59
16:A:172:VAL:HG12	16:A:223:THR:HG23	1.83	0.59
19:E:269:THR:HG1	19:E:271:HIS:HD1	1.50	0.59
23:V:323:GLY:HA2	23:V:326:GLN:HB2	1.83	0.59
27:Z:102:HIS:HD2	27:Z:104:ASN:HB3	1.67	0.59
30:c:63:ASP:OD1	30:c:66:THR:OG1	2.20	0.59
20:F:280:PRO:HD3	20:F:325:GLN:HE21	1.66	0.59
21:C:87:VAL:HG11	21:C:116:LEU:HD13	1.84	0.59
24:W:439:VAL:HG21	30:c:232:GLN:HA	1.85	0.59
26:Y:111:LEU:HA	26:Y:114:ILE:HD13	1.83	0.59
7:L:39:LYS:HD3	7:L:144:ILE:HG12	1.85	0.58
21:C:245:ILE:HG23	21:C:290:LYS:HB2	1.85	0.58
22:U:505:ASP:HB3	22:U:508:THR:HG22	1.84	0.58
25:X:354:ILE:HG21	25:X:361:VAL:HG11	1.85	0.58
23:V:173:ILE:O	23:V:177:ASN:ND2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:436:PHE:HB3	31:d:146:GLY:H	1.68	0.58
21:C:119:ASP:OD1	21:C:119:ASP:N	2.37	0.58
22:U:474:ARG:HH21	22:U:500:ASN:HB2	1.68	0.58
27:Z:244:GLU:HG2	28:a:287:ASN:H	1.69	0.58
31:d:175:ARG:HD2	31:d:205:LYS:HZ2	1.68	0.58
23:V:349:ARG:HG3	23:V:357:LEU:HD21	1.85	0.58
24:W:13:ILE:HG22	24:W:54:THR:HG21	1.85	0.58
26:Y:190:ALA:O	26:Y:291:HIS:NE2	2.35	0.58
27:Z:96:HIS:HE1	27:Z:121:LEU:HD13	1.68	0.58
1:f:662:LEU:N	1:f:663:VAL:HA	2.19	0.58
2:G:184:LYS:HA	2:G:185:LYS:C	2.29	0.58
8:M:99:ARG:O	15:T:65:GLN:NE2	2.34	0.58
10:O:133:ALA:HB3	10:O:162:GLY:HA2	1.86	0.58
18:D:200:ARG:HD2	18:D:296:MET:HE3	1.86	0.58
19:E:354:ALA:HB1	19:E:362:VAL:HG21	1.83	0.58
21:C:65:LEU:HA	30:c:190:GLN:HE22	1.69	0.58
22:U:637:VAL:HG13	22:U:652:ALA:HB1	1.85	0.58
27:Z:14:LEU:HA	30:c:39:LEU:HD13	1.86	0.58
30:c:272:ILE:HG13	30:c:275:VAL:HG23	1.86	0.58
2:G:53:GLN:HA	2:G:215:ILE:HA	1.84	0.58
16:A:183:GLN:NE2	16:A:342:GLU:O	2.36	0.58
22:U:610:VAL:HG11	27:Z:177:ARG:HG3	1.86	0.58
5:J:137:ASP:OD1	5:J:143:ARG:NE	2.34	0.58
12:Q:148:THR:HB	12:Q:151:ILE:HB	1.86	0.58
22:U:14:GLU:O	22:U:20:LYS:NZ	2.37	0.58
23:V:337:LEU:O	23:V:401:ASN:ND2	2.37	0.58
25:X:414:LEU:HD23	25:X:417:LYS:HD2	1.83	0.58
26:Y:51:ALA:HB2	26:Y:116:ASP:H	1.68	0.58
27:Z:168:GLU:HA	30:c:42:LEU:HD13	1.86	0.58
1:f:108:ARG:HH21	1:f:141:ARG:HD3	1.67	0.58
8:M:15:SER:OG	8:M:19:ARG:O	2.22	0.58
16:A:351:ARG:HH11	16:A:379:ASN:H	1.52	0.58
21:C:14:GLY:O	21:C:18:SER:N	2.27	0.58
23:V:211:TYR:HB3	23:V:253:LEU:HD11	1.85	0.58
23:V:357:LEU:O	23:V:361:PHE:N	2.37	0.58
8:M:99:ARG:HB3	15:T:69:GLN:HE22	1.68	0.58
23:V:326:GLN:HB3	23:V:353:LEU:HD22	1.86	0.58
24:W:374:THR:HG23	28:a:327:VAL:HA	1.85	0.58
26:Y:179:ARG:NH2	26:Y:212:GLU:OE2	2.34	0.58
27:Z:266:ILE:HG12	30:c:256:ASN:HB3	1.86	0.58
1:f:111:LEU:HA	1:f:116:MET:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:385:LEU:HD22	18:D:402:ALA:HB2	1.86	0.57
26:Y:194:PHE:HB3	26:Y:230:ALA:HB2	1.84	0.57
21:C:13:GLU:N	21:C:14:GLY:HA3	2.18	0.57
1:f:106:ALA:HB1	1:f:107:LEU:HA	1.87	0.57
1:f:392:LYS:O	1:f:433:ASN:ND2	2.36	0.57
2:G:37:LEU:HD23	2:G:81:THR:HA	1.84	0.57
5:J:96:LEU:HA	12:Q:62:LYS:HE2	1.86	0.57
6:K:16:SER:HB3	6:K:20:ARG:H	1.68	0.57
22:U:215:ASN:OD1	22:U:216:VAL:N	2.36	0.57
26:Y:192:ARG:NH2	26:Y:291:HIS:O	2.37	0.57
26:Y:301:ILE:HD12	26:Y:342:ARG:HB3	1.85	0.57
24:W:135:LYS:HB3	24:W:136:ILE:C	2.30	0.57
2:G:119:ALA:HA	2:G:122:SER:HB2	1.87	0.57
4:I:154:GLY:O	5:J:81:ARG:NH1	2.37	0.57
13:R:12:VAL:H	13:R:179:VAL:HB	1.68	0.57
17:B:274:ALA:O	17:B:278:ALA:N	2.38	0.57
18:D:200:ARG:HE	18:D:305:VAL:HG11	1.70	0.57
22:U:220:LEU:HD11	22:U:252:LEU:HD13	1.85	0.57
23:V:283:ASN:HB2	23:V:317:PRO:HD2	1.87	0.57
28:a:112:ILE:HD13	28:a:151:VAL:HG11	1.87	0.57
8:M:35:THR:HA	8:M:166:GLY:HA3	1.86	0.57
8:M:149:TYR:HD1	8:M:159:GLY:HA3	1.70	0.57
18:D:179:GLU:HA	18:D:183:LEU:HD22	1.85	0.57
18:D:283:ARG:HE	21:C:222:LYS:HD3	1.69	0.57
21:C:151:ILE:HD12	21:C:198:LEU:HB3	1.87	0.57
21:C:167:LEU:HD11	21:C:174:LEU:HD11	1.86	0.57
1:f:615:GLY:HA2	1:f:619:LEU:N	2.17	0.57
3:H:222:THR:OG1	3:H:225:GLU:OE1	2.22	0.57
8:M:54:LEU:H	8:M:57:LEU:HD11	1.69	0.57
10:O:100:LEU:HB2	10:O:113:ILE:HD11	1.86	0.57
17:B:131:HIS:NE2	17:B:156:VAL:O	2.37	0.57
18:D:196:ILE:HD13	21:C:367:GLY:HA3	1.86	0.57
21:C:89:VAL:HG12	21:C:91:PRO:HD2	1.87	0.57
27:Z:138:TYR:HB3	27:Z:155:PHE:HB3	1.85	0.57
1:f:270:ILE:HD12	1:f:274:LEU:HD12	1.87	0.57
16:A:406:GLU:H	16:A:407:LYS:HB3	1.69	0.57
17:B:106:PRO:O	17:B:154:HIS:NE2	2.38	0.57
18:D:202:VAL:HB	18:D:308:ILE:HA	1.86	0.57
18:D:389:GLU:HB3	18:D:391:ARG:N	2.20	0.57
20:F:94:ILE:HB	20:F:123:VAL:HB	1.86	0.57
29:b:8:VAL:HA	29:b:110:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:251:ALA:HA	1:f:254:SER:HB2	1.86	0.57
2:G:86:ASP:HB2	2:G:136:CYS:HB3	1.87	0.57
4:I:86:LEU:HD22	4:I:114:LEU:HD11	1.87	0.57
22:U:649:ARG:HB3	22:U:675:MET:HE1	1.87	0.57
23:V:483:CYS:HA	23:V:486:ILE:HD12	1.87	0.57
12:Q:168:GLN:NE2	12:Q:174:ASN:O	2.38	0.57
14:S:35:ILE:O	15:T:151:ARG:NH2	2.37	0.57
16:A:339:ARG:NH2	20:F:402:GLU:OE1	2.38	0.57
24:W:136:ILE:H	24:W:141:GLU:HG2	1.70	0.57
26:Y:68:ASP:HA	26:Y:71:ASN:HB2	1.85	0.57
26:Y:356:THR:HA	26:Y:357:ASN:CG	2.29	0.57
4:I:62:SER:OG	4:I:65:ILE:O	2.18	0.56
8:M:15:SER:OG	8:M:17:ASP:OD1	2.17	0.56
15:T:112:ILE:O	15:T:123:GLY:N	2.35	0.56
17:B:219:PRO:O	17:B:346:ARG:NH2	2.38	0.56
24:W:223:LYS:HA	24:W:226:TYR:HB3	1.86	0.56
24:W:235:GLN:NE2	24:W:247:TYR:OH	2.37	0.56
3:H:34:PRO:HB3	3:H:165:LYS:H	1.70	0.56
19:E:97:ARG:HD2	19:E:111:LEU:HD11	1.88	0.56
27:Z:176:LEU:HB2	30:c:218:LEU:HD12	1.86	0.56
30:c:161:ARG:NH1	30:c:162:LEU:O	2.38	0.56
3:H:46:LEU:O	3:H:211:GLY:N	2.33	0.56
4:I:83:ALA:HB2	4:I:132:VAL:HG11	1.87	0.56
14:S:46:LEU:HB3	14:S:72:LEU:HD11	1.88	0.56
18:D:388:ARG:O	18:D:390:ASN:ND2	2.38	0.56
19:E:241:ARG:HG2	19:E:243:PHE:H	1.71	0.56
22:U:800:VAL:HG21	22:U:914:LEU:HD21	1.86	0.56
24:W:44:ILE:HB	24:W:93:ARG:HD2	1.88	0.56
25:X:255:LEU:HD12	25:X:287:LEU:HB3	1.88	0.56
27:Z:113:LYS:NZ	27:Z:117:PRO:O	2.31	0.56
11:P:190:ILE:HG22	11:P:195:ILE:HG23	1.86	0.56
19:E:56:ILE:O	19:E:100:LEU:N	2.37	0.56
24:W:125:ILE:HD12	24:W:128:LEU:HD12	1.86	0.56
26:Y:13:LYS:O	26:Y:17:LEU:N	2.35	0.56
3:H:50:LYS:NZ	3:H:62:VAL:O	2.38	0.56
6:K:52:LYS:NZ	6:K:215:ILE:O	2.39	0.56
18:D:88:VAL:N	18:D:132:LEU:O	2.29	0.56
24:W:92:LYS:N	24:W:93:ARG:HB3	2.19	0.56
21:C:184:LYS:HD3	21:C:280:LEU:HB2	1.88	0.56
24:W:151:THR:O	24:W:155:GLN:NE2	2.38	0.56
15:T:136:SER:HB2	15:T:150:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:82:LEU:O	22:U:129:ARG:NE	2.39	0.56
22:U:522:GLY:O	22:U:559:ARG:NH2	2.39	0.56
23:V:148:ARG:HH22	23:V:193:GLN:HB2	1.71	0.56
23:V:415:SER:O	23:V:460:SER:OG	2.22	0.56
1:f:335:ARG:N	1:f:336:GLU:OE1	2.31	0.56
4:I:99:LEU:O	12:Q:86:ARG:NH2	2.39	0.56
16:A:333:ARG:O	16:A:337:LEU:N	2.39	0.56
25:X:258:LYS:HD3	25:X:267:VAL:HG22	1.88	0.56
15:T:49:THR:HA	15:T:114:GLY:HA3	1.88	0.56
16:A:140:VAL:HG12	16:A:152:PRO:HB3	1.88	0.56
16:A:210:LYS:HA	16:A:316:LYS:HG2	1.88	0.56
17:B:191:ASP:HA	17:B:194:ILE:HG22	1.88	0.56
18:D:251:PHE:HB3	18:D:299:PHE:HZ	1.70	0.56
20:F:415:LEU:HD23	20:F:416:THR:HG22	1.87	0.56
26:Y:174:TRP:O	26:Y:178:ASN:ND2	2.38	0.56
32:e:1:MET:H3	32:e:2:SER:HA	1.71	0.56
1:f:335:ARG:HB2	1:f:336:GLU:HA	1.88	0.56
3:H:46:LEU:HD13	3:H:75:VAL:HG22	1.88	0.56
5:J:81:ARG:O	5:J:85:ASN:ND2	2.39	0.56
6:K:101:PHE:HA	13:R:57:ARG:HH21	1.70	0.56
7:L:152:ASN:HA	8:M:85:ARG:HH22	1.70	0.56
10:O:163:ILE:HG12	10:O:169:SER:HB3	1.88	0.56
20:F:293:THR:HA	20:F:337:ILE:HG21	1.88	0.56
21:C:248:MET:HG3	21:C:269:VAL:HG11	1.88	0.56
22:U:799:LYS:HA	22:U:843:GLU:HG3	1.88	0.56
27:Z:240:VAL:HG21	28:a:285:PRO:HB2	1.88	0.56
28:a:290:GLN:HE21	28:a:330:ARG:HB2	1.70	0.56
31:d:44:THR:O	31:d:47:GLN:NE2	2.39	0.56
1:f:52:ILE:HG13	1:f:64:GLU:HG2	1.88	0.55
3:H:22:ILE:HG23	3:H:129:PRO:HB3	1.86	0.55
4:I:14:PRO:N	5:J:21:TYR:CZ	2.74	0.55
11:P:189:ILE:HG23	11:P:196:THR:HB	1.88	0.55
13:R:18:SER:OG	13:R:173:ALA:N	2.35	0.55
18:D:381:GLU:HA	18:D:384:MET:HB2	1.88	0.55
1:f:6:GLU:HG2	1:f:8:ALA:H	1.71	0.55
7:L:91:GLU:HB3	7:L:108:LEU:HD11	1.87	0.55
15:T:114:GLY:HA2	15:T:192:VAL:HG21	1.88	0.55
22:U:94:SER:OG	22:U:95:GLU:OE1	2.24	0.55
23:V:81:GLN:HB3	23:V:83:GLU:N	2.21	0.55
23:V:447:ILE:HG13	23:V:449:ALA:H	1.71	0.55
24:W:40:LEU:HB2	24:W:41:GLN:CA	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:182:GLU:HB2	17:B:239:VAL:HG21	1.87	0.55
18:D:208:PRO:HB2	18:D:375:ILE:HG12	1.88	0.55
19:E:182:LEU:HD21	33:E:401:ATP:H2'	1.88	0.55
20:F:92:ASN:HB3	20:F:125:LYS:HB2	1.88	0.55
22:U:73:ALA:HB1	22:U:76:GLU:HB3	1.89	0.55
17:B:284:ILE:HB	17:B:329:MET:HA	1.88	0.55
22:U:792:ASN:OD1	22:U:793:LYS:N	2.39	0.55
27:Z:224:HIS:CG	27:Z:225:GLN:HA	2.41	0.55
28:a:273:GLN:HE22	28:a:302:ILE:HD13	1.71	0.55
31:d:214:GLY:N	31:d:215:TRP:HB3	2.21	0.55
3:H:40:ALA:HB1	3:H:184:LEU:HA	1.89	0.55
12:Q:100:VAL:H	12:Q:120:TYR:HB3	1.71	0.55
15:T:54:SER:HB2	15:T:109:THR:HB	1.89	0.55
18:D:376:ASN:HD22	19:E:291:ARG:HH21	1.55	0.55
27:Z:186:THR:HG23	27:Z:187:LEU:H	1.71	0.55
1:f:333:SER:O	1:f:334:ASN:ND2	2.38	0.55
4:I:15:GLU:O	5:J:28:LYS:NZ	2.37	0.55
8:M:34:SER:OG	8:M:65:ARG:NH2	2.39	0.55
12:Q:107:TYR:HA	12:Q:113:PRO:HA	1.88	0.55
17:B:116:ILE:HG22	17:B:118:ASP:H	1.72	0.55
18:D:283:ARG:HH11	21:C:222:LYS:HB2	1.70	0.55
23:V:241:ARG:HG3	23:V:242:HIS:H	1.72	0.55
27:Z:208:ILE:HD11	28:a:350:LYS:HA	1.88	0.55
30:c:98:MET:O	30:c:102:THR:OG1	2.21	0.55
30:c:295:ASN:HA	30:c:298:GLN:HG2	1.87	0.55
2:G:47:CYS:HB3	2:G:221:THR:HG23	1.89	0.55
24:W:220:GLU:N	24:W:221:LYS:HA	2.20	0.55
27:Z:193:ASN:HB3	30:c:307:VAL:HG11	1.89	0.55
29:b:25:ARG:HA	29:b:28:ALA:HB3	1.88	0.55
1:f:18:GLU:OE1	1:f:79:ASN:ND2	2.40	0.55
8:M:37:ILE:HD11	8:M:193:VAL:HG13	1.88	0.55
10:O:209:THR:OG1	11:P:169:GLN:NE2	2.40	0.55
21:C:21:ARG:HH22	22:U:106:ASP:HB2	1.71	0.55
21:C:165:ILE:HG23	21:C:207:THR:HG23	1.88	0.55
23:V:322:VAL:HG13	23:V:323:GLY:H	1.72	0.55
23:V:365:GLN:OE1	32:e:54:ASN:ND2	2.38	0.55
25:X:203:PRO:HB2	25:X:204:PRO:C	2.31	0.55
28:a:31:LYS:HG3	29:b:176:GLY:HA2	1.88	0.55
2:G:63:SER:O	2:G:67:THR:OG1	2.17	0.55
7:L:137:TYR:HE1	7:L:215:VAL:HG13	1.72	0.55
12:Q:55:GLN:HE21	13:R:85:ASN:HD22	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:612:ASP:HA	22:U:615:ARG:HD3	1.89	0.55
23:V:54:LYS:N	23:V:55:THR:OG1	2.40	0.55
31:d:227:SER:C	31:d:229:GLN:HA	2.32	0.55
13:R:179:VAL:HA	13:R:184:TRP:HA	1.89	0.54
23:V:62:HIS:HA	23:V:65:ARG:HB3	1.89	0.54
23:V:212:TYR:CE1	32:e:4:LYS:CG	2.90	0.54
28:a:327:VAL:HG13	28:a:328:ASP:H	1.71	0.54
4:I:218:ARG:NH1	4:I:223:THR:OG1	2.39	0.54
13:R:167:ASP:HB3	13:R:170:SER:HB2	1.89	0.54
17:B:386:ALA:O	17:B:429:LYS:NZ	2.40	0.54
19:E:269:THR:OG1	19:E:271:HIS:ND1	2.36	0.54
30:c:157:ILE:HG12	30:c:158:ASP:H	1.72	0.54
32:e:1:MET:N	32:e:2:SER:HA	2.22	0.54
7:L:41:LYS:NZ	7:L:180:MET:O	2.39	0.54
15:T:92:LEU:HG	15:T:125:VAL:HG11	1.90	0.54
17:B:99:VAL:HA	17:B:102:LEU:HD13	1.89	0.54
19:E:349:GLU:HA	19:E:352:MET:HE3	1.89	0.54
28:a:33:LEU:HB3	29:b:20:ASP:HB3	1.89	0.54
15:T:8:GLY:HA3	15:T:55:GLY:H	1.73	0.54
19:E:264:MET:HE3	19:E:294:ARG:HB3	1.90	0.54
22:U:772:TRP:HB3	22:U:775:LEU:HG	1.90	0.54
24:W:186:ILE:O	24:W:189:GLN:NE2	2.40	0.54
2:G:96:TYR:O	2:G:100:ASN:ND2	2.41	0.54
18:D:336:PRO:HG2	18:D:375:ILE:HD11	1.89	0.54
19:E:61:LEU:HD11	19:E:72:LYS:HB2	1.90	0.54
20:F:89:LEU:HB3	20:F:153:VAL:HG13	1.89	0.54
22:U:380:THR:HG23	22:U:382:SER:H	1.72	0.54
1:f:392:LYS:NZ	1:f:418:LEU:O	2.33	0.54
4:I:143:TYR:HB2	4:I:146:GLN:HE21	1.73	0.54
5:J:88:ARG:NH2	12:Q:66:LEU:O	2.40	0.54
8:M:123:THR:HG22	8:M:130:PRO:HB3	1.90	0.54
16:A:176:ASP:HA	16:A:357:ILE:HD13	1.90	0.54
23:V:212:TYR:CD2	32:e:4:LYS:NZ	2.76	0.54
7:L:72:ILE:HG22	7:L:134:ILE:HA	1.90	0.54
16:A:94:GLN:HE22	17:B:157:HIS:HB2	1.72	0.54
18:D:401:LYS:HA	18:D:404:LYS:HE2	1.90	0.54
22:U:242:LEU:HB2	22:U:793:LYS:HD2	1.88	0.54
26:Y:92:GLU:HA	26:Y:100:ILE:HD13	1.90	0.54
30:c:57:MET:N	30:c:110:GLY:O	2.38	0.54
8:M:66:LEU:HD13	8:M:214:SER:HB2	1.90	0.54
17:B:110:GLY:H	17:B:152:LEU:HD13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:220:LYS:HD3	17:B:346:ARG:HH21	1.71	0.54
20:F:431:LYS:HA	20:F:432:LYS:HB3	1.89	0.54
22:U:173:VAL:HG13	22:U:176:MET:HB2	1.89	0.54
1:f:339:LEU:HD12	1:f:340:THR:HG23	1.89	0.54
4:I:69:ASN:OD1	4:I:70:GLU:N	2.41	0.54
13:R:164:THR:HG22	13:R:170:SER:HB3	1.90	0.54
27:Z:225:GLN:HB2	27:Z:228:TYR:CE1	2.43	0.54
17:B:345:GLY:HA3	17:B:346:ARG:HD2	1.90	0.54
19:E:165:ILE:HD12	19:E:166:PRO:HD2	1.89	0.54
21:C:187:LEU:HD21	21:C:307:ARG:HB2	1.90	0.54
22:U:494:TYR:OH	22:U:531:ASP:OD2	2.25	0.54
22:U:740:GLY:HA3	22:U:744:VAL:HG22	1.90	0.54
24:W:440:ASN:O	24:W:443:THR:OG1	2.16	0.54
1:f:450:VAL:HG21	1:f:473:LYS:HB2	1.89	0.53
17:B:105:THR:HG23	17:B:106:PRO:HD3	1.89	0.53
19:E:353:PHE:HA	19:E:356:ARG:HD3	1.89	0.53
23:V:259:LEU:HD21	23:V:294:ARG:HD2	1.90	0.53
9:N:127:ILE:O	15:T:35:ARG:NH2	2.41	0.53
17:B:139:VAL:HA	17:B:140:ASP:HB3	1.90	0.53
23:V:30:PRO:HA	23:V:33:GLN:HB2	1.89	0.53
23:V:208:ALA:O	32:e:4:LYS:NZ	2.39	0.53
24:W:56:THR:HG21	24:W:103:LYS:HE3	1.91	0.53
30:c:250:GLU:HA	30:c:253:LYS:HE2	1.89	0.53
2:G:86:ASP:OD1	8:M:120:HIS:NE2	2.41	0.53
3:H:19:LEU:O	3:H:23:GLU:HB2	2.08	0.53
3:H:79:MET:HE3	3:H:131:GLY:HA3	1.89	0.53
4:I:26:GLU:O	4:I:30:HIS:ND1	2.30	0.53
8:M:99:ARG:HD3	8:M:103:GLY:HA2	1.90	0.53
1:f:676:GLU:HB3	1:f:691:VAL:HG22	1.89	0.53
2:G:34:GLN:NE2	8:M:17:ASP:O	2.41	0.53
17:B:397:ALA:HB3	21:C:311:ILE:HD12	1.90	0.53
18:D:72:PHE:HD2	21:C:49:ARG:HH21	1.56	0.53
18:D:151:ILE:HB	18:D:152:MET:HA	1.91	0.53
22:U:384:GLN:HG2	22:U:385:PHE:H	1.73	0.53
23:V:59:ALA:N	23:V:60:ALA:HB3	2.24	0.53
24:W:66:ILE:HD13	24:W:67:LEU:HD13	1.90	0.53
27:Z:33:LYS:HD3	27:Z:60:GLU:N	2.24	0.53
28:a:122:LYS:HE3	28:a:134:THR:HG21	1.91	0.53
8:M:100:SER:O	15:T:65:GLN:NE2	2.41	0.53
22:U:126:ILE:HG23	22:U:130:LEU:HD11	1.89	0.53
27:Z:244:GLU:HG2	28:a:287:ASN:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:195:LYS:HD2	8:M:241:GLU:HB2	1.91	0.53
18:D:149:SER:HB3	19:E:61:LEU:HD13	1.90	0.53
20:F:172:VAL:HG21	20:F:266:LYS:HE3	1.91	0.53
27:Z:37:GLY:HA2	27:Z:56:VAL:HG12	1.90	0.53
27:Z:102:HIS:CD2	27:Z:104:ASN:HB3	2.44	0.53
2:G:179:LEU:HA	2:G:182:LYS:HB3	1.90	0.53
4:I:73:ALA:HB3	4:I:137:ILE:HD11	1.91	0.53
17:B:133:VAL:HG11	17:B:159:VAL:HG12	1.91	0.53
23:V:319:HIS:HB2	23:V:320:THR:HA	1.91	0.53
25:X:194:ARG:HD2	25:X:210:LEU:HD11	1.90	0.53
27:Z:111:LEU:HD12	29:b:59:GLU:HB3	1.90	0.53
31:d:75:MET:HG2	31:d:102:ASN:HB2	1.91	0.53
3:H:150:ASP:OD2	3:H:152:SER:OG	2.26	0.53
20:F:225:MET:HG2	20:F:233:LYS:HD2	1.90	0.53
23:V:441:ALA:HB1	23:V:446:VAL:HB	1.91	0.53
24:W:135:LYS:HB3	24:W:136:ILE:HB	1.90	0.53
26:Y:251:HIS:HA	26:Y:257:ARG:HD3	1.90	0.53
28:a:163:TYR:HE1	28:a:169:HIS:HA	1.72	0.53
16:A:244:GLU:OE2	17:B:314:ASN:ND2	2.42	0.53
24:W:5:GLY:HA2	24:W:34:LEU:HD13	1.90	0.53
24:W:178:GLU:OE1	24:W:181:GLU:N	2.42	0.53
28:a:335:TRP:CG	28:a:336:VAL:H	2.27	0.53
5:J:121:SER:C	5:J:123:GLY:HA3	2.33	0.53
8:M:231:ILE:O	8:M:232:ARG:HG2	2.08	0.53
11:P:36:THR:OG1	11:P:38:ASP:OD1	2.22	0.53
12:Q:38:MET:O	12:Q:65:GLN:NE2	2.42	0.53
22:U:808:PRO:HD3	22:U:836:THR:HB	1.90	0.53
23:V:47:SER:HA	23:V:50:GLU:HB2	1.91	0.53
27:Z:194:GLN:HG2	28:a:368:GLU:HG2	1.90	0.53
28:a:145:LEU:HD12	28:a:146:PRO:HD2	1.90	0.53
1:f:559:ASP:HB3	1:f:562:VAL:HG22	1.91	0.52
1:f:644:PHE:HE1	1:f:648:ARG:HH21	1.57	0.52
2:G:172:GLN:OE1	2:G:172:GLN:N	2.40	0.52
11:P:11:VAL:HG11	11:P:52:GLY:HA3	1.90	0.52
12:Q:38:MET:HG3	12:Q:44:LEU:HB2	1.92	0.52
12:Q:43:LEU:HD12	12:Q:183:ILE:HD11	1.91	0.52
16:A:95:VAL:HB	16:A:144:ARG:H	1.74	0.52
20:F:391:PHE:CE2	20:F:424:ILE:HG23	2.44	0.52
22:U:265:ILE:HG23	22:U:269:ARG:HH12	1.74	0.52
28:a:28:LEU:HD23	28:a:37:LEU:HA	1.91	0.52
7:L:82:ARG:O	7:L:86:ASN:ND2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:84:LEU:O	7:L:88:MET:N	2.42	0.52
12:Q:41:LYS:O	12:Q:107:TYR:N	2.43	0.52
17:B:278:ALA:HB1	17:B:279:PRO:HA	1.92	0.52
20:F:153:VAL:HG23	20:F:158:TYR:HA	1.91	0.52
22:U:446:LEU:O	22:U:450:HIS:ND1	2.38	0.52
22:U:497:LEU:HD23	22:U:516:LEU:HB2	1.91	0.52
1:f:439:CYS:HB3	1:f:475:LYS:HE2	1.91	0.52
4:I:72:MET:HE1	4:I:105:ILE:HG23	1.92	0.52
7:L:196:ARG:HE	7:L:239:ARG:HH21	1.55	0.52
20:F:124:ILE:O	20:F:132:TYR:N	2.36	0.52
21:C:90:HIS:HB2	21:C:91:PRO:HD3	1.91	0.52
22:U:803:LYS:HA	22:U:839:ALA:H	1.74	0.52
24:W:187:LEU:HD22	24:W:226:TYR:CD1	2.45	0.52
24:W:372:ARG:HG2	24:W:414:ASN:HB3	1.92	0.52
26:Y:14:ASN:HA	26:Y:17:LEU:HB3	1.91	0.52
26:Y:102:ASP:HA	26:Y:105:MET:HG2	1.91	0.52
31:d:139:LEU:HD11	31:d:151:VAL:HG22	1.90	0.52
7:L:39:LYS:HE2	7:L:157:ARG:HA	1.92	0.52
16:A:161:VAL:HG13	16:A:162:THR:HG23	1.92	0.52
17:B:286:GLU:N	17:B:330:ALA:O	2.43	0.52
18:D:54:LEU:HA	18:D:57:GLN:HB2	1.90	0.52
20:F:327:LYS:H	20:F:327:LYS:HD2	1.74	0.52
22:U:738:ASP:OD1	22:U:742:HIS:NE2	2.42	0.52
27:Z:222:ILE:HG23	27:Z:224:HIS:HB2	1.90	0.52
2:G:155:ASP:HB2	18:D:418:LYS:HE2	1.91	0.52
5:J:36:ARG:HE	5:J:157:LYS:HA	1.73	0.52
7:L:204:ASP:HA	7:L:205:LEU:HB3	1.92	0.52
8:M:56:LYS:H	8:M:57:LEU:HA	1.74	0.52
9:N:18:SER:HB2	9:N:30:VAL:HA	1.90	0.52
18:D:53:PHE:HB3	22:U:632:GLN:HE22	1.74	0.52
20:F:74:LYS:O	20:F:78:GLU:N	2.38	0.52
22:U:643:SER:O	22:U:649:ARG:NH1	2.38	0.52
10:O:51:ASP:HB3	10:O:94:ILE:HG23	1.92	0.52
15:T:5:MET:HB3	15:T:30:TYR:HE1	1.72	0.52
18:D:47:LEU:HB2	21:C:25:LEU:HD23	1.92	0.52
20:F:91:SER:OG	20:F:124:ILE:HG23	2.10	0.52
22:U:203:LYS:O	22:U:207:ASN:ND2	2.43	0.52
23:V:349:ARG:HH11	23:V:354:LYS:HB2	1.74	0.52
5:J:66:ASP:OD1	5:J:67:ASP:N	2.40	0.52
5:J:195:LEU:O	5:J:201:SER:OG	2.21	0.52
7:L:215:VAL:HB	7:L:221:PHE:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:166:LEU:HA	14:S:170:ARG:HD3	1.92	0.52
16:A:100:LYS:HB3	16:A:115:VAL:HG23	1.92	0.52
20:F:314:LEU:HD11	20:F:342:LEU:HD23	1.91	0.52
22:U:623:GLY:HA2	22:U:659:CYS:HB2	1.91	0.52
23:V:302:TYR:HB3	23:V:339:LEU:HD23	1.92	0.52
23:V:346:LEU:HD11	32:e:47:ASN:HB2	1.91	0.52
24:W:312:MET:SD	24:W:361:HIS:ND1	2.83	0.52
28:a:125:ILE:HG22	28:a:126:GLY:C	2.35	0.52
31:d:45:LYS:HG2	31:d:48:LEU:HD12	1.91	0.52
7:L:104:PRO:HB3	7:L:138:ASP:HB3	1.91	0.52
14:S:4:PRO:O	15:T:100:ARG:NH2	2.42	0.52
23:V:56:ALA:O	23:V:59:ALA:HB3	2.10	0.52
26:Y:293:ARG:NH1	32:e:49:GLU:OE2	2.41	0.52
17:B:170:LEU:HD13	17:B:255:LEU:HD21	1.92	0.52
17:B:265:LYS:O	17:B:269:GLU:N	2.32	0.52
19:E:312:ILE:HD11	33:E:401:ATP:HN62	1.75	0.52
23:V:197:THR:HG21	23:V:200:ARG:HG3	1.92	0.52
23:V:372:LEU:H	23:V:427:GLN:NE2	2.08	0.52
23:V:412:LEU:O	26:Y:346:LYS:NZ	2.34	0.52
26:Y:330:ILE:HA	26:Y:333:GLU:HB3	1.92	0.52
27:Z:182:THR:N	27:Z:183:THR:HA	2.25	0.52
1:f:493:VAL:HG12	1:f:495:VAL:HG23	1.92	0.52
3:H:231:ALA:N	3:H:232:ALA:HB3	2.25	0.52
18:D:218:ALA:O	18:D:222:HIS:ND1	2.36	0.52
19:E:171:LEU:N	19:E:297:ARG:O	2.38	0.52
20:F:249:LEU:HB2	20:F:283:ILE:HG13	1.92	0.52
22:U:154:ALA:HB2	22:U:166:THR:HG21	1.91	0.52
22:U:483:LEU:HD11	22:U:781:LEU:HD11	1.91	0.52
23:V:404:LYS:HA	23:V:407:VAL:HG12	1.91	0.52
6:K:209:LYS:O	6:K:214:ASN:ND2	2.43	0.51
10:O:50:ALA:HB2	11:P:129:CYS:HB2	1.90	0.51
17:B:400:THR:O	17:B:404:LEU:N	2.39	0.51
21:C:232:ARG:O	21:C:236:VAL:N	2.34	0.51
23:V:349:ARG:HH21	32:e:43:TRP:CD1	2.28	0.51
27:Z:67:VAL:HG13	29:b:92:VAL:HG23	1.92	0.51
28:a:342:ASP:HB2	28:a:345:GLN:HG2	1.92	0.51
1:f:664:ALA:H	1:f:668:PRO:HD2	1.75	0.51
9:N:164:MET:HB3	9:N:171:GLY:HA2	1.91	0.51
10:O:213:THR:HG22	10:O:214:GLU:H	1.75	0.51
14:S:169:ASP:OD2	14:S:173:ARG:NH2	2.44	0.51
22:U:510:GLU:OE2	22:U:546:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:68:TRP:CD2	27:Z:108:ILE:HG13	2.45	0.51
28:a:230:ARG:HE	28:a:233:LEU:HD22	1.74	0.51
16:A:164:MET:HG2	17:B:264:PRO:HD2	1.92	0.51
16:A:334:PRO:HB3	20:F:398:ALA:HB2	1.92	0.51
21:C:252:ASP:CG	21:C:296:ASN:H	2.18	0.51
21:C:336:MET:HE1	21:C:363:CYS:HB3	1.91	0.51
22:U:208:LEU:HD23	22:U:210:LYS:H	1.75	0.51
23:V:98:LEU:HD12	23:V:107:ARG:HH21	1.76	0.51
25:X:251:LEU:HA	25:X:254:MET:HG2	1.92	0.51
27:Z:21:ASP:HB2	30:c:36:LEU:HD22	1.92	0.51
27:Z:190:ARG:NH1	28:a:371:ALA:O	2.36	0.51
31:d:35:PHE:HD2	31:d:36:LEU:HD23	1.74	0.51
1:f:438:VAL:HG13	1:f:472:LYS:HD3	1.93	0.51
6:K:36:THR:HA	6:K:171:GLY:HA3	1.91	0.51
6:K:45:GLY:HA3	6:K:221:GLN:HG3	1.92	0.51
17:B:193:GLN:NE2	17:B:352:GLU:O	2.44	0.51
18:D:64:GLU:HB2	22:U:603:LEU:HD11	1.92	0.51
18:D:113:VAL:HA	21:C:66:LEU:HD11	1.92	0.51
22:U:154:ALA:HB1	22:U:163:PHE:HD1	1.74	0.51
4:I:156:TYR:HE1	5:J:58:THR:HB	1.75	0.51
5:J:77:THR:HA	5:J:80:ALA:HB3	1.92	0.51
6:K:74:ILE:HG12	6:K:109:VAL:HG22	1.93	0.51
11:P:155:GLU:HB2	11:P:158:MET:HG2	1.93	0.51
17:B:232:LYS:HB3	21:C:278:ASN:HD22	1.76	0.51
21:C:321:ASN:OD1	21:C:322:GLU:N	2.42	0.51
24:W:359:VAL:O	24:W:363:ILE:HG12	2.11	0.51
5:J:9:VAL:HG21	6:K:12:VAL:HG11	1.93	0.51
5:J:97:THR:HA	13:R:81:LYS:HG2	1.92	0.51
19:E:109:ARG:NH1	20:F:98:ASP:OD2	2.40	0.51
19:E:357:ALA:O	19:E:359:HIS:ND1	2.43	0.51
23:V:101:LEU:HB3	23:V:102:PRO:HD2	1.90	0.51
23:V:179:LYS:HD2	23:V:214:HIS:CE1	2.45	0.51
23:V:416:ARG:HH12	23:V:418:SER:HB2	1.75	0.51
25:X:225:TRP:HB3	25:X:261:LEU:HG	1.93	0.51
31:d:109:GLN:O	31:d:111:ARG:NH2	2.43	0.51
1:f:523:GLY:HA3	1:f:527:LEU:HD23	1.93	0.51
4:I:90:LEU:HD12	4:I:114:LEU:HB2	1.93	0.51
11:P:175:VAL:HG13	11:P:181:SER:HB3	1.92	0.51
16:A:95:VAL:HB	16:A:143:ASP:HA	1.91	0.51
20:F:281:SER:H	20:F:326:VAL:HG13	1.76	0.51
22:U:570:LEU:HD22	22:U:578:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:139:GLU:HG2	24:W:142:ARG:HD2	1.92	0.51
24:W:366:MET:HB3	24:W:370:TYR:CE2	2.45	0.51
29:b:140:ILE:HD13	29:b:157:VAL:HG22	1.93	0.51
30:c:248:MET:O	30:c:252:ALA:N	2.44	0.51
2:G:52:THR:HG22	2:G:53:GLN:H	1.75	0.51
8:M:31:GLU:OE1	8:M:169:ARG:NH1	2.44	0.51
11:P:169:GLN:O	11:P:173:ASN:ND2	2.35	0.51
13:R:191:ASN:OD1	13:R:192:VAL:N	2.44	0.51
14:S:5:TYR:OH	14:S:103:PRO:O	2.26	0.51
16:A:210:LYS:HG2	16:A:336:ARG:HH11	1.76	0.51
17:B:305:ILE:HA	17:B:308:THR:HG22	1.93	0.51
20:F:406:ILE:HG22	20:F:410:ARG:HH21	1.76	0.51
22:U:748:LEU:HD23	22:U:760:VAL:HG22	1.92	0.51
25:X:395:LYS:NZ	26:Y:366:TYR:OH	2.43	0.51
31:d:106:LEU:HD11	31:d:114:GLU:HB3	1.92	0.51
5:J:11:SER:OG	5:J:15:HIS:O	2.29	0.51
5:J:154:HIS:CE1	6:K:59:MET:HG3	2.45	0.51
10:O:7:VAL:HG22	10:O:12:ILE:HG12	1.91	0.51
15:T:51:LEU:HD11	15:T:110:MET:HB3	1.93	0.51
23:V:33:GLN:HB3	23:V:115:LYS:HD3	1.93	0.51
26:Y:74:LYS:HA	26:Y:77:ASN:HB3	1.92	0.51
30:c:56:LEU:HA	30:c:111:TRP:HA	1.93	0.51
11:P:54:ALA:HB3	11:P:106:GLU:HB2	1.93	0.51
23:V:372:LEU:HD13	23:V:427:GLN:HE21	1.76	0.51
25:X:356:LEU:HD13	25:X:359:ALA:HB3	1.93	0.51
1:f:11:TRP:HB3	1:f:12:GLN:HB3	1.93	0.50
1:f:401:LEU:HD23	1:f:672:VAL:HG12	1.93	0.50
5:J:20:GLU:OE1	5:J:20:GLU:N	2.40	0.50
11:P:135:ASP:OD1	11:P:135:ASP:N	2.43	0.50
12:Q:17:SER:OG	12:Q:179:SER:OG	2.22	0.50
17:B:264:PRO:HG3	17:B:315:GLN:HA	1.92	0.50
18:D:186:THR:HG23	18:D:187:HIS:H	1.76	0.50
22:U:112:CYS:SG	22:U:159:ARG:NH1	2.84	0.50
23:V:101:LEU:O	23:V:103:SER:N	2.44	0.50
23:V:294:ARG:HH21	23:V:331:LEU:HD23	1.76	0.50
29:b:34:ASN:O	29:b:38:HIS:ND1	2.31	0.50
31:d:237:ILE:N	31:d:238:PRO:HD2	2.26	0.50
5:J:11:SER:OG	5:J:13:ASP:OD1	2.19	0.50
9:N:173:VAL:HG23	9:N:190:LEU:HB3	1.93	0.50
13:R:73:ARG:NH2	13:R:105:ASP:OD1	2.43	0.50
17:B:189:GLY:HA3	17:B:360:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:50:ASN:HD21	22:U:643:SER:HA	1.76	0.50
21:C:245:ILE:HG22	21:C:246:ILE:H	1.74	0.50
23:V:234:ARG:HG3	23:V:250:LEU:HD11	1.92	0.50
25:X:360:ASP:OD1	25:X:361:VAL:N	2.44	0.50
28:a:291:LEU:O	28:a:331:VAL:N	2.44	0.50
3:H:38:ILE:N	3:H:45:VAL:O	2.39	0.50
4:I:48:GLU:H	4:I:64:LYS:HD2	1.77	0.50
7:L:204:ASP:HB3	7:L:205:LEU:C	2.36	0.50
15:T:138:ALA:HB3	15:T:147:GLN:HB2	1.92	0.50
15:T:153:VAL:HG21	15:T:168:LEU:HD11	1.94	0.50
19:E:55:GLN:O	20:F:133:PHE:N	2.36	0.50
19:E:285:LEU:HB3	19:E:289:LEU:HB2	1.93	0.50
23:V:200:ARG:O	23:V:204:ASP:N	2.39	0.50
24:W:431:LYS:O	24:W:435:LEU:HB2	2.10	0.50
26:Y:144:LEU:HD22	26:Y:160:ASN:HB3	1.93	0.50
9:N:63:LEU:O	9:N:67:SER:N	2.43	0.50
12:Q:85:ARG:HA	12:Q:88:LEU:HB2	1.93	0.50
14:S:28:ARG:NH2	14:S:211:ARG:O	2.44	0.50
17:B:109:VAL:HG22	17:B:151:LEU:HD23	1.93	0.50
21:C:229:ARG:HH11	21:C:232:ARG:HD2	1.77	0.50
24:W:221:LYS:HG3	24:W:224:LEU:HB2	1.93	0.50
26:Y:191:ILE:HG13	26:Y:192:ARG:H	1.76	0.50
12:Q:44:LEU:HD21	12:Q:57:ALA:HA	1.93	0.50
18:D:45:LYS:O	18:D:48:GLN:NE2	2.45	0.50
18:D:83:GLN:HE21	18:D:87:LEU:HD21	1.76	0.50
19:E:180:LYS:HG3	19:E:181:THR:H	1.77	0.50
23:V:362:LEU:HB3	23:V:382:PHE:HE2	1.77	0.50
23:V:474:LEU:HA	23:V:477:HIS:HD2	1.77	0.50
26:Y:66:ASP:HB3	26:Y:70:LEU:HD12	1.92	0.50
27:Z:241:SER:HB2	27:Z:242:LEU:HD12	1.93	0.50
28:a:290:GLN:HA	28:a:332:HIS:HA	1.92	0.50
29:b:12:ASN:ND2	29:b:53:THR:OG1	2.44	0.50
31:d:209:TYR:HB3	31:d:213:ARG:HE	1.77	0.50
31:d:256:ILE:N	31:d:257:VAL:HA	2.25	0.50
4:I:234:GLU:HA	4:I:237:ILE:HD12	1.93	0.50
9:N:103:TRP:HA	9:N:109:GLY:HA2	1.94	0.50
12:Q:47:VAL:HB	12:Q:102:LEU:HG	1.93	0.50
16:A:333:ARG:HH22	16:A:340:LYS:HD3	1.76	0.50
19:E:130:VAL:O	19:E:134:GLU:HG2	2.12	0.50
26:Y:301:ILE:HA	26:Y:304:TYR:HB2	1.92	0.50
26:Y:349:LYS:O	26:Y:350:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:685:VAL:HG23	1:f:686:ARG:H	1.76	0.50
21:C:84:LYS:HA	21:C:98:ASP:HA	1.93	0.50
27:Z:94:TRP:HB3	27:Z:112:MET:HE1	1.94	0.50
3:H:72:ILE:HD11	3:H:107:THR:HG22	1.94	0.50
4:I:44:LEU:HD21	4:I:189:ALA:HB3	1.94	0.50
5:J:96:LEU:HD23	5:J:97:THR:HG23	1.93	0.50
6:K:79:SER:HB2	6:K:140:ALA:HB3	1.93	0.50
8:M:92:ARG:HH21	15:T:73:ASP:HA	1.76	0.50
12:Q:8:GLN:HE21	12:Q:115:LEU:HB2	1.77	0.50
16:A:183:GLN:HB3	16:A:341:ILE:HD12	1.93	0.50
23:V:99:ARG:HH22	23:V:146:GLN:HB3	1.76	0.50
24:W:436:MET:HA	24:W:439:VAL:HG22	1.92	0.50
26:Y:316:LEU:HG	26:Y:352:GLU:HG3	1.93	0.50
28:a:129:GLN:HG3	28:a:130:VAL:H	1.76	0.50
3:H:74:LEU:HD11	3:H:134:LEU:HD13	1.94	0.50
10:O:138:PHE:O	10:O:142:PHE:HB3	2.12	0.50
17:B:242:GLN:HG2	17:B:247:PHE:CD2	2.47	0.50
31:d:36:LEU:HB2	31:d:37:PRO:HA	1.94	0.50
1:f:565:ASN:ND2	1:f:681:LEU:HD22	2.26	0.49
3:H:183:GLU:HB3	3:H:186:ASP:HB2	1.92	0.49
4:I:105:ILE:HG12	4:I:110:LEU:HD13	1.93	0.49
16:A:183:GLN:HG3	16:A:341:ILE:HB	1.94	0.49
19:E:44:GLU:HG3	20:F:73:ILE:HG22	1.94	0.49
23:V:201:ARG:HG2	23:V:244:ALA:HB3	1.93	0.49
27:Z:204:LYS:HE3	28:a:353:LEU:HG	1.93	0.49
30:c:261:GLU:O	30:c:265:MET:HG2	2.12	0.49
1:f:350:LYS:HD2	1:f:390:GLU:HA	1.93	0.49
7:L:11:THR:HG23	8:M:129:ARG:HB3	1.94	0.49
15:T:89:HIS:CE1	15:T:131:ALA:HB1	2.47	0.49
19:E:185:ARG:NH2	20:F:319:GLY:HA2	2.27	0.49
21:C:250:GLU:O	21:C:251:ILE:HG22	2.12	0.49
22:U:115:ASN:HA	22:U:118:LEU:HD13	1.94	0.49
22:U:465:LEU:HD11	22:U:477:GLY:HA3	1.94	0.49
22:U:908:ILE:HG12	22:U:909:GLY:H	1.76	0.49
28:a:54:ASP:HA	28:a:57:ILE:HG22	1.94	0.49
30:c:191:ALA:O	30:c:194:HIS:ND1	2.45	0.49
1:f:301:ASP:OD1	1:f:301:ASP:N	2.29	0.49
10:O:215:LYS:HB3	11:P:197:THR:HB	1.93	0.49
15:T:92:LEU:HD23	15:T:112:ILE:HD11	1.94	0.49
16:A:407:LYS:HA	16:A:410:LEU:HG	1.93	0.49
19:E:47:LEU:HD22	20:F:76:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:299:ILE:HG22	24:W:301:LYS:H	1.78	0.49
25:X:223:LYS:HZ3	26:Y:244:ALA:HB2	1.75	0.49
31:d:159:PRO:N	31:d:160:ALA:HA	2.27	0.49
6:K:94:VAL:O	6:K:98:ASN:ND2	2.44	0.49
12:Q:85:ARG:O	12:Q:89:ALA:N	2.34	0.49
14:S:145:LEU:O	14:S:149:LEU:N	2.37	0.49
16:A:104:ALA:O	16:A:112:ILE:HG22	2.12	0.49
16:A:239:ARG:HA	16:A:273:PHE:HB3	1.94	0.49
16:A:406:GLU:N	16:A:407:LYS:HB3	2.28	0.49
21:C:247:PHE:HE2	21:C:249:ASP:HB2	1.77	0.49
22:U:184:CYS:O	22:U:188:MET:N	2.46	0.49
22:U:757:MET:HG3	22:U:758:PRO:HD3	1.94	0.49
24:W:91:SER:HB2	24:W:92:LYS:HA	1.94	0.49
28:a:31:LYS:HG3	29:b:177:PRO:HD3	1.95	0.49
14:S:16:ALA:HA	14:S:21:ALA:HA	1.93	0.49
21:C:74:GLY:N	21:C:114:VAL:O	2.42	0.49
22:U:571:CYS:HB2	22:U:601:ARG:HH21	1.78	0.49
23:V:106:ARG:O	23:V:110:HIS:ND1	2.32	0.49
1:f:350:LYS:HA	1:f:356:ALA:HB3	1.94	0.49
1:f:397:ARG:HG2	1:f:433:ASN:HA	1.95	0.49
1:f:400:PRO:HB2	1:f:440:ALA:HB3	1.94	0.49
6:K:181:LEU:HD23	6:K:182:GLN:HG3	1.93	0.49
18:D:45:LYS:HB2	22:U:187:LEU:HD22	1.93	0.49
19:E:76:GLY:N	19:E:77:PRO:HD2	2.28	0.49
25:X:410:VAL:HG11	26:Y:376:LEU:HD21	1.95	0.49
1:f:617:LEU:HB3	1:f:618:THR:CB	2.37	0.49
9:N:176:LEU:HD12	9:N:187:GLN:HE21	1.76	0.49
15:T:23:ALA:HB3	15:T:169:VAL:HG11	1.94	0.49
18:D:356:GLU:C	18:D:358:VAL:H	2.19	0.49
18:D:367:PRO:HA	18:D:370:ILE:HG22	1.95	0.49
22:U:541:HIS:HB2	22:U:544:ILE:HG22	1.94	0.49
23:V:320:THR:HG23	23:V:321:ALA:HB2	1.95	0.49
25:X:356:LEU:HD11	25:X:360:ASP:OD1	2.13	0.49
26:Y:101:ARG:HD3	26:Y:130:LYS:HD3	1.94	0.49
27:Z:106:ILE:HG13	27:Z:153:LYS:HD2	1.94	0.49
31:d:60:GLN:OE1	31:d:162:SER:OG	2.19	0.49
1:f:369:GLY:O	1:f:372:ASN:ND2	2.46	0.49
1:f:463:SER:HA	1:f:466:LYS:HE3	1.94	0.49
2:G:159:TYR:HA	3:H:84:ARG:HH21	1.77	0.49
5:J:98:VAL:HG13	13:R:78:ALA:HB2	1.94	0.49
6:K:51:GLU:HA	6:K:215:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:34:LEU:HD22	9:N:177:ALA:HB2	1.94	0.49
10:O:35:HIS:NE2	10:O:53:ASP:OD1	2.46	0.49
16:A:76:ALA:HA	17:B:138:PHE:HD1	1.78	0.49
21:C:267:SER:HA	21:C:270:GLN:HB2	1.95	0.49
23:V:237:THR:O	23:V:241:ARG:NE	2.36	0.49
26:Y:46:ARG:C	26:Y:48:ASN:H	2.20	0.49
27:Z:222:ILE:N	27:Z:223:ASN:HA	2.27	0.49
29:b:19:GLY:HA2	29:b:24:THR:HA	1.95	0.49
6:K:16:SER:OG	6:K:18:GLU:OE1	2.25	0.49
7:L:123:TYR:N	8:M:127:ALA:O	2.44	0.49
8:M:106:ILE:HD12	8:M:107:PRO:HD2	1.93	0.49
17:B:126:SER:HA	17:B:127:VAL:HA	1.54	0.49
25:X:228:ALA:HA	25:X:231:TYR:HD2	1.78	0.49
27:Z:256:GLN:HG3	27:Z:260:VAL:HG23	1.95	0.49
1:f:458:SER:HB2	1:f:461:PHE:HA	1.95	0.49
19:E:360:ASP:OD1	19:E:360:ASP:N	2.41	0.49
23:V:362:LEU:HD12	23:V:365:GLN:HB3	1.94	0.49
26:Y:197:ALA:HB3	26:Y:226:VAL:HG21	1.95	0.49
26:Y:346:LYS:O	26:Y:355:GLU:N	2.39	0.49
27:Z:238:PRO:HG2	27:Z:240:VAL:HG22	1.93	0.49
28:a:193:GLN:HB3	28:a:225:LEU:HD13	1.94	0.49
28:a:208:GLU:HG2	28:a:271:LYS:HD2	1.94	0.49
28:a:252:LYS:HA	28:a:255:TRP:HD1	1.78	0.49
1:f:192:THR:HA	1:f:193:HIS:HB2	1.95	0.48
1:f:446:ASN:C	1:f:448:LEU:H	2.21	0.48
16:A:210:LYS:HB3	16:A:317:VAL:HG22	1.95	0.48
16:A:234:ASP:HA	16:A:235:ALA:HA	1.51	0.48
18:D:50:GLU:HA	18:D:53:PHE:HB2	1.94	0.48
19:E:266:GLY:HA3	19:E:268:ASP:H	1.77	0.48
20:F:77:SER:O	20:F:81:LYS:N	2.45	0.48
21:C:29:GLU:O	21:C:33:LEU:N	2.40	0.48
23:V:26:PRO:O	23:V:29:PRO:HD2	2.13	0.48
23:V:80:LYS:HB3	23:V:81:GLN:C	2.38	0.48
23:V:466:ILE:HG23	23:V:467:TYR:H	1.77	0.48
24:W:202:THR:HG21	24:W:233:LEU:HD11	1.95	0.48
25:X:200:ILE:HG22	25:X:201:TYR:H	1.77	0.48
25:X:262:ASN:O	25:X:297:ARG:NH2	2.37	0.48
25:X:370:LEU:HD13	26:Y:306:GLN:HB2	1.93	0.48
26:Y:48:ASN:ND2	26:Y:77:ASN:HB2	2.28	0.48
27:Z:82:PHE:HA	27:Z:85:VAL:HG12	1.95	0.48
3:H:93:LEU:HD11	3:H:117:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:94:GLU:OE1	8:M:118:TYR:OH	2.24	0.48
18:D:200:ARG:NH1	18:D:296:MET:O	2.46	0.48
18:D:300:ASP:HA	18:D:301:GLN:HA	1.52	0.48
20:F:334:ARG:HG2	20:F:336:ASP:H	1.77	0.48
21:C:183:PRO:HG2	21:C:290:LYS:HE3	1.95	0.48
22:U:27:LEU:O	22:U:31:VAL:HB	2.14	0.48
22:U:485:ALA:O	22:U:488:THR:OG1	2.31	0.48
29:b:17:ARG:HG2	29:b:80:PRO:HG2	1.95	0.48
1:f:225:ALA:HB1	1:f:230:LYS:HD2	1.95	0.48
4:I:107:CYS:HA	4:I:110:LEU:HB3	1.95	0.48
6:K:73:HIS:ND1	6:K:146:VAL:O	2.46	0.48
10:O:40:ASN:HB3	10:O:73:LEU:HD11	1.95	0.48
12:Q:20:VAL:HG21	12:Q:175:LEU:HA	1.95	0.48
21:C:139:MET:HB3	21:C:211:PHE:HB3	1.94	0.48
21:C:312:ASP:OD1	21:C:313:ARG:N	2.41	0.48
21:C:397:LYS:HG2	21:C:398:ASN:HA	1.95	0.48
23:V:25:GLU:HG2	23:V:84:LYS:HD2	1.95	0.48
26:Y:300:ARG:HH12	32:e:63:HIS:CD2	2.30	0.48
31:d:238:PRO:HA	31:d:241:GLU:HG2	1.94	0.48
1:f:69:LYS:HE2	17:B:413:LYS:HB2	1.95	0.48
5:J:120:GLN:O	6:K:134:SER:OG	2.31	0.48
7:L:95:SER:O	7:L:100:ASP:N	2.46	0.48
14:S:2:PHE:H	15:T:2:GLN:HE22	1.62	0.48
17:B:248:LEU:HD23	17:B:282:VAL:HG13	1.95	0.48
19:E:385:ASP:HB3	19:E:386:TYR:HA	1.94	0.48
20:F:183:GLU:HG2	20:F:239:ALA:HB2	1.95	0.48
2:G:17:SER:O	3:H:24:TYR:HB3	2.14	0.48
3:H:89:ARG:O	3:H:93:LEU:N	2.39	0.48
16:A:313:GLY:C	16:A:315:ILE:H	2.21	0.48
23:V:273:LYS:HA	23:V:274:SER:HB2	1.95	0.48
24:W:364:ARG:HG2	24:W:402:ILE:HD11	1.95	0.48
26:Y:380:VAL:HA	26:Y:383:LEU:HB2	1.96	0.48
28:a:284:ARG:NH1	28:a:291:LEU:HD21	2.29	0.48
28:a:285:PRO:HB3	28:a:352:ARG:HD3	1.95	0.48
29:b:157:VAL:HG21	29:b:170:LEU:HB2	1.96	0.48
30:c:273:LYS:HD2	30:c:274:ASN:HB2	1.96	0.48
1:f:370:SER:HA	1:f:371:CYS:SG	2.54	0.48
2:G:44:GLY:N	2:G:47:CYS:O	2.45	0.48
2:G:189:TRP:HE3	2:G:194:THR:HG22	1.78	0.48
7:L:205:LEU:H	7:L:209:ASN:HD21	1.61	0.48
18:D:413:GLU:HG2	18:D:414:HIS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:235:ILE:HG22	19:E:279:THR:HB	1.95	0.48
20:F:188:ILE:HA	20:F:365:ILE:HG22	1.95	0.48
21:C:255:GLY:N	21:C:256:SER:HB2	2.28	0.48
22:U:697:GLN:NE2	22:U:786:THR:OG1	2.47	0.48
22:U:802:TYR:HB3	22:U:895:PRO:HG3	1.95	0.48
24:W:243:ILE:HA	24:W:246:HIS:HB3	1.96	0.48
25:X:264:PRO:HG2	25:X:267:VAL:HG23	1.95	0.48
27:Z:134:PRO:HG3	30:c:220:LEU:HG	1.95	0.48
31:d:201:ASN:N	31:d:201:ASN:OD1	2.46	0.48
5:J:94:HIS:CE1	5:J:103:THR:H	2.31	0.48
6:K:28:ILE:HG21	20:F:437:TYR:HD1	1.78	0.48
10:O:34:ILE:HD12	10:O:185:PHE:HE1	1.78	0.48
17:B:290:ILE:HG21	17:B:336:THR:HG21	1.94	0.48
18:D:366:ARG:HB3	18:D:367:PRO:HD3	1.94	0.48
20:F:433:ALA:HA	20:F:434:ASN:CG	2.39	0.48
24:W:55:ARG:NH1	24:W:75:TYR:HB3	2.29	0.48
26:Y:16:ASP:HB2	26:Y:113:ARG:HE	1.79	0.48
26:Y:215:ASP:O	26:Y:218:THR:OG1	2.26	0.48
27:Z:34:ARG:NE	27:Z:98:GLY:O	2.39	0.48
6:K:94:VAL:HG22	13:R:65:ILE:HD13	1.94	0.48
17:B:262:ASP:OD1	17:B:262:ASP:N	2.47	0.48
21:C:238:ALA:O	21:C:244:SER:OG	2.30	0.48
22:U:9:ILE:HG12	22:U:41:SER:HB2	1.94	0.48
22:U:16:GLU:HB3	22:U:18:GLN:HG2	1.95	0.48
1:f:109:LEU:HA	1:f:110:ALA:HB3	1.96	0.48
1:f:611:HIS:HB2	1:f:614:LYS:HB2	1.95	0.48
4:I:220:ASN:HA	4:I:221:GLY:HA2	1.54	0.48
5:J:92:GLN:HG3	12:Q:62:LYS:HB3	1.95	0.48
7:L:40:SER:OG	7:L:43:HIS:O	2.26	0.48
13:R:171:GLY:HA2	13:R:192:VAL:HG21	1.95	0.48
15:T:54:SER:O	15:T:108:ASN:ND2	2.39	0.48
16:A:200:ARG:HA	16:A:204:LEU:HD13	1.95	0.48
16:A:219:GLY:HA2	16:A:220:THR:HA	1.58	0.48
18:D:69:LYS:HG3	21:C:49:ARG:HH22	1.79	0.48
25:X:206:LEU:O	25:X:210:LEU:N	2.37	0.48
25:X:299:LEU:HA	25:X:302:PHE:HB3	1.95	0.48
27:Z:142:GLU:OE2	27:Z:153:LYS:NZ	2.47	0.48
5:J:34:GLY:HA2	5:J:43:LEU:HA	1.94	0.48
6:K:225:ASN:HB2	6:K:226:PHE:CD2	2.49	0.48
9:N:99:ILE:HG23	9:N:113:SER:HA	1.96	0.48
18:D:235:PHE:HZ	18:D:270:ILE:HD13	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:102:ASN:O	27:Z:45:LYS:NZ	2.29	0.48
20:F:233:LYS:N	33:F:501:ATP:O1B	2.47	0.48
24:W:12:ARG:HA	24:W:15:LYS:HD3	1.96	0.48
24:W:409:LEU:HD23	25:X:384:VAL:HG21	1.95	0.48
4:I:49:ARG:N	4:I:210:LYS:O	2.41	0.47
15:T:192:VAL:HG12	15:T:197:VAL:HG22	1.96	0.47
16:A:217:PRO:HD2	16:A:343:PHE:HB2	1.96	0.47
16:A:362:MET:HG2	16:A:363:SER:H	1.79	0.47
18:D:242:GLU:OE1	19:E:78:ARG:NH1	2.39	0.47
19:E:196:LEU:HB3	19:E:230:ILE:HG12	1.96	0.47
22:U:343:ILE:HG23	22:U:344:ARG:HG2	1.96	0.47
22:U:509:GLY:HA3	22:U:544:ILE:HD13	1.96	0.47
24:W:16:MET:HG2	24:W:27:ARG:HH22	1.79	0.47
24:W:141:GLU:HB3	24:W:172:GLU:HG2	1.95	0.47
24:W:247:TYR:HA	24:W:250:ILE:HG23	1.96	0.47
24:W:316:ARG:O	24:W:319:THR:OG1	2.25	0.47
29:b:48:ASN:HA	29:b:66:PRO:HA	1.96	0.47
30:c:261:GLU:HA	30:c:264:LYS:HG2	1.96	0.47
31:d:184:LYS:HB2	31:d:185:ALA:HB2	1.96	0.47
2:G:119:ALA:HB1	2:G:158:GLY:C	2.38	0.47
6:K:40:ILE:HG23	6:K:185:TYR:HE1	1.79	0.47
12:Q:13:VAL:HB	12:Q:183:ILE:HD12	1.97	0.47
18:D:301:GLN:HA	18:D:302:ASN:HA	1.62	0.47
20:F:339:ASP:HB3	20:F:342:LEU:HG	1.94	0.47
22:U:756:HIS:HD2	22:U:759:SER:HB2	1.79	0.47
25:X:366:SER:HA	25:X:369:ILE:HD12	1.96	0.47
26:Y:134:LEU:HB2	26:Y:168:ILE:HG23	1.95	0.47
30:c:247:GLU:OE1	30:c:247:GLU:N	2.47	0.47
2:G:159:TYR:HA	3:H:84:ARG:NH2	2.29	0.47
13:R:7:LYS:O	13:R:143:TYR:OH	2.32	0.47
18:D:181:VAL:C	18:D:184:PRO:HD2	2.39	0.47
19:E:135:ILE:HA	19:E:312:ILE:HD13	1.96	0.47
1:f:223:ASN:HA	1:f:254:SER:HB3	1.96	0.47
1:f:681:LEU:HB2	1:f:682:PRO:HD3	1.96	0.47
2:G:97:GLU:HA	2:G:100:ASN:HD22	1.78	0.47
6:K:212:ALA:HA	6:K:234:LEU:HD22	1.96	0.47
7:L:27:GLU:O	7:L:31:GLN:N	2.48	0.47
11:P:11:VAL:HG23	11:P:54:ALA:HB2	1.96	0.47
16:A:345:LEU:HG	16:A:346:PRO:HD2	1.96	0.47
18:D:39:ASP:N	22:U:148:LYS:O	2.48	0.47
18:D:172:ILE:HG13	18:D:173:GLN:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:303:VAL:HA	18:D:304:ASN:HA	1.78	0.47
20:F:94:ILE:HD11	20:F:125:LYS:HG2	1.95	0.47
21:C:147:THR:HA	21:C:205:HIS:CD2	2.48	0.47
21:C:241:HIS:HB2	21:C:244:SER:HB3	1.96	0.47
21:C:298:ILE:HG22	21:C:299:ASP:H	1.80	0.47
28:a:359:ASP:O	28:a:362:SER:OG	2.33	0.47
1:f:400:PRO:HG2	1:f:437:ASP:HA	1.96	0.47
3:H:6:TYR:HB2	3:H:13:PHE:HB3	1.95	0.47
6:K:227:HIS:HA	6:K:228:MET:C	2.39	0.47
8:M:20:VAL:HG12	8:M:22:GLN:H	1.79	0.47
10:O:110:LEU:HD21	10:O:125:VAL:HG22	1.97	0.47
15:T:44:ARG:HA	15:T:50:MET:HG3	1.95	0.47
17:B:106:PRO:HB3	21:C:120:SER:HB2	1.97	0.47
18:D:146:GLU:CD	18:D:147:ALA:H	2.22	0.47
18:D:287:ARG:O	18:D:291:GLU:N	2.44	0.47
21:C:310:ARG:HA	21:C:311:ILE:HA	1.53	0.47
22:U:69:TYR:OH	23:V:239:THR:O	2.22	0.47
22:U:345:ASN:HD21	22:U:883:ARG:HG2	1.80	0.47
22:U:564:ASP:HA	22:U:567:ILE:HB	1.97	0.47
30:c:96:LEU:HD23	30:c:99:LEU:HD12	1.96	0.47
31:d:160:ALA:N	31:d:161:GLU:HA	2.27	0.47
31:d:226:ALA:HA	31:d:227:SER:HA	1.65	0.47
19:E:232:MET:O	19:E:278:ALA:N	2.48	0.47
19:E:309:ARG:HA	19:E:312:ILE:HG22	1.96	0.47
20:F:154:ASN:O	20:F:157:SER:OG	2.29	0.47
23:V:197:THR:C	23:V:199:ASN:H	2.22	0.47
23:V:451:ILE:HD13	31:d:186:TYR:CE1	2.50	0.47
27:Z:128:PRO:HD3	30:c:216:MET:HE3	1.95	0.47
27:Z:148:GLY:HA2	28:a:181:GLY:C	2.40	0.47
1:f:371:CYS:C	1:f:373:GLY:HA2	2.39	0.47
3:H:6:TYR:H	3:H:13:PHE:HB3	1.79	0.47
4:I:43:VAL:HG12	4:I:216:LEU:HB3	1.95	0.47
4:I:93:ILE:HA	4:I:96:ARG:HG2	1.96	0.47
4:I:143:TYR:HB2	4:I:146:GLN:NE2	2.30	0.47
7:L:164:ARG:HH21	20:F:430:LYS:HE2	1.80	0.47
13:R:173:ALA:HA	13:R:191:ASN:HA	1.96	0.47
16:A:115:VAL:HG13	16:A:117:GLN:H	1.79	0.47
23:V:221:LEU:HD12	23:V:222:ASP:H	1.80	0.47
23:V:227:VAL:HA	23:V:230:PHE:HB3	1.97	0.47
23:V:394:LEU:HD13	23:V:398:LEU:HD13	1.96	0.47
24:W:216:GLU:CD	24:W:217:GLU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:173:ASP:N	26:Y:177:ARG:HD3	2.29	0.47
26:Y:174:TRP:CE3	26:Y:175:ASP:HB2	2.49	0.47
27:Z:240:VAL:O	27:Z:243:GLN:N	2.44	0.47
31:d:54:ILE:HA	31:d:57:ILE:HG22	1.96	0.47
1:f:567:ILE:HG13	1:f:605:LEU:HD22	1.97	0.47
8:M:80:LEU:HD23	8:M:83:ASP:H	1.80	0.47
16:A:210:LYS:HG2	16:A:336:ARG:NH1	2.30	0.47
17:B:262:ASP:H	17:B:266:LEU:HD11	1.80	0.47
26:Y:232:GLU:O	26:Y:236:LEU:N	2.39	0.47
27:Z:223:ASN:HB2	27:Z:227:ILE:HG12	1.97	0.47
30:c:34:SER:HB3	30:c:208:ARG:NH2	2.30	0.47
32:e:63:HIS:HA	32:e:66:LYS:HE2	1.96	0.47
1:f:106:ALA:HB1	1:f:107:LEU:CA	2.45	0.47
1:f:320:LEU:HD23	1:f:689:GLN:HG2	1.97	0.47
4:I:57:ASP:HB3	4:I:59:VAL:HG13	1.96	0.47
16:A:273:PHE:CD1	16:A:318:LEU:HD22	2.49	0.47
19:E:240:GLY:O	19:E:254:GLN:NE2	2.47	0.47
22:U:346:ASN:HA	22:U:743:ASN:HD21	1.79	0.47
22:U:787:CYS:HB2	22:U:881:PRO:HB2	1.97	0.47
23:V:280:ALA:HA	23:V:281:ASN:HA	1.54	0.47
26:Y:131:THR:O	26:Y:137:ARG:NH1	2.48	0.47
26:Y:286:TRP:O	26:Y:287:LEU:HG	2.14	0.47
26:Y:357:ASN:HB2	26:Y:359:PRO:HD3	1.97	0.47
30:c:229:LEU:O	30:c:230:THR:OG1	2.25	0.47
1:f:479:ASP:HB3	1:f:506:GLU:H	1.80	0.47
3:H:34:PRO:HB3	3:H:165:LYS:N	2.29	0.47
3:H:136:ILE:N	3:H:147:PHE:O	2.43	0.47
16:A:365:GLU:HG2	16:A:366:ARG:H	1.80	0.47
21:C:213:ARG:NE	21:C:249:ASP:O	2.28	0.47
24:W:373:ILE:HG12	24:W:374:THR:N	2.29	0.47
25:X:409:LYS:HE2	30:c:264:LYS:HG3	1.97	0.47
27:Z:39:LEU:HD11	27:Z:50:VAL:HG11	1.97	0.47
28:a:308:GLU:OE1	28:a:308:GLU:N	2.41	0.47
1:f:281:ILE:HG13	1:f:282:LYS:H	1.80	0.46
2:G:39:SER:H	2:G:172:GLN:NE2	2.13	0.46
4:I:13:SER:O	5:J:21:TYR:CD1	2.68	0.46
5:J:96:LEU:C	13:R:81:LYS:HZ3	2.24	0.46
5:J:211:MET:HB2	5:J:217:LEU:HB3	1.96	0.46
14:S:68:ILE:O	14:S:72:LEU:N	2.47	0.46
18:D:326:ARG:HH22	21:C:141:GLU:HB3	1.79	0.46
21:C:186:VAL:HG23	21:C:312:ASP:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:896:GLU:O	22:U:901:GLN:NE2	2.49	0.46
24:W:422:ASN:OD1	24:W:423:ASN:N	2.48	0.46
31:d:215:TRP:CG	31:d:216:VAL:H	2.32	0.46
1:f:297:ARG:HA	1:f:298:ASN:C	2.39	0.46
2:G:77:GLY:H	2:G:141:ILE:HD11	1.80	0.46
4:I:140:ASP:OD1	4:I:144:GLY:N	2.49	0.46
14:S:193:LEU:HB3	14:S:208:VAL:HB	1.97	0.46
19:E:90:SER:O	19:E:93:LYS:NZ	2.43	0.46
22:U:625:ILE:HG13	22:U:626:LEU:HG	1.97	0.46
23:V:89:LYS:HD3	23:V:92:ARG:HH11	1.81	0.46
23:V:221:LEU:HD12	23:V:222:ASP:N	2.30	0.46
24:W:169:LEU:HD22	24:W:186:ILE:HG13	1.97	0.46
31:d:122:LEU:HB3	31:d:125:LYS:HB2	1.96	0.46
2:G:71:LYS:HE2	2:G:74:GLU:HA	1.97	0.46
3:H:65:VAL:HG22	3:H:75:VAL:HG12	1.98	0.46
5:J:93:SER:O	5:J:97:THR:N	2.47	0.46
8:M:37:ILE:HG22	8:M:164:ALA:HA	1.96	0.46
16:A:164:MET:HA	17:B:265:LYS:HE2	1.97	0.46
16:A:343:PHE:HA	16:A:344:SER:OG	2.15	0.46
16:A:349:GLU:O	16:A:353:HIS:ND1	2.32	0.46
16:A:401:ARG:HH12	16:A:414:ASN:HD22	1.63	0.46
18:D:213:THR:HG22	18:D:217:LYS:HE3	1.96	0.46
22:U:214:ILE:HA	22:U:217:CYS:HB3	1.97	0.46
22:U:632:GLN:O	22:U:635:SER:OG	2.29	0.46
2:G:56:VAL:HA	2:G:61:LEU:HD13	1.96	0.46
5:J:180:ALA:HA	5:J:181:ILE:HA	1.46	0.46
8:M:77:VAL:HG21	8:M:84:ALA:HB1	1.98	0.46
10:O:146:MET:HE2	10:O:154:LEU:HD22	1.97	0.46
11:P:62:THR:OG1	12:Q:85:ARG:NH2	2.31	0.46
16:A:167:GLU:HB2	16:A:239:ARG:HG2	1.96	0.46
18:D:274:ARG:NH1	19:E:248:SER:OG	2.49	0.46
18:D:285:VAL:HA	18:D:288:ILE:HD12	1.96	0.46
22:U:68:PHE:HB3	22:U:73:ALA:HB3	1.96	0.46
26:Y:20:ALA:HB2	26:Y:150:PHE:HD1	1.80	0.46
27:Z:32:GLN:HG3	27:Z:33:LYS:H	1.79	0.46
27:Z:228:TYR:CE2	28:a:338:PRO:HB2	2.51	0.46
30:c:282:ARG:HG3	30:c:284:LEU:HD13	1.96	0.46
3:H:136:ILE:HB	3:H:147:PHE:HB2	1.97	0.46
6:K:167:ALA:HB3	6:K:181:LEU:HD21	1.98	0.46
7:L:84:LEU:HA	7:L:87:PHE:HB3	1.98	0.46
17:B:203:LEU:HG	17:B:211:TYR:HD1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:343:ARG:HB2	17:B:344:PRO:HD3	1.96	0.46
21:C:186:VAL:HG12	21:C:292:ILE:HG12	1.98	0.46
21:C:192:PRO:HD3	21:C:296:ASN:O	2.16	0.46
21:C:207:THR:HG21	21:C:245:ILE:HG12	1.97	0.46
22:U:195:ASN:HB2	22:U:223:LEU:HD13	1.98	0.46
22:U:664:GLY:HA2	22:U:698:GLN:HE22	1.81	0.46
23:V:148:ARG:NH1	23:V:193:GLN:OE1	2.36	0.46
23:V:256:ARG:HG3	32:e:5:LYS:HD3	1.97	0.46
27:Z:196:HIS:HB2	30:c:231:LEU:HG	1.97	0.46
28:a:31:LYS:HA	29:b:177:PRO:HD3	1.97	0.46
28:a:219:HIS:ND1	28:a:221:VAL:HG22	2.30	0.46
30:c:32:TYR:HE1	30:c:206:ASN:HD21	1.62	0.46
1:f:414:ILE:HG12	1:f:418:LEU:HD13	1.97	0.46
5:J:45:VAL:HG13	5:J:46:GLU:H	1.80	0.46
9:N:42:PHE:HB2	9:N:179:ILE:HD11	1.98	0.46
17:B:324:ASP:N	17:B:324:ASP:OD1	2.49	0.46
19:E:223:ARG:HA	19:E:226:GLN:HE21	1.80	0.46
20:F:397:LYS:HA	20:F:400:CYS:HB3	1.97	0.46
22:U:789:ILE:HB	22:U:911:ILE:HA	1.97	0.46
22:U:885:MET:HG2	22:U:887:ALA:H	1.80	0.46
28:a:19:PRO:HA	28:a:22:TRP:HB2	1.96	0.46
31:d:225:PHE:HA	31:d:226:ALA:HA	1.69	0.46
2:G:93:ARG:HH22	2:G:121:ILE:HB	1.80	0.46
2:G:199:ILE:HD13	2:G:242:LEU:HD21	1.97	0.46
6:K:46:VAL:HG23	6:K:151:PRO:HB2	1.97	0.46
13:R:55:TRP:O	13:R:59:LEU:N	2.39	0.46
13:R:95:LEU:HD21	14:S:100:ARG:HG2	1.97	0.46
15:T:11:VAL:HG13	15:T:24:ALA:HB2	1.97	0.46
17:B:144:LEU:HD11	17:B:162:VAL:HG21	1.98	0.46
19:E:57:VAL:HA	19:E:99:ALA:HA	1.98	0.46
19:E:264:MET:HB3	19:E:294:ARG:HA	1.98	0.46
20:F:298:SER:HB2	20:F:299:GLU:HG3	1.98	0.46
23:V:98:LEU:N	23:V:99:ARG:HA	2.31	0.46
23:V:263:LEU:HG	23:V:264:TYR:H	1.80	0.46
24:W:370:TYR:OH	24:W:373:ILE:HD12	2.15	0.46
26:Y:181:LYS:HA	26:Y:200:LEU:HD23	1.97	0.46
27:Z:62:ASP:OD2	27:Z:63:LYS:NZ	2.39	0.46
29:b:16:MET:HA	29:b:25:ARG:HD2	1.98	0.46
29:b:97:LEU:O	29:b:100:ARG:NE	2.48	0.46
30:c:154:LYS:HG2	30:c:156:VAL:H	1.80	0.46
18:D:341:LYS:NZ	18:D:374:ASP:O	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:409:LYS:HB2	18:D:410:ASP:C	2.41	0.46
21:C:99:VAL:HA	21:C:100:ASP:HB2	1.98	0.46
22:U:107:HIS:HA	22:U:110:LYS:HE3	1.98	0.46
23:V:486:ILE:HG21	26:Y:377:LEU:HD21	1.97	0.46
25:X:377:ILE:HG12	26:Y:312:ARG:HB3	1.96	0.46
5:J:98:VAL:HG12	5:J:100:ASP:OD1	2.16	0.46
9:N:132:SER:HA	9:N:135:ILE:HG12	1.97	0.46
12:Q:20:VAL:HG21	12:Q:176:PRO:HD2	1.97	0.46
16:A:107:GLU:HB2	16:A:110:LYS:HG2	1.97	0.46
16:A:253:GLY:HA3	16:A:298:THR:HG22	1.98	0.46
20:F:83:ASN:O	20:F:154:ASN:ND2	2.49	0.46
22:U:573:ASP:OD1	22:U:574:LYS:N	2.49	0.46
24:W:59:ASP:O	24:W:63:THR:OG1	2.21	0.46
28:a:70:ARG:HH21	29:b:80:PRO:HD2	1.81	0.46
31:d:135:HIS:HB3	31:d:136:PRO:HD3	1.98	0.46
31:d:198:LEU:HD22	31:d:205:LYS:HE3	1.98	0.46
32:e:4:LYS:HD2	32:e:4:LYS:HA	1.83	0.46
1:f:635:ALA:C	1:f:637:LEU:HA	2.41	0.46
2:G:109:ILE:HD13	2:G:114:LEU:HB2	1.98	0.46
3:H:11:THR:HG22	3:H:12:THR:H	1.81	0.46
3:H:80:GLY:O	3:H:82:ASP:N	2.48	0.46
16:A:94:GLN:HA	17:B:131:HIS:CD2	2.50	0.46
18:D:116:LEU:HB2	18:D:140:VAL:HA	1.98	0.46
22:U:494:TYR:HD1	22:U:516:LEU:HD11	1.81	0.46
22:U:540:GLN:HG3	22:U:541:HIS:CD2	2.50	0.46
22:U:557:TYR:HD1	22:U:588:MET:HB3	1.79	0.46
26:Y:349:LYS:C	26:Y:351:ASN:H	2.24	0.46
27:Z:7:GLN:OE1	27:Z:46:LYS:NZ	2.34	0.46
27:Z:171:GLY:HA3	30:c:38:LEU:HD21	1.98	0.46
27:Z:208:ILE:HD12	28:a:353:LEU:HB3	1.97	0.46
27:Z:237:LEU:HB2	27:Z:239:ASP:OD1	2.16	0.46
28:a:244:ASN:ND2	28:a:272:ILE:O	2.49	0.46
16:A:97:ARG:HA	16:A:98:CYS:HA	1.66	0.45
17:B:176:VAL:HG23	17:B:177:GLU:HB2	1.97	0.45
18:D:267:ILE:HD13	18:D:309:MET:SD	2.55	0.45
18:D:345:PHE:HA	18:D:348:ILE:HG22	1.97	0.45
20:F:221:LYS:HD2	20:F:327:LYS:HG3	1.98	0.45
30:c:191:ALA:HA	30:c:194:HIS:HD1	1.81	0.45
30:c:272:ILE:HB	30:c:273:LYS:HA	1.99	0.45
1:f:220:GLY:HA2	1:f:223:ASN:HD21	1.80	0.45
1:f:269:GLN:HE21	1:f:272:LYS:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:392:LYS:HD3	1:f:421:LEU:HB2	1.98	0.45
2:G:157:ALA:HB3	18:D:418:LYS:HG2	1.97	0.45
7:L:148:CYS:SG	7:L:150:SER:OG	2.62	0.45
7:L:156:CYS:HA	8:M:59:GLU:H	1.80	0.45
17:B:176:VAL:HA	17:B:177:GLU:HA	1.60	0.45
18:D:268:ASP:HA	18:D:271:ALA:HB3	1.98	0.45
26:Y:71:ASN:HA	26:Y:74:LYS:HG2	1.97	0.45
28:a:50:PHE:N	28:a:51:ALA:HA	2.30	0.45
29:b:48:ASN:OD1	29:b:48:ASN:N	2.46	0.45
30:c:164:ASN:HB2	30:c:167:MET:HG3	1.98	0.45
30:c:213:GLU:O	30:c:216:MET:HG2	2.16	0.45
6:K:17:PRO:HA	7:L:24:TYR:CZ	2.50	0.45
8:M:200:VAL:HG22	8:M:201:HIS:H	1.81	0.45
10:O:8:TYR:CE1	10:O:13:VAL:HG23	2.52	0.45
17:B:139:VAL:HA	17:B:140:ASP:CB	2.46	0.45
18:D:198:PRO:HD2	18:D:302:ASN:ND2	2.29	0.45
18:D:313:ARG:HH11	19:E:242:ARG:HG3	1.81	0.45
18:D:412:GLN:O	18:D:415:GLU:N	2.47	0.45
20:F:317:LEU:HD13	20:F:347:ARG:HA	1.98	0.45
21:C:215:SER:HA	21:C:216:GLY:HA3	1.59	0.45
22:U:377:HIS:HB3	22:U:411:ILE:HG23	1.98	0.45
1:f:371:CYS:O	1:f:372:ASN:HB2	2.16	0.45
3:H:71:HIS:HA	3:H:217:GLY:HA2	1.97	0.45
5:J:22:ALA:HB1	5:J:128:GLY:HA2	1.99	0.45
17:B:104:GLY:HA3	17:B:105:THR:HA	1.76	0.45
17:B:175:LYS:HB3	17:B:176:VAL:HB	1.99	0.45
18:D:154:LEU:C	18:D:156:SER:H	2.25	0.45
20:F:342:LEU:HD13	20:F:348:LEU:HD12	1.97	0.45
21:C:224:ILE:HD13	21:C:237:MET:HG3	1.98	0.45
22:U:32:ASN:OD1	22:U:33:ASP:N	2.49	0.45
26:Y:300:ARG:O	26:Y:304:TYR:N	2.41	0.45
27:Z:54:PHE:HB3	27:Z:82:PHE:HE2	1.82	0.45
2:G:184:LYS:HA	2:G:186:LYS:N	2.31	0.45
5:J:10:PHE:H	6:K:23:GLN:NE2	2.14	0.45
5:J:131:ALA:N	5:J:147:THR:OG1	2.44	0.45
13:R:25:TYR:OH	14:S:142:SER:O	2.29	0.45
17:B:362:LYS:HB2	17:B:384:ILE:HD13	1.99	0.45
21:C:161:ILE:HD13	21:C:315:ILE:HD11	1.98	0.45
21:C:338:LEU:HD21	21:C:342:ILE:HD13	1.99	0.45
22:U:568:GLU:OE2	22:U:572:ARG:NH2	2.48	0.45
23:V:31:ALA:HB3	23:V:32:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:78:HIS:HB3	23:V:161:PRO:HB3	1.99	0.45
23:V:372:LEU:HD21	23:V:399:ARG:HH22	1.80	0.45
6:K:68:VAL:HG23	6:K:76:CYS:HB3	1.99	0.45
18:D:145:PRO:O	18:D:252:ARG:NH1	2.49	0.45
20:F:434:ASN:CG	20:F:435:LEU:H	2.23	0.45
23:V:419:LEU:HD23	23:V:458:VAL:HG23	1.99	0.45
26:Y:85:ASP:O	26:Y:88:LEU:HG	2.15	0.45
2:G:153:LYS:O	2:G:161:CYS:HB3	2.16	0.45
3:H:71:HIS:CD2	3:H:72:ILE:HG13	2.52	0.45
5:J:76:LEU:HB3	17:B:440:LEU:HD23	1.98	0.45
10:O:176:CYS:HB2	10:O:185:PHE:HD1	1.82	0.45
14:S:28:ARG:NH1	14:S:187:VAL:O	2.49	0.45
19:E:226:GLN:HE22	19:E:273:VAL:HB	1.80	0.45
19:E:378:LYS:HE3	20:F:343:LEU:HD22	1.98	0.45
20:F:266:LYS:O	20:F:270:ASP:HB2	2.16	0.45
21:C:11:LEU:HD23	22:U:149:GLN:HE21	1.82	0.45
23:V:131:LEU:HD23	23:V:134:PHE:HD2	1.82	0.45
24:W:70:VAL:HA	24:W:73:MET:HE3	1.99	0.45
24:W:397:VAL:HG13	25:X:341:PRO:HB2	1.99	0.45
31:d:82:TYR:CZ	31:d:95:MET:HG3	2.52	0.45
1:f:194:LEU:HB3	1:f:195:GLU:H	1.54	0.45
1:f:390:GLU:HB3	1:f:391:LEU:HA	1.99	0.45
2:G:43:ARG:HG3	2:G:48:ALA:HB2	1.99	0.45
3:H:183:GLU:OE1	3:H:186:ASP:N	2.38	0.45
4:I:100:GLN:HG3	12:Q:86:ARG:HG3	1.98	0.45
5:J:104:VAL:HB	5:J:143:ARG:HD3	1.98	0.45
6:K:167:ALA:HB1	6:K:181:LEU:HD11	1.99	0.45
14:S:108:ASN:HB2	14:S:124:PHE:HD2	1.81	0.45
15:T:49:THR:HB	15:T:85:PRO:HG3	1.98	0.45
16:A:113:ILE:HB	16:A:121:PHE:HB3	1.98	0.45
18:D:190:LEU:HD21	21:C:371:LEU:HG	1.98	0.45
19:E:65:THR:HG22	19:E:66:GLU:H	1.81	0.45
21:C:35:VAL:HA	21:C:38:LYS:HB2	1.99	0.45
22:U:31:VAL:HG22	22:U:35:TRP:CD1	2.51	0.45
24:W:403:PHE:HB3	24:W:416:GLN:HG3	1.97	0.45
29:b:68:THR:HA	29:b:71:ILE:HD13	1.98	0.45
1:f:462:ASP:C	1:f:464:LYS:H	2.25	0.45
1:f:656:HIS:C	1:f:658:VAL:H	2.25	0.45
2:G:61:LEU:HG	2:G:66:VAL:HG21	1.98	0.45
2:G:128:ASN:HA	3:H:127:VAL:HG11	1.99	0.45
2:G:144:ASP:HB3	2:G:147:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:191:PHE:HE1	2:G:219:VAL:HG21	1.82	0.45
3:H:9:SER:HA	3:H:10:LEU:HA	1.72	0.45
4:I:105:ILE:HD12	4:I:106:PRO:HD2	1.99	0.45
7:L:160:SER:O	7:L:169:ARG:NH2	2.50	0.45
7:L:229:VAL:HG12	7:L:233:LEU:HG	1.98	0.45
10:O:103:VAL:HG21	10:O:179:SER:HA	1.99	0.45
13:R:35:ILE:HD11	13:R:45:MET:HE3	1.99	0.45
14:S:60:ASP:HB3	14:S:104:TYR:HB3	1.98	0.45
14:S:150:ASP:O	14:S:155:PHE:N	2.50	0.45
15:T:41:ARG:HH21	15:T:54:SER:HA	1.82	0.45
18:D:45:LYS:HE3	22:U:158:ARG:HH12	1.82	0.45
18:D:380:GLN:O	18:D:384:MET:N	2.46	0.45
18:D:409:LYS:NZ	18:D:413:GLU:OE1	2.49	0.45
19:E:55:GLN:HA	19:E:102:MET:HG2	1.98	0.45
20:F:205:PRO:O	20:F:209:LYS:HB2	2.16	0.45
21:C:130:LYS:HB2	21:C:133:PRO:HG2	1.99	0.45
21:C:321:ASN:H	21:C:324:ALA:HB3	1.82	0.45
22:U:666:LYS:HZ3	22:U:703:CYS:HB2	1.81	0.45
23:V:378:VAL:HG13	23:V:382:PHE:HD2	1.81	0.45
24:W:234:ASP:OD2	24:W:246:HIS:NE2	2.50	0.45
25:X:410:VAL:HB	26:Y:376:LEU:HD11	1.99	0.45
29:b:109:ILE:HB	29:b:138:VAL:HG22	1.99	0.45
1:f:510:GLU:C	1:f:512:ALA:H	2.25	0.45
3:H:45:VAL:HG22	3:H:212:ILE:HG22	1.99	0.45
4:I:232:GLU:O	4:I:235:GLN:HG2	2.17	0.45
5:J:94:HIS:HE1	5:J:103:THR:H	1.63	0.45
5:J:158:ALA:HB3	5:J:172:LEU:HD13	1.97	0.45
6:K:174:SER:HA	6:K:177:ALA:HB3	1.99	0.45
8:M:40:ARG:HA	8:M:45:VAL:HA	2.00	0.45
8:M:197:ILE:HG21	8:M:211:LEU:HD13	1.98	0.45
15:T:20:VAL:HG11	15:T:122:LEU:HD13	1.99	0.45
15:T:51:LEU:HD13	15:T:112:ILE:HG12	1.98	0.45
18:D:197:ASP:O	18:D:199:PRO:HD3	2.17	0.45
21:C:247:PHE:CE2	21:C:249:ASP:HB2	2.51	0.45
22:U:682:TYR:HB3	22:U:725:MET:SD	2.57	0.45
22:U:842:LYS:HE3	22:U:843:GLU:O	2.17	0.45
24:W:78:LYS:HA	24:W:81:ASP:HB3	1.99	0.45
26:Y:387:ILE:HA	26:Y:388:ASN:HA	1.56	0.45
30:c:252:ALA:O	30:c:256:ASN:N	2.49	0.45
31:d:109:GLN:HG3	31:d:111:ARG:HG2	1.98	0.45
17:B:205:LEU:HG	17:B:279:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:436:GLU:CB	17:B:437:GLY:HA2	2.47	0.44
18:D:151:ILE:HB	18:D:152:MET:CA	2.46	0.44
18:D:161:ASP:OD2	18:D:229:ARG:NH2	2.50	0.44
24:W:76:GLU:HA	24:W:79:GLU:HB2	1.99	0.44
25:X:346:GLN:HA	25:X:384:VAL:HA	1.99	0.44
26:Y:43:ALA:O	26:Y:49:ASN:ND2	2.40	0.44
28:a:24:ARG:O	28:a:28:LEU:HD13	2.17	0.44
5:J:88:ARG:HH22	12:Q:69:MET:HB2	1.82	0.44
7:L:50:LYS:HB2	7:L:209:ASN:HA	1.99	0.44
16:A:164:MET:SD	17:B:265:LYS:HG3	2.57	0.44
16:A:351:ARG:HA	16:A:354:ILE:HD12	1.98	0.44
17:B:256:ILE:HD12	17:B:312:LEU:HD13	1.98	0.44
17:B:319:PHE:HA	17:B:320:ASP:HA	1.55	0.44
17:B:397:ALA:HB3	21:C:311:ILE:HB	2.00	0.44
21:C:229:ARG:HE	21:C:232:ARG:HB3	1.81	0.44
23:V:244:ALA:C	23:V:246:GLY:H	2.24	0.44
27:Z:58:PHE:CZ	27:Z:68:TRP:HB2	2.51	0.44
28:a:244:ASN:ND2	28:a:276:CYS:HB3	2.32	0.44
31:d:246:VAL:HA	31:d:249:TYR:HB3	1.99	0.44
1:f:314:ASN:HA	1:f:319:ARG:HD2	1.99	0.44
1:f:376:THR:HG21	1:f:410:LYS:HE2	1.98	0.44
1:f:669:ARG:HB3	1:f:674:PHE:HE2	1.83	0.44
3:H:50:LYS:HD2	3:H:64:LYS:HG2	1.99	0.44
14:S:21:ALA:HB3	14:S:198:VAL:HB	2.00	0.44
22:U:361:ARG:HG3	22:U:365:CYS:HB2	1.99	0.44
31:d:198:LEU:HD13	31:d:206:MET:HB3	1.99	0.44
7:L:171:TYR:O	7:L:175:HIS:ND1	2.50	0.44
8:M:185:THR:O	8:M:189:ILE:HG12	2.18	0.44
12:Q:19:ARG:HD2	12:Q:179:SER:HB3	1.99	0.44
12:Q:77:PRO:HG2	12:Q:108:ASP:HB2	1.99	0.44
16:A:80:LEU:HD13	17:B:99:VAL:HG21	1.99	0.44
17:B:408:ARG:NH2	21:C:159:LYS:HD2	2.33	0.44
18:D:136:SER:HB2	21:C:66:LEU:HD23	1.99	0.44
20:F:336:ASP:OD1	20:F:337:ILE:N	2.49	0.44
21:C:99:VAL:HG13	21:C:101:LYS:N	2.32	0.44
21:C:117:ARG:HG3	21:C:124:HIS:HB2	1.99	0.44
22:U:195:ASN:HA	22:U:198:LEU:HB3	2.00	0.44
26:Y:357:ASN:OD1	26:Y:358:ARG:N	2.50	0.44
27:Z:84:LYS:HG2	30:c:76:PRO:HB3	1.99	0.44
27:Z:212:LEU:HB2	28:a:350:LYS:HD2	1.99	0.44
31:d:30:LEU:HA	31:d:34:ASN:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:146:LEU:HG	1:f:178:LEU:HD13	1.98	0.44
1:f:191:LYS:O	1:f:193:HIS:ND1	2.50	0.44
7:L:184:LEU:H	7:L:184:LEU:HD12	1.82	0.44
11:P:33:GLN:HE22	12:Q:136:ALA:HB1	1.82	0.44
18:D:129:SER:HB3	18:D:143:LEU:HD12	1.99	0.44
18:D:266:GLU:HA	18:D:311:THR:HA	2.00	0.44
23:V:94:VAL:HG13	23:V:95:LEU:HD12	1.99	0.44
26:Y:138:LEU:HD23	26:Y:176:ARG:HD3	1.99	0.44
26:Y:210:SER:H	26:Y:213:LEU:HB2	1.83	0.44
28:a:139:GLU:HA	28:a:142:LEU:HB3	1.99	0.44
2:G:93:ARG:NH2	2:G:97:GLU:OE2	2.43	0.44
18:D:86:PRO:O	18:D:87:LEU:HD12	2.17	0.44
22:U:167:ILE:HB	22:U:177:LEU:HD21	2.00	0.44
24:W:397:VAL:HG22	25:X:341:PRO:HB2	1.99	0.44
1:f:11:TRP:HA	1:f:12:GLN:HA	1.75	0.44
1:f:266:GLY:HA3	1:f:267:LEU:HA	1.72	0.44
1:f:282:LYS:NZ	1:f:283:SER:O	2.51	0.44
5:J:132:LEU:HA	5:J:146:GLN:HA	1.99	0.44
7:L:85:CYS:HG	7:L:89:ARG:HH12	1.64	0.44
17:B:177:GLU:N	17:B:178:LYS:HA	2.22	0.44
18:D:270:ILE:HD12	18:D:289:LEU:HB2	1.98	0.44
19:E:171:LEU:HD22	19:E:295:LEU:HD13	2.00	0.44
21:C:35:VAL:HA	21:C:38:LYS:HD3	2.00	0.44
21:C:130:LYS:HB2	21:C:133:PRO:HD2	1.98	0.44
21:C:273:MET:HB2	21:C:307:ARG:NH1	2.31	0.44
25:X:421:LEU:HD13	26:Y:386:VAL:HG21	2.00	0.44
26:Y:186:LEU:HA	26:Y:189:VAL:HG12	2.00	0.44
30:c:174:PRO:HB2	30:c:175:ARG:HH11	1.81	0.44
30:c:227:GLU:HB3	30:c:233:ASP:HB2	1.98	0.44
31:d:68:ILE:HB	31:d:69:PRO:HD3	1.99	0.44
31:d:118:GLU:HG2	31:d:121:ARG:HH12	1.82	0.44
2:G:86:ASP:HA	8:M:120:HIS:CE1	2.52	0.44
4:I:42:GLY:HA3	4:I:186:LEU:HD21	2.00	0.44
16:A:269:ALA:H	16:A:315:ILE:HG22	1.83	0.44
17:B:229:GLY:HA2	21:C:274:LEU:HD13	1.99	0.44
18:D:167:ILE:HG23	33:D:501:ATP:HN62	1.83	0.44
20:F:91:SER:HB3	20:F:151:VAL:HG23	1.99	0.44
20:F:344:ARG:HH11	20:F:346:GLY:H	1.66	0.44
27:Z:10:VAL:N	27:Z:48:LEU:O	2.50	0.44
4:I:184:MET:HA	4:I:185:THR:OG1	2.18	0.44
18:D:361:GLU:O	18:D:364:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:384:LEU:HG	19:E:385:ASP:OD1	2.18	0.44
22:U:26:LYS:HD2	31:d:34:ASN:ND2	2.33	0.44
22:U:806:CYS:SG	22:U:891:VAL:HG21	2.57	0.44
23:V:104:THR:HA	23:V:107:ARG:HG2	2.00	0.44
23:V:212:TYR:CG	32:e:4:LYS:NZ	2.86	0.44
26:Y:50:MET:HA	26:Y:53:TYR:CE2	2.53	0.44
26:Y:116:ASP:HB2	26:Y:118:GLU:OE1	2.18	0.44
30:c:64:ASP:HA	30:c:139:ARG:HH21	1.82	0.44
1:f:525:PRO:O	1:f:526:THR:HG22	2.17	0.43
2:G:43:ARG:HA	2:G:48:ALA:HA	2.00	0.43
2:G:159:TYR:CE1	18:D:418:LYS:HD2	2.53	0.43
3:H:83:TYR:N	3:H:132:VAL:HG21	2.33	0.43
10:O:113:ILE:HA	10:O:119:THR:HG22	1.98	0.43
15:T:50:MET:N	15:T:113:GLY:O	2.50	0.43
16:A:191:VAL:HG23	16:A:316:LYS:HE2	2.00	0.43
21:C:186:VAL:HG22	21:C:187:LEU:H	1.83	0.43
22:U:685:GLN:HG3	22:U:729:GLY:HA3	1.99	0.43
23:V:46:GLY:HA3	23:V:62:HIS:HE1	1.83	0.43
23:V:80:LYS:HA	23:V:80:LYS:HD3	1.84	0.43
23:V:144:ASP:N	23:V:145:LEU:HA	2.32	0.43
24:W:418:PRO:O	24:W:421:PRO:HD3	2.17	0.43
29:b:161:ASN:ND2	29:b:168:SER:H	2.16	0.43
29:b:184:ILE:H	29:b:184:ILE:HG13	1.70	0.43
30:c:272:ILE:HD12	30:c:277:LYS:HB3	1.99	0.43
1:f:314:ASN:HD21	1:f:355:VAL:HG13	1.82	0.43
1:f:481:LYS:O	1:f:484:PRO:HD2	2.18	0.43
4:I:100:GLN:O	12:Q:82:ASN:ND2	2.51	0.43
5:J:88:ARG:HB3	12:Q:66:LEU:HD11	2.00	0.43
10:O:8:TYR:HE2	10:O:10:ASP:HB2	1.83	0.43
16:A:210:LYS:HD3	16:A:336:ARG:HG3	2.00	0.43
17:B:178:LYS:HG3	17:B:180:PRO:HG3	2.00	0.43
20:F:80:ILE:O	20:F:84:LYS:N	2.51	0.43
21:C:380:GLN:HA	21:C:383:PHE:HD1	1.83	0.43
22:U:167:ILE:HD12	22:U:204:ILE:HG21	2.00	0.43
22:U:789:ILE:HG22	22:U:791:LEU:H	1.83	0.43
23:V:97:ALA:N	23:V:98:LEU:HA	2.33	0.43
27:Z:236:LEU:HD11	28:a:335:TRP:CD1	2.52	0.43
30:c:229:LEU:HB2	30:c:232:GLN:HG3	2.00	0.43
1:f:318:MET:HA	1:f:689:GLN:HE22	1.83	0.43
4:I:47:ALA:HB2	4:I:65:ILE:HD11	2.00	0.43
16:A:100:LYS:NZ	16:A:142:VAL:HB	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:105:ASP:OD1	16:A:105:ASP:N	2.50	0.43
16:A:159:PRO:HD2	16:A:162:THR:OG1	2.18	0.43
19:E:359:HIS:HB2	19:E:362:VAL:HG22	2.01	0.43
20:F:188:ILE:HD13	20:F:191:LEU:HB2	2.00	0.43
22:U:645:ASN:HD21	22:U:648:VAL:HG23	1.82	0.43
22:U:794:ASP:OD1	22:U:795:LEU:N	2.52	0.43
23:V:212:TYR:CE1	32:e:4:LYS:HG3	2.53	0.43
24:W:86:ASN:HD22	24:W:88:MET:HE2	1.84	0.43
24:W:417:ARG:O	24:W:419:LYS:N	2.51	0.43
26:Y:297:ARG:HD3	32:e:52:PHE:CE1	2.53	0.43
27:Z:33:LYS:HE3	27:Z:33:LYS:HB3	1.83	0.43
28:a:253:THR:HG23	28:a:261:LEU:HD21	2.00	0.43
30:c:116:PRO:HA	30:c:147:PRO:HD2	1.99	0.43
18:D:239:TYR:CE2	19:E:76:GLY:HA3	2.54	0.43
18:D:322:LEU:HD23	18:D:330:LYS:HZ3	1.84	0.43
21:C:184:LYS:HB2	21:C:277:LEU:HD23	2.00	0.43
22:U:20:LYS:HG3	22:U:54:PHE:HE1	1.84	0.43
22:U:146:LYS:HE2	22:U:148:LYS:HD3	2.00	0.43
22:U:472:ILE:HA	22:U:475:HIS:CE1	2.53	0.43
23:V:419:LEU:HA	23:V:422:ILE:HG22	1.99	0.43
28:a:36:GLN:H	28:a:36:GLN:CD	2.25	0.43
28:a:245:VAL:HA	28:a:246:GLU:C	2.44	0.43
1:f:248:MET:O	1:f:254:SER:OG	2.37	0.43
1:f:606:ALA:HA	1:f:609:LEU:HD13	1.98	0.43
11:P:15:LYS:HD3	11:P:119:PRO:HG2	2.00	0.43
14:S:63:THR:HG23	15:T:94:ARG:HH12	1.82	0.43
20:F:144:LYS:HA	20:F:145:LEU:HA	1.68	0.43
20:F:167:GLU:HB3	20:F:168:TYR:H	1.60	0.43
21:C:142:LYS:HB3	21:C:213:ARG:NH1	2.33	0.43
21:C:255:GLY:CA	21:C:256:SER:HB2	2.48	0.43
23:V:372:LEU:H	23:V:427:GLN:HE22	1.65	0.43
28:a:4:VAL:HB	28:a:5:PRO:HD3	2.01	0.43
30:c:75:MET:HE3	30:c:76:PRO:HD2	2.01	0.43
1:f:567:ILE:HB	1:f:602:MET:SD	2.59	0.43
4:I:228:LEU:HB3	4:I:229:LYS:HA	1.99	0.43
5:J:79:ASP:HB3	5:J:127:PHE:CE1	2.54	0.43
12:Q:42:ILE:HA	12:Q:106:GLY:HA2	1.99	0.43
12:Q:59:TYR:O	12:Q:63:ASN:ND2	2.47	0.43
17:B:320:ASP:OD1	17:B:320:ASP:N	2.50	0.43
20:F:281:SER:OG	20:F:282:ILE:N	2.51	0.43
21:C:189:TYR:HD2	21:C:300:ILE:HG23	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:370:TYR:HA	24:W:371:THR:HB	2.01	0.43
26:Y:384:SER:HB2	27:Z:279:LYS:HD3	2.00	0.43
26:Y:387:ILE:HD13	27:Z:283:ARG:HG3	2.00	0.43
29:b:33:VAL:HA	29:b:36:VAL:HG22	2.00	0.43
31:d:244:LYS:HD3	31:d:247:ILE:HD12	2.00	0.43
1:f:281:ILE:HG23	1:f:282:LYS:N	2.34	0.43
1:f:298:ASN:HA	1:f:299:GLU:HA	1.75	0.43
2:G:9:PHE:O	2:G:13:ILE:HG12	2.18	0.43
2:G:153:LYS:HZ1	2:G:167:ALA:HA	1.84	0.43
3:H:182:LEU:HD23	3:H:183:GLU:H	1.83	0.43
4:I:228:LEU:HB3	4:I:229:LYS:CA	2.48	0.43
6:K:157:ASP:OD1	6:K:161:THR:N	2.48	0.43
7:L:82:ARG:HA	7:L:85:CYS:HB3	2.00	0.43
9:N:16:ALA:HB1	9:N:33:LYS:HB2	2.01	0.43
11:P:21:ALA:HB2	11:P:189:ILE:HD13	2.00	0.43
16:A:303:ILE:HA	16:A:306:LEU:HB2	2.01	0.43
19:E:355:ILE:HD11	20:F:211:LYS:HE3	1.99	0.43
22:U:138:PHE:CZ	22:U:166:THR:HG22	2.54	0.43
26:Y:67:VAL:O	26:Y:71:ASN:N	2.50	0.43
28:a:97:LEU:HD22	28:a:118:ILE:HG13	2.00	0.43
30:c:87:VAL:HG21	30:c:133:PHE:HZ	1.83	0.43
31:d:3:GLU:HB3	31:d:4:GLN:CA	2.41	0.43
1:f:251:ALA:HB1	1:f:255:LEU:HG	2.01	0.43
6:K:86:LYS:HA	6:K:89:ILE:HB	2.01	0.43
9:N:2:THR:HA	9:N:129:GLY:HA3	1.99	0.43
13:R:167:ASP:OD1	13:R:168:ALA:N	2.52	0.43
19:E:385:ASP:HB3	19:E:386:TYR:CD1	2.54	0.43
21:C:246:ILE:HB	21:C:291:VAL:HG12	2.00	0.43
22:U:154:ALA:HB1	22:U:163:PHE:CD1	2.52	0.43
22:U:172:ASP:HA	22:U:173:VAL:HB	2.01	0.43
23:V:266:GLN:HG3	23:V:295:ILE:HD12	2.01	0.43
24:W:135:LYS:HB3	24:W:136:ILE:CA	2.49	0.43
24:W:419:LYS:HE2	25:X:388:PHE:HA	2.01	0.43
24:W:435:LEU:HA	24:W:438:LEU:HG	2.00	0.43
26:Y:47:ASP:HB3	26:Y:49:ASN:ND2	2.33	0.43
26:Y:203:ASP:N	26:Y:203:ASP:OD1	2.52	0.43
27:Z:191:ILE:O	27:Z:195:VAL:HG23	2.18	0.43
28:a:166:ILE:N	28:a:167:GLY:HA3	2.33	0.43
1:f:458:SER:O	1:f:459:GLU:HB2	2.17	0.43
4:I:44:LEU:HD22	4:I:190:LEU:HG	2.00	0.43
7:L:26:MET:HE1	7:L:148:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:203:ASN:HB3	16:A:204:LEU:HD12	2.01	0.43
17:B:187:ILE:HD12	17:B:190:LEU:HD21	2.01	0.43
19:E:327:ASP:H	19:E:364:GLN:CD	2.27	0.43
21:C:84:LYS:HE3	21:C:96:VAL:HG22	2.01	0.43
21:C:249:ASP:HA	21:C:250:GLU:HA	1.72	0.43
23:V:48:THR:HG23	23:V:147:PHE:HE2	1.83	0.43
23:V:186:LYS:NZ	23:V:234:ARG:HD3	2.33	0.43
24:W:428:TRP:HZ2	30:c:245:VAL:H	1.67	0.43
26:Y:268:TYR:CZ	26:Y:307:LEU:HD12	2.54	0.43
27:Z:39:LEU:HB2	27:Z:95:TYR:HD2	1.82	0.43
1:f:382:THR:HG22	1:f:386:LYS:NZ	2.34	0.43
3:H:111:VAL:HG22	3:H:136:ILE:HG21	2.00	0.43
4:I:18:LEU:HD13	4:I:21:VAL:HG21	2.00	0.43
6:K:236:GLU:HA	6:K:239:LYS:HE3	2.00	0.43
10:O:25:VAL:HG11	11:P:147:TYR:CZ	2.54	0.43
16:A:249:TYR:N	17:B:304:GLU:OE2	2.38	0.43
19:E:349:GLU:HG2	19:E:374:VAL:HG11	1.99	0.43
21:C:194:THR:HG22	21:C:195:GLY:H	1.83	0.43
23:V:484:LEU:HA	23:V:487:HIS:HD2	1.83	0.43
24:W:215:GLN:NE2	24:W:227:TYR:OH	2.44	0.43
25:X:223:LYS:HD3	26:Y:244:ALA:HA	2.01	0.43
30:c:170:LEU:HG	30:c:171:GLY:H	1.83	0.43
2:G:140:LEU:N	2:G:152:TYR:O	2.37	0.42
3:H:86:LEU:HD13	3:H:134:LEU:HD11	2.00	0.42
13:R:13:ILE:HD12	13:R:176:LEU:HD11	2.01	0.42
15:T:24:ALA:H	15:T:42:ILE:HD11	1.84	0.42
16:A:291:GLY:H	16:A:294:GLU:HG2	1.83	0.42
16:A:316:LYS:O	16:A:317:VAL:HG13	2.19	0.42
16:A:373:LEU:HD23	16:A:415:LYS:HG2	2.01	0.42
18:D:356:GLU:HG2	18:D:357:GLU:H	1.83	0.42
19:E:381:GLU:OE1	20:F:351:LYS:HE3	2.19	0.42
23:V:91:PRO:HA	23:V:94:VAL:HG12	2.00	0.42
26:Y:324:GLY:N	26:Y:325:VAL:HA	2.33	0.42
31:d:183:GLU:CD	31:d:186:TYR:HB2	2.45	0.42
31:d:191:PHE:O	31:d:195:THR:OG1	2.34	0.42
1:f:683:VAL:HA	1:f:687:VAL:HG21	2.00	0.42
4:I:187:LYS:HA	4:I:190:LEU:HB2	2.00	0.42
6:K:96:THR:HG22	6:K:107:MET:HB3	2.01	0.42
6:K:206:MET:HE1	6:K:210:LEU:HD13	2.00	0.42
8:M:8:ASP:O	8:M:22:GLN:NE2	2.32	0.42
8:M:49:VAL:O	8:M:212:GLU:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:113:ASP:OD1	11:P:114:PRO:HD2	2.19	0.42
18:D:92:PHE:HA	18:D:103:VAL:HG23	2.01	0.42
19:E:37:THR:HG21	20:F:66:LEU:HD22	2.00	0.42
21:C:277:LEU:HD22	21:C:311:ILE:HD11	2.01	0.42
22:U:525:ASN:HB3	22:U:528:ALA:HB2	2.01	0.42
22:U:681:ASN:OD1	22:U:681:ASN:N	2.51	0.42
23:V:367:VAL:HG22	23:V:398:LEU:HD21	2.01	0.42
26:Y:289:ALA:HB3	26:Y:290:PRO:HD3	2.01	0.42
26:Y:336:ARG:CZ	32:e:56:LEU:HD23	2.49	0.42
28:a:100:THR:HA	28:a:103:LYS:HG2	2.01	0.42
30:c:64:ASP:HA	30:c:139:ARG:NH2	2.34	0.42
31:d:183:GLU:OE1	31:d:224:SER:HB2	2.20	0.42
31:d:225:PHE:HB3	31:d:226:ALA:HB2	2.00	0.42
32:e:59:GLU:HB3	32:e:63:HIS:CE1	2.54	0.42
4:I:47:ALA:HB1	4:I:64:LYS:HB3	2.01	0.42
12:Q:43:LEU:HD21	12:Q:188:ILE:HG12	2.02	0.42
18:D:114:ARG:NH2	21:C:62:GLU:HG2	2.34	0.42
23:V:455:LYS:H	23:V:456:GLY:HA2	1.80	0.42
24:W:406:VAL:HA	24:W:413:ILE:HG22	2.01	0.42
25:X:366:SER:HB2	26:Y:310:SER:HB3	2.02	0.42
26:Y:42:MET:HG3	26:Y:46:ARG:HH12	1.84	0.42
27:Z:68:TRP:HH2	27:Z:111:LEU:HD22	1.84	0.42
30:c:157:ILE:HG23	30:c:158:ASP:N	2.34	0.42
30:c:266:THR:HB	30:c:283:HIS:CD2	2.55	0.42
31:d:147:SER:HG	31:d:151:VAL:HG23	1.83	0.42
31:d:150:LYS:HD2	31:d:153:LEU:HD12	2.01	0.42
2:G:110:PRO:O	2:G:111:VAL:HG12	2.19	0.42
8:M:68:ASN:ND2	8:M:224:HIS:O	2.53	0.42
11:P:58:THR:OG1	12:Q:121:LEU:O	2.23	0.42
16:A:164:MET:HE2	17:B:264:PRO:HD2	2.00	0.42
16:A:180:CYS:HB3	16:A:184:ILE:HB	2.00	0.42
16:A:292:ASP:O	16:A:296:GLN:HG2	2.19	0.42
17:B:166:ASP:OD1	21:C:78:ARG:NH1	2.52	0.42
17:B:296:ASP:HA	17:B:297:SER:HA	1.56	0.42
21:C:175:PHE:CE2	21:C:182:GLN:HG3	2.55	0.42
24:W:162:ALA:O	24:W:166:LEU:HG	2.20	0.42
25:X:245:PRO:HA	25:X:248:ILE:HG22	2.02	0.42
26:Y:80:GLU:O	26:Y:84:LEU:HG	2.20	0.42
1:f:61:ASP:C	1:f:63:ASP:H	2.27	0.42
1:f:246:HIS:CE1	1:f:250:SER:HB3	2.55	0.42
1:f:370:SER:HB3	1:f:372:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:ASP:HB3	2:G:156:PRO:HD2	2.02	0.42
6:K:114:GLN:HA	6:K:117:SER:HB2	2.00	0.42
7:L:158:ALA:HB3	7:L:176:MET:HE3	2.00	0.42
16:A:121:PHE:CE1	20:F:86:LEU:HD22	2.55	0.42
17:B:144:LEU:HD21	17:B:162:VAL:HB	2.02	0.42
17:B:217:LYS:C	17:B:219:PRO:HD3	2.45	0.42
17:B:224:LEU:O	17:B:330:ALA:HA	2.19	0.42
18:D:381:GLU:O	18:D:385:LEU:N	2.47	0.42
20:F:293:THR:HG23	20:F:337:ILE:HG21	2.01	0.42
21:C:219:LEU:HD23	21:C:219:LEU:O	2.19	0.42
22:U:257:SER:O	22:U:261:LEU:HG	2.20	0.42
22:U:479:LEU:HD13	22:U:511:ALA:HA	2.02	0.42
22:U:607:VAL:O	22:U:615:ARG:NH1	2.53	0.42
23:V:306:ARG:HB3	23:V:339:LEU:HD21	2.00	0.42
26:Y:63:TRP:HB3	26:Y:64:GLN:CB	2.49	0.42
1:f:304:LEU:HD11	1:f:326:LEU:HD12	2.02	0.42
1:f:335:ARG:NH2	1:f:372:ASN:OD1	2.52	0.42
1:f:483:ALA:HB1	1:f:500:LEU:HG	2.02	0.42
1:f:663:VAL:HA	1:f:664:ALA:HA	1.67	0.42
2:G:159:TYR:CD2	18:D:418:LYS:HG3	2.54	0.42
3:H:115:ALA:HA	3:H:118:MET:HB3	2.01	0.42
16:A:94:GLN:NE2	17:B:157:HIS:HB2	2.34	0.42
20:F:170:SER:OG	20:F:171:ARG:N	2.50	0.42
20:F:234:THR:HG22	20:F:238:ARG:HH22	1.85	0.42
22:U:357:LYS:NZ	22:U:389:ASN:HD22	2.18	0.42
22:U:792:ASN:HA	22:U:914:LEU:HB3	2.01	0.42
24:W:92:LYS:HB2	24:W:93:ARG:HB2	2.02	0.42
24:W:347:GLY:O	24:W:351:TRP:N	2.51	0.42
26:Y:192:ARG:NH2	26:Y:294:TYR:HB3	2.33	0.42
26:Y:356:THR:HA	26:Y:357:ASN:OD1	2.19	0.42
27:Z:210:SER:O	27:Z:214:LYS:HG2	2.18	0.42
28:a:148:VAL:C	28:a:150:SER:H	2.27	0.42
30:c:272:ILE:HG21	30:c:276:GLY:N	2.22	0.42
1:f:610:THR:HG23	1:f:611:HIS:CD2	2.54	0.42
4:I:79:ILE:HG22	4:I:82:ASP:H	1.85	0.42
16:A:164:MET:HE1	17:B:319:PHE:O	2.19	0.42
16:A:191:VAL:C	16:A:194:PRO:HD2	2.45	0.42
18:D:82:ILE:HA	18:D:83:GLN:HA	1.68	0.42
18:D:130:VAL:HB	18:D:142:VAL:HG12	2.01	0.42
19:E:54:GLY:H	20:F:158:TYR:HB2	1.85	0.42
22:U:56:SER:O	22:U:60:ALA:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:266:GLN:O	22:U:270:THR:OG1	2.32	0.42
23:V:90:GLU:OE1	23:V:90:GLU:N	2.46	0.42
23:V:157:THR:OG1	23:V:158:PRO:HD3	2.20	0.42
25:X:391:PRO:HG2	25:X:392:PRO:HD3	2.02	0.42
26:Y:84:LEU:HD12	26:Y:111:LEU:HD11	2.02	0.42
26:Y:170:GLU:CG	26:Y:171:GLY:HA3	2.43	0.42
1:f:297:ARG:HA	1:f:298:ASN:O	2.20	0.42
2:G:43:ARG:HD2	2:G:149:PRO:HG2	2.02	0.42
3:H:3:GLU:HA	3:H:4:ARG:HB2	2.01	0.42
5:J:109:ARG:NH2	13:R:69:ARG:HH11	2.18	0.42
19:E:228:CYS:HB3	19:E:273:VAL:HG23	2.01	0.42
21:C:200:ALA:HB1	21:C:211:PHE:CZ	2.55	0.42
24:W:353:ASP:OD1	24:W:357:ARG:NH2	2.52	0.42
25:X:332:GLU:HA	25:X:335:LEU:HB2	2.02	0.42
25:X:389:ASP:HB2	25:X:391:PRO:HD3	2.01	0.42
26:Y:191:ILE:HD12	26:Y:191:ILE:HA	1.91	0.42
28:a:243:GLY:HA3	28:a:244:ASN:HA	1.63	0.42
29:b:146:GLU:HG2	29:b:147:GLU:H	1.85	0.42
30:c:32:TYR:HB3	30:c:208:ARG:HD3	2.01	0.42
10:O:83:LEU:HD13	10:O:113:ILE:HD13	2.02	0.42
12:Q:16:ALA:HA	12:Q:180:VAL:HA	2.02	0.42
12:Q:29:LYS:HE3	12:Q:32:HIS:HA	2.02	0.42
19:E:75:ASN:C	19:E:77:PRO:HD2	2.45	0.42
21:C:168:PRO:HB2	21:C:288:ASN:ND2	2.35	0.42
23:V:212:TYR:CZ	32:e:4:LYS:CG	3.02	0.42
23:V:470:ARG:O	23:V:473:GLN:HG2	2.19	0.42
30:c:88:ASP:HB3	30:c:91:PHE:HB2	2.02	0.42
31:d:227:SER:N	31:d:230:GLN:H	2.18	0.42
1:f:662:LEU:H	1:f:663:VAL:HA	1.85	0.42
14:S:71:ARG:NE	14:S:91:MET:SD	2.75	0.42
16:A:121:PHE:CD2	16:A:123:VAL:HB	2.54	0.42
17:B:217:LYS:HG2	17:B:219:PRO:HD3	2.00	0.42
17:B:364:ILE:O	17:B:368:HIS:ND1	2.48	0.42
19:E:61:LEU:HD12	19:E:70:ILE:HG22	2.01	0.42
19:E:309:ARG:HD2	19:E:332:VAL:HG13	2.02	0.42
20:F:228:PRO:O	20:F:231:THR:HG23	2.19	0.42
23:V:295:ILE:O	23:V:298:ILE:HG22	2.20	0.42
24:W:70:VAL:O	24:W:73:MET:HG2	2.20	0.42
24:W:306:LEU:O	24:W:310:THR:HG22	2.20	0.42
24:W:455:LEU:HD12	24:W:456:GLN:N	2.35	0.42
25:X:264:PRO:C	25:X:266:ASP:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:409:LYS:HG3	30:c:268:GLU:HG3	2.02	0.42
27:Z:187:LEU:HA	27:Z:190:ARG:HG2	2.02	0.42
27:Z:199:LYS:HA	27:Z:202:ASN:ND2	2.35	0.42
27:Z:242:LEU:C	27:Z:244:GLU:H	2.28	0.42
29:b:25:ARG:CZ	29:b:144:GLY:HA2	2.50	0.42
29:b:164:ASP:H	29:b:165:GLY:HA2	1.81	0.42
1:f:23:GLU:HB3	1:f:24:PRO:HD3	2.02	0.41
2:G:11:ARG:O	2:G:24:GLN:NE2	2.35	0.41
3:H:103:GLU:OE2	11:P:86:THR:OG1	2.23	0.41
6:K:33:LEU:HB2	16:A:431:THR:HB	2.02	0.41
7:L:95:SER:HB3	7:L:103:LEU:HG	2.01	0.41
16:A:237:PHE:HA	16:A:270:CYS:SG	2.60	0.41
16:A:293:ASN:ND2	20:F:303:ASP:HB2	2.35	0.41
17:B:155:LYS:HA	17:B:156:VAL:HA	1.61	0.41
17:B:394:ASP:HA	21:C:311:ILE:HD13	2.02	0.41
20:F:275:ALA:HB1	20:F:326:VAL:HG21	2.02	0.41
20:F:397:LYS:HE3	20:F:397:LYS:HB3	1.95	0.41
21:C:192:PRO:HA	21:C:193:GLY:HA3	1.67	0.41
22:U:381:THR:HG22	22:U:412:HIS:HA	2.02	0.41
22:U:532:MET:HE3	22:U:552:ILE:HG22	2.02	0.41
24:W:417:ARG:HG3	24:W:420:ASP:OD1	2.21	0.41
26:Y:357:ASN:CB	26:Y:358:ARG:HA	2.47	0.41
27:Z:14:LEU:HG	30:c:39:LEU:HD22	2.01	0.41
29:b:30:GLN:HG3	29:b:75:LEU:HD13	2.02	0.41
32:e:6:GLN:N	32:e:7:PRO:HD2	2.35	0.41
1:f:73:TYR:HD2	1:f:74:LEU:HD12	1.84	0.41
1:f:397:ARG:HD3	1:f:679:ARG:HH21	1.85	0.41
2:G:101:TRP:CD2	2:G:105:TYR:HD2	2.37	0.41
11:P:67:LEU:HD21	11:P:87:LEU:HD11	2.02	0.41
16:A:100:LYS:HZ1	16:A:142:VAL:HB	1.86	0.41
16:A:316:LYS:HB3	16:A:316:LYS:HE3	1.84	0.41
16:A:325:ASP:HA	16:A:326:THR:HA	1.57	0.41
16:A:401:ARG:HH12	16:A:414:ASN:ND2	2.18	0.41
20:F:362:ARG:NH2	20:F:389:ASP:HA	2.35	0.41
21:C:331:ILE:HD13	21:C:334:ARG:HE	1.83	0.41
21:C:377:HIS:HB3	26:Y:174:TRP:CD1	2.56	0.41
23:V:277:PRO:HA	23:V:278:GLU:HA	1.74	0.41
24:W:59:ASP:HA	24:W:63:THR:HG23	2.02	0.41
24:W:135:LYS:CB	24:W:136:ILE:HB	2.50	0.41
24:W:155:GLN:HE21	24:W:161:GLU:HG3	1.85	0.41
24:W:428:TRP:O	24:W:432:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:14:ASN:HD21	26:Y:214:MET:HA	1.85	0.41
27:Z:225:GLN:NE2	27:Z:229:GLN:OE1	2.49	0.41
30:c:58:LEU:HB2	30:c:73:PHE:HE2	1.83	0.41
30:c:287:HIS:O	30:c:291:LEU:HG	2.19	0.41
1:f:61:ASP:O	1:f:62:ILE:HG22	2.20	0.41
1:f:336:GLU:HG3	1:f:337:ASP:H	1.85	0.41
1:f:544:ARG:NH1	1:f:579:ASN:OD1	2.54	0.41
2:G:12:HIS:HB3	8:M:13:THR:HG21	2.01	0.41
2:G:103:TYR:O	10:O:81:ARG:HG2	2.21	0.41
3:H:38:ILE:HD13	3:H:188:ILE:HA	2.01	0.41
5:J:36:ARG:HB3	5:J:144:LEU:HD23	2.03	0.41
5:J:43:LEU:HD23	5:J:134:VAL:HG11	2.02	0.41
12:Q:153:ARG:HH22	12:Q:184:ASP:HB3	1.85	0.41
16:A:204:LEU:HB3	16:A:205:GLY:HA3	2.02	0.41
16:A:429:TYR:HA	16:A:432:TYR:CZ	2.55	0.41
17:B:220:LYS:HB2	17:B:348:ASP:HB2	2.02	0.41
17:B:256:ILE:HG21	17:B:312:LEU:HD22	2.03	0.41
17:B:393:ALA:HB2	21:C:281:ASP:HB2	2.02	0.41
19:E:91:LYS:HD2	19:E:107:ILE:HB	2.02	0.41
21:C:379:THR:HG23	21:C:382:ASP:H	1.84	0.41
22:U:692:ALA:HB1	22:U:736:ILE:HB	2.03	0.41
23:V:296:LYS:HA	23:V:299:GLN:HB2	2.01	0.41
7:L:130:VAL:HG22	7:L:132:LEU:H	1.84	0.41
10:O:146:MET:HE3	10:O:150:GLU:HG2	2.03	0.41
14:S:211:ARG:NE	14:S:213:ASP:O	2.54	0.41
15:T:174:ARG:NH2	15:T:206:GLU:OE1	2.53	0.41
16:A:199:GLU:HA	20:F:408:LEU:HD22	2.02	0.41
16:A:206:ILE:HG13	20:F:373:MET:HB3	2.02	0.41
16:A:328:ASP:HB3	16:A:329:PRO:HD3	2.02	0.41
17:B:214:MET:HG3	17:B:216:ILE:HG12	2.02	0.41
17:B:283:PHE:HE2	17:B:285:ASP:HB2	1.84	0.41
19:E:251:ARG:NH1	19:E:255:ARG:HD3	2.36	0.41
22:U:34:PHE:O	22:U:38:ILE:HG12	2.21	0.41
23:V:25:GLU:O	23:V:28:PRO:HD2	2.19	0.41
23:V:179:LYS:HZ2	23:V:217:VAL:HG21	1.86	0.41
24:W:314:LEU:HB2	28:a:309:LEU:HD11	2.02	0.41
27:Z:205:LEU:HA	27:Z:208:ILE:HG22	2.02	0.41
30:c:226:MET:C	30:c:228:GLY:H	2.26	0.41
31:d:171:LEU:O	31:d:175:ARG:HG2	2.20	0.41
1:f:638:LEU:HA	1:f:639:THR:C	2.45	0.41
2:G:91:VAL:HG12	2:G:95:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:50:LYS:HD2	7:L:208:LYS:O	2.21	0.41
9:N:7:GLN:HA	9:N:12:VAL:HA	2.03	0.41
13:R:67:GLU:O	13:R:71:LYS:N	2.53	0.41
16:A:312:ARG:HA	16:A:313:GLY:HA2	1.58	0.41
16:A:321:THR:OG1	16:A:322:ASN:N	2.54	0.41
17:B:139:VAL:HB	17:B:141:LYS:H	1.85	0.41
17:B:139:VAL:HB	17:B:141:LYS:N	2.35	0.41
17:B:238:ALA:O	17:B:242:GLN:HG3	2.20	0.41
17:B:283:PHE:CE2	17:B:285:ASP:HB2	2.55	0.41
17:B:433:GLY:O	17:B:434:THR:OG1	2.34	0.41
18:D:373:ALA:HB1	18:D:375:ILE:HB	2.03	0.41
19:E:60:VAL:O	19:E:95:GLY:HA2	2.20	0.41
21:C:115:ALA:HB3	21:C:125:LYS:H	1.85	0.41
23:V:326:GLN:NE2	23:V:350:GLN:HE21	2.18	0.41
24:W:423:ASN:N	24:W:423:ASN:OD1	2.53	0.41
26:Y:40:GLU:O	26:Y:44:ALA:N	2.54	0.41
27:Z:196:HIS:NE2	30:c:308:VAL:HG22	2.34	0.41
27:Z:222:ILE:HG23	27:Z:223:ASN:C	2.46	0.41
2:G:61:LEU:HA	8:M:160:TYR:CD1	2.56	0.41
9:N:20:THR:HB	9:N:28:ASN:HB3	2.03	0.41
10:O:94:ILE:HA	11:P:99:ARG:HH21	1.85	0.41
19:E:101:ASP:N	19:E:106:THR:O	2.54	0.41
21:C:84:LYS:HZ1	21:C:98:ASP:N	2.18	0.41
21:C:298:ILE:C	21:C:300:ILE:H	2.29	0.41
22:U:342:LEU:HD13	22:U:378:CYS:O	2.21	0.41
22:U:697:GLN:HG3	22:U:745:THR:HB	2.03	0.41
23:V:318:GLN:O	23:V:319:HIS:CG	2.74	0.41
23:V:430:SER:OG	23:V:433:ASP:OD1	2.37	0.41
24:W:310:THR:C	24:W:312:MET:H	2.27	0.41
27:Z:196:HIS:HE1	30:c:307:VAL:HG12	1.85	0.41
28:a:286:ALA:HB1	28:a:287:ASN:CA	2.47	0.41
28:a:351:ASP:O	28:a:355:PHE:HB2	2.20	0.41
30:c:150:SER:OG	30:c:154:LYS:HB3	2.21	0.41
1:f:282:LYS:HE2	1:f:289:CYS:HB2	2.03	0.41
3:H:4:ARG:HA	3:H:13:PHE:CG	2.55	0.41
7:L:137:TYR:CZ	7:L:142:PRO:HB3	2.56	0.41
7:L:212:ILE:HD13	7:L:229:VAL:HG13	2.03	0.41
12:Q:52:ASP:OD1	13:R:88:TYR:OH	2.22	0.41
13:R:178:HIS:O	13:R:185:ILE:N	2.51	0.41
18:D:296:MET:HA	18:D:299:PHE:CD2	2.56	0.41
21:C:151:ILE:HG21	21:C:154:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:403:THR:HG23	22:U:777:HIS:HE2	1.85	0.41
23:V:344:ASP:HB2	23:V:368:ARG:HH11	1.86	0.41
24:W:375:MET:N	24:W:411:GLY:O	2.47	0.41
24:W:397:VAL:HG11	25:X:342:PHE:HD2	1.84	0.41
24:W:402:ILE:HG23	24:W:416:GLN:HE22	1.85	0.41
28:a:287:ASN:HA	28:a:288:HIS:C	2.45	0.41
6:K:85:ALA:O	6:K:89:ILE:HG12	2.20	0.41
16:A:250:VAL:HB	16:A:297:ARG:NH2	2.36	0.41
16:A:396:ALA:HA	16:A:401:ARG:HG3	2.01	0.41
20:F:145:LEU:HG	20:F:146:LYS:H	1.84	0.41
20:F:224:LEU:HB3	20:F:351:LYS:HG2	2.02	0.41
25:X:339:ILE:HG21	25:X:374:PHE:HE1	1.86	0.41
28:a:100:THR:HA	28:a:103:LYS:HE2	2.02	0.41
30:c:285:GLU:HB3	30:c:286:GLU:HA	2.02	0.41
1:f:83:GLU:HB3	1:f:84:PRO:HD3	2.02	0.41
1:f:194:LEU:HD23	1:f:199:PHE:HB3	2.03	0.41
3:H:26:LEU:O	21:C:399:MET:HE2	2.20	0.41
4:I:122:THR:HG22	4:I:129:PRO:HB3	2.03	0.41
7:L:69:HIS:HD1	7:L:137:TYR:H	1.69	0.41
10:O:21:THR:HG22	10:O:26:VAL:HA	2.03	0.41
14:S:193:LEU:N	14:S:208:VAL:O	2.49	0.41
16:A:187:LEU:O	16:A:191:VAL:HG12	2.21	0.41
16:A:188:ARG:HG3	16:A:192:GLU:HB2	2.03	0.41
17:B:364:ILE:HG21	17:B:392:GLY:HA3	2.02	0.41
18:D:48:GLN:HA	18:D:51:LEU:HB3	2.03	0.41
18:D:115:ILE:HA	18:D:139:LEU:HB2	2.02	0.41
18:D:268:ASP:OD1	18:D:268:ASP:N	2.54	0.41
18:D:293:LEU:O	18:D:296:MET:HG2	2.20	0.41
18:D:313:ARG:NH2	18:D:315:ASP:OD2	2.40	0.41
18:D:344:ILE:HA	18:D:347:THR:HG22	2.03	0.41
21:C:139:MET:O	21:C:143:VAL:HG12	2.21	0.41
21:C:165:ILE:HD12	21:C:207:THR:HG23	2.03	0.41
21:C:176:GLU:C	21:C:179:GLY:H	2.28	0.41
21:C:188:LEU:O	21:C:295:THR:OG1	2.35	0.41
22:U:374:SER:HB2	22:U:410:VAL:HB	2.01	0.41
22:U:413:LYS:HA	22:U:449:ILE:HG12	2.03	0.41
22:U:684:ARG:O	22:U:688:LEU:HG	2.21	0.41
23:V:70:VAL:O	23:V:74:ASP:N	2.46	0.41
23:V:298:ILE:HD12	23:V:298:ILE:HA	1.96	0.41
23:V:318:GLN:O	23:V:319:HIS:ND1	2.54	0.41
24:W:455:LEU:HD12	24:W:456:GLN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:17:LEU:HD13	30:c:39:LEU:HD11	2.03	0.41
28:a:238:TYR:HA	28:a:241:ASN:HB3	2.02	0.41
29:b:116:PRO:HA	29:b:146:GLU:HG3	2.03	0.41
30:c:253:LYS:HA	30:c:256:ASN:HB2	2.03	0.41
31:d:56:GLU:HA	31:d:78:LEU:HD11	2.01	0.41
32:e:64:GLY:HA2	32:e:67:MET:HE3	2.03	0.41
2:G:32:ILE:HG12	2:G:137:CYS:HB2	2.03	0.41
3:H:14:SER:HA	3:H:20:VAL:HG23	2.03	0.41
6:K:73:HIS:HA	6:K:226:PHE:CZ	2.55	0.41
6:K:178:GLN:OE1	6:K:182:GLN:NE2	2.54	0.41
6:K:227:HIS:N	6:K:228:MET:HB3	2.36	0.41
13:R:113:TYR:O	13:R:120:ARG:HA	2.21	0.41
18:D:150:SER:OG	18:D:151:ILE:N	2.54	0.41
19:E:100:LEU:HD23	19:E:107:ILE:HG13	2.02	0.41
21:C:234:LEU:HD21	21:C:246:ILE:HG21	2.03	0.41
22:U:631:GLU:O	22:U:634:PRO:HD2	2.21	0.41
24:W:205:ILE:O	24:W:209:ILE:HG12	2.21	0.41
25:X:399:ALA:HB2	30:c:257:LYS:HE3	2.01	0.41
27:Z:34:ARG:HB2	27:Z:97:THR:HG22	2.02	0.41
27:Z:227:ILE:HD13	27:Z:227:ILE:HA	1.96	0.41
29:b:84:ILE:HD11	29:b:113:VAL:HG13	2.02	0.41
1:f:653:GLY:O	1:f:656:HIS:NE2	2.54	0.40
3:H:111:VAL:HG21	3:H:147:PHE:HD2	1.86	0.40
9:N:21:THR:HG22	9:N:26:ILE:HA	2.02	0.40
9:N:50:ALA:N	10:O:118:SER:HB3	2.36	0.40
11:P:25:ASP:HA	11:P:185:VAL:HA	2.03	0.40
12:Q:18:ASP:HA	12:Q:178:PHE:HD1	1.86	0.40
19:E:135:ILE:H	19:E:135:ILE:HG13	1.70	0.40
21:C:87:VAL:O	21:C:95:PHE:N	2.49	0.40
22:U:229:VAL:HG21	22:U:252:LEU:HD22	2.03	0.40
24:W:75:TYR:HD1	24:W:78:LYS:HE2	1.86	0.40
24:W:135:LYS:HB3	24:W:137:TYR:N	2.37	0.40
1:f:193:HIS:HA	1:f:194:LEU:C	2.46	0.40
1:f:660:TYR:HB3	1:f:663:VAL:HG23	2.03	0.40
4:I:119:GLN:HE22	5:J:79:ASP:HA	1.86	0.40
13:R:40:TYR:CD2	13:R:41:LEU:HG	2.56	0.40
17:B:191:ASP:OD1	17:B:191:ASP:N	2.53	0.40
17:B:234:LEU:HD21	17:B:353:PHE:HB2	2.01	0.40
17:B:418:ASP:O	17:B:422:SER:N	2.50	0.40
22:U:574:LYS:H	22:U:574:LYS:HG2	1.66	0.40
22:U:583:MET:HA	22:U:586:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:224:LEU:HD12	23:V:224:LEU:O	2.21	0.40
26:Y:355:GLU:HG3	26:Y:357:ASN:ND2	2.36	0.40
27:Z:199:LYS:HA	27:Z:202:ASN:HD21	1.86	0.40
30:c:145:VAL:HA	30:c:157:ILE:HA	2.03	0.40
30:c:151:VAL:HG13	30:c:152:LYS:H	1.86	0.40
1:f:339:LEU:HD12	1:f:340:THR:N	2.37	0.40
2:G:74:GLU:HB3	2:G:226:LYS:HG3	2.03	0.40
5:J:76:LEU:HD13	5:J:78:ALA:HB3	2.02	0.40
6:K:211:ASN:OD1	6:K:214:ASN:N	2.55	0.40
9:N:21:THR:HA	9:N:27:ALA:H	1.87	0.40
17:B:390:LEU:HD12	17:B:390:LEU:HA	1.81	0.40
18:D:389:GLU:HB3	18:D:391:ARG:H	1.86	0.40
21:C:327:ASP:OD1	21:C:328:ILE:N	2.55	0.40
22:U:742:HIS:O	22:U:883:ARG:NH2	2.55	0.40
24:W:365:ILE:HG13	24:W:366:MET:N	2.36	0.40
26:Y:367:GLN:HG3	26:Y:371:LYS:HG2	2.03	0.40
27:Z:176:LEU:C	27:Z:178:ASP:H	2.29	0.40
29:b:18:ASN:OD1	29:b:25:ARG:NE	2.54	0.40
29:b:94:HIS:CD2	29:b:136:VAL:HG21	2.57	0.40
29:b:142:ASN:HD21	29:b:170:LEU:HD21	1.85	0.40
2:G:80:MET:HG3	2:G:87:SER:HB2	2.04	0.40
3:H:171:LYS:HD2	3:H:171:LYS:HA	1.94	0.40
4:I:68:LEU:HD22	4:I:90:LEU:HD22	2.02	0.40
6:K:152:GLN:OE1	6:K:164:GLN:NE2	2.55	0.40
8:M:110:HIS:HE2	9:N:72:GLU:CD	2.29	0.40
11:P:135:ASP:OD2	11:P:154:TRP:NE1	2.48	0.40
14:S:136:LYS:HD3	14:S:136:LYS:HA	1.96	0.40
16:A:327:LEU:O	16:A:331:LEU:HG	2.21	0.40
17:B:151:LEU:HD21	21:C:82:LYS:HE2	2.03	0.40
17:B:170:LEU:O	17:B:173:VAL:HG22	2.21	0.40
17:B:175:LYS:HA	17:B:176:VAL:HA	1.87	0.40
17:B:194:ILE:HG13	17:B:237:LYS:HD3	2.03	0.40
18:D:377:SER:HB3	19:E:292:PRO:HB2	2.02	0.40
19:E:55:GLN:HB3	19:E:100:LEU:O	2.20	0.40
19:E:101:ASP:O	19:E:105:LEU:HA	2.21	0.40
19:E:266:GLY:C	19:E:268:ASP:H	2.30	0.40
22:U:669:ILE:HG12	22:U:694:ILE:HG21	2.02	0.40
24:W:8:ARG:HD2	24:W:34:LEU:HD21	2.02	0.40
24:W:187:LEU:HA	24:W:190:MET:HE3	2.02	0.40
24:W:405:LYS:HG3	25:X:344:ARG:HG2	2.04	0.40
27:Z:69:PHE:CE2	29:b:60:VAL:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:208:SER:HA	1:f:209:ALA:HA	1.76	0.40
2:G:10:ASP:HB3	2:G:15:ILE:HD11	2.03	0.40
3:H:86:LEU:HA	3:H:89:ARG:HB3	2.03	0.40
6:K:125:GLU:O	6:K:134:SER:N	2.54	0.40
6:K:226:PHE:HA	6:K:227:HIS:C	2.47	0.40
7:L:205:LEU:N	7:L:209:ASN:HD21	2.18	0.40
9:N:26:ILE:HG21	9:N:29:ARG:HD3	2.03	0.40
13:R:54:PHE:O	13:R:58:LEU:N	2.47	0.40
16:A:108:ASP:HB2	16:A:109:PRO:HD3	2.04	0.40
17:B:220:LYS:HA	17:B:346:ARG:NH2	2.37	0.40
17:B:224:LEU:HD13	17:B:234:LEU:HB3	2.03	0.40
17:B:401:GLU:HA	17:B:404:LEU:HB3	2.03	0.40
19:E:87:LEU:H	19:E:87:LEU:HG	1.73	0.40
20:F:89:LEU:HD11	20:F:126:THR:HB	2.04	0.40
20:F:227:GLY:HA3	20:F:231:THR:HG21	2.02	0.40
22:U:32:ASN:ND2	23:V:229:SER:OG	2.55	0.40
23:V:342:ILE:HG12	23:V:343:PRO:O	2.22	0.40
26:Y:145:LEU:HD13	26:Y:183:TYR:CD1	2.56	0.40
26:Y:301:ILE:HG13	26:Y:343:LEU:HD12	2.04	0.40
27:Z:118:ASN:OD1	27:Z:118:ASN:N	2.55	0.40
27:Z:223:ASN:HD22	27:Z:227:ILE:HG12	1.86	0.40
28:a:220:PRO:HA	28:a:223:GLU:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	686/749 (92%)	575 (84%)	107 (16%)	4 (1%)	21	59
2	G	238/245 (97%)	221 (93%)	15 (6%)	2 (1%)	16	54
3	H	230/233 (99%)	200 (87%)	28 (12%)	2 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
5	J	237/247 (96%)	214 (90%)	21 (9%)	2 (1%)	16	54
6	K	224/240 (93%)	196 (88%)	27 (12%)	1 (0%)	30	67
7	L	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
8	M	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
9	N	189/238 (79%)	179 (95%)	10 (5%)	0	100	100
10	O	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
11	P	202/204 (99%)	187 (93%)	15 (7%)	0	100	100
12	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
13	R	199/262 (76%)	185 (93%)	14 (7%)	0	100	100
14	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
15	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
16	A	359/433 (83%)	307 (86%)	51 (14%)	1 (0%)	36	72
17	B	344/440 (78%)	304 (88%)	38 (11%)	2 (1%)	21	59
18	D	378/418 (90%)	323 (85%)	51 (14%)	4 (1%)	11	46
19	E	351/403 (87%)	317 (90%)	34 (10%)	0	100	100
20	F	362/439 (82%)	327 (90%)	34 (9%)	1 (0%)	36	72
21	C	390/398 (98%)	344 (88%)	42 (11%)	4 (1%)	12	49
22	U	798/953 (84%)	738 (92%)	59 (7%)	1 (0%)	48	83
23	V	478/533 (90%)	421 (88%)	57 (12%)	0	100	100
24	W	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	18	56
25	X	239/422 (57%)	213 (89%)	26 (11%)	0	100	100
26	Y	376/389 (97%)	332 (88%)	42 (11%)	2 (0%)	24	63
27	Z	284/324 (88%)	253 (89%)	30 (11%)	1 (0%)	30	67
28	a	371/376 (99%)	331 (89%)	38 (10%)	2 (0%)	24	63
29	b	189/377 (50%)	175 (93%)	14 (7%)	0	100	100
30	c	274/309 (89%)	246 (90%)	25 (9%)	3 (1%)	11	46
31	d	255/349 (73%)	229 (90%)	26 (10%)	0	100	100
32	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
All	All	9704/11269 (86%)	8711 (90%)	958 (10%)	35 (0%)	31	67

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	62	ILE
1	f	447	VAL
2	G	111	VAL
22	U	364	VAL
24	W	68	VAL
24	W	136	ILE
26	Y	350	VAL
1	f	131	VAL
30	c	157	ILE
1	f	281	ILE
5	J	199	VAL
21	C	298	ILE
28	a	340	VAL
3	H	127	VAL
6	K	12	VAL
18	D	151	ILE
21	C	68	GLU
21	C	219	LEU
24	W	138	VAL
26	Y	67	VAL
27	Z	144	VAL
30	c	156	VAL
17	B	218	PRO
18	D	411	GLU
18	D	406	VAL
18	D	259	PRO
28	a	336	VAL
30	c	189	ILE
2	G	170	VAL
3	H	20	VAL
21	C	251	ILE
16	A	206	ILE
17	B	325	VAL
20	F	326	VAL
5	J	98	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	582/628 (93%)	569 (98%)	13 (2%)	45	64
2	G	193/209 (92%)	189 (98%)	4 (2%)	47	65
3	H	164/190 (86%)	161 (98%)	3 (2%)	51	68
4	I	193/220 (88%)	190 (98%)	3 (2%)	55	70
5	J	152/210 (72%)	152 (100%)	0	100	100
6	K	186/202 (92%)	184 (99%)	2 (1%)	65	76
7	L	198/229 (86%)	196 (99%)	2 (1%)	68	78
8	M	192/211 (91%)	191 (100%)	1 (0%)	81	83
9	N	148/180 (82%)	148 (100%)	0	100	100
10	O	177/227 (78%)	177 (100%)	0	100	100
11	P	172/173 (99%)	170 (99%)	2 (1%)	63	75
12	Q	164/171 (96%)	162 (99%)	2 (1%)	63	75
13	R	153/201 (76%)	152 (99%)	1 (1%)	76	81
14	S	174/198 (88%)	173 (99%)	1 (1%)	78	83
15	T	175/214 (82%)	175 (100%)	0	100	100
16	A	308/372 (83%)	299 (97%)	9 (3%)	37	58
17	B	304/385 (79%)	295 (97%)	9 (3%)	36	57
18	D	333/366 (91%)	325 (98%)	8 (2%)	43	64
19	E	308/353 (87%)	297 (96%)	11 (4%)	31	52
20	F	312/379 (82%)	305 (98%)	7 (2%)	45	64
21	C	340/346 (98%)	334 (98%)	6 (2%)	51	68
22	U	685/816 (84%)	681 (99%)	4 (1%)	78	83
23	V	414/459 (90%)	408 (99%)	6 (1%)	59	72
24	W	416/416 (100%)	408 (98%)	8 (2%)	50	67
25	X	208/362 (58%)	207 (100%)	1 (0%)	81	83
26	Y	334/344 (97%)	330 (99%)	4 (1%)	63	75
27	Z	257/295 (87%)	253 (98%)	4 (2%)	55	70
28	a	333/336 (99%)	322 (97%)	11 (3%)	33	55
29	b	167/312 (54%)	166 (99%)	1 (1%)	78	83
30	c	243/267 (91%)	233 (96%)	10 (4%)	27	49
31	d	231/293 (79%)	225 (97%)	6 (3%)	40	62
32	e	38/63 (60%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8254/9627 (86%)	8115 (98%)	139 (2%)	52 69

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	15	ASP
1	f	29	VAL
1	f	33	VAL
1	f	129	VAL
1	f	301	ASP
1	f	334	ASN
1	f	339	LEU
1	f	342	LEU
1	f	371	CYS
1	f	391	LEU
1	f	526	THR
1	f	659	LEU
1	f	663	VAL
2	G	22	LEU
2	G	111	VAL
2	G	159	TYR
2	G	220	VAL
3	H	69	THR
3	H	182	LEU
3	H	208	ILE
4	I	34	CYS
4	I	107	CYS
4	I	232	GLU
6	K	36	THR
6	K	42	THR
7	L	46	LEU
7	L	197	GLU
8	M	179	LEU
11	P	20	VAL
11	P	189	ILE
12	Q	47	VAL
12	Q	142	ILE
13	R	13	ILE
14	S	164	VAL
16	A	94	GLN
16	A	102	ILE
16	A	125	LEU

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Mol	Chain	Res	Type
16	A	153	LEU
16	A	316	LYS
16	A	317	VAL
16	A	318	LEU
16	A	331	LEU
16	A	403	ILE
17	B	105	THR
17	B	135	ILE
17	B	156	VAL
17	B	190	LEU
17	B	235	LEU
17	B	316	LEU
17	B	348	ASP
17	B	355	LEU
17	B	436	GLU
18	D	61	ILE
18	D	82	ILE
18	D	186	THR
18	D	234	GLU
18	D	273	LYS
18	D	303	VAL
18	D	354	LEU
18	D	394	VAL
19	E	65	THR
19	E	87	LEU
19	E	104	THR
19	E	135	ILE
19	E	138	LEU
19	E	265	ASP
19	E	269	THR
19	E	273	VAL
19	E	315	ILE
19	E	326	ILE
19	E	358	ASP
20	F	73	ILE
20	F	99	VAL
20	F	153	VAL
20	F	161	LEU
20	F	166	THR
20	F	270	ASP
20	F	427	VAL
21	C	99	VAL

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Mol	Chain	Res	Type
21	C	109	THR
21	C	219	LEU
21	C	280	LEU
21	C	298	ILE
21	C	311	ILE
22	U	336	GLU
22	U	479	LEU
22	U	497	LEU
22	U	554	LEU
23	V	101	LEU
23	V	221	LEU
23	V	224	LEU
23	V	255	LEU
23	V	320	THR
23	V	322	VAL
24	W	250	ILE
24	W	333	LEU
24	W	371	THR
24	W	373	ILE
24	W	420	ASP
24	W	424	LEU
24	W	444	HIS
24	W	455	LEU
25	X	331	LEU
26	Y	114	ILE
26	Y	134	LEU
26	Y	315	THR
26	Y	350	VAL
27	Z	91	ILE
27	Z	120	VAL
27	Z	176	LEU
27	Z	186	THR
28	a	28	LEU
28	a	33	LEU
28	a	125	ILE
28	a	158	LEU
28	a	185	ILE
28	a	195	GLU
28	a	210	VAL
28	a	234	ILE
28	a	245	VAL
28	a	296	ILE

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Mol	Chain	Res	Type
28	a	340	VAL
29	b	173	VAL
30	c	25	VAL
30	c	36	LEU
30	c	42	LEU
30	c	62	VAL
30	c	69	VAL
30	c	151	VAL
30	c	178	THR
30	c	229	LEU
30	c	275	VAL
30	c	309	PHE
31	d	158	ILE
31	d	178	ILE
31	d	190	LEU
31	d	193	GLU
31	d	216	VAL
31	d	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	246	HIS
1	f	269	GLN
1	f	491	GLN
1	f	565	ASN
1	f	611	HIS
2	G	100	ASN
3	H	71	HIS
3	H	102	GLN
4	I	95	GLN
4	I	102	GLN
4	I	109	GLN
4	I	119	GLN
5	J	175	ASN
6	K	13	ASN
6	K	23	GLN
6	K	41	GLN
6	K	164	GLN
6	K	182	GLN
7	L	31	GLN
7	L	68	ASN

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Mol	Chain	Res	Type
7	L	166	GLN
7	L	190	HIS
8	M	32	ASN
9	N	158	ASN
9	N	187	GLN
10	O	57	GLN
10	O	116	HIS
11	P	33	GLN
11	P	81	GLN
11	P	188	HIS
12	Q	8	GLN
12	Q	99	HIS
13	R	29	GLN
13	R	85	ASN
13	R	162	GLN
14	S	36	HIS
14	S	159	GLN
14	S	163	HIS
15	T	2	GLN
15	T	69	GLN
16	A	231	ASN
16	A	414	ASN
17	B	120	HIS
17	B	153	ASN
17	B	157	HIS
17	B	366	GLN
18	D	286	GLN
18	D	302	ASN
18	D	376	ASN
19	E	190	GLN
19	E	226	GLN
19	E	307	GLN
20	F	116	GLN
20	F	194	GLN
20	F	255	GLN
20	F	380	ASN
21	C	50	ASN
21	C	69	GLN
21	C	270	GLN
21	C	278	ASN
21	C	288	ASN
22	U	111	GLN

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Mol	Chain	Res	Type
22	U	189	GLN
22	U	267	ASN
22	U	355	ASN
22	U	377	HIS
22	U	389	ASN
22	U	421	GLN
22	U	452	ASN
22	U	467	ASN
22	U	491	GLN
22	U	698	GLN
22	U	756	HIS
22	U	805	ASN
22	U	901	GLN
23	V	62	HIS
23	V	146	GLN
23	V	299	GLN
23	V	318	GLN
23	V	326	GLN
23	V	400	HIS
23	V	427	GLN
23	V	459	GLN
23	V	477	HIS
23	V	487	HIS
24	W	155	GLN
24	W	235	GLN
24	W	362	ASN
24	W	430	GLN
25	X	207	GLN
25	X	406	ASN
26	Y	77	ASN
26	Y	136	HIS
26	Y	251	HIS
26	Y	367	GLN
27	Z	44	GLN
27	Z	77	ASN
27	Z	102	HIS
27	Z	223	ASN
27	Z	224	HIS
27	Z	243	GLN
27	Z	256	GLN
28	a	23	HIS
28	a	164	GLN

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Mol	Chain	Res	Type
28	a	227	ASN
28	a	257	GLN
28	a	273	GLN
28	a	287	ASN
28	a	337	GLN
29	b	76	HIS
29	b	149	ASN
30	c	92	GLN
30	c	190	GLN
30	c	221	HIS
31	d	34	ASN
32	e	6	GLN
32	e	63	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
33	ATP	E	401	-	32,33,33	1.42	5 (15%)	48,52,52	1.77	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	ATP	D	501	-	32,33,33	1.40	4 (12%)	48,52,52	1.76	10 (20%)
33	ATP	A	501	-	32,33,33	1.41	4 (12%)	48,52,52	1.74	10 (20%)
33	ATP	F	501	-	32,33,33	1.40	4 (12%)	48,52,52	1.76	10 (20%)

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
33	ATP	E	401	-	-	2/22/38/38	0/3/3/3
33	ATP	D	501	-	-	3/22/38/38	0/3/3/3
33	ATP	A	501	-	-	1/22/38/38	0/3/3/3
33	ATP	F	501	-	-	4/22/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	F	501	ATP	C5-C4	4.75	1.47	1.39
33	E	401	ATP	C5-C4	4.74	1.47	1.39
33	A	501	ATP	C5-C4	4.70	1.47	1.39
33	D	501	ATP	C5-C4	4.67	1.47	1.39
33	D	501	ATP	C5-C6	2.78	1.48	1.41
33	A	501	ATP	C5-C6	2.77	1.48	1.41
33	F	501	ATP	C5-C6	2.75	1.48	1.41
33	E	401	ATP	C5-C6	2.66	1.48	1.41
33	D	501	ATP	C8-N7	2.44	1.36	1.31
33	A	501	ATP	C8-N7	2.40	1.36	1.31
33	F	501	ATP	C8-N7	2.40	1.36	1.31
33	E	401	ATP	C5-N7	-2.29	1.34	1.39
33	E	401	ATP	C8-N7	2.26	1.36	1.31
33	F	501	ATP	C5-N7	-2.23	1.35	1.39
33	A	501	ATP	C5-N7	-2.19	1.35	1.39
33	D	501	ATP	C5-N7	-2.18	1.35	1.39
33	E	401	ATP	PB-O3A	2.03	1.61	1.59

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	E	401	ATP	C5-C4-N3	-5.90	118.59	126.72
33	D	501	ATP	C5-C4-N3	-5.89	118.60	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	F	501	ATP	C5-C4-N3	-5.80	118.74	126.72
33	A	501	ATP	C5-C4-N3	-5.71	118.86	126.72
33	E	401	ATP	N3-C4-N9	4.78	135.30	127.17
33	D	501	ATP	N3-C4-N9	4.56	134.92	127.17
33	F	501	ATP	N3-C4-N9	4.56	134.92	127.17
33	A	501	ATP	N3-C4-N9	4.43	134.70	127.17
33	D	501	ATP	C2-N3-C4	3.80	121.11	111.83
33	F	501	ATP	C2-N3-C4	3.70	120.86	111.83
33	E	401	ATP	C2-N3-C4	3.69	120.84	111.83
33	A	501	ATP	C2-N3-C4	3.66	120.78	111.83
33	A	501	ATP	C4-C5-N7	-3.60	106.46	110.58
33	D	501	ATP	C4-C5-N7	-3.56	106.52	110.58
33	F	501	ATP	C4-C5-N7	-3.54	106.54	110.58
33	E	401	ATP	C4-C5-N7	-3.35	106.75	110.58
33	D	501	ATP	N3-C2-N1	-3.32	123.56	128.58
33	F	501	ATP	N3-C2-N1	-3.26	123.65	128.58
33	A	501	ATP	N3-C2-N1	-3.22	123.71	128.58
33	E	401	ATP	N3-C2-N1	-3.18	123.77	128.58
33	E	401	ATP	C4-N9-C8	2.69	108.56	105.74
33	A	501	ATP	C4-N9-C8	2.69	108.56	105.74
33	F	501	ATP	C4-N9-C8	2.67	108.54	105.74
33	E	401	ATP	C3'-C2'-C1'	2.61	106.41	101.46
33	A	501	ATP	C5-N7-C8	2.58	107.51	103.45
33	D	501	ATP	C5-N7-C8	2.58	107.50	103.45
33	F	501	ATP	C5-N7-C8	2.57	107.49	103.45
33	D	501	ATP	C4-N9-C8	2.54	108.41	105.74
33	E	401	ATP	C5-N7-C8	2.50	107.38	103.45
33	D	501	ATP	O4'-C1'-N9	2.33	112.57	108.09
33	F	501	ATP	C3'-C2'-C1'	2.27	105.75	101.46
33	D	501	ATP	C6-C5-N7	2.21	136.36	132.09
33	A	501	ATP	C6-C5-N7	2.21	136.35	132.09
33	A	501	ATP	C3'-C2'-C1'	2.13	105.49	101.46
33	F	501	ATP	C6-C5-N7	2.13	136.19	132.09
33	D	501	ATP	C3'-C2'-C1'	2.09	105.42	101.46
33	A	501	ATP	N9-C8-N7	-2.05	111.03	113.94
33	F	501	ATP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	F	501	ATP	C5'-O5'-PA-O1A

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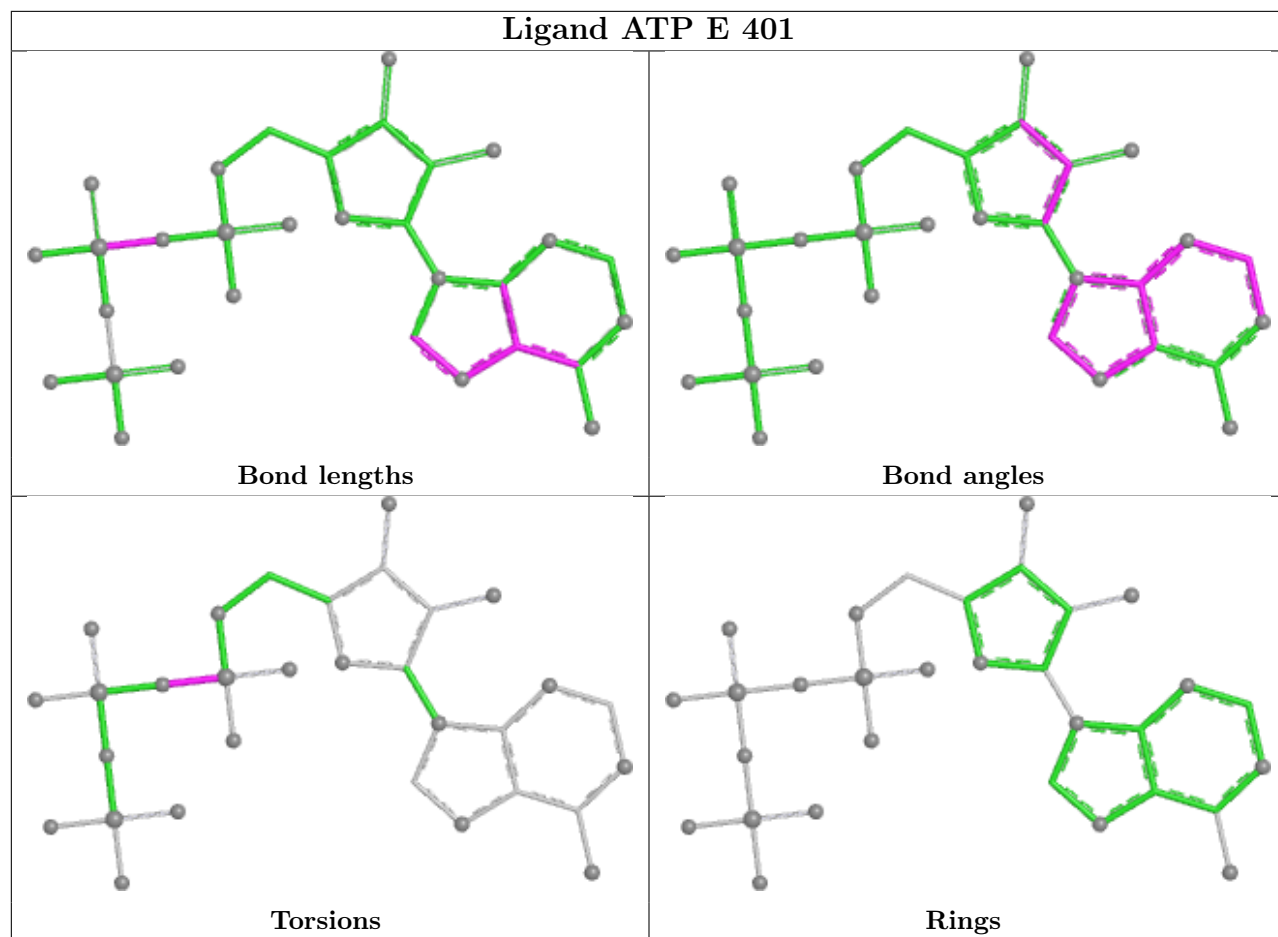
Mol	Chain	Res	Type	Atoms
33	F	501	ATP	C5'-O5'-PA-O3A
33	F	501	ATP	O4'-C4'-C5'-O5'
33	E	401	ATP	PB-O3A-PA-O1A
33	F	501	ATP	C3'-C4'-C5'-O5'
33	A	501	ATP	C5'-O5'-PA-O1A
33	D	501	ATP	C3'-C4'-C5'-O5'
33	D	501	ATP	O4'-C4'-C5'-O5'
33	E	401	ATP	PB-O3A-PA-O2A
33	D	501	ATP	C2'-C1'-N9-C8

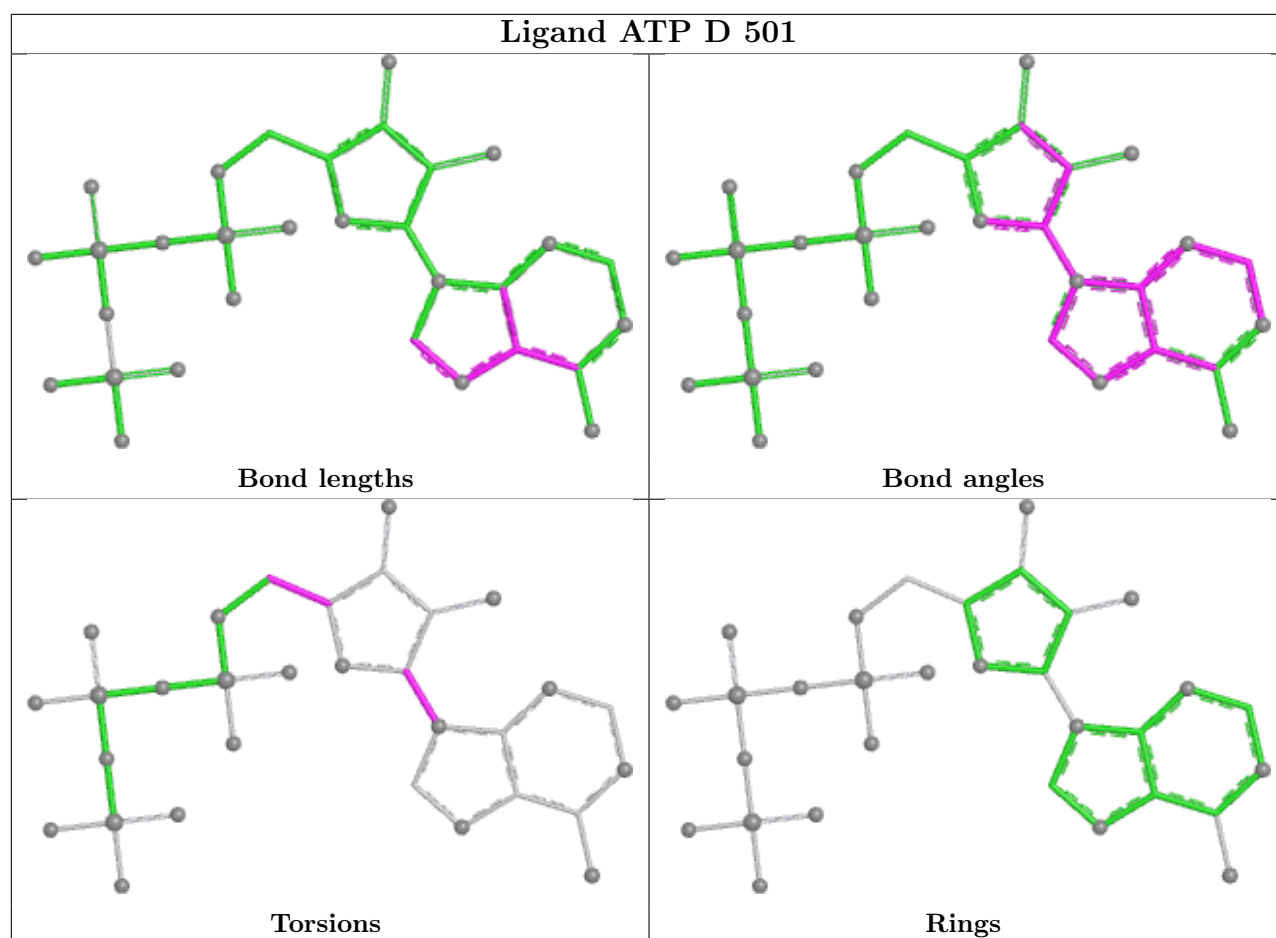
There are no ring outliers.

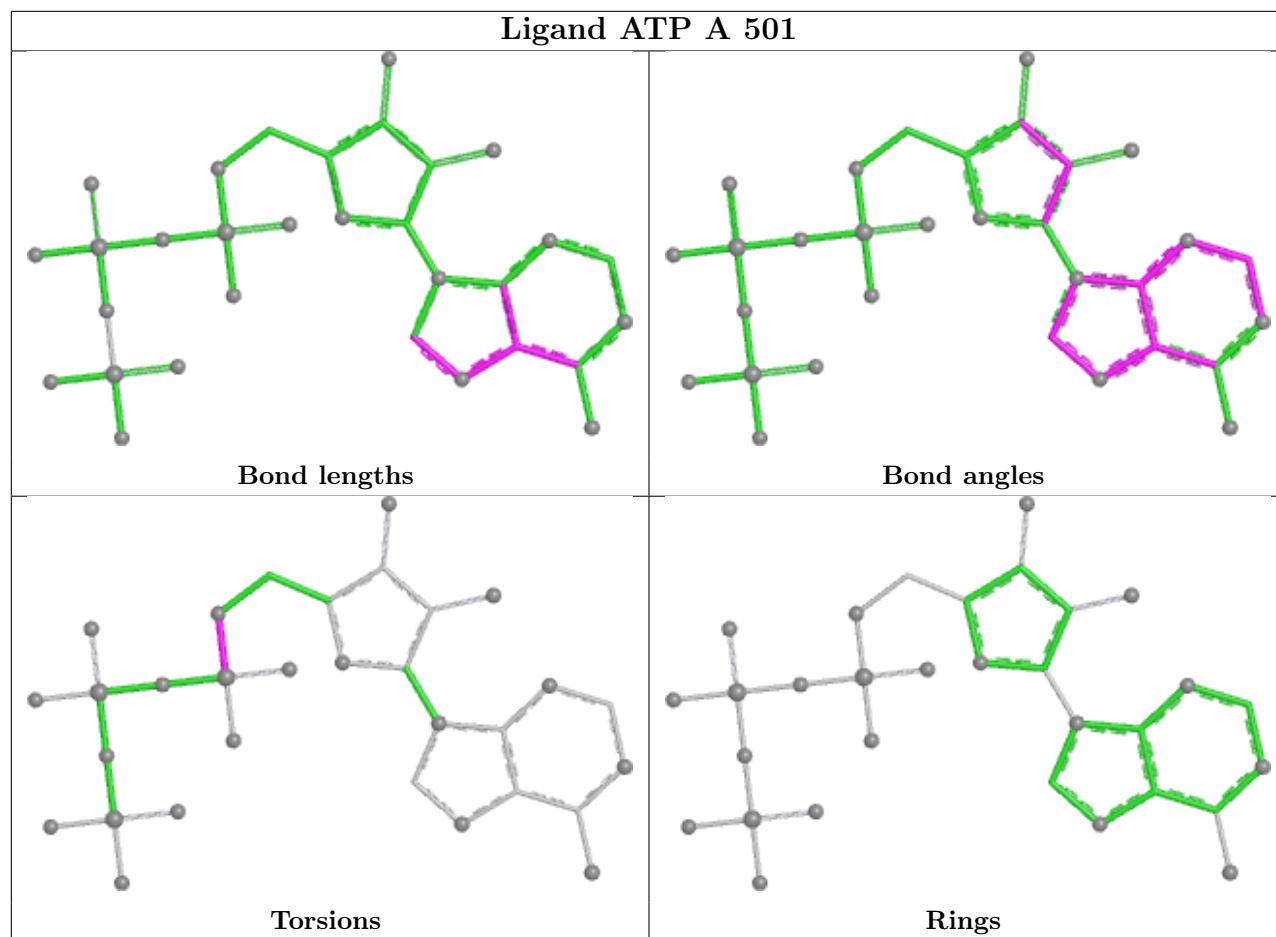
4 monomers are involved in 7 short contacts:

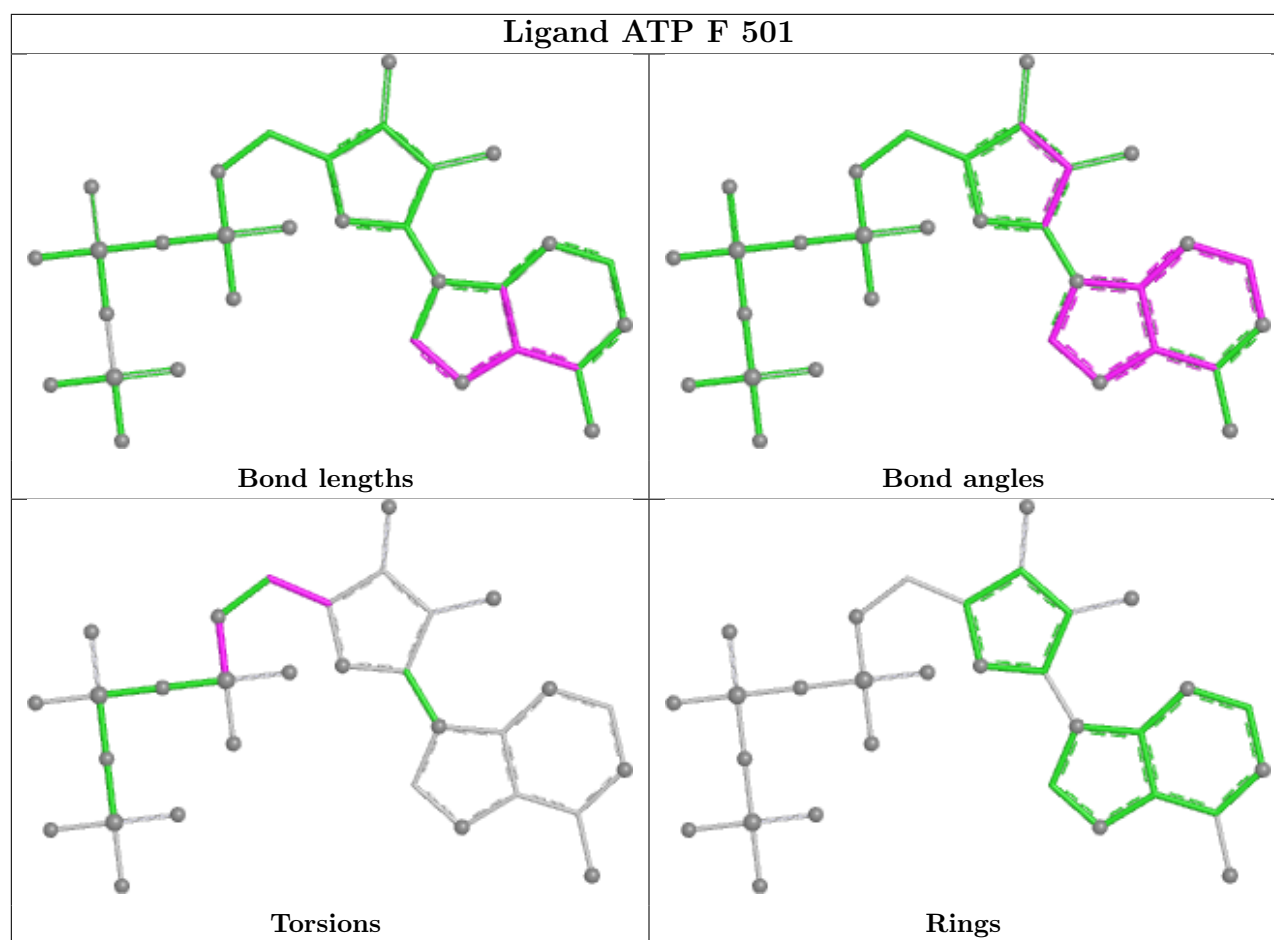
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	E	401	ATP	3	0
33	D	501	ATP	2	0
33	A	501	ATP	1	0
33	F	501	ATP	1	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	f	3
17	B	1
19	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	8.87
1	f	79:ASN	C	80:TYR	N	7.82
1	f	348:ASP	C	349:SER	N	6.24

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	216:ILE	C	217:LYS	N	4.90
1	E	175:PRO	C	176:PRO	N	1.65

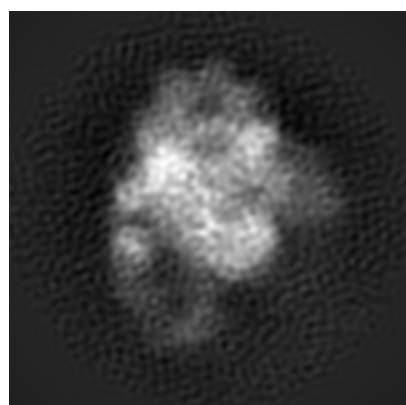
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8337. These allow visual inspection of the internal detail of the map and identification of artifacts.

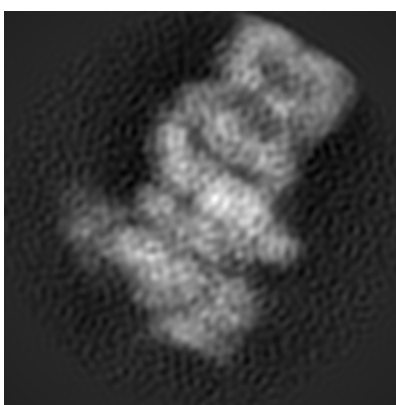
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

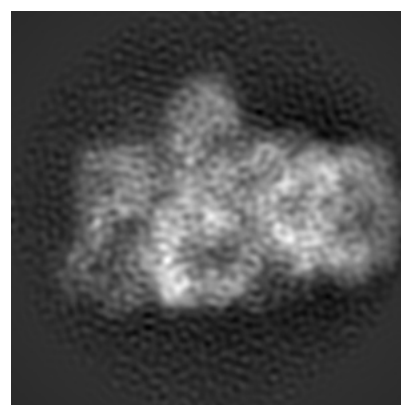
6.1.1 Primary map



X



Y

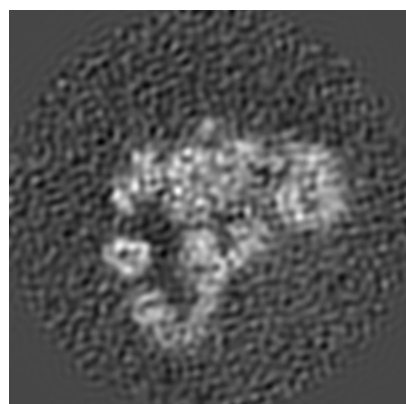


Z

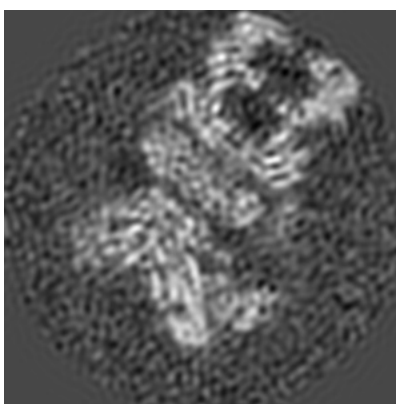
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

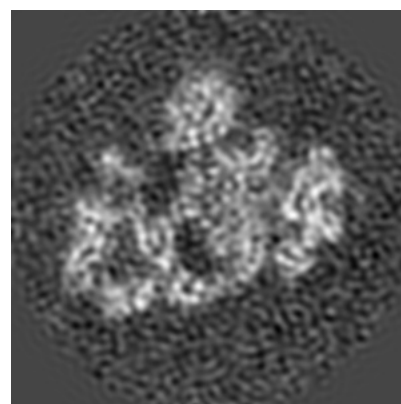
6.2.1 Primary map



X Index: 180



Y Index: 180

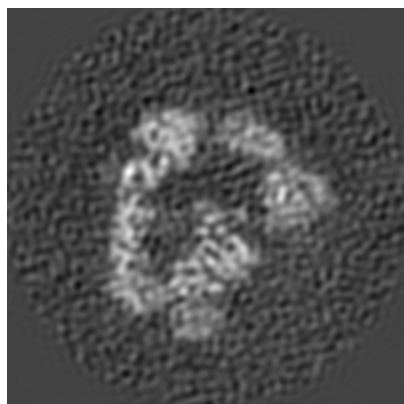


Z Index: 180

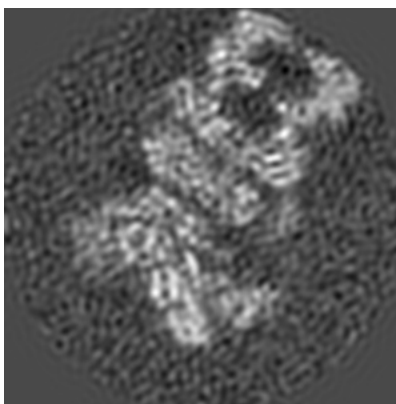
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

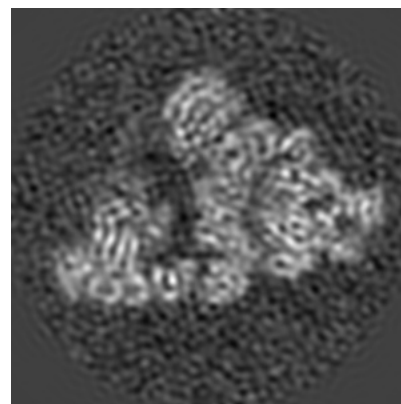
6.3.1 Primary map



X Index: 150



Y Index: 182

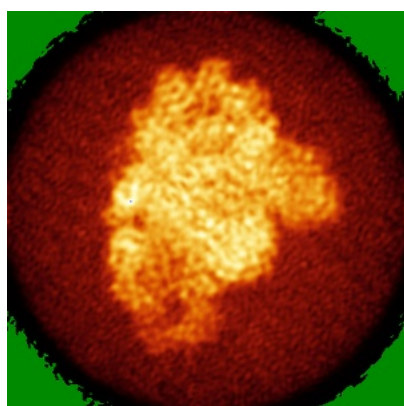


Z Index: 197

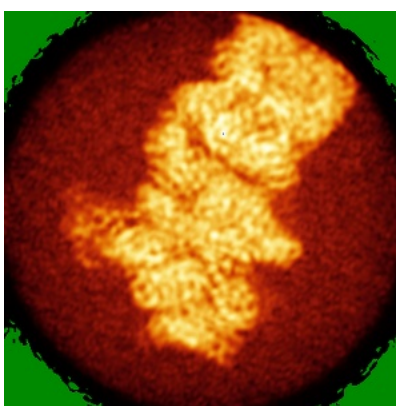
The images above show the largest variance slices of the map in three orthogonal directions.

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

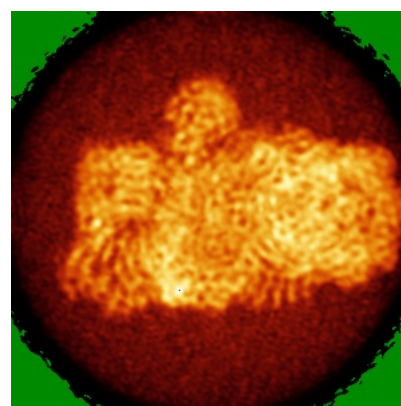
6.4.1 Primary map



X



Y

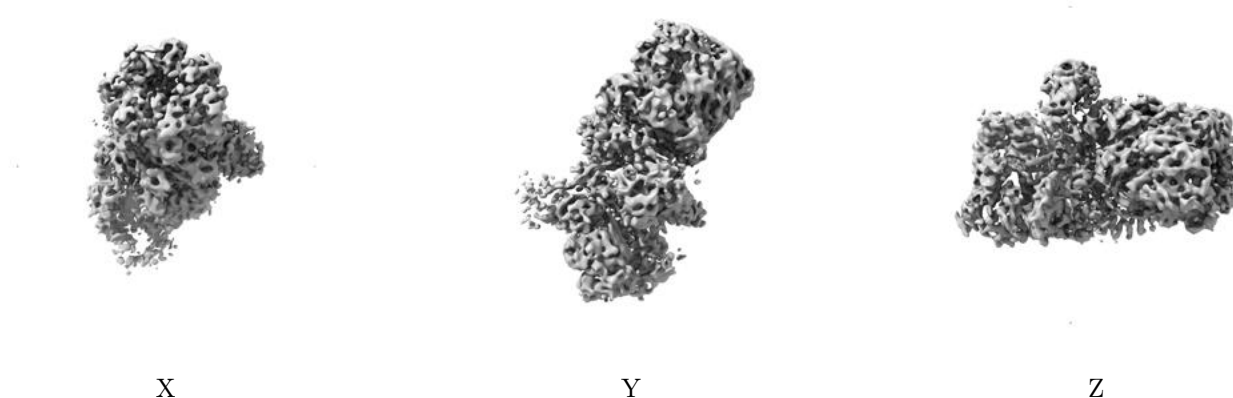


Z

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 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

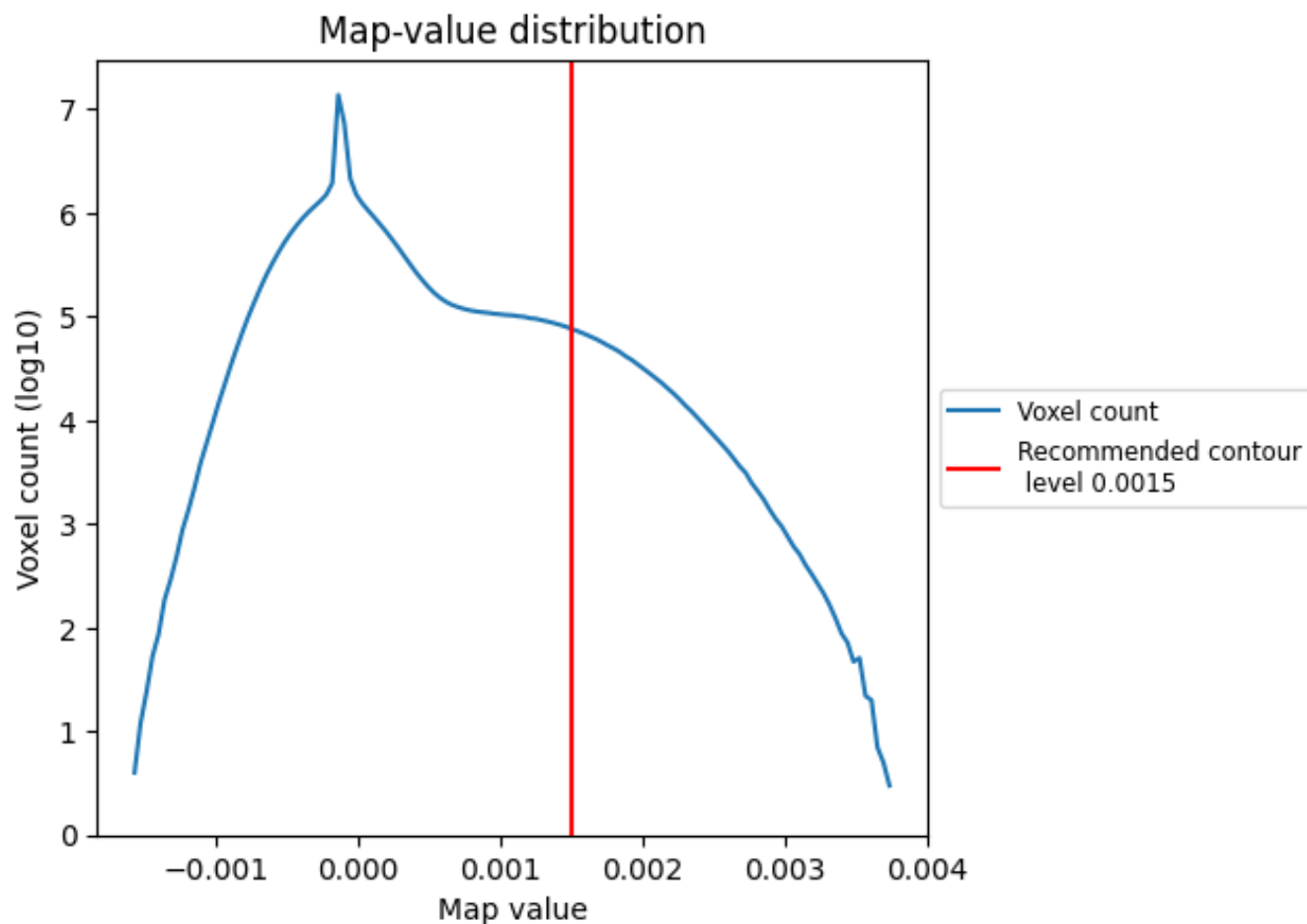
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

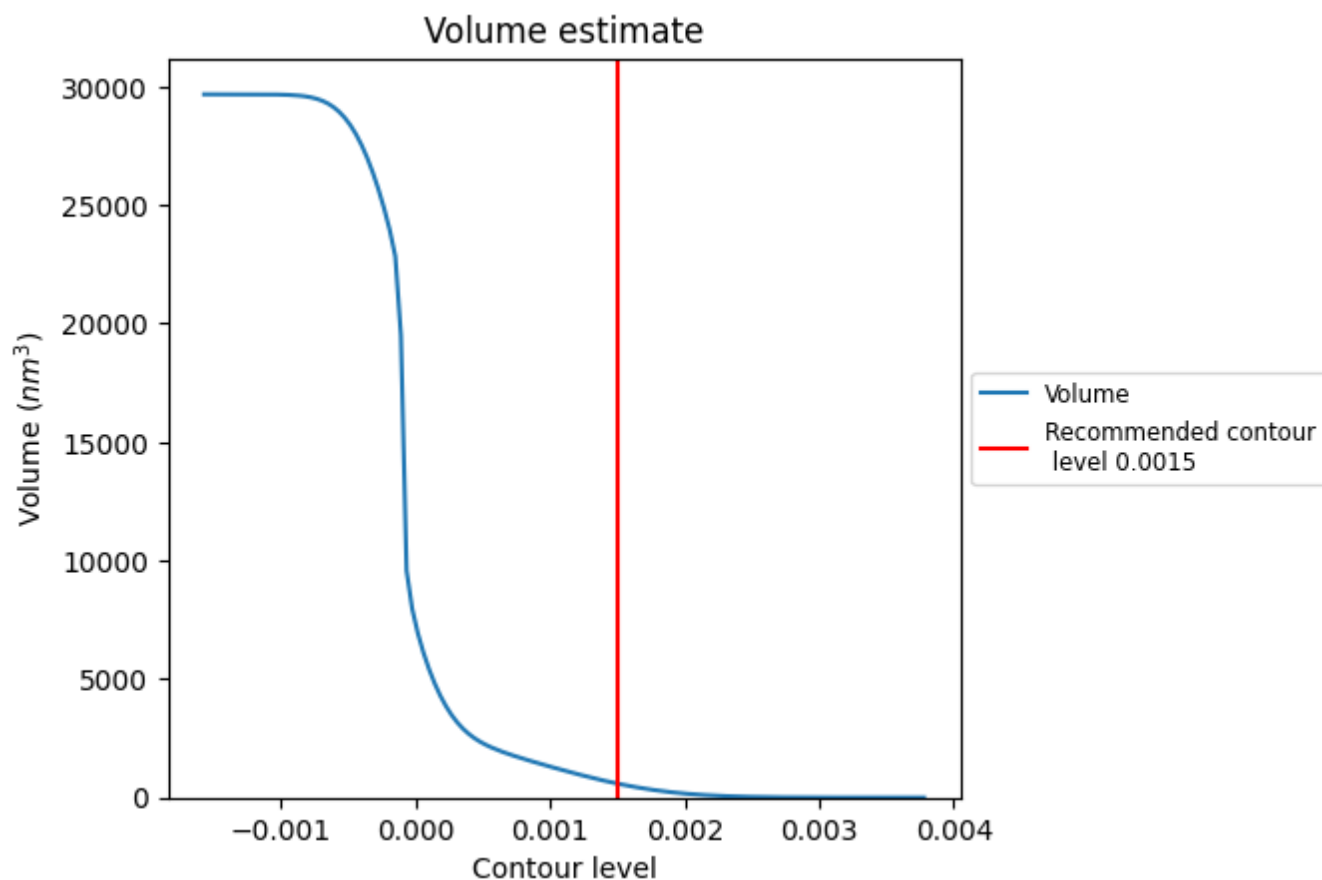
This section contains the results of statistical analysis of the map.

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.

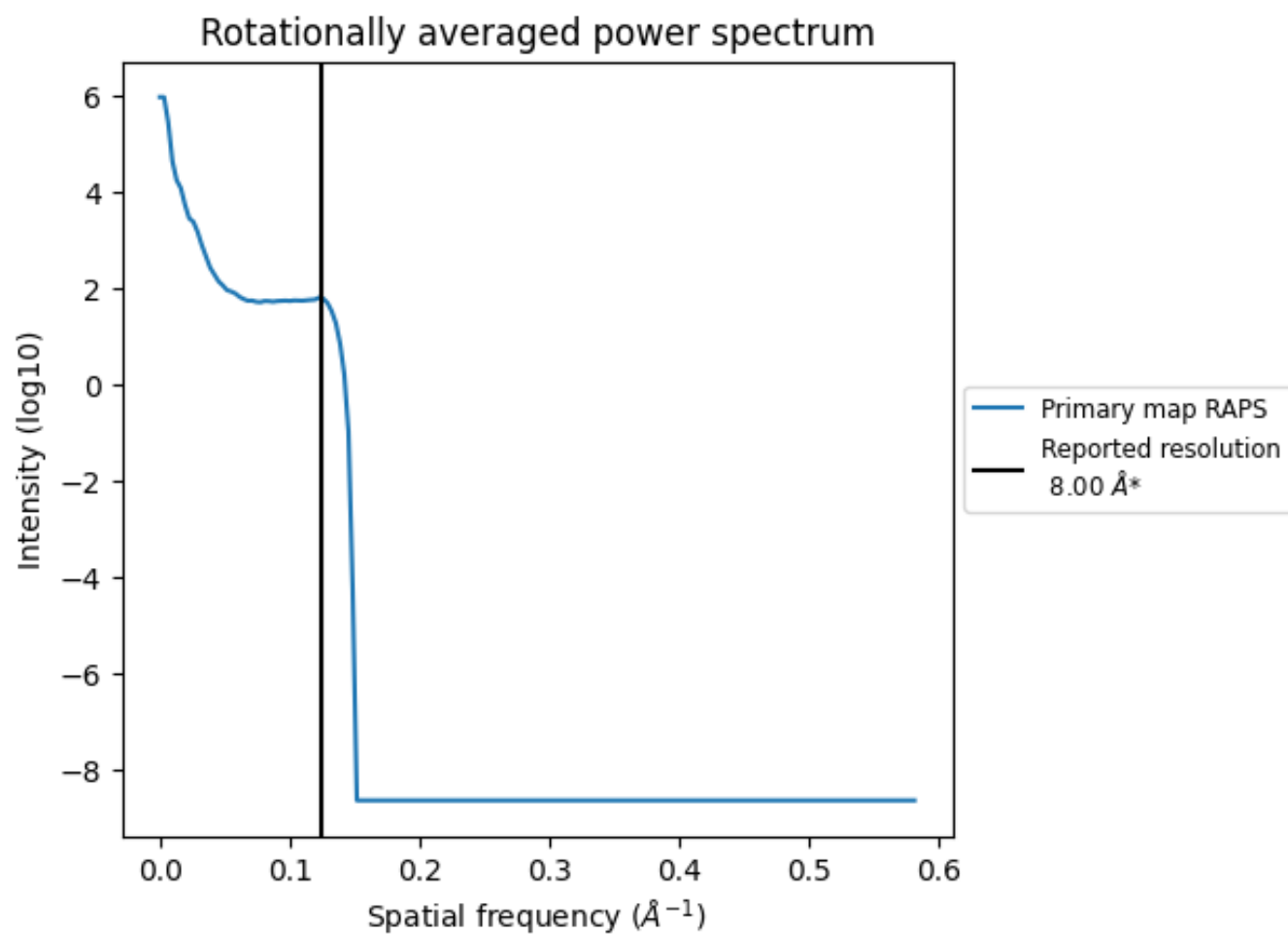
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 590 nm³; this corresponds to an approximate mass of 533 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 0.125 Å⁻¹

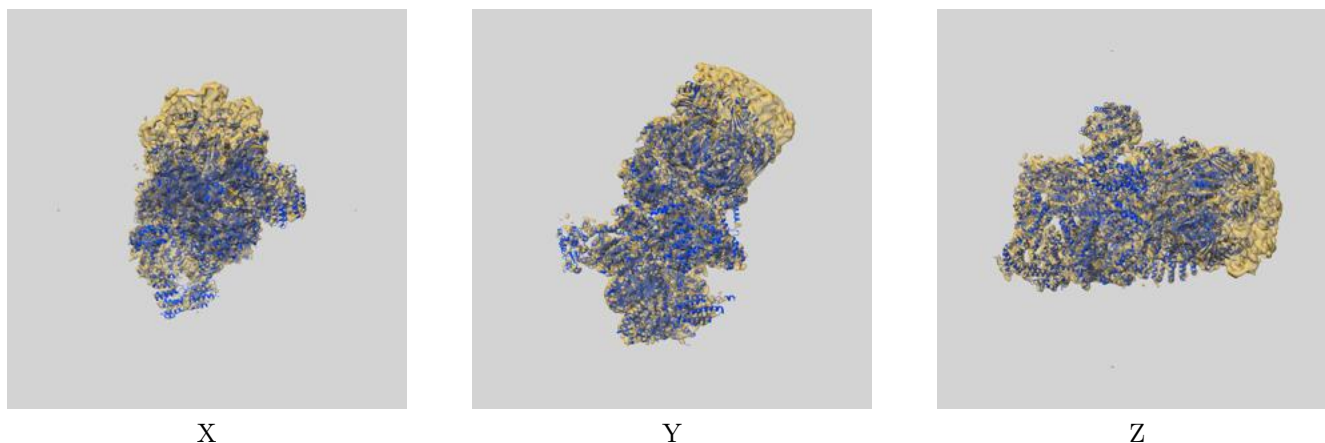
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

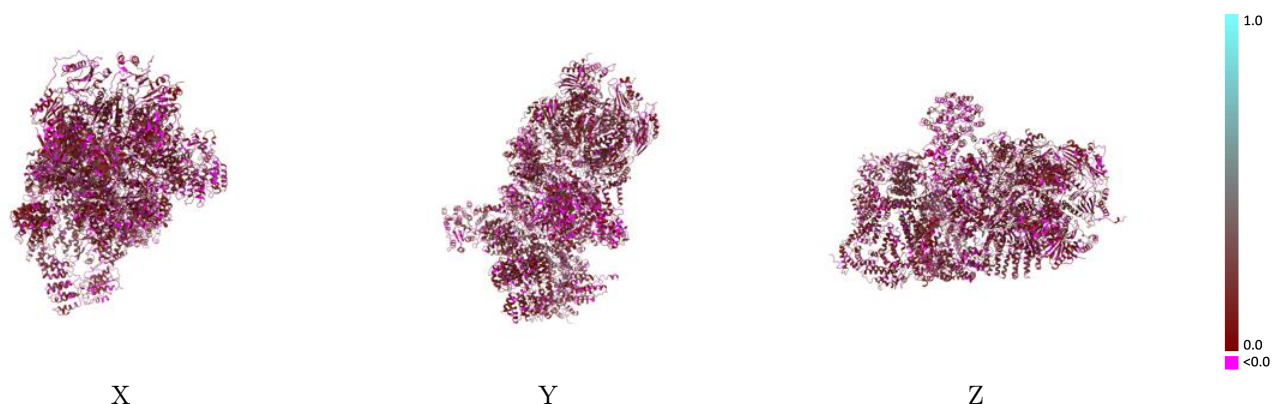
This section contains information regarding the fit between EMDB map EMD-8337 and PDB model 5T0J. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

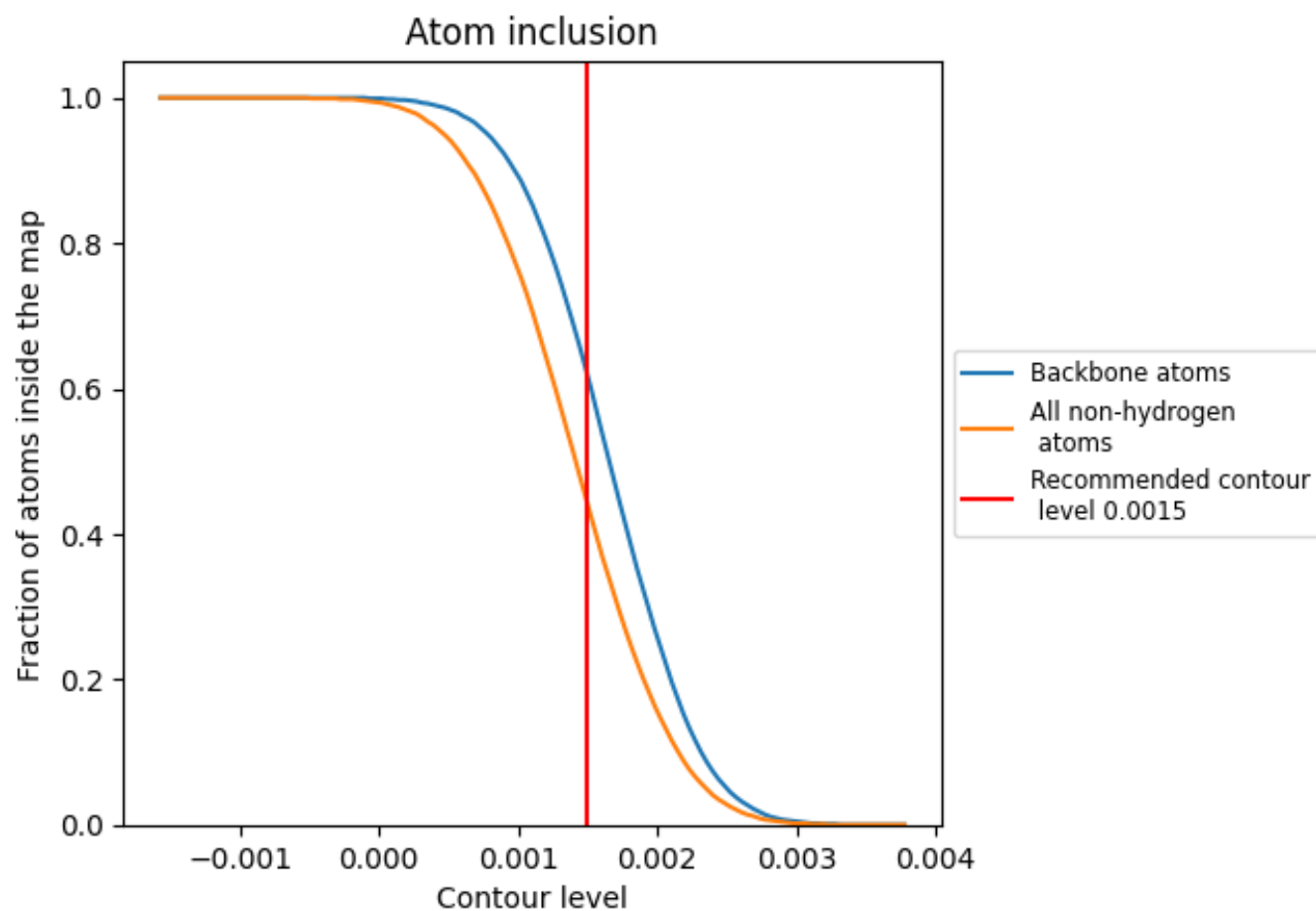


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 62% of all backbone atoms, 44% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4410	0.1160
A	0.3420	0.1020
B	0.2650	0.0920
C	0.3460	0.1040
D	0.3310	0.1040
E	0.3040	0.1130
F	0.3190	0.0980
G	0.5310	0.1330
H	0.4920	0.1230
I	0.4770	0.1330
J	0.5460	0.1470
K	0.5390	0.1500
L	0.5570	0.1390
M	0.5620	0.1380
N	0.5390	0.1190
O	0.5450	0.1130
P	0.5530	0.1160
Q	0.5570	0.1320
R	0.5630	0.1260
S	0.4690	0.1140
T	0.5510	0.1280
U	0.5970	0.1300
V	0.4370	0.1210
W	0.4440	0.1300
X	0.4100	0.1040
Y	0.5830	0.1320
Z	0.4460	0.1170
a	0.3730	0.1160
b	0.1300	0.0790
c	0.4680	0.1300
d	0.3760	0.1200
e	0.4550	0.1270
f	0.3070	0.0710

