



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:17 PM UTC

PDB ID : 5T0I / pdb_00005t0i
EMDB ID : EMD-8336
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:

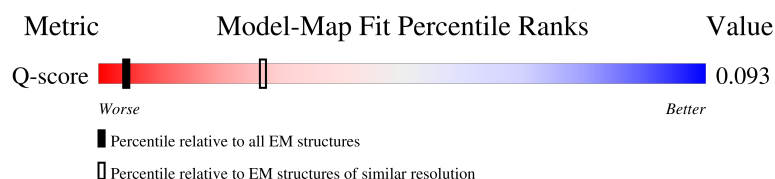
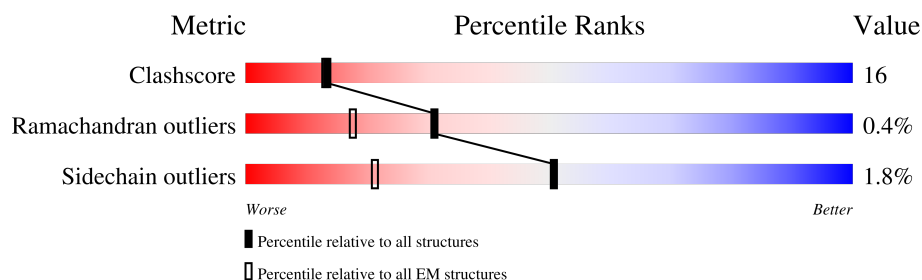
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

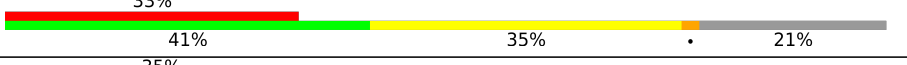
The reported resolution of this entry is 8.00 Å.

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	A	433	
2	B	440	
3	C	398	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	245	
8	H	233	
9	I	260	
10	J	247	
11	K	240	
12	L	268	
13	M	254	
14	N	238	
15	O	276	
16	P	204	
17	Q	201	
18	R	262	
19	S	240	
20	T	263	
21	U	953	
22	V	533	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	309	

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Mol	Chain	Length	Quality of chain
30	d	349	30%46%27%•26%
31	e	70	17%24%31%•43%
32	f	749	49%66%25%•7%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 76616 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 protease regulatory subunit 7.

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

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

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

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

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

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

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

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	233	Total	C	N	O	S	0	0
			1713	1084	290	334	5		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

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

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

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

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 14 is a protein called Proteasome subunit beta type-6.

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

- Molecule 15 is a protein called Proteasome subunit beta type-7.

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

- Molecule 16 is a protein called Proteasome subunit beta type-3.

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

- Molecule 17 is a protein called Proteasome subunit beta type-2.

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

- Molecule 18 is a protein called Proteasome subunit beta type-5.

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

- Molecule 19 is a protein called Proteasome subunit beta type-1.

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

- Molecule 20 is a protein called Proteasome subunit beta type-4.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

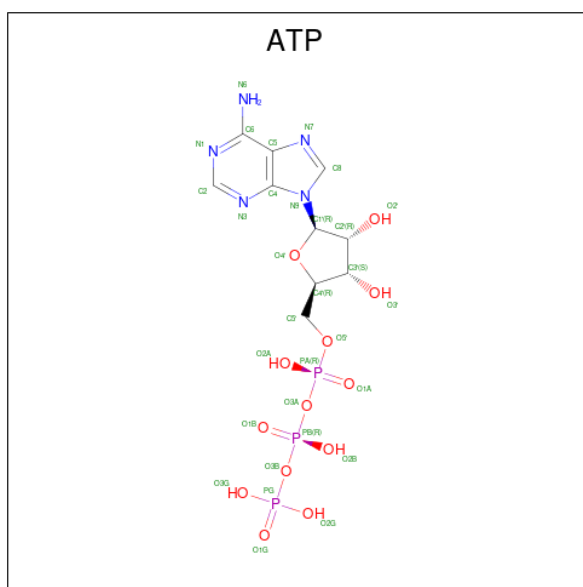
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

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

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

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

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



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

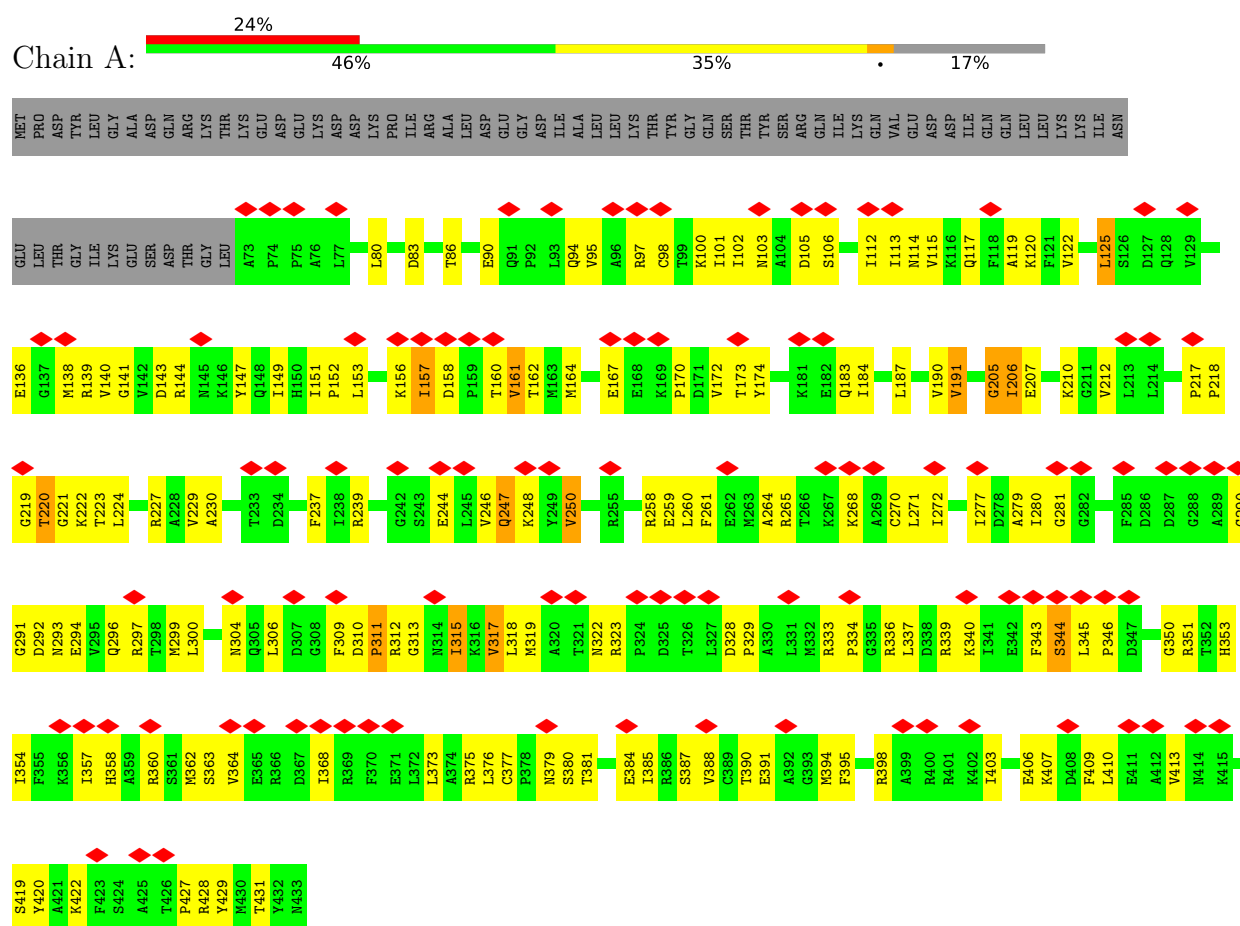
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

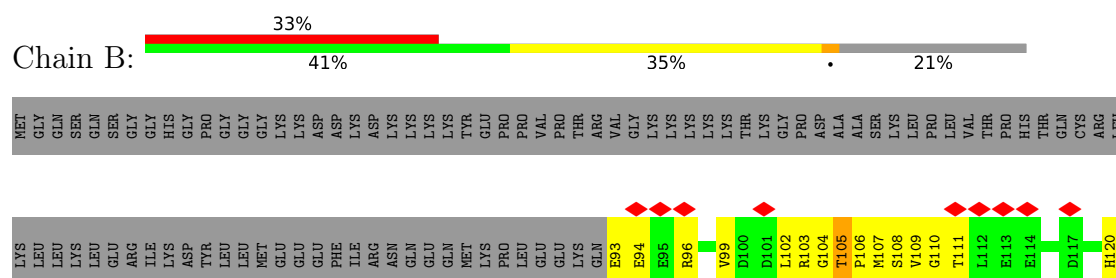
3 Residue-property plots

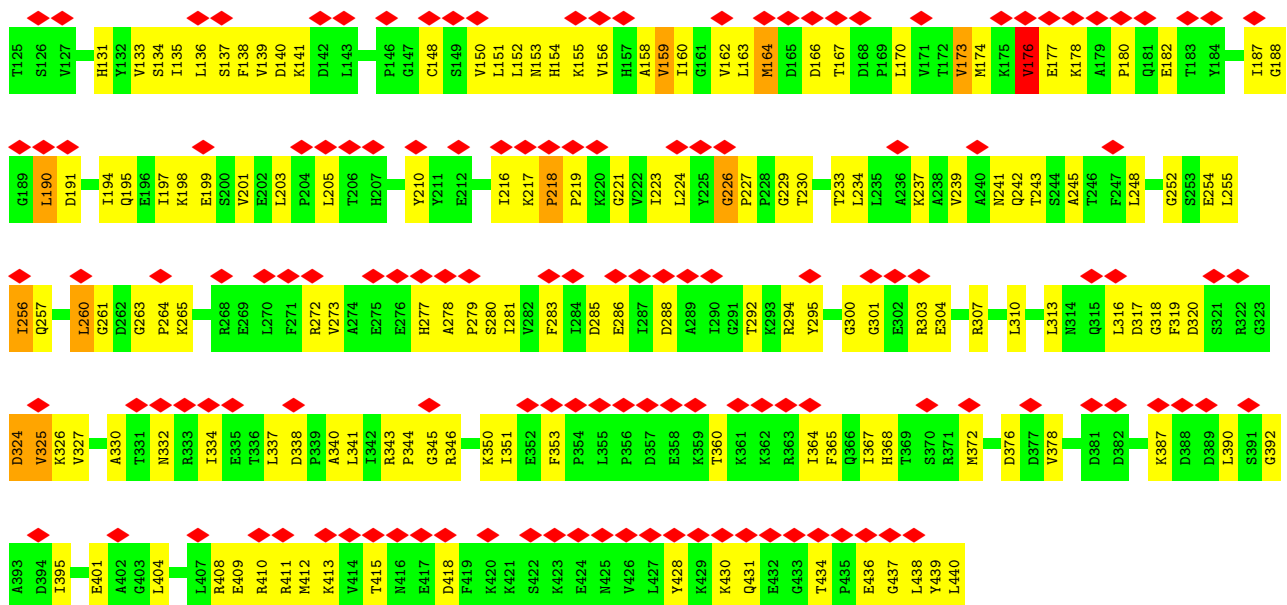
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 protease regulatory subunit 7

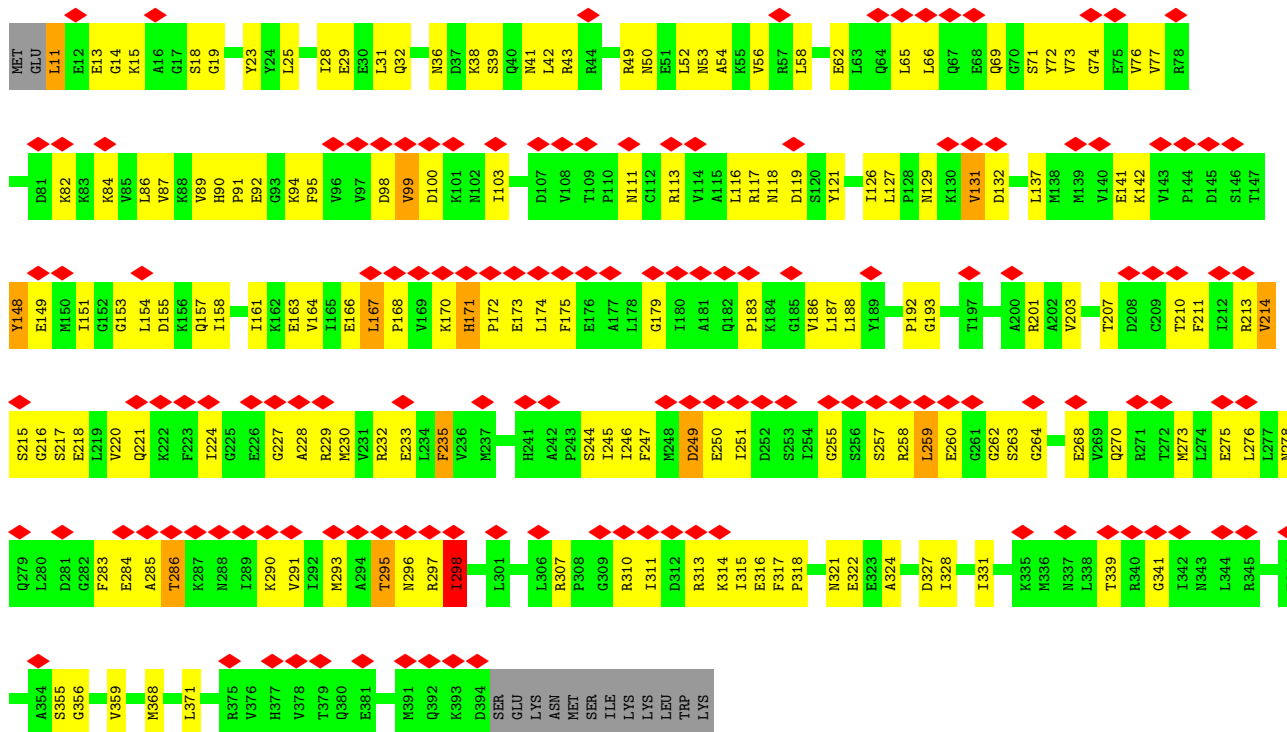


- Molecule 2: 26S protease regulatory subunit 4



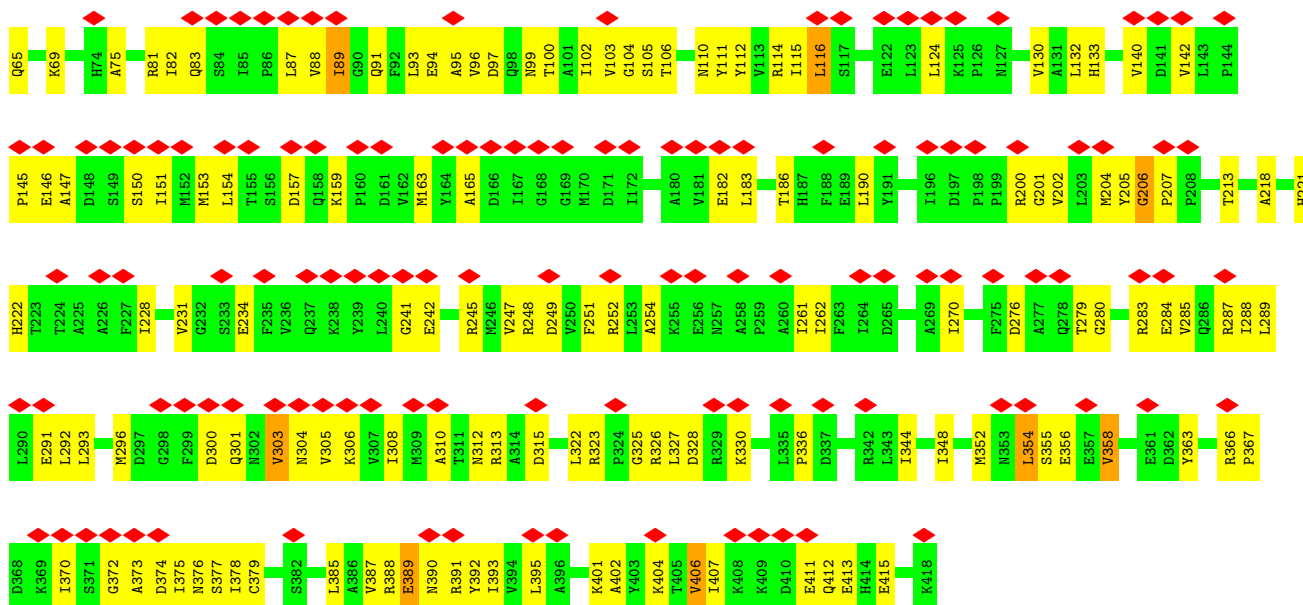


• Molecule 3: 26S protease regulatory subunit 8

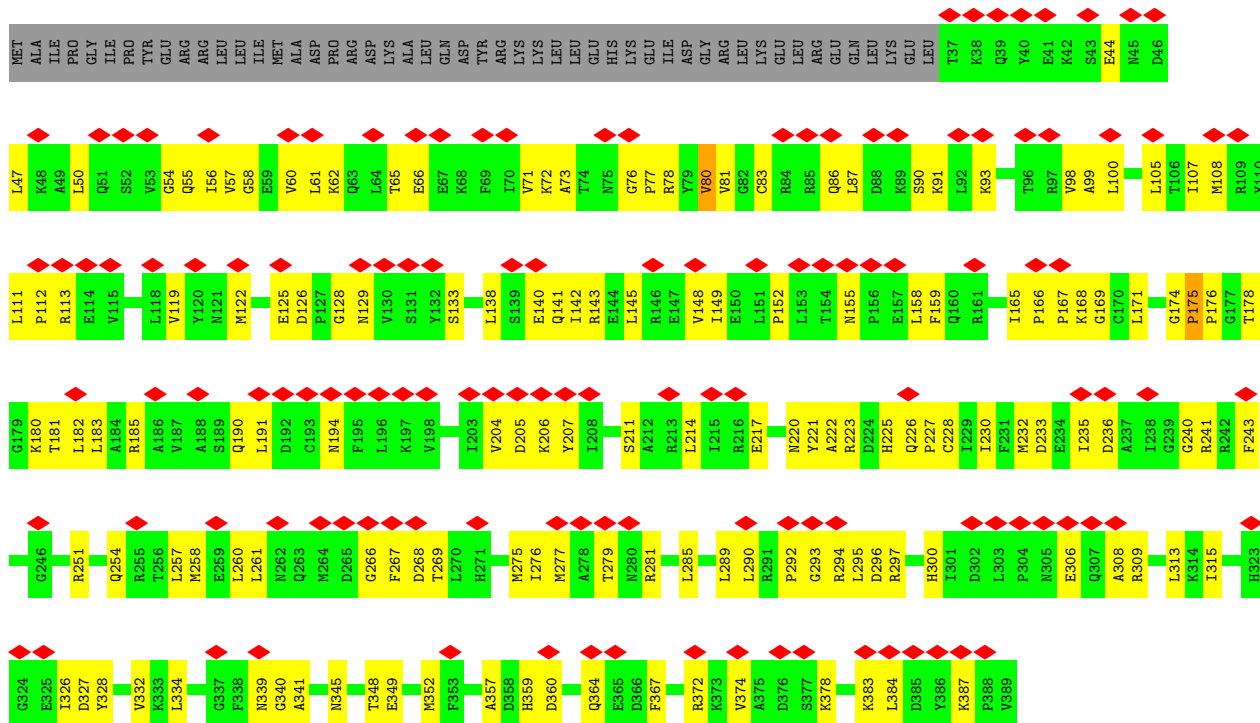


• Molecule 4: 26S protease regulatory subunit 6B

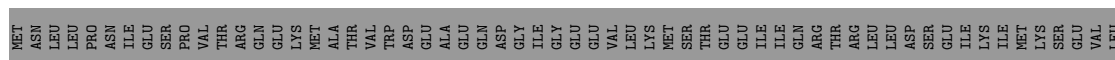


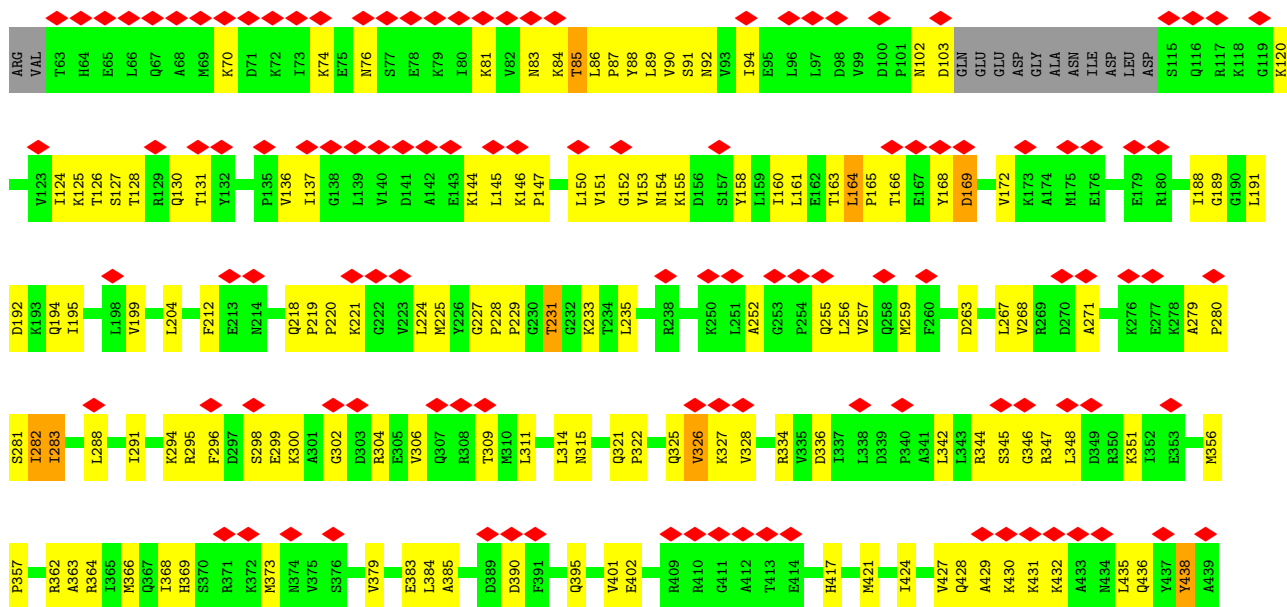


• Molecule 5: 26S protease regulatory subunit 10B

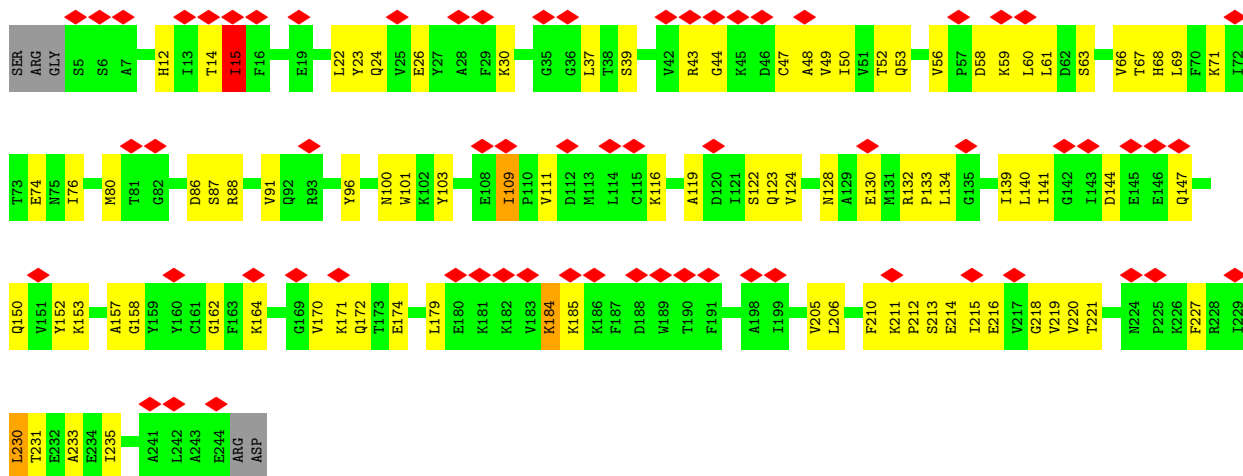


• Molecule 6: 26S protease regulatory subunit 6A

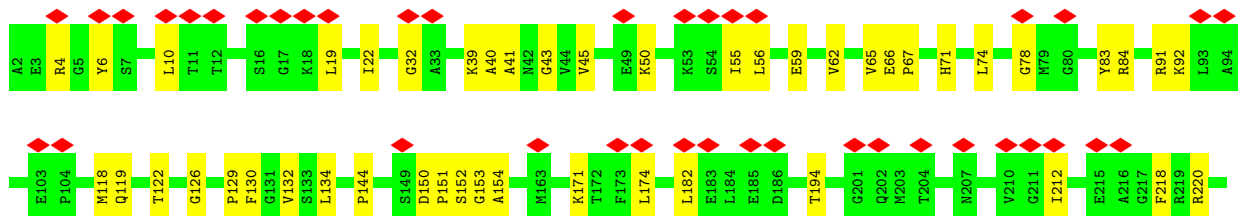
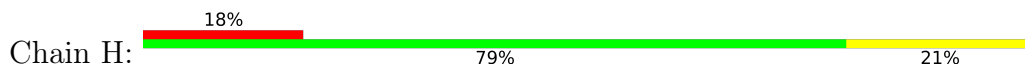




• Molecule 7: Proteasome subunit alpha type-6

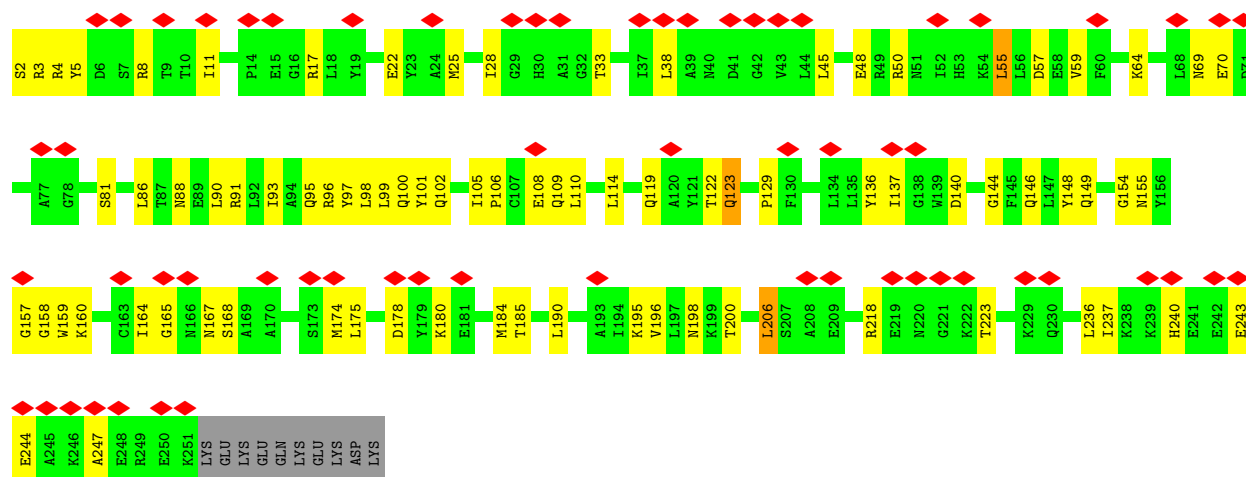


• Molecule 8: Proteasome subunit alpha type-2

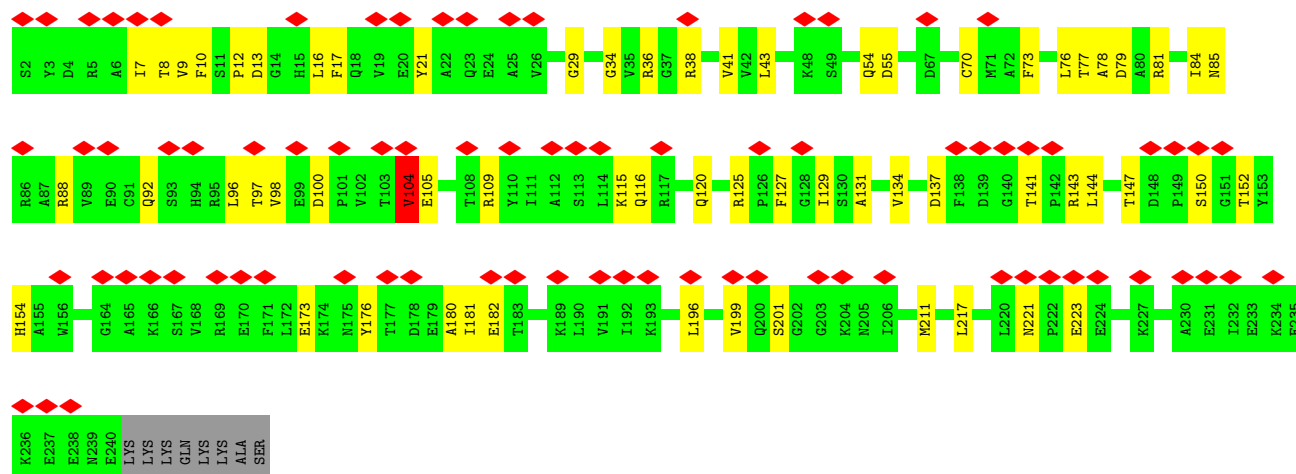




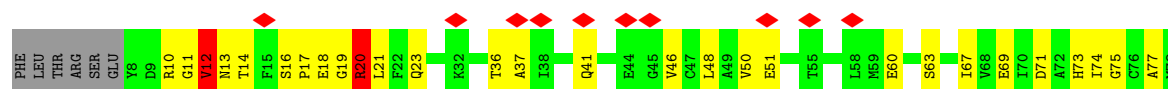
• Molecule 9: Proteasome subunit alpha type-4

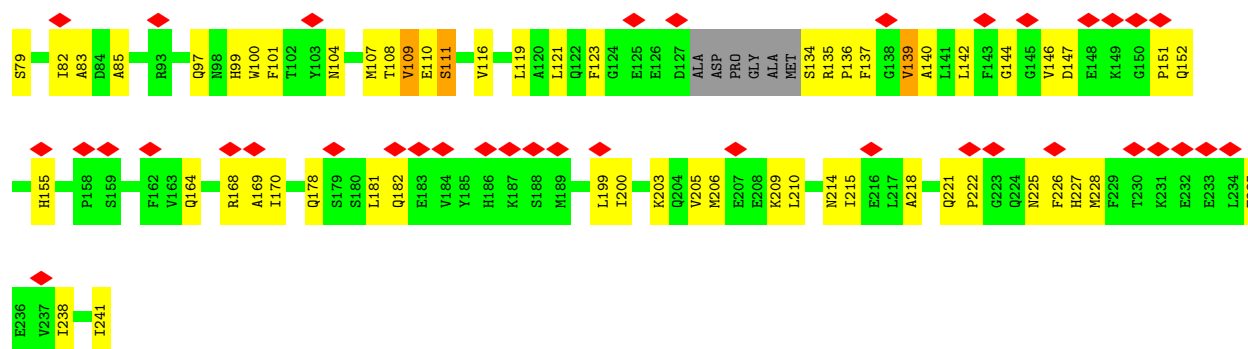


• Molecule 10: Proteasome subunit alpha type-7

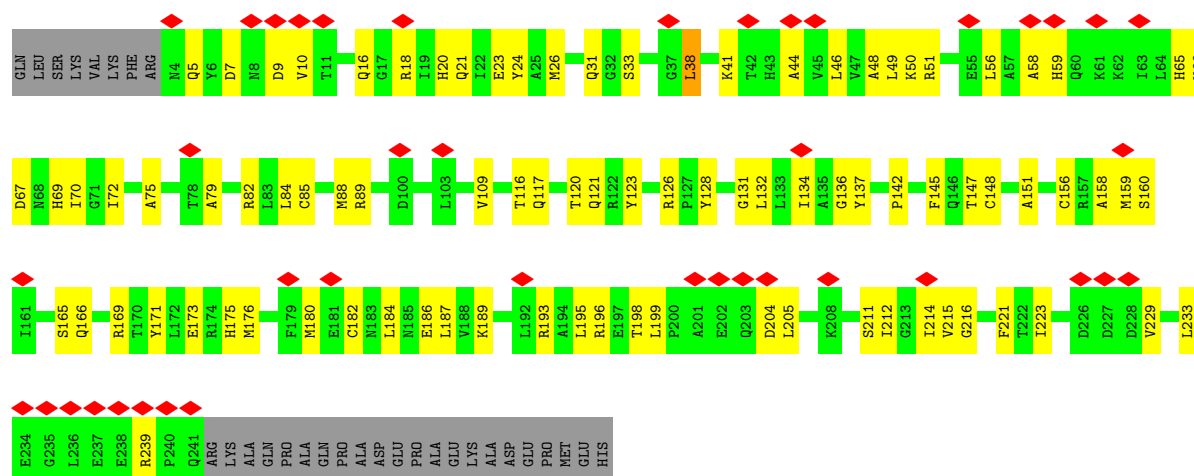


• Molecule 11: Proteasome subunit alpha type-5

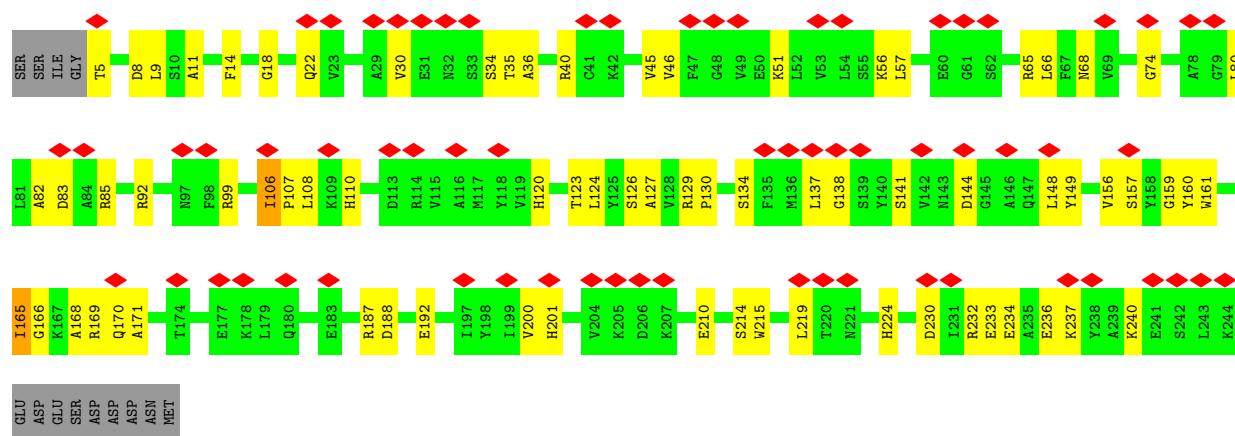




• Molecule 12: Proteasome subunit alpha type-1

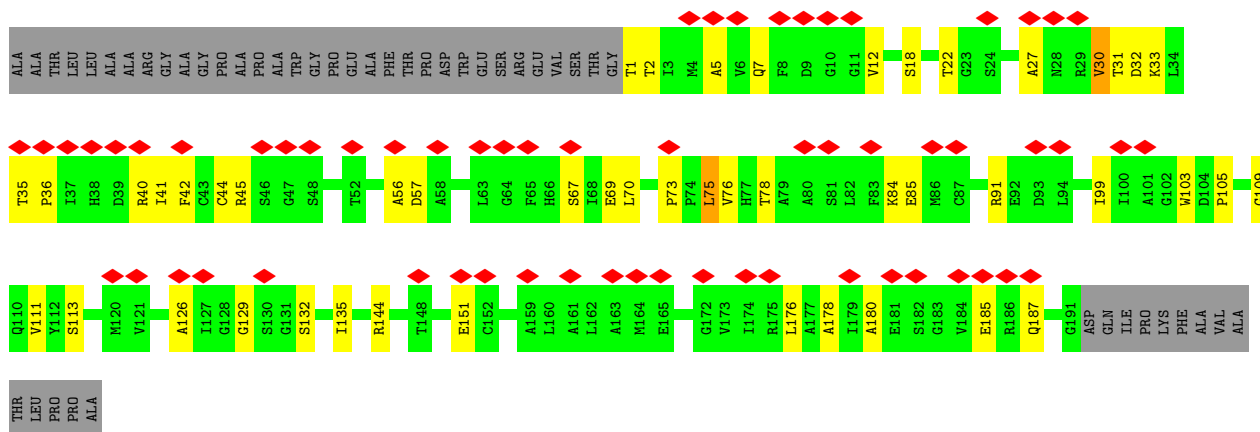


• Molecule 13: Proteasome subunit alpha type-3

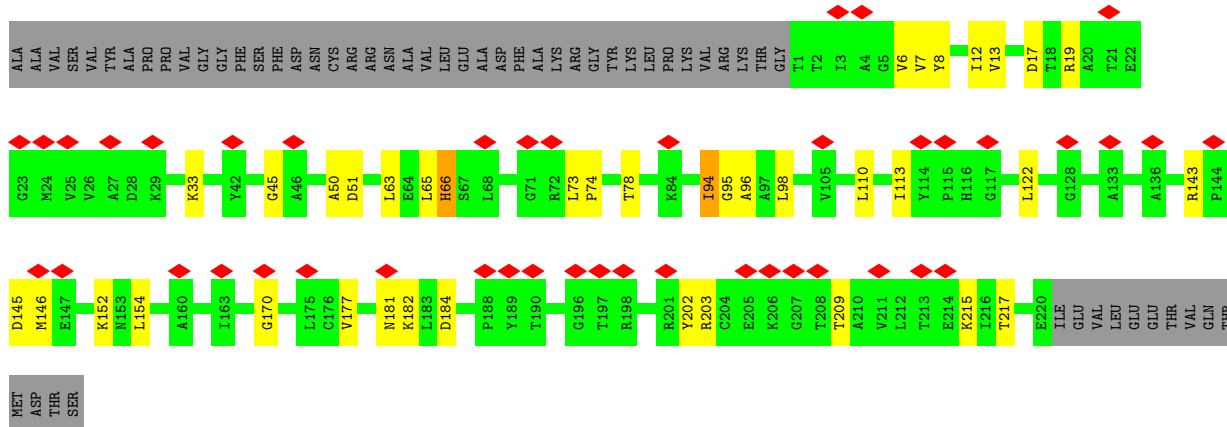


• Molecule 14: Proteasome subunit beta type-6

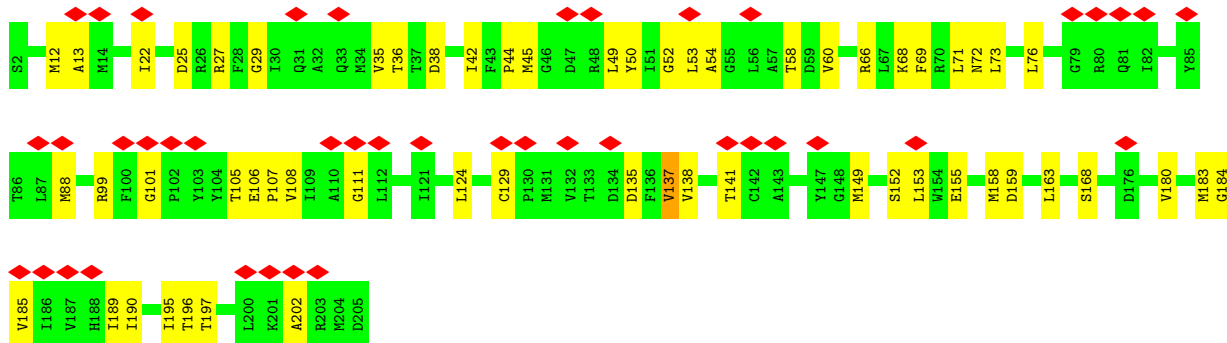




• Molecule 15: Proteasome subunit beta type-7

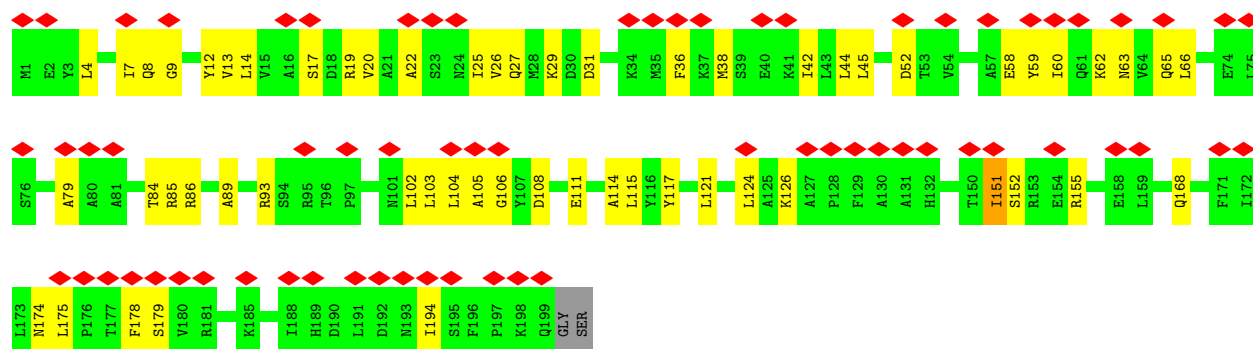


• Molecule 16: Proteasome subunit beta type-3

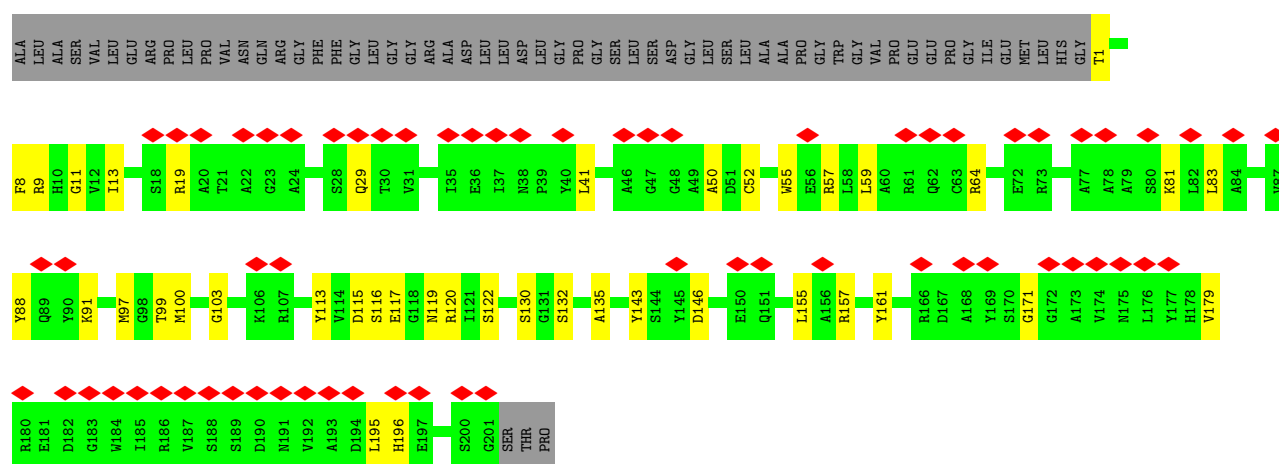


• Molecule 17: Proteasome subunit beta type-2

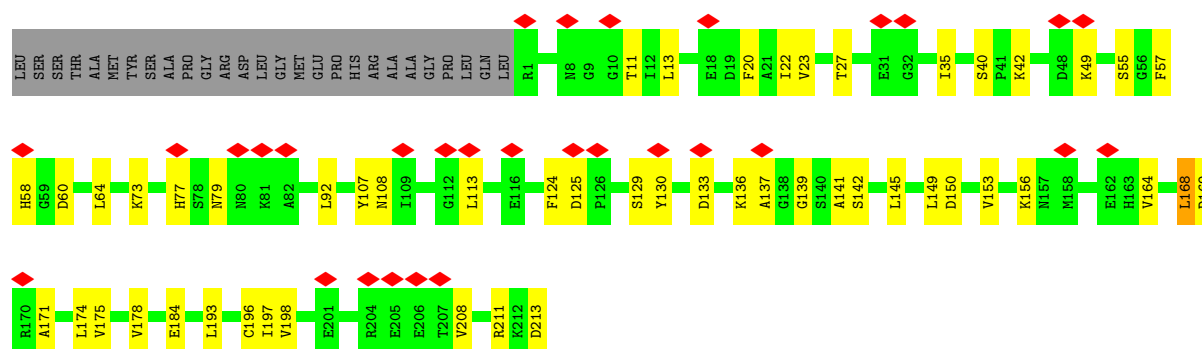




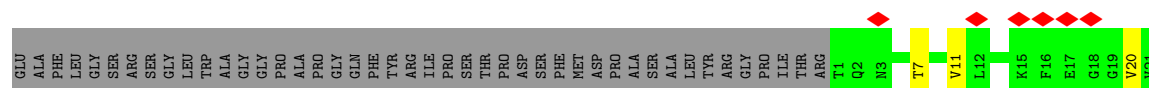
• Molecule 18: Proteasome subunit beta type-5



• Molecule 19: Proteasome subunit beta type-1

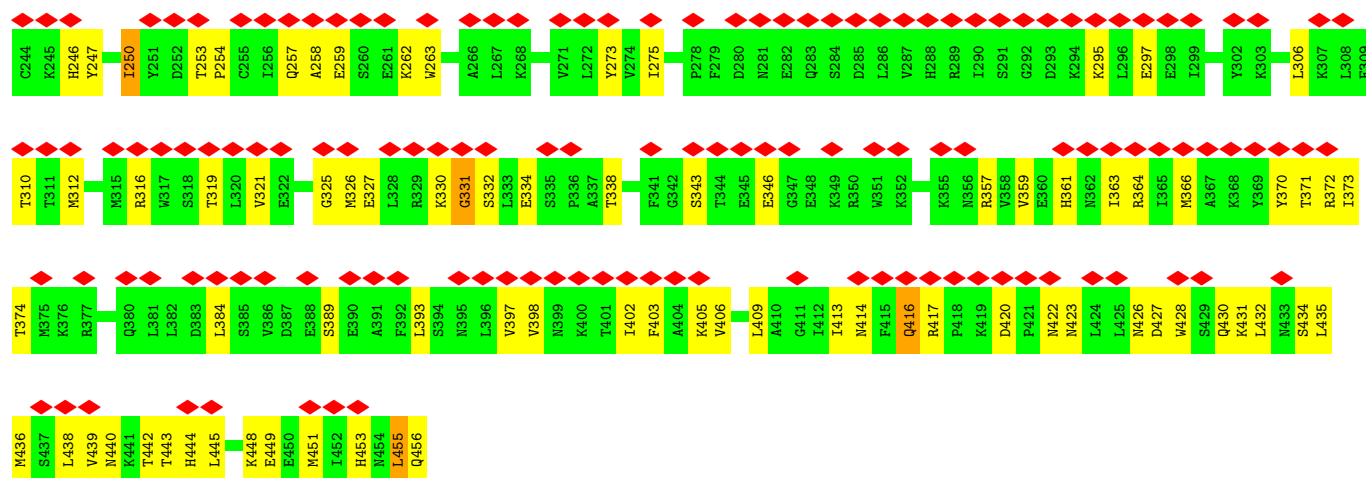


• Molecule 20: Proteasome subunit beta type-4

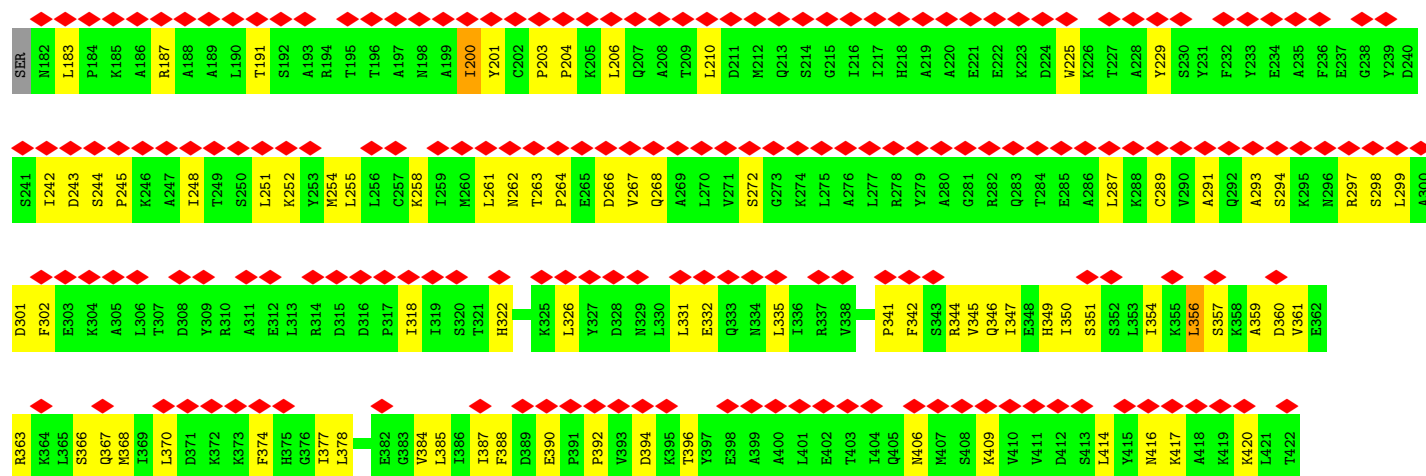
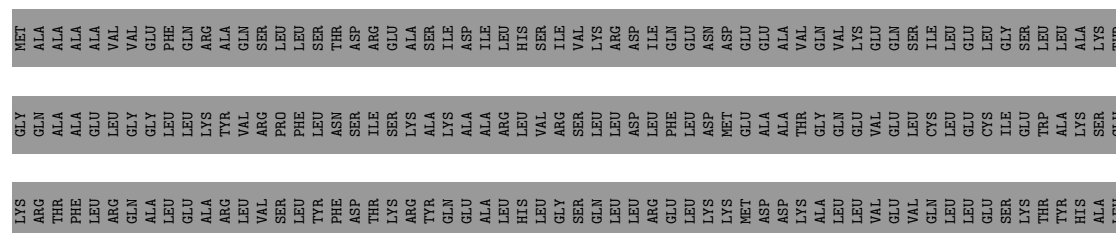
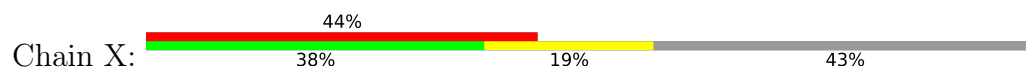


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

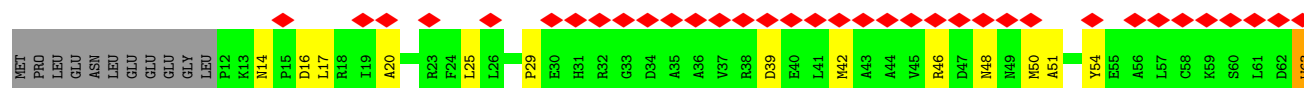


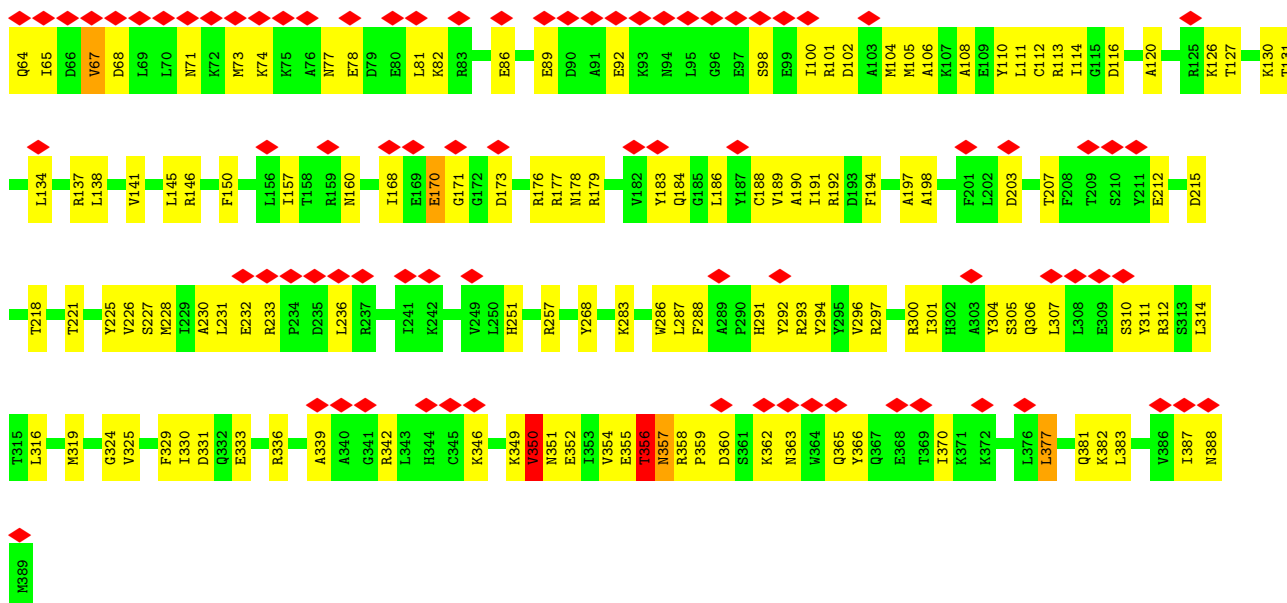


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

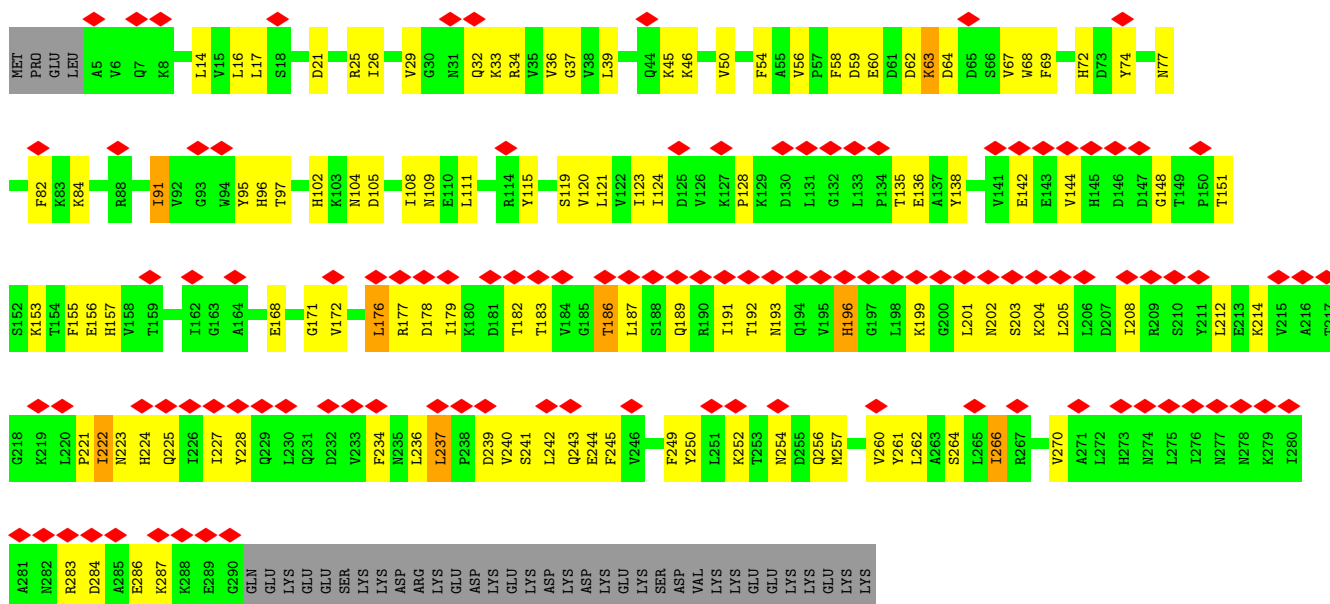


• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

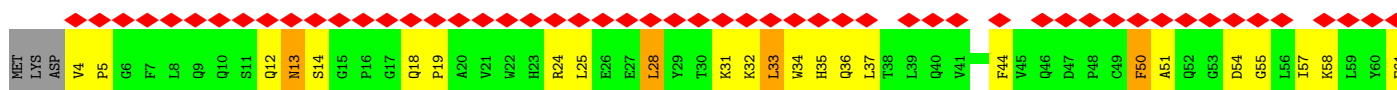


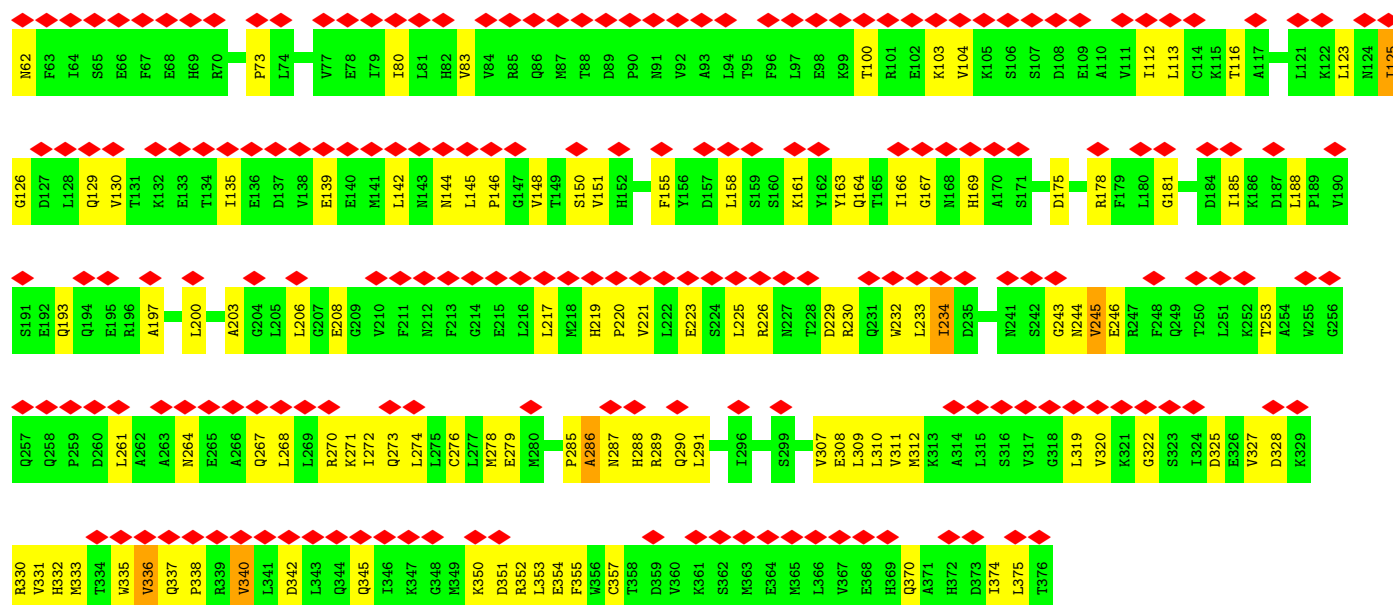


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

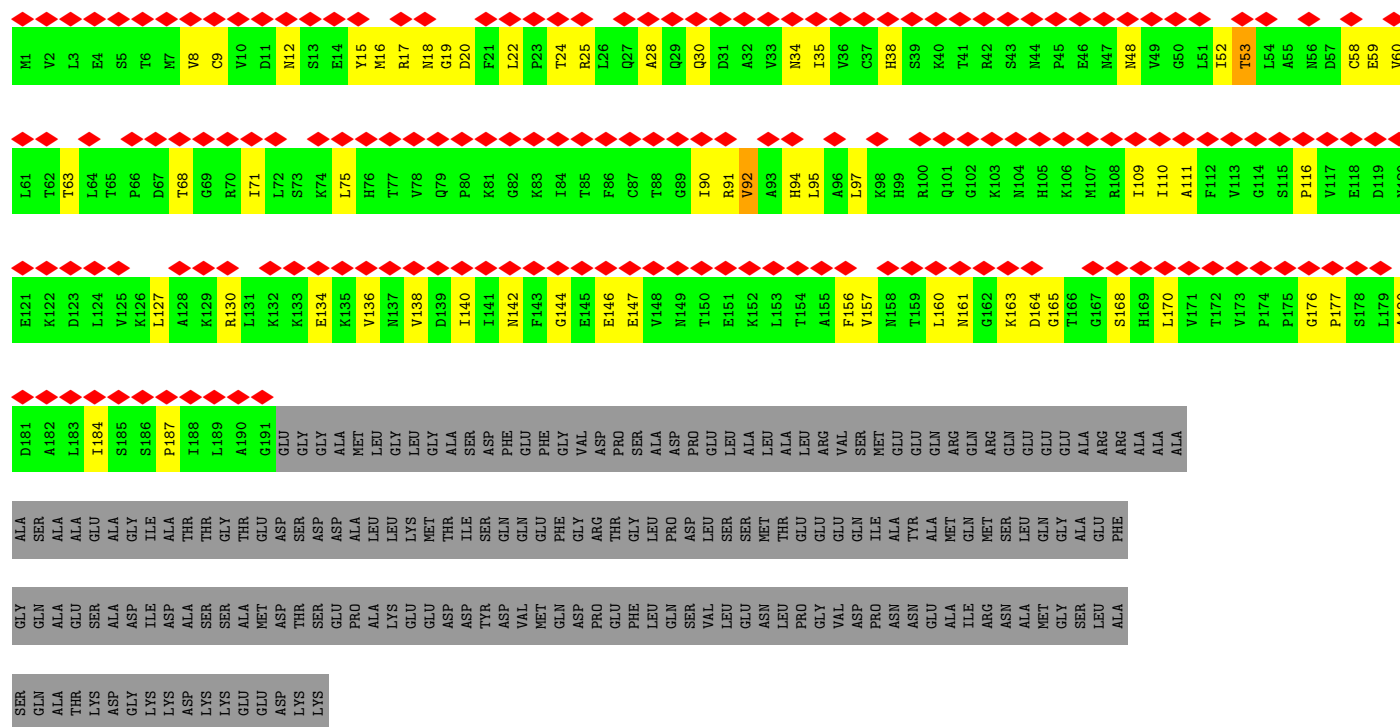
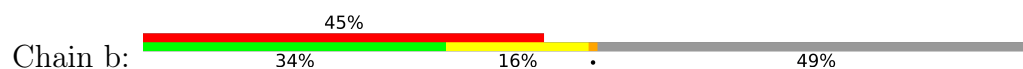


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

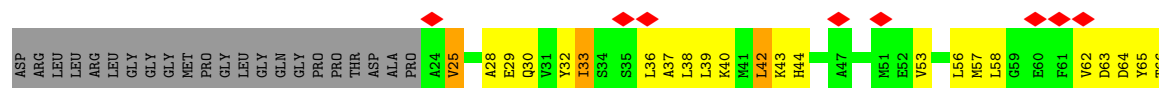


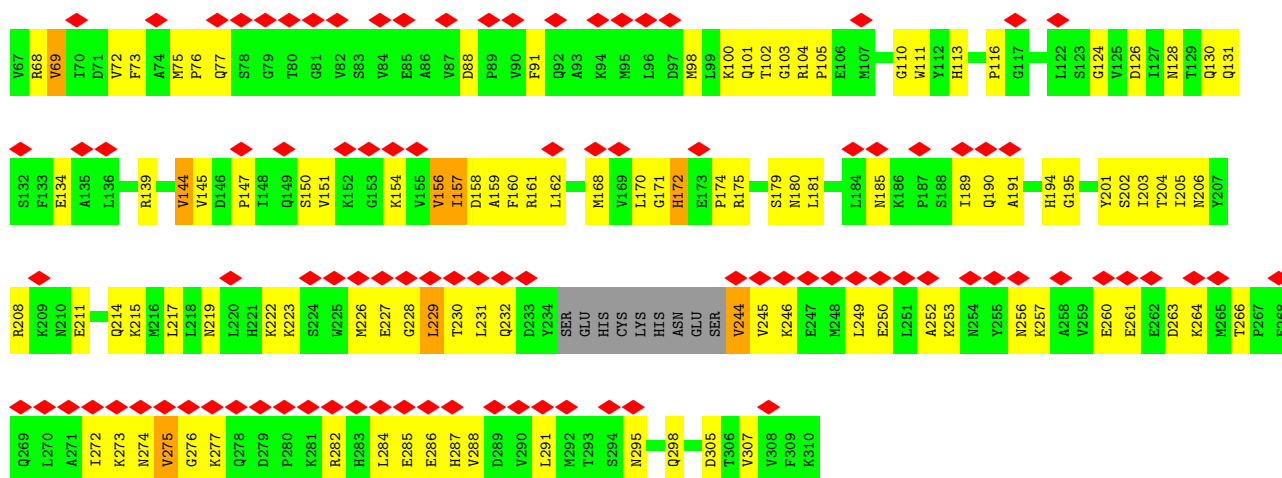


• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

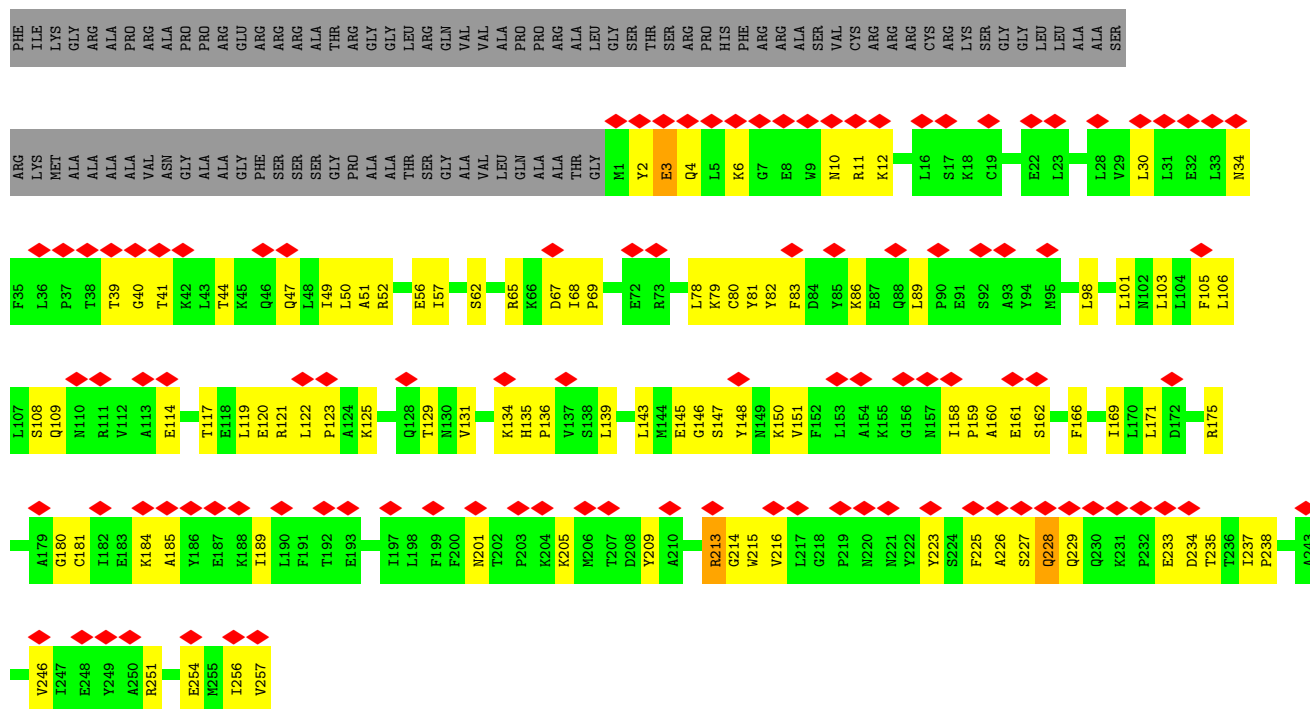


• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

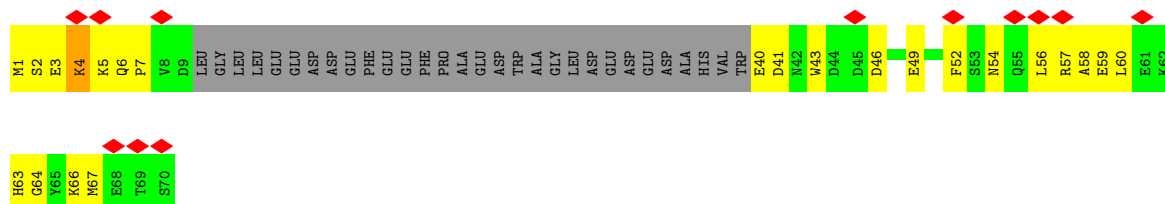
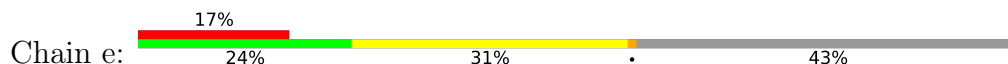




• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit DSS1



Chain f:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10622	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	0.005	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size ($\text{\AA}$)	309.6, 309.6, 309.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ATP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/2886	0.54	6/3899 (0.2%)
2	B	0.24	0/2757	0.69	5/3724 (0.1%)
3	C	0.18	0/3054	0.54	0/4107
4	D	0.18	0/3090	0.56	6/4168 (0.1%)
5	E	0.15	0/2835	0.47	0/3821
6	F	0.77	6/2903 (0.2%)	0.54	2/3912 (0.1%)
7	G	0.13	0/1859	0.43	2/2523 (0.1%)
8	H	0.14	0/1747	0.43	3/2376 (0.1%)
9	I	0.14	0/1942	0.44	0/2628
10	J	0.14	0/1728	0.47	0/2358
11	K	1.39	1/1747 (0.1%)	0.56	2/2364 (0.1%)
12	L	0.13	0/1885	0.42	0/2552
13	M	0.16	0/1891	0.41	0/2552
14	N	0.10	0/1454	0.33	0/1967
15	O	0.12	0/1669	0.40	0/2262
16	P	0.11	0/1613	0.32	0/2174
17	Q	0.13	0/1603	0.37	0/2174
18	R	0.10	0/1579	0.35	0/2134
19	S	0.11	0/1671	0.33	0/2253
20	T	0.11	0/1700	0.35	0/2305
21	U	0.13	0/6396	0.42	1/8646 (0.0%)
22	V	0.69	6/3929 (0.2%)	0.61	11/5309 (0.2%)
23	W	0.18	0/3751	0.54	5/5042 (0.1%)
24	X	0.15	0/1936	0.46	0/2614
25	Y	0.16	0/3173	0.55	5/4273 (0.1%)
26	Z	0.18	0/2324	0.56	4/3150 (0.1%)
27	a	0.15	0/3053	0.48	2/4133 (0.0%)
28	b	0.17	0/1478	0.38	0/2001
29	c	0.20	1/2226 (0.0%)	0.53	0/3007
30	d	0.20	0/2162	0.56	2/2919 (0.1%)
31	e	3.04	1/338 (0.3%)	0.82	2/450 (0.4%)
32	f	0.27	1/5413 (0.0%)	0.58	10/7317 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
All	All	0.39	16/77792 (0.0%)	0.50	68/105114 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
3	C	0	2
22	V	0	2
23	W	0	1
25	Y	0	1
27	a	0	1
30	d	0	1
32	f	0	1
All	All	0	12

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	20	ARG	CB-CG	57.77	3.25	1.52
31	e	4	LYS	CD-CE	55.72	3.19	1.52
22	V	212	TYR	CD2-CE2	20.41	1.99	1.38
22	V	212	TYR	CD1-CE1	20.31	1.99	1.38
6	F	438	TYR	CD2-CE2	19.95	1.98	1.38
6	F	438	TYR	CD1-CE1	19.50	1.97	1.38
22	V	212	TYR	CE1-CZ	16.02	1.76	1.38
6	F	438	TYR	CE2-CZ	15.70	1.75	1.38
6	F	438	TYR	CE1-CZ	15.64	1.75	1.38
22	V	212	TYR	CE2-CZ	15.64	1.75	1.38
32	f	681	LEU	C-N	14.85	1.68	1.33
22	V	212	TYR	CG-CD2	14.11	1.69	1.39
22	V	212	TYR	CG-CD1	14.00	1.68	1.39
6	F	438	TYR	CG-CD2	13.56	1.67	1.39
6	F	438	TYR	CG-CD1	13.32	1.67	1.39
29	c	104	ARG	C-N	5.50	1.46	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	20	ARG	CA-CB-CG	10.89	135.88	114.10
32	f	636	GLY	N-CA-C	10.71	126.32	113.79
4	D	206	GLY	CA-C-N	-9.84	112.58	119.66
4	D	206	GLY	C-N-CA	-9.84	112.58	119.66
31	e	4	LYS	CG-CD-CE	9.82	133.88	111.30
2	B	226	GLY	CA-C-N	9.69	130.37	120.38
2	B	226	GLY	C-N-CA	9.69	130.37	120.38
11	K	20	ARG	CB-CG-CD	9.50	133.16	111.30
32	f	459	GLU	N-CA-C	9.38	127.77	113.51
26	Z	63	LYS	N-CA-C	7.99	121.15	111.40
25	Y	63	TRP	CA-C-N	7.73	135.62	121.70
25	Y	63	TRP	C-N-CA	7.73	135.62	121.70
23	W	92	LYS	CA-C-N	7.30	134.84	121.70
23	W	92	LYS	C-N-CA	7.30	134.84	121.70
23	W	135	LYS	CA-C-N	7.28	134.80	121.70
23	W	135	LYS	C-N-CA	7.28	134.80	121.70
22	V	57	ALA	CA-C-N	6.78	133.91	121.70
22	V	57	ALA	C-N-CA	6.78	133.91	121.70
30	d	228	GLN	N-CA-C	6.77	124.01	113.72
32	f	459	GLU	CA-C-N	6.76	133.86	121.70
32	f	459	GLU	C-N-CA	6.76	133.86	121.70
25	Y	356	THR	CA-C-N	6.43	133.27	121.70
25	Y	356	THR	C-N-CA	6.43	133.27	121.70
25	Y	170	GLU	N-CA-C	6.24	118.59	111.11
26	Z	63	LYS	CA-C-N	6.14	132.75	121.70
26	Z	63	LYS	C-N-CA	6.14	132.75	121.70
2	B	260	LEU	N-CA-C	6.07	119.87	112.23
32	f	617	LEU	CA-C-N	6.05	132.59	121.70
32	f	617	LEU	C-N-CA	6.05	132.59	121.70
6	F	164	LEU	CA-C-N	5.95	127.28	119.84
6	F	164	LEU	C-N-CA	5.95	127.28	119.84
32	f	459	GLU	N-CA-CB	-5.91	108.19	114.10
23	W	331	GLY	CA-C-O	-5.90	118.38	122.22
31	e	4	LYS	CD-CE-NZ	5.83	130.57	111.90
22	V	81	GLN	CA-C-N	5.81	132.16	121.70
22	V	81	GLN	C-N-CA	5.81	132.16	121.70
2	B	324	ASP	CA-C-N	5.63	131.84	121.70
2	B	324	ASP	C-N-CA	5.63	131.84	121.70
22	V	316	ALA	CA-C-N	5.60	126.84	119.84
22	V	316	ALA	C-N-CA	5.60	126.84	119.84
32	f	459	GLU	CB-CA-C	-5.58	104.31	109.83
21	U	468	ALA	CB-CA-C	-5.53	109.71	117.23
8	H	231	ALA	CA-C-N	5.50	131.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	231	ALA	C-N-CA	5.50	131.59	121.70
32	f	617	LEU	N-CA-C	5.49	117.12	111.03
8	H	41	ALA	CB-CA-C	-5.47	109.79	117.23
26	Z	222	ILE	N-CA-C	5.45	118.74	111.44
1	A	344	SER	CA-C-N	5.36	131.35	121.70
1	A	344	SER	C-N-CA	5.36	131.35	121.70
27	a	13	ASN	N-CA-C	5.34	117.69	107.75
1	A	247	GLN	CA-C-N	5.25	131.15	121.70
1	A	247	GLN	C-N-CA	5.25	131.15	121.70
32	f	459	GLU	CA-C-O	-5.22	114.90	119.18
22	V	54	LYS	CA-C-N	5.18	131.03	121.70
22	V	54	LYS	C-N-CA	5.18	131.03	121.70
30	d	2	TYR	CB-CA-C	-5.18	110.19	117.23
4	D	389	GLU	CA-C-N	5.14	130.96	121.70
4	D	389	GLU	C-N-CA	5.14	130.96	121.70
1	A	205	GLY	CA-C-N	5.11	130.90	121.70
1	A	205	GLY	C-N-CA	5.11	130.90	121.70
22	V	193	GLN	CB-CA-C	-5.07	110.33	117.23
4	D	354	LEU	CA-C-N	5.07	130.83	121.70
4	D	354	LEU	C-N-CA	5.07	130.83	121.70
27	a	50	PHE	N-CA-C	5.05	117.18	111.11
22	V	80	LYS	CA-C-N	5.05	130.79	121.70
22	V	80	LYS	C-N-CA	5.05	130.79	121.70
7	G	184	LYS	CA-C-N	5.03	130.76	121.70
7	G	184	LYS	C-N-CA	5.03	130.76	121.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	PRO	Peptide
2	B	176	VAL	Peptide
2	B	278	ALA	Peptide
3	C	171	HIS	Peptide
3	C	255	GLY	Peptide
22	V	101	LEU	Peptide
22	V	319	HIS	Peptide
23	W	416	GLN	Peptide
25	Y	357	ASN	Peptide
27	a	286	ALA	Peptide
30	d	3	GLU	Peptide
32	f	459	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2835	0	2879	146	0
2	B	2717	0	2756	132	0
3	C	3015	0	3125	142	0
4	D	3040	0	3076	124	0
5	E	2790	0	2846	110	0
6	F	2863	0	2931	140	0
7	G	1826	0	1796	68	0
8	H	1713	0	1598	30	0
9	I	1912	0	1851	66	0
10	J	1704	0	1517	59	0
11	K	1722	0	1673	106	0
12	L	1850	0	1822	65	0
13	M	1856	0	1814	63	0
14	N	1430	0	1398	29	0
15	O	1643	0	1643	32	0
16	P	1585	0	1597	42	0
17	Q	1570	0	1547	39	0
18	R	1548	0	1499	27	0
19	S	1641	0	1618	32	0
20	T	1667	0	1628	32	0
21	U	6287	0	6338	163	0
22	V	3852	0	3893	201	0
23	W	3703	0	3822	133	0
24	X	1905	0	1951	63	0
25	Y	3115	0	3120	136	0
26	Z	2281	0	2312	122	0
27	a	2995	0	3012	113	0
28	b	1458	0	1505	49	0
29	c	2187	0	2215	113	0
30	d	2116	0	2146	70	0
31	e	334	0	294	47	0
32	f	5331	0	5344	135	0
33	A	31	0	12	1	0
33	D	31	0	12	2	0
33	E	31	0	12	2	0
33	F	31	0	12	2	0
34	c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	76616	0	76614	2472	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 16.

All (2472) 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)
6:F:438:TYR:CZ	6:F:438:TYR:CE2	1.75	1.68
6:F:438:TYR:CZ	6:F:438:TYR:CE1	1.75	1.67
22:V:212:TYR:CZ	22:V:212:TYR:CE2	1.75	1.64
22:V:212:TYR:CZ	22:V:212:TYR:CE1	1.76	1.63
6:F:438:TYR:CE1	6:F:438:TYR:CD1	1.97	1.51
22:V:212:TYR:CE1	22:V:212:TYR:CD1	1.99	1.49
22:V:212:TYR:CE2	22:V:212:TYR:CD2	1.99	1.49
32:f:681:LEU:C	32:f:682:PRO:N	1.68	1.49
6:F:438:TYR:CE2	6:F:438:TYR:CD2	1.98	1.47
27:a:13:ASN:OD1	27:a:19:PRO:HG3	1.41	1.18
27:a:13:ASN:OD1	27:a:19:PRO:CG	1.95	1.13
6:F:438:TYR:CZ	11:K:20:ARG:CG	2.34	1.11
6:F:438:TYR:CE1	11:K:20:ARG:CG	2.35	1.10
22:V:212:TYR:CE1	31:e:4:LYS:CE	2.35	1.10
22:V:212:TYR:CZ	31:e:4:LYS:CE	2.36	1.08
22:V:212:TYR:CD2	31:e:4:LYS:CD	2.37	1.07
6:F:438:TYR:CD2	11:K:20:ARG:CB	2.38	1.06
6:F:438:TYR:CE2	11:K:20:ARG:CG	2.39	1.05
22:V:212:TYR:CE2	31:e:4:LYS:CE	2.39	1.04
22:V:212:TYR:CD1	31:e:4:LYS:CE	2.40	1.04
22:V:212:TYR:CE2	31:e:4:LYS:CD	2.41	1.04
6:F:438:TYR:CD1	11:K:20:ARG:CB	2.43	1.02
6:F:438:TYR:CD1	11:K:20:ARG:CG	2.43	1.01
22:V:212:TYR:CD1	31:e:4:LYS:CD	2.43	1.01
6:F:438:TYR:CE2	11:K:20:ARG:CB	2.42	1.01
22:V:212:TYR:CD2	31:e:4:LYS:CE	2.44	1.01
6:F:438:TYR:CZ	11:K:20:ARG:HG2	1.94	1.00
6:F:438:TYR:CD2	11:K:20:ARG:HB3	1.97	1.00
22:V:212:TYR:CG	31:e:4:LYS:CD	2.44	1.00
6:F:438:TYR:CG	11:K:20:ARG:CB	2.45	0.99
22:V:212:TYR:CZ	31:e:4:LYS:CD	2.46	0.99
6:F:438:TYR:CZ	11:K:20:ARG:CB	2.47	0.97
22:V:212:TYR:CG	31:e:4:LYS:CE	2.48	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:438:TYR:CE1	11:K:20:ARG:CB	2.46	0.97
22:V:212:TYR:CE1	31:e:4:LYS:CD	2.47	0.96
6:F:438:TYR:CD2	11:K:20:ARG:CG	2.49	0.96
22:V:212:TYR:CZ	31:e:4:LYS:HE2	2.02	0.93
6:F:438:TYR:CG	11:K:20:ARG:CG	2.53	0.92
6:F:438:TYR:CD1	11:K:20:ARG:HB2	2.03	0.91
22:V:212:TYR:CG	31:e:4:LYS:HD2	2.07	0.90
6:F:438:TYR:CD1	11:K:20:ARG:HG3	2.07	0.90
22:V:212:TYR:CE1	31:e:4:LYS:HE3	2.08	0.89
23:W:40:LEU:HB2	23:W:41:GLN:HA	1.56	0.87
32:f:617:LEU:HB3	32:f:618:THR:HB	1.57	0.86
9:I:33:THR:H	9:I:64:LYS:HZ3	1.23	0.86
8:H:231:ALA:HB3	8:H:232:ALA:HB3	1.55	0.85
4:D:389:GLU:HA	4:D:390:ASN:HB2	1.57	0.84
3:C:214:VAL:HG21	3:C:249:ASP:H	1.41	0.83
17:Q:8:GLN:HE21	17:Q:115:LEU:HB2	1.43	0.83
22:V:212:TYR:CE2	31:e:4:LYS:HD3	2.12	0.82
32:f:615:GLY:HA2	32:f:619:LEU:H	1.43	0.82
2:B:230:THR:HG23	2:B:353:PHE:HB3	1.60	0.82
23:W:416:GLN:HB3	23:W:417:ARG:HA	1.61	0.82
22:V:212:TYR:CD2	31:e:4:LYS:HD3	2.15	0.82
1:A:333:ARG:HH12	1:A:340:LYS:HD3	1.43	0.82
4:D:100:THR:HB	4:D:114:ARG:HD2	1.63	0.81
29:c:273:LYS:HD2	29:c:274:ASN:HB2	1.61	0.81
6:F:165:PRO:HB2	6:F:166:THR:HG22	1.63	0.80
4:D:354:LEU:HA	4:D:355:SER:HB3	1.62	0.80
2:B:265:LYS:HD3	3:C:227:GLY:HA3	1.63	0.80
11:K:225:ASN:HA	11:K:227:HIS:HB3	1.62	0.80
22:V:212:TYR:CD1	31:e:4:LYS:HE3	2.16	0.80
29:c:272:ILE:HG21	29:c:276:GLY:H	1.47	0.80
2:B:176:VAL:HG22	2:B:177:GLU:HA	1.63	0.79
21:U:361:ARG:HG3	21:U:365:CYS:HB2	1.64	0.79
22:V:81:GLN:HB3	22:V:82:LEU:C	2.07	0.79
4:D:104:GLY:HA2	4:D:110:ASN:HA	1.65	0.79
22:V:212:TYR:CE2	31:e:4:LYS:HE2	2.17	0.78
8:H:92:LYS:HG2	15:O:65:LEU:HD21	1.65	0.78
22:V:212:TYR:CD1	31:e:4:LYS:HD2	2.19	0.78
5:E:191:LEU:HD21	5:E:227:PRO:HG2	1.64	0.78
5:E:174:GLY:HA2	5:E:176:PRO:HD2	1.65	0.78
5:E:372:ARG:NH2	13:M:168:ALA:O	2.16	0.78
29:c:211:GLU:HA	29:c:214:GLN:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:256:LEU:HB2	6:F:306:VAL:HG22	1.66	0.78
22:V:57:ALA:HB3	22:V:58:ALA:HB3	1.64	0.78
3:C:187:LEU:HA	3:C:293:MET:HB3	1.67	0.77
1:A:103:ASN:ND2	6:F:169:ASP:OD1	2.17	0.77
23:W:92:LYS:H	23:W:93:ARG:HB3	1.49	0.77
9:I:167:ASN:ND2	9:I:200:THR:O	2.17	0.76
32:f:450:VAL:HG21	32:f:473:LYS:HB2	1.67	0.76
6:F:92:ASN:HB3	6:F:125:LYS:HB2	1.66	0.76
6:F:299:GLU:HB3	6:F:300:LYS:HB2	1.68	0.76
22:V:99:ARG:HH22	22:V:147:PHE:H	1.34	0.76
4:D:293:LEU:O	4:D:326:ARG:NH1	2.20	0.75
5:E:113:ARG:HH11	5:E:220:ASN:HD21	1.34	0.75
24:X:370:LEU:HD13	25:Y:306:GLN:HB2	1.68	0.74
4:D:348:ILE:HG21	4:D:379:CYS:HB3	1.68	0.74
17:Q:4:LEU:HD22	17:Q:17:SER:HA	1.68	0.74
21:U:173:VAL:HG13	21:U:176:MET:HB2	1.70	0.74
8:H:39:LYS:HE2	8:H:144:PRO:HG2	1.69	0.74
25:Y:170:GLU:HG3	25:Y:171:GLY:HA3	1.70	0.74
6:F:137:ILE:HG21	6:F:160:ILE:HB	1.69	0.73
21:U:799:LYS:HA	21:U:843:GLU:HG3	1.69	0.73
1:A:170:PRO:HA	1:A:229:VAL:HG12	1.70	0.73
9:I:2:SER:N	12:L:123:TYR:HH	1.85	0.73
21:U:424:ALA:HA	21:U:427:LEU:HD13	1.69	0.73
22:V:255:LEU:HD22	22:V:291:TYR:HB3	1.70	0.73
1:A:312:ARG:HG3	1:A:336:ARG:HH11	1.53	0.73
32:f:503:MET:SD	32:f:669:ARG:NH1	2.62	0.73
21:U:337:LEU:HD13	21:U:789:ILE:HG12	1.70	0.73
14:N:75:LEU:HD13	14:N:78:THR:HB	1.71	0.73
32:f:662:LEU:H	32:f:664:ALA:HA	1.53	0.72
12:L:67:ASP:HB3	12:L:70:ILE:HB	1.71	0.72
11:K:10:ARG:NH2	12:L:7:ASP:O	2.21	0.72
15:O:8:TYR:HA	15:O:145:ASP:HB2	1.70	0.72
9:I:100:GLN:HG3	17:Q:86:ARG:HG3	1.70	0.72
29:c:272:ILE:HG13	29:c:275:VAL:HG23	1.70	0.72
27:a:34:TRP:HD1	28:b:19:GLY:H	1.38	0.72
32:f:296:VAL:HG12	32:f:297:ARG:HG2	1.71	0.72
29:c:272:ILE:HD12	29:c:277:LYS:HB3	1.72	0.72
4:D:387:VAL:HG11	5:E:167:PRO:HD3	1.72	0.72
21:U:413:LYS:HA	21:U:449:ILE:HG12	1.71	0.72
24:X:366:SER:HB2	25:Y:310:SER:HB3	1.71	0.72
3:C:258:ARG:HD2	3:C:260:GLU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:303:VAL:HG23	4:D:304:ASN:HB2	1.71	0.72
24:X:416:ASN:OD1	29:c:273:LYS:NZ	2.23	0.72
6:F:357:PRO:O	6:F:362:ARG:NH1	2.22	0.72
26:Z:102:HIS:HD2	26:Z:104:ASN:HB3	1.52	0.72
1:A:315:ILE:HD12	1:A:317:VAL:H	1.53	0.72
24:X:229:TYR:OH	24:X:258:LYS:NZ	2.23	0.72
25:Y:101:ARG:HB3	25:Y:130:LYS:HD3	1.72	0.72
32:f:65:ASN:ND2	32:f:115:ASP:OD1	2.23	0.71
18:R:52:CYS:HA	18:R:97:MET:HE3	1.72	0.71
25:Y:190:ALA:O	25:Y:291:HIS:NE2	2.23	0.71
2:B:436:GLU:H	2:B:437:GLY:C	1.98	0.71
3:C:229:ARG:HH11	3:C:232:ARG:HH11	1.35	0.71
9:I:154:GLY:O	10:J:81:ARG:NH1	2.24	0.71
23:W:417:ARG:NH1	23:W:420:ASP:OD1	2.23	0.71
27:a:286:ALA:HB1	27:a:287:ASN:HA	1.72	0.71
4:D:270:ILE:HG22	5:E:251:ARG:HH21	1.55	0.71
30:d:215:TRP:CD1	30:d:216:VAL:H	2.08	0.71
27:a:188:LEU:HD11	27:a:193:GLN:HG3	1.72	0.71
13:M:34:SER:OG	13:M:65:ARG:NH1	2.24	0.71
32:f:361:LEU:HD13	32:f:398:TRP:HB3	1.71	0.71
26:Z:176:LEU:HD12	26:Z:177:ARG:H	1.54	0.71
23:W:44:ILE:HB	23:W:93:ARG:HD2	1.73	0.70
30:d:12:LYS:HG2	30:d:57:ILE:HD11	1.73	0.70
29:c:261:GLU:HA	29:c:264:LYS:HG2	1.73	0.70
25:Y:101:ARG:HE	25:Y:127:THR:HA	1.56	0.70
27:a:244:ASN:ND2	27:a:272:ILE:O	2.23	0.70
30:d:3:GLU:HB3	30:d:4:GLN:HA	1.73	0.70
22:V:447:ILE:HG13	22:V:449:ALA:H	1.56	0.70
24:X:225:TRP:HB3	24:X:261:LEU:HG	1.72	0.70
28:b:15:TYR:O	28:b:25:ARG:NH1	2.24	0.70
1:A:80:LEU:HD23	2:B:137:SER:HB3	1.73	0.70
23:W:257:GLN:HA	23:W:258:ALA:HB3	1.72	0.70
22:V:80:LYS:HA	22:V:81:GLN:HB2	1.73	0.70
23:W:436:MET:O	23:W:440:ASN:ND2	2.22	0.70
5:E:175:PRO:HD2	5:E:387:LYS:HE3	1.74	0.70
21:U:510:GLU:OE2	21:U:546:ARG:NH2	2.25	0.70
22:V:416:ARG:HG3	22:V:459:GLN:HA	1.73	0.70
30:d:147:SER:HA	30:d:148:TYR:HB2	1.74	0.69
32:f:371:CYS:SG	32:f:372:ASN:N	2.65	0.69
6:F:153:VAL:HB	6:F:160:ILE:HG13	1.74	0.69
25:Y:357:ASN:HB2	25:Y:359:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:PRO:HA	3:C:172:PRO:HG3	1.74	0.69
24:X:417:LYS:HD3	25:Y:383:LEU:HD23	1.74	0.69
4:D:105:SER:O	4:D:245:ARG:NH1	2.25	0.69
8:H:71:HIS:HA	8:H:218:PHE:H	1.56	0.69
23:W:91:SER:HB2	23:W:92:LYS:HD2	1.73	0.69
6:F:438:TYR:CE1	11:K:20:ARG:HG3	2.28	0.69
22:V:455:LYS:N	22:V:456:GLY:HA2	2.07	0.69
1:A:157:ILE:HG23	1:A:158:ASP:HB2	1.75	0.69
2:B:105:THR:HG23	2:B:106:PRO:HD3	1.74	0.69
8:H:40:ALA:HB1	8:H:182:LEU:H	1.57	0.69
22:V:283:ASN:HB2	22:V:317:PRO:HD2	1.75	0.69
26:Z:244:GLU:HG2	27:a:287:ASN:H	1.58	0.69
30:d:214:GLY:N	30:d:215:TRP:HB3	2.08	0.69
32:f:391:LEU:HD12	32:f:392:LYS:H	1.57	0.69
17:Q:59:TYR:O	17:Q:63:ASN:ND2	2.22	0.69
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.74	0.69
7:G:63:SER:O	7:G:67:THR:OG1	2.11	0.68
25:Y:111:LEU:HA	25:Y:114:ILE:HD13	1.75	0.68
1:A:102:ILE:HA	1:A:113:ILE:HA	1.74	0.68
16:P:105:THR:HG23	16:P:107:PRO:HD3	1.75	0.68
25:Y:77:ASN:O	25:Y:81:LEU:N	2.27	0.68
6:F:84:LYS:HA	6:F:161:LEU:HD22	1.74	0.68
22:V:440:LYS:NZ	30:d:143:LEU:O	2.27	0.68
25:Y:64:GLN:HG2	25:Y:65:ILE:HG22	1.75	0.68
25:Y:358:ARG:HD2	25:Y:359:PRO:HD2	1.76	0.68
13:M:92:ARG:NH2	20:T:73:ASP:OD1	2.27	0.68
1:A:258:ARG:HD2	6:F:255:GLN:HE22	1.59	0.68
1:A:100:LYS:HZ3	1:A:140:VAL:HG23	1.59	0.68
6:F:221:LYS:HD2	6:F:327:LYS:HG3	1.76	0.68
27:a:286:ALA:HA	27:a:288:HIS:HB2	1.76	0.68
5:E:138:LEU:HD22	5:E:140:GLU:HG2	1.76	0.68
22:V:212:TYR:OH	22:V:287:ARG:NH2	2.26	0.68
21:U:842:LYS:HA	21:U:843:GLU:HB3	1.74	0.68
24:X:406:ASN:HA	24:X:409:LYS:HD3	1.75	0.68
2:B:372:MET:HB3	3:C:179:GLY:HA2	1.76	0.67
17:Q:168:GLN:NE2	17:Q:174:ASN:O	2.26	0.67
19:S:168:LEU:HD23	19:S:169:ASP:H	1.59	0.67
27:a:270:ARG:NH1	27:a:310:LEU:O	2.27	0.67
28:b:12:ASN:ND2	28:b:53:THR:OG1	2.27	0.67
2:B:166:ASP:HB3	2:B:167:THR:HA	1.75	0.67
6:F:314:LEU:HD21	6:F:342:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:35:THR:HA	13:M:166:GLY:HA3	1.75	0.67
24:X:252:LYS:HD3	24:X:287:LEU:HD21	1.75	0.67
25:Y:145:LEU:HG	25:Y:160:ASN:HD21	1.59	0.67
18:R:19:ARG:HE	18:R:29:GLN:HE22	1.43	0.67
23:W:90:LEU:HA	23:W:94:ARG:HD2	1.75	0.67
9:I:198:ASN:HB2	9:I:206:LEU:HD12	1.75	0.67
27:a:13:ASN:OD1	27:a:19:PRO:CB	2.43	0.67
6:F:188:ILE:HD11	6:F:195:ILE:HD12	1.76	0.67
6:F:427:VAL:HA	6:F:431:LYS:HZ2	1.59	0.67
2:B:217:LYS:HG3	2:B:219:PRO:HD3	1.76	0.67
12:L:38:LEU:HD11	12:L:187:LEU:HD11	1.77	0.67
15:O:17:ASP:O	15:O:33:LYS:NZ	2.28	0.67
19:S:55:SER:HB3	19:S:107:TYR:HB2	1.75	0.67
7:G:132:ARG:NH1	13:M:11:ALA:O	2.28	0.67
21:U:212:ASP:O	21:U:215:ASN:ND2	2.28	0.67
27:a:13:ASN:CG	27:a:19:PRO:HG3	2.19	0.67
4:D:89:ILE:HD11	5:E:80:VAL:HG13	1.77	0.66
26:Z:111:LEU:HD12	28:b:59:GLU:HB3	1.75	0.66
23:W:430:GLN:O	23:W:434:SER:OG	2.14	0.66
5:E:223:ARG:O	5:E:226:GLN:NE2	2.28	0.66
22:V:294:ARG:HH21	22:V:331:LEU:HD23	1.60	0.66
27:a:197:ALA:HA	27:a:200:LEU:HB3	1.78	0.66
10:J:196:LEU:O	10:J:201:SER:OG	2.12	0.66
21:U:112:CYS:SG	21:U:159:ARG:NH1	2.68	0.66
21:U:155:LEU:O	21:U:158:ARG:NH1	2.28	0.66
31:e:58:ALA:HB3	31:e:59:GLU:HA	1.77	0.66
7:G:30:LYS:HG3	13:M:18:GLY:HA3	1.76	0.66
30:d:147:SER:OG	30:d:151:VAL:N	2.22	0.66
32:f:399:LEU:HD23	32:f:418:LEU:HD21	1.78	0.66
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.76	0.66
13:M:46:VAL:HG22	13:M:215:TRP:HD1	1.61	0.66
23:W:331:GLY:HA2	23:W:332:SER:HB3	1.78	0.66
23:W:427:ASP:HB3	29:c:245:VAL:HG21	1.78	0.66
27:a:320:VAL:HG22	27:a:322:GLY:H	1.60	0.66
32:f:372:ASN:N	32:f:373:GLY:HA2	2.11	0.66
1:A:304:ASN:HD21	6:F:252:ALA:HB1	1.61	0.66
5:E:171:LEU:HB2	5:E:295:LEU:HD22	1.78	0.66
20:T:54:SER:HB2	20:T:109:THR:HB	1.78	0.66
23:W:397:VAL:HG13	24:X:341:PRO:HB2	1.78	0.65
32:f:154:GLU:HB3	32:f:184:LYS:HD3	1.78	0.65
2:B:197:ILE:HG21	2:B:234:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:VAL:HG11	5:E:105:LEU:HB2	1.78	0.65
5:E:266:GLY:HA2	5:E:267:PHE:HB2	1.77	0.65
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.77	0.65
32:f:294:SER:O	32:f:298:ASN:ND2	2.29	0.65
3:C:153:GLY:HA3	3:C:324:ALA:HA	1.79	0.65
23:W:123:ARG:HH12	23:W:127:THR:HB	1.62	0.65
9:I:174:MET:SD	9:I:195:LYS:NZ	2.69	0.65
23:W:219:THR:HA	23:W:220:GLU:HB2	1.79	0.65
5:E:206:LYS:NZ	6:F:263:ASP:OD1	2.26	0.65
32:f:311:VAL:HB	32:f:319:ARG:HG2	1.78	0.65
2:B:103:ARG:HD3	2:B:160:ILE:HG12	1.79	0.65
11:K:71:ASP:HB3	11:K:74:ILE:HB	1.78	0.65
22:V:266:GLN:HB3	22:V:299:GLN:HE22	1.61	0.65
25:Y:312:ARG:HA	25:Y:356:THR:HG22	1.78	0.65
12:L:10:VAL:HG13	12:L:21:GLN:HG3	1.79	0.65
21:U:327:LYS:HE3	21:U:333:MET:HE2	1.78	0.65
21:U:338:HIS:CD2	21:U:785:PRO:HB2	2.32	0.65
2:B:221:GLY:O	2:B:346:ARG:NE	2.28	0.65
5:E:83:CYS:HB3	5:E:87:LEU:HD21	1.78	0.65
12:L:41:LYS:HG3	12:L:180:MET:HB3	1.78	0.65
4:D:411:GLU:OE1	4:D:412:GLN:NE2	2.30	0.65
26:Z:168:GLU:HA	29:c:42:LEU:HD13	1.79	0.65
1:A:306:LEU:O	1:A:336:ARG:NE	2.29	0.64
5:E:277:MET:HB2	5:E:295:LEU:HD21	1.78	0.64
9:I:17:ARG:HD2	9:I:22:GLU:HG3	1.79	0.64
21:U:540:GLN:OE1	29:c:68:ARG:NH1	2.30	0.64
25:Y:51:ALA:HA	25:Y:54:TYR:HB2	1.79	0.64
3:C:270:GLN:HA	3:C:273:MET:HE3	1.79	0.64
15:O:143:ARG:HH12	15:O:146:MET:HG2	1.62	0.64
19:S:193:LEU:HB3	19:S:208:VAL:HB	1.80	0.64
22:V:101:LEU:O	22:V:103:SER:N	2.31	0.64
1:A:100:LYS:NZ	1:A:141:GLY:O	2.30	0.64
1:A:246:VAL:HG23	2:B:260:LEU:HD23	1.79	0.64
8:H:231:ALA:H	8:H:232:ALA:C	2.05	0.64
23:W:442:THR:HB	29:c:229:LEU:HD11	1.80	0.64
12:L:137:TYR:HE2	12:L:215:VAL:HG13	1.63	0.64
24:X:242:ILE:HG22	24:X:243:ASP:H	1.63	0.64
4:D:374:ASP:HB3	4:D:378:ILE:HD12	1.79	0.64
22:V:99:ARG:NH1	22:V:144:ASP:O	2.31	0.64
26:Z:14:LEU:HG	29:c:39:LEU:HD22	1.80	0.64
29:c:229:LEU:HD22	29:c:231:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:301:ASP:OD1	32:f:301:ASP:N	2.27	0.64
1:A:293:ASN:HB2	6:F:295:ARG:HH11	1.61	0.64
9:I:119:GLN:HE22	10:J:79:ASP:HA	1.62	0.64
22:V:197:THR:HG21	22:V:200:ARG:HG3	1.78	0.64
4:D:91:GLN:O	4:D:104:GLY:N	2.31	0.64
4:D:204:MET:HE3	4:D:310:ALA:HB2	1.80	0.64
3:C:164:VAL:O	3:C:290:LYS:NZ	2.28	0.63
10:J:38:ARG:HH22	10:J:182:GLU:HA	1.63	0.63
25:Y:98:SER:HA	25:Y:130:LYS:HD2	1.79	0.63
29:c:124:GLY:O	29:c:128:ASN:ND2	2.30	0.63
3:C:69:GLN:HB2	3:C:118:ASN:HB2	1.80	0.63
5:E:91:LYS:HD2	5:E:107:ILE:HB	1.80	0.63
1:A:345:LEU:HG	1:A:346:PRO:HD2	1.79	0.63
3:C:213:ARG:HG3	3:C:214:VAL:HG12	1.80	0.63
14:N:41:ILE:HG12	14:N:76:VAL:HG22	1.80	0.63
26:Z:16:LEU:HD11	26:Z:135:THR:HG21	1.79	0.63
32:f:629:MET:HE2	32:f:649:ASN:HD21	1.62	0.63
2:B:248:LEU:HD22	2:B:273:VAL:HG11	1.79	0.63
3:C:259:LEU:HD23	3:C:263:SER:HB3	1.79	0.63
13:M:99:ARG:HB3	20:T:69:GLN:HE22	1.64	0.63
11:K:164:GLN:HB3	12:L:58:ALA:HB3	1.81	0.63
22:V:252:ASN:ND2	22:V:284:GLU:OE2	2.31	0.63
26:Z:202:ASN:OD1	26:Z:203:SER:N	2.31	0.63
28:b:19:GLY:HA2	28:b:24:THR:HA	1.80	0.63
13:M:169:ARG:HD3	13:M:201:HIS:HB2	1.81	0.63
17:Q:60:ILE:HD12	17:Q:84:THR:HG22	1.78	0.63
22:V:211:TYR:HB3	22:V:253:LEU:HD11	1.81	0.63
25:Y:138:LEU:HD23	25:Y:176:ARG:HB2	1.80	0.63
26:Z:212:LEU:HB2	27:a:350:LYS:HD2	1.80	0.63
1:A:346:PRO:HD3	1:A:381:THR:HA	1.79	0.63
2:B:218:PRO:HB2	2:B:346:ARG:HH12	1.64	0.63
4:D:50:GLU:HA	4:D:53:PHE:HB2	1.80	0.63
11:K:13:ASN:HD21	12:L:126:ARG:HH11	1.47	0.63
12:L:18:ARG:NH1	12:L:23:GLU:OE2	2.32	0.63
22:V:346:LEU:O	31:e:43:TRP:NE1	2.29	0.63
23:W:312:MET:SD	23:W:361:HIS:ND1	2.72	0.63
26:Z:245:PHE:O	26:Z:249:PHE:N	2.32	0.63
30:d:49:ILE:HD11	30:d:89:LEU:HD22	1.81	0.63
10:J:81:ARG:O	10:J:85:ASN:ND2	2.32	0.63
15:O:177:VAL:HB	15:O:184:ASP:HB2	1.81	0.63
22:V:275:VAL:H	22:V:276:PHE:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:139:GLU:HA	27:a:142:LEU:HB3	1.80	0.63
10:J:211:MET:HB2	10:J:217:LEU:HD23	1.81	0.62
11:K:74:ILE:HD11	11:K:109:VAL:H	1.64	0.62
26:Z:142:GLU:OE2	26:Z:153:LYS:NZ	2.32	0.62
22:V:80:LYS:HE2	22:V:87:SER:HA	1.81	0.62
2:B:411:ARG:HG2	2:B:412:MET:HG2	1.81	0.62
4:D:373:ALA:HA	4:D:374:ASP:HB2	1.80	0.62
22:V:266:GLN:O	22:V:269:LYS:NZ	2.32	0.62
23:W:76:GLU:HA	23:W:79:GLU:HB2	1.81	0.62
29:c:160:PHE:HA	29:c:202:SER:HA	1.81	0.62
2:B:252:GLY:O	2:B:257:GLN:NE2	2.33	0.62
11:K:16:SER:O	11:K:19:GLY:HA3	2.00	0.62
11:K:104:ASN:ND2	19:S:130:TYR:OH	2.33	0.62
22:V:353:LEU:HG	22:V:357:LEU:HD23	1.81	0.62
22:V:415:SER:O	22:V:460:SER:OG	2.16	0.62
27:a:230:ARG:HE	27:a:233:LEU:HD22	1.65	0.62
1:A:122:VAL:HG23	6:F:90:VAL:HG22	1.81	0.62
3:C:111:ASN:O	3:C:129:ASN:ND2	2.32	0.62
6:F:83:ASN:O	6:F:154:ASN:ND2	2.32	0.62
6:F:280:PRO:HB3	6:F:326:VAL:HA	1.82	0.62
7:G:43:ARG:HH11	7:G:150:GLN:HA	1.62	0.62
2:B:139:VAL:HA	2:B:140:ASP:HB3	1.81	0.62
2:B:408:ARG:O	2:B:410:ARG:NH1	2.33	0.62
6:F:224:LEU:HB3	6:F:351:LYS:HG2	1.80	0.62
17:Q:38:MET:O	17:Q:65:GLN:NE2	2.33	0.62
21:U:773:PHE:O	21:U:776:SER:OG	2.18	0.62
25:Y:190:ALA:HA	25:Y:287:LEU:HD13	1.82	0.62
30:d:235:THR:HG22	30:d:237:ILE:H	1.63	0.62
1:A:112:ILE:HD12	6:F:150:LEU:HG	1.81	0.61
10:J:81:ARG:HA	10:J:84:ILE:HB	1.82	0.61
22:V:321:ALA:HB1	22:V:322:VAL:HB	1.81	0.61
23:W:78:LYS:HA	23:W:81:ASP:HB3	1.81	0.61
25:Y:138:LEU:HD12	25:Y:141:VAL:HB	1.82	0.61
32:f:369:GLY:O	32:f:372:ASN:ND2	2.32	0.61
3:C:214:VAL:HG22	3:C:215:SER:H	1.65	0.61
4:D:64:GLU:HB2	21:U:603:LEU:HD11	1.81	0.61
4:D:247:VAL:HG21	4:D:288:ILE:HG23	1.82	0.61
26:Z:199:LYS:HD3	26:Z:202:ASN:HD21	1.65	0.61
32:f:108:ARG:HH21	32:f:141:ARG:HD3	1.64	0.61
32:f:339:LEU:HD12	32:f:340:THR:HG23	1.82	0.61
25:Y:293:ARG:NH1	31:e:49:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:226:ARG:HB3	27:a:234:ILE:HG12	1.82	0.61
9:I:206:LEU:HD13	9:I:237:ILE:HG23	1.81	0.61
26:Z:208:ILE:HD11	27:a:350:LYS:HA	1.82	0.61
27:a:290:GLN:HE21	27:a:330:ARG:HB2	1.65	0.61
22:V:99:ARG:HB2	22:V:104:THR:HG22	1.82	0.61
22:V:337:LEU:O	22:V:401:ASN:ND2	2.33	0.61
23:W:55:ARG:NH1	23:W:75:TYR:O	2.33	0.61
26:Z:193:ASN:HB3	29:c:307:VAL:HG11	1.81	0.61
1:A:141:GLY:N	1:A:151:ILE:O	2.29	0.61
2:B:440:LEU:HG	10:J:29:GLY:HA2	1.82	0.61
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.81	0.61
22:V:241:ARG:HG3	22:V:242:HIS:H	1.65	0.61
25:Y:349:LYS:HG3	25:Y:350:VAL:HG13	1.82	0.61
24:X:251:LEU:HA	24:X:254:MET:HG2	1.83	0.61
30:d:78:LEU:HA	30:d:81:TYR:HD2	1.65	0.61
6:F:438:TYR:CG	11:K:20:ARG:HB2	2.32	0.61
7:G:211:LYS:NZ	7:G:213:SER:OG	2.27	0.61
27:a:287:ASN:HB3	27:a:289:ARG:HB2	1.82	0.61
3:C:246:ILE:HB	3:C:291:VAL:HG12	1.83	0.61
6:F:256:LEU:HD12	6:F:306:VAL:HG13	1.83	0.61
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.83	0.61
19:S:35:ILE:H	20:T:151:ARG:HH22	1.47	0.61
22:V:62:HIS:HA	22:V:65:ARG:HB3	1.81	0.61
27:a:34:TRP:H	28:b:18:ASN:HB2	1.65	0.61
30:d:131:VAL:HG23	30:d:134:LYS:HE2	1.83	0.61
32:f:20:VAL:HG12	32:f:24:PRO:HD3	1.81	0.61
14:N:5:ALA:HB3	14:N:126:ALA:HB3	1.81	0.61
3:C:214:VAL:HG11	3:C:249:ASP:HB3	1.83	0.60
2:B:313:LEU:O	2:B:317:ASP:N	2.34	0.60
6:F:438:TYR:CE1	11:K:20:ARG:HG2	2.32	0.60
22:V:54:LYS:N	22:V:55:THR:OG1	2.33	0.60
23:W:224:LEU:O	23:W:253:THR:OG1	2.19	0.60
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	1.81	0.60
28:b:164:ASP:N	28:b:165:GLY:HA2	2.15	0.60
31:e:1:MET:H3	31:e:2:SER:HA	1.66	0.60
22:V:416:ARG:HH12	22:V:418:SER:HB2	1.65	0.60
23:W:220:GLU:N	23:W:221:LYS:HA	2.15	0.60
27:a:290:GLN:HA	27:a:332:HIS:HA	1.82	0.60
30:d:215:TRP:CG	30:d:216:VAL:H	2.19	0.60
32:f:335:ARG:N	32:f:336:GLU:OE1	2.30	0.60
1:A:264:ALA:O	1:A:268:LYS:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:12:LEU:HB2	21:U:44:LYS:HE3	1.83	0.60
23:W:397:VAL:HG21	24:X:342:PHE:HB3	1.83	0.60
24:X:262:ASN:HD21	24:X:326:LEU:HG	1.66	0.60
3:C:157:GLN:NE2	3:C:316:GLU:O	2.34	0.60
4:D:130:VAL:HB	4:D:142:VAL:HG12	1.82	0.60
10:J:116:GLN:NE2	10:J:150:SER:O	2.34	0.60
24:X:406:ASN:HD21	29:c:264:LYS:HD2	1.64	0.60
15:O:209:THR:HG21	16:P:168:SER:HB3	1.82	0.60
21:U:789:ILE:HG22	21:U:791:LEU:H	1.65	0.60
27:a:125:ILE:N	27:a:126:GLY:HA2	2.17	0.60
31:e:63:HIS:HA	31:e:66:LYS:HE2	1.81	0.60
2:B:170:LEU:HD22	2:B:265:LYS:HE3	1.84	0.60
2:B:401:GLU:HA	2:B:404:LEU:HB3	1.83	0.60
8:H:32:GLY:HA3	8:H:78:GLY:HA2	1.83	0.60
10:J:154:HIS:HE1	11:K:60:GLU:H	1.49	0.60
19:S:145:LEU:HD21	19:S:178:VAL:HG21	1.84	0.60
5:E:334:LEU:HD23	5:E:372:ARG:HB2	1.83	0.60
16:P:58:THR:OG1	17:Q:121:LEU:O	2.17	0.60
7:G:144:ASP:HB3	7:G:147:GLN:HB2	1.84	0.60
23:W:135:LYS:HB3	23:W:136:ILE:HB	1.83	0.60
30:d:227:SER:C	30:d:229:GLN:HA	2.26	0.60
32:f:62:ILE:HD12	32:f:99:LYS:HB3	1.84	0.60
11:K:235:GLU:HA	11:K:238:ILE:HD12	1.84	0.60
24:X:332:GLU:HA	24:X:335:LEU:HB2	1.82	0.60
21:U:14:GLU:HG2	21:U:16:GLU:H	1.67	0.59
22:V:262:SER:HB2	22:V:263:LEU:HB2	1.82	0.59
3:C:11:LEU:N	21:U:144:ASP:OD2	2.35	0.59
4:D:370:ILE:HD13	4:D:404:LYS:HA	1.83	0.59
17:Q:85:ARG:HB2	17:Q:124:LEU:HD11	1.82	0.59
21:U:189:GLN:NE2	21:U:595:ASN:OD1	2.31	0.59
24:X:346:GLN:HE21	24:X:349:HIS:HB2	1.67	0.59
26:Z:97:THR:HA	26:Z:124:ILE:HG13	1.83	0.59
29:c:131:GLN:HA	29:c:134:GLU:HG2	1.85	0.59
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.85	0.59
23:W:125:ILE:HD12	23:W:128:LEU:HD12	1.84	0.59
23:W:431:LYS:O	23:W:435:LEU:HB2	2.02	0.59
26:Z:54:PHE:HB3	26:Z:82:PHE:HE2	1.67	0.59
26:Z:222:ILE:HG23	26:Z:224:HIS:HB2	1.85	0.59
1:A:339:ARG:NH2	6:F:402:GLU:OE1	2.35	0.59
23:W:92:LYS:N	23:W:93:ARG:HB3	2.15	0.59
23:W:187:LEU:HA	23:W:190:MET:HE3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:GLU:HB3	2:B:437:GLY:HA3	1.85	0.59
3:C:297:ARG:HG3	3:C:298:ILE:H	1.68	0.59
7:G:111:VAL:HG11	7:G:144:ASP:HB2	1.83	0.59
21:U:94:SER:OG	21:U:95:GLU:OE1	2.19	0.59
22:V:486:ILE:HD13	25:Y:377:LEU:HD22	1.84	0.59
4:D:391:ARG:HG2	4:D:395:LEU:HG	1.85	0.59
21:U:39:SER:HA	21:U:67:VAL:HG23	1.85	0.59
21:U:524:LYS:HE3	21:U:556:MET:HA	1.83	0.59
1:A:222:LYS:HD2	2:B:319:PHE:HB2	1.84	0.59
3:C:158:ILE:HA	3:C:161:ILE:HG22	1.84	0.59
6:F:87:PRO:HB2	6:F:152:GLY:HA3	1.84	0.59
23:W:235:GLN:NE2	23:W:247:TYR:OH	2.36	0.59
25:Y:101:ARG:NH2	25:Y:126:LYS:O	2.35	0.59
1:A:357:ILE:HG13	1:A:360:ARG:HH21	1.68	0.59
16:P:49:LEU:HG	16:P:111:GLY:HA3	1.84	0.59
22:V:349:ARG:HG3	22:V:357:LEU:HD21	1.84	0.59
26:Z:204:LYS:HE3	27:a:353:LEU:HG	1.85	0.59
30:d:233:GLU:N	30:d:234:ASP:HA	2.16	0.59
32:f:600:LEU:HD13	32:f:600:LEU:H	1.67	0.59
32:f:615:GLY:HA2	32:f:619:LEU:N	2.16	0.59
7:G:14:THR:HG22	7:G:24:GLN:HG3	1.83	0.59
11:K:225:ASN:HB2	11:K:226:PHE:CG	2.38	0.59
24:X:203:PRO:HB3	24:X:206:LEU:HB2	1.85	0.59
30:d:145:GLU:N	30:d:146:GLY:HA2	2.17	0.59
1:A:281:GLY:HA2	1:A:299:MET:HB3	1.83	0.59
13:M:40:ARG:NH1	13:M:160:TYR:O	2.36	0.59
22:V:331:LEU:HD12	22:V:334:VAL:HG21	1.85	0.59
32:f:414:ILE:HG13	32:f:417:ILE:HD11	1.85	0.59
11:K:18:GLU:HB2	11:K:19:GLY:HA2	1.84	0.58
15:O:8:TYR:HE2	15:O:13:VAL:HG23	1.69	0.58
32:f:676:GLU:HB3	32:f:691:VAL:HG22	1.84	0.58
1:A:381:THR:OG1	2:B:343:ARG:NH1	2.37	0.58
3:C:127:LEU:HD22	4:D:96:VAL:HG11	1.85	0.58
4:D:411:GLU:HB3	4:D:412:GLN:HB2	1.85	0.58
21:U:376:MET:HA	21:U:741:GLY:H	1.67	0.58
23:W:16:MET:HG2	23:W:27:ARG:HH22	1.67	0.58
24:X:255:LEU:HD12	24:X:287:LEU:HB3	1.85	0.58
25:Y:81:LEU:HD12	25:Y:111:LEU:HD13	1.85	0.58
26:Z:63:LYS:HB2	26:Z:64:ASP:HB2	1.84	0.58
32:f:662:LEU:N	32:f:663:VAL:HA	2.18	0.58
2:B:223:ILE:HD12	2:B:346:ARG:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:36:ALA:HB2	13:M:65:ARG:HH21	1.67	0.58
20:T:185:ASN:ND2	20:T:205:THR:OG1	2.34	0.58
32:f:371:CYS:SG	32:f:406:ASN:ND2	2.76	0.58
3:C:270:GLN:O	3:C:307:ARG:NH1	2.36	0.58
6:F:231:THR:OG1	6:F:233:LYS:NZ	2.27	0.58
8:H:50:LYS:NZ	8:H:62:VAL:O	2.37	0.58
16:P:36:THR:OG1	16:P:38:ASP:OD1	2.18	0.58
22:V:91:PRO:HG3	22:V:126:ALA:HB3	1.84	0.58
23:W:422:ASN:O	23:W:426:ASN:ND2	2.35	0.58
26:Z:102:HIS:CD2	26:Z:104:ASN:HB3	2.36	0.58
28:b:25:ARG:HA	28:b:28:ALA:HB3	1.86	0.58
32:f:191:LYS:O	32:f:193:HIS:ND1	2.33	0.58
1:A:103:ASN:HB2	1:A:112:ILE:HG23	1.83	0.58
5:E:285:LEU:HB3	5:E:289:LEU:HB2	1.85	0.58
9:I:48:GLU:OE1	9:I:50:ARG:NH1	2.36	0.58
15:O:143:ARG:NH1	15:O:146:MET:HG2	2.18	0.58
21:U:759:SER:HA	21:U:782:ALA:HA	1.85	0.58
26:Z:21:ASP:HB2	29:c:36:LEU:HD22	1.86	0.58
30:d:184:LYS:HB2	30:d:185:ALA:HB2	1.85	0.58
3:C:113:ARG:HG2	3:C:127:LEU:HD12	1.85	0.58
22:V:259:LEU:HD21	22:V:294:ARG:HD2	1.85	0.58
6:F:94:ILE:HA	6:F:147:PRO:HB3	1.84	0.58
10:J:176:TYR:HB3	10:J:180:ALA:HB3	1.84	0.58
12:L:66:VAL:HG13	12:L:89:ARG:HD3	1.86	0.58
24:X:262:ASN:O	24:X:297:ARG:NH2	2.33	0.58
25:Y:16:ASP:HB2	25:Y:113:ARG:HE	1.68	0.58
25:Y:357:ASN:HB2	25:Y:358:ARG:HA	1.86	0.58
27:a:33:LEU:HB3	28:b:20:ASP:HB3	1.84	0.58
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.86	0.58
32:f:33:VAL:HG23	32:f:34:PRO:HD3	1.84	0.58
2:B:229:GLY:O	2:B:233:THR:N	2.37	0.58
21:U:68:PHE:HB3	21:U:73:ALA:HB3	1.85	0.58
25:Y:178:ASN:HB3	25:Y:207:THR:HG22	1.85	0.58
26:Z:34:ARG:HH12	26:Z:102:HIS:HE1	1.51	0.58
26:Z:212:LEU:HD22	27:a:350:LYS:HE2	1.86	0.58
2:B:316:LEU:HD11	2:B:327:VAL:HG11	1.86	0.58
3:C:230:MET:O	3:C:233:GLU:N	2.36	0.58
4:D:248:ARG:NH2	4:D:291:GLU:OE2	2.37	0.58
7:G:71:LYS:HE2	7:G:74:GLU:HA	1.85	0.58
9:I:123:GLN:NE2	10:J:79:ASP:OD1	2.37	0.58
12:L:215:VAL:HB	12:L:221:PHE:HD1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:38:MET:HG3	17:Q:44:LEU:HB2	1.86	0.58
23:W:52:LYS:HD3	23:W:55:ARG:HD3	1.86	0.58
2:B:133:VAL:HG11	2:B:159:VAL:HG12	1.85	0.58
2:B:190:LEU:HD12	2:B:194:ILE:HB	1.84	0.58
22:V:365:GLN:OE1	31:e:54:ASN:ND2	2.37	0.58
28:b:91:ARG:HH22	28:b:130:ARG:HE	1.52	0.58
4:D:389:GLU:HB3	4:D:391:ARG:N	2.18	0.57
13:M:141:SER:HB3	13:M:144:ASP:HB2	1.86	0.57
21:U:213:PHE:HE2	21:U:244:MET:HB2	1.69	0.57
23:W:40:LEU:HB2	23:W:41:GLN:CA	2.31	0.57
27:a:278:MET:HE2	27:a:279:GLU:HG3	1.86	0.57
1:A:310:ASP:N	1:A:312:ARG:HB2	2.19	0.57
2:B:280:SER:HB2	2:B:325:VAL:N	2.19	0.57
5:E:357:ALA:O	5:E:359:HIS:ND1	2.30	0.57
21:U:203:LYS:O	21:U:207:ASN:ND2	2.36	0.57
1:A:391:GLU:HA	1:A:394:MET:HB3	1.86	0.57
2:B:148:CYS:HB3	2:B:150:VAL:HG13	1.86	0.57
10:J:115:LYS:NZ	10:J:129:ILE:O	2.37	0.57
26:Z:182:THR:H	26:Z:183:THR:HA	1.68	0.57
3:C:42:LEU:HD21	4:D:65:GLN:HE22	1.69	0.57
4:D:87:LEU:HB2	5:E:80:VAL:HG23	1.86	0.57
4:D:94:GLU:HG2	4:D:102:ILE:HD11	1.85	0.57
6:F:227:GLY:HA3	6:F:231:THR:HG21	1.87	0.57
19:S:35:ILE:O	20:T:151:ARG:NH2	2.37	0.57
21:U:740:GLY:HA3	21:U:744:VAL:HG22	1.86	0.57
22:V:383:GLY:O	22:V:392:TYR:OH	2.21	0.57
22:V:479:ARG:HD2	25:Y:370:ILE:HG12	1.86	0.57
25:Y:330:ILE:HA	25:Y:333:GLU:HB3	1.85	0.57
3:C:229:ARG:HE	3:C:232:ARG:HG3	1.68	0.57
3:C:245:ILE:HD12	3:C:290:LYS:HB2	1.87	0.57
11:K:101:PHE:HA	18:R:57:ARG:HE	1.69	0.57
22:V:28:PRO:HG2	22:V:84:LYS:HE2	1.87	0.57
1:A:380:SER:O	2:B:343:ARG:NH1	2.38	0.57
13:M:169:ARG:HD2	13:M:200:VAL:HG13	1.87	0.57
29:c:157:ILE:HG12	29:c:158:ASP:H	1.69	0.57
12:L:5:GLN:HE21	13:M:5:THR:HA	1.70	0.57
12:L:48:ALA:HB3	12:L:211:SER:HB2	1.85	0.57
15:O:94:ILE:HG22	15:O:95:GLY:H	1.69	0.57
23:W:223:LYS:HA	23:W:226:TYR:HB3	1.86	0.57
30:d:254:GLU:HA	30:d:257:VAL:HG23	1.87	0.57
1:A:296:GLN:HB3	1:A:300:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:16:GLN:OE1	12:L:18:ARG:NH2	2.28	0.57
27:a:14:SER:HB2	27:a:18:GLN:HG2	1.87	0.57
32:f:644:PHE:HE1	32:f:648:ARG:HH21	1.51	0.57
32:f:663:VAL:HG13	32:f:664:ALA:HB2	1.87	0.57
3:C:15:LYS:HZ1	21:U:149:GLN:HG2	1.69	0.57
12:L:151:ALA:O	13:M:85:ARG:NH2	2.38	0.57
18:R:91:LYS:NZ	18:R:117:GLU:OE1	2.38	0.57
22:V:175:MET:O	22:V:178:SER:OG	2.21	0.57
24:X:203:PRO:HB2	24:X:204:PRO:C	2.30	0.57
26:Z:34:ARG:HB2	26:Z:97:THR:HG22	1.87	0.57
29:c:175:ARG:NH2	29:c:201:TYR:OH	2.37	0.57
1:A:94:GLN:OE1	2:B:131:HIS:NE2	2.37	0.56
1:A:167:GLU:HB2	1:A:239:ARG:HG2	1.87	0.56
4:D:372:GLY:HA3	4:D:374:ASP:HB2	1.87	0.56
13:M:149:TYR:HA	13:M:159:GLY:HA3	1.87	0.56
28:b:109:ILE:HB	28:b:138:VAL:HG13	1.87	0.56
1:A:138:MET:SD	1:A:156:LYS:NZ	2.69	0.56
9:I:122:THR:O	10:J:125:ARG:NH1	2.38	0.56
25:Y:388:ASN:ND2	26:Z:286:GLU:OE2	2.38	0.56
27:a:129:GLN:HG3	27:a:130:VAL:H	1.70	0.56
30:d:6:LYS:HD3	30:d:50:LEU:HG	1.87	0.56
1:A:140:VAL:HA	1:A:152:PRO:HA	1.86	0.56
2:B:317:ASP:HB3	2:B:318:GLY:HA2	1.86	0.56
11:K:23:GLN:HE22	11:K:135:ARG:HB2	1.71	0.56
11:K:210:LEU:HG	11:K:238:ILE:HG23	1.87	0.56
12:L:158:ALA:HB3	12:L:176:MET:HE3	1.87	0.56
15:O:96:ALA:HB1	15:O:98:LEU:HG	1.87	0.56
21:U:474:ARG:HH21	21:U:500:ASN:HB2	1.71	0.56
23:W:144:ARG:HA	23:W:147:LYS:HE2	1.86	0.56
24:X:318:ILE:O	24:X:322:HIS:ND1	2.38	0.56
25:Y:82:LYS:O	25:Y:86:GLU:N	2.36	0.56
25:Y:314:LEU:HD21	25:Y:319:MET:HG2	1.87	0.56
27:a:31:LYS:HA	28:b:177:PRO:HD3	1.88	0.56
28:b:34:ASN:O	28:b:38:HIS:ND1	2.32	0.56
30:d:80:CYS:HA	30:d:83:PHE:HB3	1.88	0.56
33:E:401:ATP:O3'	6:F:344:ARG:NH2	2.37	0.56
10:J:10:PHE:CG	10:J:16:LEU:HD23	2.40	0.56
21:U:792:ASN:OD1	21:U:793:LYS:N	2.38	0.56
24:X:359:ALA:O	24:X:363:ARG:NE	2.37	0.56
1:A:364:VAL:HG13	1:A:368:ILE:HD12	1.86	0.56
2:B:198:LYS:HD3	2:B:237:LYS:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.86	0.56
23:W:334:GLU:OE1	23:W:338:THR:OG1	2.23	0.56
26:Z:224:HIS:CG	26:Z:225:GLN:HA	2.39	0.56
2:B:221:GLY:HA2	2:B:326:LYS:HE3	1.88	0.56
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.39	0.56
17:Q:45:LEU:HB3	17:Q:102:LEU:HD13	1.88	0.56
22:V:73:GLU:HB3	22:V:78:HIS:HA	1.87	0.56
25:Y:14:ASN:HA	25:Y:17:LEU:HB3	1.87	0.56
1:A:139:ARG:H	1:A:156:LYS:HE3	1.71	0.56
1:A:343:PHE:HA	1:A:344:SER:OG	2.06	0.56
3:C:157:GLN:HE22	3:C:318:PRO:HD3	1.71	0.56
12:L:121:GLN:HG3	13:M:129:ARG:HG2	1.86	0.56
13:M:8:ASP:O	13:M:22:GLN:NE2	2.39	0.56
32:f:251:ALA:HA	32:f:254:SER:HB2	1.86	0.56
32:f:390:GLU:HG3	32:f:395:TYR:HB3	1.86	0.56
2:B:205:LEU:HD21	2:B:245:ALA:HB2	1.87	0.56
6:F:89:LEU:HG	6:F:153:VAL:HG13	1.86	0.56
9:I:106:PRO:HD2	9:I:109:GLN:HE21	1.70	0.56
13:M:200:VAL:HG22	13:M:201:HIS:H	1.70	0.56
18:R:55:TRP:HB3	18:R:83:LEU:HD11	1.87	0.56
23:W:142:ARG:HH21	23:W:178:GLU:HB2	1.71	0.56
26:Z:225:GLN:HB2	26:Z:228:TYR:CE2	2.41	0.56
27:a:285:PRO:HB3	27:a:352:ARG:HD3	1.86	0.56
29:c:191:ALA:O	29:c:195:GLY:N	2.39	0.56
5:E:261:LEU:HD13	5:E:294:ARG:HE	1.69	0.56
5:E:327:ASP:O	5:E:364:GLN:NE2	2.38	0.56
22:V:200:ARG:O	22:V:204:ASP:N	2.36	0.56
22:V:302:TYR:HB3	22:V:339:LEU:HD23	1.87	0.56
23:W:440:ASN:O	23:W:443:THR:OG1	2.19	0.56
24:X:299:LEU:HA	24:X:302:PHE:HB3	1.88	0.56
29:c:64:ASP:HA	29:c:139:ARG:HH21	1.70	0.56
32:f:109:LEU:HG	32:f:141:ARG:HH22	1.71	0.56
2:B:188:GLY:HA3	2:B:367:ILE:HD12	1.87	0.56
10:J:73:PHE:HA	10:J:131:ALA:HA	1.88	0.56
22:V:410:ILE:HD13	22:V:425:LYS:HE3	1.88	0.56
2:B:170:LEU:HD13	3:C:228:ALA:HA	1.87	0.55
5:E:57:VAL:HA	5:E:99:ALA:HA	1.87	0.55
9:I:149:GLN:O	9:I:157:GLY:N	2.38	0.55
11:K:109:VAL:HG11	11:K:152:GLN:HB2	1.87	0.55
14:N:32:ASP:O	14:N:45:ARG:NH1	2.39	0.55
21:U:506:ALA:HB3	29:c:65:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:62:ASP:OD2	26:Z:63:LYS:NZ	2.39	0.55
26:Z:236:LEU:HD11	27:a:335:TRP:HD1	1.72	0.55
4:D:88:VAL:N	4:D:132:LEU:O	2.30	0.55
5:E:122:MET:SD	5:E:225:HIS:NE2	2.79	0.55
6:F:256:LEU:HD13	6:F:309:THR:HG21	1.88	0.55
11:K:100:TRP:O	18:R:57:ARG:NH2	2.39	0.55
11:K:178:GLN:HE22	11:K:181:LEU:HD22	1.71	0.55
22:V:319:HIS:HB2	22:V:320:THR:HA	1.88	0.55
25:Y:105:MET:HG3	25:Y:106:ALA:H	1.71	0.55
25:Y:179:ARG:NH2	25:Y:212:GLU:OE2	2.38	0.55
8:H:171:LYS:HE3	9:I:55:LEU:HD13	1.88	0.55
13:M:169:ARG:HG3	13:M:170:GLN:H	1.70	0.55
22:V:30:PRO:HA	22:V:33:GLN:HB2	1.88	0.55
23:W:259:GLU:HG2	23:W:262:LYS:HB3	1.88	0.55
29:c:253:LYS:O	29:c:257:LYS:N	2.40	0.55
2:B:257:GLN:OE1	2:B:257:GLN:N	2.37	0.55
3:C:32:GLN:O	3:C:36:ASN:N	2.36	0.55
6:F:438:TYR:CD2	11:K:20:ARG:CD	2.88	0.55
12:L:69:HIS:HD1	12:L:137:TYR:H	1.54	0.55
16:P:52:GLY:N	16:P:108:VAL:O	2.33	0.55
21:U:842:LYS:HG2	21:U:882:ALA:HB2	1.89	0.55
25:Y:225:TYR:HA	25:Y:228:MET:HE3	1.88	0.55
26:Z:33:LYS:HD3	26:Z:60:GLU:N	2.21	0.55
30:d:101:LEU:HD22	30:d:166:PHE:HE2	1.70	0.55
3:C:90:HIS:HB2	3:C:91:PRO:HD3	1.89	0.55
3:C:164:VAL:HG21	3:C:313:ARG:HB2	1.89	0.55
3:C:171:HIS:O	3:C:173:GLU:N	2.39	0.55
4:D:39:ASP:N	21:U:148:LYS:O	2.39	0.55
6:F:280:PRO:HA	6:F:281:SER:HB2	1.89	0.55
10:J:96:LEU:HG	17:Q:58:GLU:HB3	1.88	0.55
12:L:166:GLN:OE1	12:L:169:ARG:NH1	2.40	0.55
22:V:38:LYS:HA	22:V:41:ALA:HB3	1.88	0.55
22:V:67:LEU:O	22:V:71:THR:OG1	2.21	0.55
25:Y:232:GLU:O	25:Y:236:LEU:N	2.39	0.55
25:Y:301:ILE:HD12	25:Y:342:ARG:HB3	1.88	0.55
1:A:373:LEU:HD21	1:A:413:VAL:HG21	1.88	0.55
3:C:84:LYS:NZ	3:C:98:ASP:OD1	2.32	0.55
9:I:4:ARG:NH2	9:I:5:TYR:OH	2.40	0.55
21:U:685:GLN:HB2	21:U:726:ALA:HA	1.88	0.55
24:X:345:VAL:HG21	24:X:350:ILE:HD13	1.87	0.55
24:X:351:SER:OG	24:X:357:SER:OG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:194:PHE:HB3	25:Y:230:ALA:HB2	1.89	0.55
27:a:264:ASN:ND2	27:a:267:GLN:OE1	2.39	0.55
23:W:216:GLU:CD	23:W:217:GLU:H	2.15	0.55
26:Z:241:SER:HB2	26:Z:242:LEU:HD12	1.88	0.55
14:N:7:GLN:HB3	14:N:111:VAL:HG23	1.89	0.55
20:T:92:LEU:HG	20:T:125:VAL:HG11	1.88	0.55
21:U:82:LEU:O	21:U:129:ARG:NE	2.40	0.55
22:V:317:PRO:HD3	25:Y:382:LYS:HD2	1.89	0.55
24:X:414:LEU:HD23	24:X:417:LYS:HD2	1.87	0.55
3:C:87:VAL:O	3:C:95:PHE:N	2.26	0.55
5:E:293:GLY:N	5:E:296:ASP:OD1	2.40	0.55
22:V:173:ILE:O	22:V:177:ASN:ND2	2.40	0.55
23:W:135:LYS:HB3	23:W:136:ILE:C	2.32	0.55
26:Z:25:ARG:HB3	29:c:103:GLY:HA3	1.89	0.55
29:c:170:LEU:HG	29:c:171:GLY:H	1.71	0.55
6:F:306:VAL:HA	6:F:309:THR:HB	1.88	0.55
10:J:116:GLN:HE21	11:K:83:ALA:HB3	1.72	0.55
21:U:428:PRO:HB3	21:U:439:GLU:HB2	1.88	0.55
22:V:159:LEU:HD13	22:V:178:SER:HB3	1.88	0.55
23:W:435:LEU:HA	23:W:438:LEU:HG	1.88	0.55
24:X:183:LEU:HD22	25:Y:251:HIS:HD2	1.72	0.55
28:b:94:HIS:HD2	28:b:136:VAL:HG21	1.71	0.55
28:b:161:ASN:ND2	28:b:168:SER:H	2.03	0.55
1:A:323:ARG:HE	1:A:431:THR:HB	1.72	0.54
4:D:287:ARG:O	4:D:291:GLU:N	2.40	0.54
4:D:354:LEU:HD23	4:D:356:GLU:HB3	1.88	0.54
7:G:124:VAL:O	7:G:128:ASN:ND2	2.40	0.54
9:I:25:MET:HA	9:I:28:ILE:HD13	1.88	0.54
15:O:13:VAL:HG21	15:O:152:LYS:HG2	1.89	0.54
26:Z:240:VAL:O	26:Z:243:GLN:N	2.39	0.54
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.89	0.54
29:c:272:ILE:HG21	29:c:276:GLY:N	2.20	0.54
32:f:106:ALA:HB1	32:f:107:LEU:HA	1.89	0.54
11:K:37:ALA:HB2	11:K:50:VAL:HG23	1.88	0.54
22:V:484:LEU:HA	22:V:487:HIS:HD2	1.71	0.54
23:W:66:ILE:HA	23:W:67:LEU:HB2	1.89	0.54
23:W:178:GLU:OE1	23:W:181:GLU:N	2.40	0.54
25:Y:63:TRP:HB3	25:Y:64:GLN:HB3	1.88	0.54
27:a:327:VAL:HG13	27:a:328:ASP:H	1.72	0.54
32:f:230:LYS:NZ	32:f:666:MET:SD	2.80	0.54
1:A:143:ASP:O	1:A:147:TYR:N	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ILE:HG12	3:C:268:GLU:HG3	1.88	0.54
3:C:371:LEU:HG	4:D:190:LEU:HD21	1.90	0.54
5:E:60:VAL:HG22	5:E:71:VAL:HG12	1.88	0.54
6:F:126:THR:OG1	6:F:130:GLN:O	2.25	0.54
19:S:13:LEU:HD23	19:S:175:VAL:HG22	1.89	0.54
22:V:451:ILE:HG13	22:V:458:VAL:HG13	1.89	0.54
2:B:390:LEU:HD13	2:B:430:LYS:HE2	1.89	0.54
3:C:321:ASN:OD1	3:C:322:GLU:N	2.40	0.54
6:F:369:HIS:NE2	33:F:501:ATP:N3	2.56	0.54
8:H:45:VAL:HG22	8:H:212:ILE:HG22	1.88	0.54
10:J:70:CYS:HB2	10:J:134:VAL:HB	1.89	0.54
21:U:208:LEU:HD23	21:U:210:LYS:H	1.72	0.54
21:U:356:THR:HG22	21:U:717:ILE:HG21	1.89	0.54
23:W:423:ASN:HD22	29:c:246:LYS:HD2	1.72	0.54
32:f:590:ALA:HB2	32:f:603:VAL:HG11	1.87	0.54
32:f:681:LEU:C	32:f:682:PRO:CA	2.74	0.54
1:A:380:SER:HB3	1:A:384:GLU:HB3	1.89	0.54
4:D:81:ARG:HH21	29:c:151:VAL:HG12	1.72	0.54
5:E:241:ARG:HG2	5:E:243:PHE:H	1.73	0.54
6:F:168:TYR:HB2	6:F:169:ASP:HB2	1.88	0.54
8:H:119:GLN:NE2	8:H:152:SER:O	2.40	0.54
16:P:190:ILE:HG22	16:P:195:ILE:HG23	1.90	0.54
20:T:7:THR:OG1	20:T:182:ARG:NH2	2.41	0.54
22:V:466:ILE:HD11	22:V:471:GLU:HB2	1.88	0.54
24:X:417:LYS:HZ2	26:Z:283:ARG:HH12	1.55	0.54
25:Y:67:VAL:O	25:Y:71:ASN:N	2.41	0.54
28:b:90:ILE:HD13	28:b:127:LEU:HD13	1.90	0.54
3:C:72:TYR:HB2	3:C:116:LEU:HD23	1.90	0.54
15:O:63:LEU:HA	15:O:66:HIS:HB2	1.89	0.54
17:Q:17:SER:OG	17:Q:179:SER:OG	2.25	0.54
21:U:220:LEU:HD11	21:U:252:LEU:HD13	1.90	0.54
22:V:372:LEU:HD21	22:V:399:ARG:HH22	1.73	0.54
1:A:344:SER:N	1:A:345:LEU:HB3	2.22	0.54
2:B:111:THR:OG1	2:B:124:SER:O	2.21	0.54
6:F:267:LEU:O	6:F:271:ALA:N	2.35	0.54
7:G:132:ARG:HG3	7:G:134:LEU:H	1.73	0.54
19:S:184:GLU:OE2	19:S:211:ARG:NH1	2.40	0.54
21:U:505:ASP:OD1	29:c:65:TYR:OH	2.26	0.54
22:V:131:LEU:HD23	22:V:134:PHE:HD2	1.72	0.54
22:V:372:LEU:H	22:V:427:GLN:NE2	2.05	0.54
22:V:443:ARG:NH2	30:d:180:GLY:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:SER:HB2	2:B:325:VAL:H	1.73	0.54
9:I:69:ASN:OD1	9:I:70:GLU:N	2.41	0.54
13:M:46:VAL:HG22	13:M:215:TRP:CD1	2.41	0.54
16:P:45:MET:HE3	16:P:71:LEU:HD22	1.89	0.54
30:d:44:THR:O	30:d:47:GLN:NE2	2.41	0.54
32:f:6:GLU:HG2	32:f:8:ALA:H	1.72	0.54
3:C:155:ASP:HA	3:C:158:ILE:HG12	1.88	0.54
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.90	0.54
22:V:320:THR:HG23	22:V:321:ALA:HB2	1.90	0.54
26:Z:266:ILE:HB	29:c:295:ASN:HD21	1.72	0.54
3:C:19:GLY:O	3:C:23:TYR:N	2.37	0.54
3:C:153:GLY:N	3:C:327:ASP:OD2	2.41	0.54
10:J:77:THR:O	10:J:81:ARG:NH2	2.41	0.54
22:V:468:SER:O	22:V:472:PRO:HD2	2.07	0.54
25:Y:46:ARG:C	25:Y:48:ASN:H	2.16	0.54
25:Y:74:LYS:HA	25:Y:77:ASN:HB3	1.90	0.54
26:Z:17:LEU:HD13	29:c:39:LEU:HD21	1.89	0.54
29:c:229:LEU:O	29:c:230:THR:OG1	2.23	0.54
1:A:218:PRO:HD3	1:A:428:ARG:HH21	1.73	0.53
1:A:427:PRO:HB2	1:A:429:TYR:HD2	1.71	0.53
7:G:184:LYS:NZ	8:H:55:ILE:O	2.38	0.53
12:L:184:LEU:H	12:L:184:LEU:HD12	1.74	0.53
22:V:379:LEU:HD13	22:V:395:ILE:HG12	1.89	0.53
26:Z:179:ILE:HG12	29:c:222:LYS:HE3	1.90	0.53
26:Z:270:VAL:HG13	29:c:288:VAL:HG13	1.90	0.53
29:c:63:ASP:OD1	29:c:66:THR:OG1	2.23	0.53
32:f:493:VAL:HG12	32:f:495:VAL:HG23	1.90	0.53
3:C:49:ARG:HA	3:C:52:LEU:HB2	1.90	0.53
4:D:56:VAL:HG23	21:U:600:ARG:HE	1.74	0.53
5:E:285:LEU:HB2	5:E:290:LEU:HG	1.90	0.53
7:G:88:ARG:NH2	13:M:157:SER:O	2.41	0.53
19:S:108:ASN:HB2	19:S:124:PHE:HD2	1.73	0.53
21:U:375:PHE:O	21:U:740:GLY:N	2.30	0.53
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.90	0.53
23:W:65:ARG:HB2	23:W:66:ILE:HD13	1.88	0.53
23:W:247:TYR:HD2	23:W:273:TYR:HD2	1.56	0.53
24:X:394:ASP:N	24:X:394:ASP:OD1	2.41	0.53
6:F:88:TYR:CD2	6:F:155:LYS:HG3	2.43	0.53
6:F:257:VAL:HG23	6:F:306:VAL:HG23	1.89	0.53
20:T:112:ILE:O	20:T:123:GLY:N	2.37	0.53
25:Y:68:ASP:HA	25:Y:71:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:253:LYS:HA	29:c:256:ASN:HB2	1.89	0.53
3:C:28:ILE:HA	3:C:31:LEU:HB3	1.89	0.53
5:E:285:LEU:HD12	5:E:290:LEU:HD23	1.90	0.53
11:K:210:LEU:HD11	11:K:215:ILE:HG12	1.90	0.53
12:L:204:ASP:HA	12:L:205:LEU:HB3	1.89	0.53
22:V:212:TYR:CD2	31:e:4:LYS:NZ	2.76	0.53
22:V:345:ARG:HH12	22:V:357:LEU:HB2	1.72	0.53
25:Y:329:PHE:HB3	31:e:66:LYS:HZ2	1.74	0.53
26:Z:91:ILE:HD13	26:Z:115:TYR:HB3	1.89	0.53
26:Z:214:LYS:HE3	26:Z:221:PRO:HG2	1.89	0.53
26:Z:244:GLU:HG2	27:a:287:ASN:N	2.21	0.53
27:a:145:LEU:HD12	27:a:146:PRO:HD2	1.91	0.53
32:f:535:LEU:HD22	32:f:569:ALA:HB1	1.90	0.53
1:A:428:ARG:HH22	2:B:340:ALA:HB2	1.72	0.53
4:D:201:GLY:HA3	4:D:327:LEU:HA	1.91	0.53
21:U:616:ARG:HH21	21:U:647:HIS:HA	1.73	0.53
22:V:412:LEU:O	25:Y:346:LYS:NZ	2.31	0.53
1:A:205:GLY:HA2	1:A:206:ILE:HG22	1.89	0.53
3:C:142:LYS:HB2	3:C:213:ARG:HG2	1.90	0.53
4:D:182:GLU:HG3	4:D:183:LEU:HD12	1.90	0.53
4:D:280:GLY:O	4:D:284:GLU:N	2.41	0.53
4:D:354:LEU:HB3	4:D:356:GLU:H	1.73	0.53
8:H:122:THR:HG22	8:H:129:PRO:HB3	1.90	0.53
21:U:774:PRO:HA	21:U:777:HIS:CD2	2.44	0.53
21:U:802:TYR:HB3	21:U:895:PRO:HD3	1.89	0.53
22:V:234:ARG:HG3	22:V:250:LEU:HD11	1.91	0.53
25:Y:197:ALA:HB3	25:Y:226:VAL:HG21	1.89	0.53
27:a:28:LEU:HD23	27:a:37:LEU:HA	1.90	0.53
3:C:119:ASP:OD1	3:C:119:ASP:N	2.41	0.53
11:K:48:LEU:HB3	11:K:218:ALA:HB3	1.91	0.53
3:C:28:ILE:O	3:C:32:GLN:N	2.26	0.53
4:D:91:GLN:HB2	4:D:245:ARG:HE	1.74	0.53
7:G:53:GLN:HA	7:G:215:ILE:HA	1.89	0.53
8:H:65:VAL:HB	8:H:220:ARG:HE	1.74	0.53
10:J:116:GLN:OE1	11:K:135:ARG:NH2	2.42	0.53
16:P:58:THR:O	17:Q:85:ARG:NH2	2.42	0.53
16:P:88:MET:HG3	16:P:124:LEU:HD11	1.90	0.53
22:V:322:VAL:HG13	22:V:323:GLY:H	1.73	0.53
26:Z:68:TRP:CD2	26:Z:108:ILE:HG13	2.43	0.53
32:f:223:ASN:HA	32:f:254:SER:HB3	1.90	0.53
32:f:401:LEU:HD23	32:f:672:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:PRO:HB2	2:B:154:HIS:HD2	1.73	0.53
3:C:11:LEU:HD12	3:C:14:GLY:HA2	1.90	0.53
3:C:50:ASN:HD21	21:U:643:SER:HA	1.72	0.53
6:F:195:ILE:HG12	6:F:199:VAL:HG23	1.91	0.53
11:K:11:GLY:C	11:K:13:ASN:H	2.16	0.53
20:T:92:LEU:HD23	20:T:112:ILE:HD11	1.90	0.53
21:U:649:ARG:HB3	21:U:675:MET:HE1	1.90	0.53
1:A:120:LYS:H	6:F:127:SER:HB2	1.73	0.53
2:B:304:GLU:HA	2:B:307:ARG:HG2	1.90	0.53
3:C:82:LYS:HE2	3:C:84:LYS:HD3	1.90	0.53
3:C:99:VAL:HA	3:C:100:ASP:HB3	1.91	0.53
4:D:242:GLU:OE2	5:E:78:ARG:NH2	2.42	0.53
14:N:18:SER:HB2	14:N:30:VAL:HA	1.90	0.53
25:Y:192:ARG:NH2	25:Y:294:TYR:HB3	2.24	0.53
27:a:13:ASN:OD1	27:a:19:PRO:HB3	2.08	0.53
27:a:58:LYS:HD2	27:a:83:VAL:HG11	1.91	0.53
29:c:252:ALA:O	29:c:256:ASN:N	2.42	0.53
32:f:270:ILE:HD12	32:f:274:LEU:HD12	1.89	0.53
3:C:11:LEU:HD23	21:U:146:LYS:HB3	1.91	0.52
4:D:293:LEU:O	4:D:296:MET:HG2	2.09	0.52
7:G:86:ASP:HA	13:M:120:HIS:CE1	2.44	0.52
12:L:75:ALA:HB3	12:L:131:GLY:HA3	1.90	0.52
26:Z:33:LYS:HG2	26:Z:34:ARG:HG2	1.90	0.52
28:b:28:ALA:HB1	28:b:180:ALA:HB2	1.91	0.52
1:A:334:PRO:HB3	6:F:395:GLN:HE21	1.74	0.52
1:A:384:GLU:H	2:B:343:ARG:HH11	1.57	0.52
3:C:214:VAL:HG13	3:C:215:SER:O	2.09	0.52
6:F:383:GLU:HB3	6:F:417:HIS:NE2	2.24	0.52
13:M:56:LYS:HB3	13:M:57:LEU:C	2.34	0.52
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.23	0.52
21:U:474:ARG:NH2	21:U:496:LEU:O	2.41	0.52
22:V:338:LEU:HD21	22:V:394:LEU:HB2	1.91	0.52
22:V:362:LEU:HD12	22:V:365:GLN:HB3	1.92	0.52
27:a:73:PRO:HG2	27:a:113:LEU:HD21	1.89	0.52
32:f:559:ASP:HB3	32:f:562:VAL:HG22	1.91	0.52
5:E:145:LEU:HA	5:E:148:VAL:HB	1.91	0.52
9:I:195:LYS:HB2	9:I:240:HIS:CD2	2.45	0.52
17:Q:84:THR:HG21	17:Q:104:LEU:HD11	1.91	0.52
21:U:643:SER:O	21:U:649:ARG:NH1	2.43	0.52
22:V:33:GLN:HB3	22:V:115:LYS:HD3	1.91	0.52
23:W:389:SER:O	23:W:393:LEU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:173:ASP:H	25:Y:177:ARG:HD3	1.74	0.52
1:A:102:ILE:HD11	1:A:136:GLU:HA	1.92	0.52
5:E:348:THR:HG21	6:F:218:GLN:HB2	1.92	0.52
22:V:59:ALA:N	22:V:60:ALA:HB3	2.25	0.52
23:W:55:ARG:NH1	23:W:79:GLU:HG3	2.24	0.52
4:D:153:MET:HG3	4:D:154:LEU:HD13	1.90	0.52
6:F:438:TYR:CZ	11:K:20:ARG:CA	2.93	0.52
16:P:184:GLY:H	16:P:202:ALA:HB3	1.75	0.52
21:U:237:VAL:HG13	21:U:321:GLN:HG3	1.91	0.52
22:V:212:TYR:CE1	31:e:4:LYS:CG	2.93	0.52
22:V:480:ILE:HD11	26:Z:264:SER:HA	1.92	0.52
26:Z:189:GLN:O	26:Z:192:THR:OG1	2.27	0.52
28:b:30:GLN:HG3	28:b:75:LEU:HD13	1.91	0.52
30:d:225:PHE:HB3	30:d:226:ALA:HB2	1.92	0.52
32:f:392:LYS:O	32:f:433:ASN:ND2	2.39	0.52
3:C:221:GLN:HB2	4:D:283:ARG:NH1	2.25	0.52
23:W:361:HIS:CD2	23:W:364:ARG:HH11	2.27	0.52
32:f:288:ALA:HB1	32:f:651:ILE:HD11	1.91	0.52
3:C:193:GLY:H	3:C:355:SER:HB2	1.75	0.52
3:C:229:ARG:HB3	3:C:232:ARG:HB2	1.92	0.52
5:E:292:PRO:HA	5:E:295:LEU:O	2.10	0.52
9:I:95:GLN:HE21	16:P:69:PHE:HA	1.75	0.52
21:U:57:ARG:HA	21:U:60:ALA:HB3	1.91	0.52
21:U:628:ARG:NH1	21:U:749:GLN:OE1	2.38	0.52
23:W:5:GLY:HA3	23:W:47:LEU:HD13	1.91	0.52
25:Y:16:ASP:HB3	25:Y:146:ARG:HH21	1.75	0.52
28:b:52:ILE:HD11	28:b:58:CYS:HB3	1.90	0.52
32:f:191:LYS:HD2	32:f:478:LYS:HE2	1.92	0.52
1:A:427:PRO:HB3	10:J:13:ASP:HB3	1.91	0.52
7:G:74:GLU:O	7:G:227:PHE:N	2.42	0.52
10:J:17:PHE:O	10:J:21:TYR:HB3	2.09	0.52
10:J:131:ALA:N	10:J:147:THR:OG1	2.42	0.52
14:N:178:ALA:HB3	14:N:185:GLU:HB2	1.92	0.52
15:O:215:LYS:HB3	16:P:197:THR:HB	1.92	0.52
21:U:806:CYS:SG	21:U:888:GLN:HG2	2.50	0.52
1:A:220:THR:HB	33:A:501:ATP:C5	2.45	0.52
2:B:261:GLY:C	2:B:263:GLY:H	2.17	0.52
4:D:251:PHE:CE2	4:D:292:LEU:HB2	2.45	0.52
6:F:279:ALA:HA	6:F:325:GLN:HE21	1.73	0.52
8:H:150:ASP:OD1	8:H:154:ALA:N	2.43	0.52
11:K:146:VAL:HG11	11:K:222:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:204:ASP:HB3	12:L:205:LEU:C	2.34	0.52
13:M:187:ARG:O	13:M:232:ARG:NH1	2.41	0.52
21:U:764:LEU:HA	21:U:767:THR:HG23	1.92	0.52
27:a:335:TRP:CG	27:a:336:VAL:H	2.28	0.52
27:a:370:GLN:O	30:d:251:ARG:NH1	2.43	0.52
30:d:228:GLN:N	30:d:229:GLN:HA	2.25	0.52
2:B:338:ASP:H	2:B:341:LEU:HG	1.74	0.52
3:C:49:ARG:HH22	4:D:69:LYS:HG3	1.75	0.52
5:E:152:PRO:HG3	5:E:159:PHE:HE2	1.74	0.52
10:J:10:PHE:HB2	10:J:16:LEU:HA	1.91	0.52
14:N:35:THR:HG21	14:N:56:ALA:HB1	1.92	0.52
22:V:137:GLU:O	22:V:141:THR:N	2.40	0.52
26:Z:192:THR:O	26:Z:196:HIS:N	2.37	0.52
28:b:116:PRO:HA	28:b:146:GLU:HG3	1.91	0.52
32:f:109:LEU:HB2	32:f:141:ARG:HH12	1.75	0.52
8:H:4:ARG:HD2	8:H:6:TYR:HB3	1.91	0.51
12:L:70:ILE:HG12	12:L:136:GLY:HA3	1.91	0.51
12:L:156:CYS:SG	12:L:159:MET:HG2	2.51	0.51
19:S:73:LYS:O	19:S:77:HIS:ND1	2.35	0.51
23:W:445:LEU:HA	23:W:448:LYS:HZ3	1.75	0.51
32:f:502:ALA:HB1	32:f:537:LEU:HD12	1.92	0.51
1:A:277:ILE:HG13	1:A:280:ILE:HD11	1.93	0.51
4:D:41:TYR:HA	4:D:44:TYR:HB3	1.92	0.51
5:E:56:ILE:HG23	5:E:100:LEU:HB2	1.90	0.51
16:P:13:ALA:HB3	16:P:137:VAL:HG23	1.92	0.51
25:Y:346:LYS:HB2	25:Y:355:GLU:HB3	1.93	0.51
26:Z:17:LEU:HB3	29:c:39:LEU:HD11	1.92	0.51
29:c:37:ALA:HB1	29:c:72:VAL:HG23	1.90	0.51
29:c:57:MET:N	29:c:110:GLY:O	2.38	0.51
30:d:106:LEU:HG	30:d:109:GLN:HE21	1.75	0.51
4:D:336:PRO:HG2	4:D:375:ILE:HG21	1.91	0.51
8:H:74:LEU:HD21	8:H:134:LEU:HD22	1.91	0.51
20:T:11:VAL:HG13	20:T:24:ALA:HB2	1.91	0.51
21:U:774:PRO:O	21:U:778:PHE:N	2.43	0.51
22:V:474:LEU:HA	22:V:477:HIS:HD2	1.76	0.51
4:D:163:MET:HG3	4:D:165:ALA:H	1.75	0.51
6:F:435:LEU:HD13	12:L:31:GLN:HG3	1.90	0.51
7:G:172:GLN:OE1	7:G:172:GLN:N	2.42	0.51
9:I:2:SER:HA	9:I:5:TYR:HD2	1.74	0.51
9:I:69:ASN:HA	16:P:76:LEU:HD22	1.90	0.51
10:J:137:ASP:N	10:J:141:THR:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:69:THR:O	22:V:73:GLU:N	2.36	0.51
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.91	0.51
9:I:11:ILE:HG21	10:J:7:ILE:HD12	1.92	0.51
10:J:96:LEU:HD23	10:J:97:THR:HG23	1.93	0.51
12:L:184:LEU:HD23	12:L:214:ILE:HG21	1.92	0.51
13:M:30:VAL:HG11	13:M:134:SER:HB3	1.91	0.51
17:Q:19:ARG:NH2	17:Q:31:ASP:O	2.44	0.51
22:V:378:VAL:HG13	22:V:382:PHE:HD2	1.76	0.51
23:W:374:THR:HG23	27:a:327:VAL:HA	1.93	0.51
24:X:420:LYS:O	26:Z:287:LYS:NZ	2.28	0.51
25:Y:191:ILE:HG13	25:Y:192:ARG:H	1.74	0.51
32:f:335:ARG:HB2	32:f:336:GLU:HA	1.91	0.51
32:f:403:LEU:HD11	32:f:410:LYS:HG2	1.93	0.51
3:C:89:VAL:HG12	3:C:91:PRO:HD2	1.92	0.51
3:C:137:LEU:O	3:C:141:GLU:HG3	2.11	0.51
3:C:246:ILE:HG22	3:C:247:PHE:H	1.76	0.51
6:F:70:LYS:HE2	6:F:74:LYS:HE3	1.93	0.51
6:F:334:ARG:HG2	6:F:336:ASP:H	1.75	0.51
10:J:36:ARG:HB3	10:J:144:LEU:HD23	1.93	0.51
11:K:182:GLN:HA	12:L:56:LEU:HD23	1.92	0.51
21:U:403:THR:HA	21:U:406:ALA:HB3	1.93	0.51
21:U:908:ILE:HG12	21:U:909:GLY:H	1.76	0.51
22:V:227:VAL:O	22:V:231:LEU:N	2.43	0.51
24:X:298:SER:O	24:X:301:ASP:N	2.43	0.51
1:A:95:VAL:HB	1:A:144:ARG:H	1.76	0.51
1:A:260:LEU:HD13	1:A:272:ILE:HG13	1.92	0.51
9:I:155:ASN:OD1	10:J:81:ARG:NH2	2.44	0.51
12:L:132:LEU:HB2	12:L:147:THR:HG21	1.93	0.51
16:P:12:MET:HG3	16:P:138:VAL:HG12	1.92	0.51
18:R:132:SER:O	18:R:135:ALA:N	2.34	0.51
22:V:227:VAL:HA	22:V:230:PHE:HB3	1.92	0.51
25:Y:20:ALA:HB2	25:Y:150:PHE:HD1	1.75	0.51
25:Y:356:THR:HA	25:Y:357:ASN:CG	2.35	0.51
29:c:130:GLN:HE21	29:c:162:LEU:HB2	1.76	0.51
1:A:270:CYS:O	1:A:315:ILE:HG12	2.10	0.51
2:B:224:LEU:O	2:B:330:ALA:HA	2.11	0.51
2:B:337:LEU:HA	2:B:341:LEU:HD12	1.93	0.51
3:C:193:GLY:H	3:C:356:GLY:H	1.58	0.51
5:E:165:ILE:HD12	5:E:166:PRO:HD2	1.93	0.51
11:K:227:HIS:HA	11:K:228:MET:C	2.36	0.51
17:Q:22:ALA:HB2	17:Q:27:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:27:THR:HB	19:S:40:SER:H	1.74	0.51
20:T:20:VAL:HG11	20:T:122:LEU:HD13	1.92	0.51
21:U:574:LYS:HD2	29:c:211:GLU:HG3	1.93	0.51
29:c:88:ASP:HB3	29:c:91:PHE:HB2	1.93	0.51
30:d:98:LEU:HA	30:d:101:LEU:HG	1.93	0.51
32:f:333:SER:O	32:f:334:ASN:ND2	2.43	0.51
32:f:397:ARG:HD3	32:f:679:ARG:HE	1.75	0.51
1:A:191:VAL:HG21	1:A:271:LEU:HD21	1.93	0.51
4:D:202:VAL:HB	4:D:308:ILE:HA	1.92	0.51
7:G:130:GLU:OE1	13:M:126:SER:OG	2.29	0.51
11:K:108:THR:O	11:K:110:GLU:N	2.44	0.51
14:N:2:THR:HA	14:N:129:GLY:HA3	1.93	0.51
23:W:316:ARG:O	23:W:319:THR:OG1	2.27	0.51
29:c:29:GLU:HB2	29:c:203:ILE:HD11	1.93	0.51
2:B:110:GLY:HA3	2:B:152:LEU:HD13	1.93	0.51
7:G:205:VAL:HG12	7:G:206:LEU:HG	1.92	0.51
12:L:84:LEU:O	12:L:88:MET:N	2.44	0.51
13:M:214:SER:OG	13:M:224:HIS:NE2	2.41	0.51
18:R:1:THR:O	18:R:130:SER:N	2.35	0.51
20:T:45:VAL:HB	20:T:49:THR:HG23	1.93	0.51
23:W:141:GLU:HB3	23:W:172:GLU:HG3	1.93	0.51
26:Z:256:GLN:HG3	26:Z:260:VAL:HG23	1.93	0.51
27:a:112:ILE:HD13	27:a:151:VAL:HG11	1.92	0.51
27:a:219:HIS:ND1	27:a:221:VAL:HG22	2.26	0.51
7:G:60:LEU:HD22	13:M:161:TRP:HB2	1.93	0.50
15:O:203:ARG:NH2	16:P:155:GLU:OE1	2.44	0.50
21:U:885:MET:HG2	21:U:887:ALA:H	1.75	0.50
29:c:56:LEU:HA	29:c:111:TRP:HA	1.92	0.50
3:C:201:ARG:HH11	3:C:211:PHE:HB3	1.76	0.50
6:F:325:GLN:HG2	6:F:326:VAL:HG23	1.93	0.50
9:I:105:ILE:HG12	9:I:110:LEU:HD13	1.93	0.50
15:O:98:LEU:HB2	15:O:113:ILE:HD12	1.92	0.50
18:R:50:ALA:HB2	19:S:129:SER:HB2	1.93	0.50
22:V:203:LEU:O	22:V:207:ALA:N	2.25	0.50
23:W:442:THR:HA	23:W:445:LEU:HB2	1.94	0.50
26:Z:199:LYS:HA	26:Z:202:ASN:ND2	2.25	0.50
30:d:209:TYR:HB3	30:d:213:ARG:HE	1.76	0.50
1:A:160:THR:C	1:A:162:THR:H	2.19	0.50
1:A:333:ARG:O	1:A:337:LEU:N	2.45	0.50
23:W:5:GLY:HA2	23:W:34:LEU:HD13	1.92	0.50
30:d:30:LEU:HA	30:d:34:ASN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:159:PRO:N	30:d:160:ALA:HA	2.27	0.50
2:B:254:GLU:HG3	2:B:292:THR:HG22	1.94	0.50
10:J:92:GLN:HE21	17:Q:66:LEU:HB2	1.75	0.50
21:U:20:LYS:HE2	21:U:48:LEU:HD21	1.94	0.50
27:a:103:LYS:HG3	27:a:104:VAL:HG23	1.94	0.50
28:b:25:ARG:CZ	28:b:144:GLY:HA2	2.42	0.50
30:d:40:GLY:HA3	30:d:41:THR:C	2.36	0.50
32:f:304:LEU:HD11	32:f:326:LEU:HD12	1.94	0.50
12:L:79:ALA:HA	12:L:82:ARG:HH21	1.77	0.50
13:M:234:GLU:HA	13:M:237:LYS:HB3	1.92	0.50
15:O:73:LEU:HD12	15:O:74:PRO:HD2	1.94	0.50
21:U:529:ILE:HD11	21:U:555:VAL:HG11	1.93	0.50
25:Y:73:MET:O	25:Y:77:ASN:N	2.28	0.50
26:Z:33:LYS:HZ1	26:Z:34:ARG:C	2.18	0.50
26:Z:77:ASN:HB2	29:c:98:MET:HE1	1.94	0.50
29:c:145:VAL:HA	29:c:157:ILE:HA	1.92	0.50
30:d:52:ARG:NH2	30:d:82:TYR:OH	2.44	0.50
3:C:13:GLU:N	3:C:14:GLY:HA3	2.27	0.50
4:D:231:VAL:HG11	5:E:258:MET:HB3	1.94	0.50
6:F:436:GLN:C	6:F:438:TYR:H	2.19	0.50
11:K:137:PHE:HB3	11:K:139:VAL:HG12	1.93	0.50
19:S:11:THR:HA	19:S:139:GLY:HA3	1.94	0.50
21:U:576:PRO:HB3	21:U:611:ASN:HD22	1.76	0.50
22:V:80:LYS:HB3	22:V:81:GLN:C	2.37	0.50
23:W:321:VAL:O	23:W:325:GLY:N	2.43	0.50
23:W:366:MET:HB3	23:W:370:TYR:CE2	2.47	0.50
26:Z:223:ASN:HB2	26:Z:227:ILE:HG12	1.93	0.50
32:f:483:ALA:HB1	32:f:500:LEU:HG	1.93	0.50
32:f:567:ILE:HG13	32:f:605:LEU:HD22	1.93	0.50
1:A:205:GLY:HA2	1:A:206:ILE:CG2	2.41	0.50
1:A:333:ARG:HG3	1:A:334:PRO:HD3	1.92	0.50
5:E:206:LYS:HG3	5:E:207:TYR:H	1.77	0.50
7:G:12:HIS:CD2	13:M:9:LEU:HD12	2.46	0.50
16:P:13:ALA:HA	16:P:22:ILE:HA	1.92	0.50
18:R:97:MET:HE2	18:R:99:THR:HG21	1.93	0.50
19:S:49:LYS:HB3	19:S:113:LEU:HB2	1.94	0.50
29:c:63:ASP:O	29:c:139:ARG:NH2	2.45	0.50
32:f:192:THR:HA	32:f:193:HIS:HB2	1.94	0.50
7:G:171:LYS:HB3	7:G:205:VAL:HG11	1.94	0.50
13:M:123:THR:HG22	13:M:130:PRO:HB3	1.94	0.50
3:C:71:SER:HB2	4:D:112:TYR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:217:THR:HB	16:P:195:ILE:HB	1.94	0.50
2:B:199:GLU:O	2:B:203:LEU:N	2.45	0.49
3:C:163:GLU:OE1	3:C:163:GLU:N	2.44	0.49
9:I:196:VAL:O	9:I:200:THR:OG1	2.22	0.49
10:J:104:VAL:HG23	10:J:143:ARG:HD3	1.94	0.49
12:L:33:SER:HB2	12:L:49:LEU:HB3	1.94	0.49
12:L:72:ILE:HG22	12:L:134:ILE:HA	1.94	0.49
23:W:438:LEU:HD22	26:Z:234:PHE:CD1	2.47	0.49
29:c:180:ASN:HB2	29:c:204:THR:HG21	1.94	0.49
30:d:147:SER:HG	30:d:151:VAL:H	1.52	0.49
32:f:146:LEU:HG	32:f:178:LEU:HD13	1.93	0.49
1:A:354:ILE:O	1:A:358:HIS:ND1	2.40	0.49
14:N:84:LYS:NZ	14:N:85:GLU:OE2	2.40	0.49
17:Q:151:ILE:HG13	17:Q:152:SER:HB2	1.94	0.49
24:X:258:LYS:HD3	24:X:267:VAL:HG22	1.93	0.49
25:Y:233:ARG:NH1	25:Y:306:GLN:OE1	2.45	0.49
27:a:123:LEU:HD21	27:a:161:LYS:HG3	1.94	0.49
31:e:1:MET:N	31:e:2:SER:HA	2.25	0.49
32:f:251:ALA:HB1	32:f:255:LEU:HG	1.94	0.49
32:f:392:LYS:HD3	32:f:421:LEU:HB2	1.94	0.49
1:A:218:PRO:O	1:A:221:GLY:N	2.45	0.49
1:A:373:LEU:HD13	1:A:410:LEU:HB2	1.93	0.49
5:E:141:GLN:NE2	5:E:300:HIS:O	2.41	0.49
22:V:26:PRO:O	22:V:29:PRO:HD2	2.12	0.49
23:W:170:GLN:HA	23:W:173:THR:HG23	1.94	0.49
23:W:455:LEU:HD12	23:W:456:GLN:H	1.78	0.49
25:Y:134:LEU:HD13	25:Y:168:ILE:HG23	1.94	0.49
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.34	0.49
4:D:348:ILE:HG13	4:D:352:MET:HE3	1.94	0.49
9:I:108:GLU:OE2	9:I:146:GLN:NE2	2.35	0.49
14:N:22:THR:HG22	14:N:27:ALA:HB2	1.95	0.49
20:T:25:ASP:OD1	20:T:41:ARG:NH1	2.46	0.49
21:U:792:ASN:HA	21:U:914:LEU:HB3	1.93	0.49
30:d:237:ILE:N	30:d:238:PRO:HD2	2.27	0.49
32:f:314:ASN:HA	32:f:319:ARG:HD2	1.95	0.49
1:A:86:THR:O	1:A:90:GLU:N	2.45	0.49
2:B:109:VAL:HG22	2:B:151:LEU:HD22	1.95	0.49
3:C:142:LYS:HA	4:D:323:ARG:HD2	1.95	0.49
3:C:188:LEU:HB3	3:C:317:PHE:HB2	1.93	0.49
6:F:91:SER:OG	6:F:125:LYS:O	2.20	0.49
7:G:220:VAL:HB	7:G:227:PHE:HD1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:181:ASN:OD1	15:O:182:LYS:N	2.46	0.49
21:U:842:LYS:H	21:U:882:ALA:HB2	1.76	0.49
22:V:367:VAL:HG13	22:V:402:VAL:HG22	1.93	0.49
24:X:414:LEU:HA	24:X:417:LYS:HD2	1.94	0.49
30:d:175:ARG:HD2	30:d:205:LYS:HZ2	1.76	0.49
30:d:256:ILE:N	30:d:257:VAL:HA	2.28	0.49
32:f:109:LEU:HA	32:f:110:ALA:HB3	1.95	0.49
9:I:48:GLU:O	9:I:64:LYS:NZ	2.40	0.49
21:U:27:LEU:O	21:U:31:VAL:N	2.45	0.49
27:a:193:GLN:HB3	27:a:225:LEU:HD13	1.93	0.49
1:A:217:PRO:HD2	1:A:343:PHE:HB2	1.94	0.49
2:B:364:ILE:O	2:B:368:HIS:ND1	2.32	0.49
4:D:89:ILE:O	4:D:106:THR:OG1	2.29	0.49
5:E:360:ASP:OD1	5:E:360:ASP:N	2.44	0.49
13:M:56:LYS:H	13:M:57:LEU:HA	1.77	0.49
20:T:46:ASN:OD1	20:T:48:SER:N	2.29	0.49
21:U:345:ASN:ND2	21:U:743:ASN:OD1	2.45	0.49
21:U:472:ILE:HG22	21:U:475:HIS:CE1	2.47	0.49
21:U:885:MET:HB3	21:U:888:GLN:HG3	1.94	0.49
22:V:326:GLN:HB3	22:V:353:LEU:HD22	1.93	0.49
23:W:372:ARG:HG2	23:W:414:ASN:HB3	1.93	0.49
26:Z:39:LEU:HD11	26:Z:50:VAL:HG11	1.94	0.49
26:Z:254:ASN:O	29:c:246:LYS:NZ	2.37	0.49
27:a:13:ASN:CG	27:a:19:PRO:CG	2.82	0.49
30:d:39:THR:HG23	30:d:86:LYS:HE3	1.94	0.49
1:A:151:ILE:HD12	1:A:152:PRO:HD2	1.94	0.49
1:A:297:ARG:NE	6:F:302:GLY:O	2.45	0.49
9:I:175:LEU:HA	9:I:178:ASP:HB2	1.94	0.49
9:I:190:LEU:HB3	9:I:236:LEU:HD21	1.95	0.49
16:P:72:ASN:O	16:P:76:LEU:HG	2.13	0.49
17:Q:7:ILE:HD13	17:Q:14:LEU:HD23	1.94	0.49
22:V:219:GLU:OE2	22:V:256:ARG:NH1	2.45	0.49
24:X:368:MET:HB3	24:X:374:PHE:HB3	1.95	0.49
27:a:32:LYS:HD3	28:b:22:LEU:HD11	1.94	0.49
32:f:252:ALA:HA	32:f:334:ASN:HB2	1.95	0.49
32:f:371:CYS:C	32:f:373:GLY:HA2	2.38	0.49
1:A:120:LYS:HE2	6:F:90:VAL:HG11	1.95	0.49
3:C:131:VAL:HG13	3:C:132:ASP:H	1.78	0.49
3:C:328:ILE:HG23	3:C:359:VAL:HG11	1.95	0.49
4:D:285:VAL:HA	4:D:288:ILE:HB	1.94	0.49
5:E:133:SER:HA	5:E:142:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:36:PHE:HB2	17:Q:44:LEU:HB3	1.95	0.49
21:U:118:LEU:HD21	21:U:123:LYS:HA	1.95	0.49
21:U:612:ASP:HA	21:U:615:ARG:HD3	1.95	0.49
23:W:2:ALA:HA	23:W:47:LEU:HD11	1.95	0.49
29:c:282:ARG:HG3	29:c:284:LEU:HD13	1.94	0.49
32:f:458:SER:HB2	32:f:461:PHE:HA	1.93	0.49
32:f:656:HIS:C	32:f:658:VAL:H	2.19	0.49
2:B:103:ARG:HG3	2:B:104:GLY:H	1.78	0.49
4:D:300:ASP:HA	4:D:301:GLN:HA	1.64	0.49
5:E:178:THR:HG21	5:E:340:GLY:H	1.77	0.49
11:K:99:HIS:HB2	11:K:107:MET:HE3	1.95	0.49
18:R:115:ASP:HB2	18:R:119:ASN:HD22	1.78	0.49
19:S:133:ASP:OD2	19:S:136:LYS:NZ	2.39	0.49
26:Z:105:ASP:HA	26:Z:108:ILE:HD13	1.94	0.49
29:c:174:PRO:HB3	29:c:175:ARG:HD3	1.93	0.49
3:C:89:VAL:HB	3:C:92:GLU:HB2	1.95	0.48
4:D:116:LEU:HD12	4:D:140:VAL:HG22	1.94	0.48
6:F:438:TYR:CE2	11:K:20:ARG:HG2	2.40	0.48
11:K:46:VAL:HG23	11:K:151:PRO:HB2	1.95	0.48
11:K:210:LEU:HA	11:K:214:ASN:HD22	1.77	0.48
13:M:74:GLY:HA3	13:M:224:HIS:CE1	2.48	0.48
21:U:520:MET:HE2	21:U:525:ASN:HD22	1.78	0.48
23:W:405:LYS:HG3	24:X:344:ARG:HG2	1.95	0.48
24:X:420:LYS:NZ	26:Z:284:ASP:OD1	2.40	0.48
1:A:174:TYR:HD1	1:A:227:ARG:HD2	1.78	0.48
1:A:219:GLY:HA2	1:A:220:THR:HA	1.49	0.48
7:G:52:THR:HG22	7:G:53:GLN:H	1.77	0.48
7:G:76:ILE:HA	7:G:141:ILE:HD11	1.93	0.48
11:K:221:GLN:OE1	11:K:227:HIS:NE2	2.42	0.48
12:L:85:CYS:SG	12:L:89:ARG:NH1	2.86	0.48
21:U:338:HIS:HD2	21:U:785:PRO:HB2	1.77	0.48
21:U:384:GLN:HG2	21:U:385:PHE:H	1.78	0.48
21:U:401:LYS:HB3	21:U:438:GLN:NE2	2.29	0.48
21:U:654:MET:HE1	21:U:767:THR:HG22	1.95	0.48
21:U:800:VAL:HG21	21:U:914:LEU:HD21	1.94	0.48
25:Y:131:THR:O	25:Y:137:ARG:NH1	2.45	0.48
26:Z:32:GLN:HG3	26:Z:33:LYS:H	1.78	0.48
1:A:125:LEU:HB3	1:A:149:ILE:HD12	1.94	0.48
2:B:216:ILE:O	2:B:217:LYS:HG2	2.12	0.48
4:D:254:ALA:HB1	4:D:305:VAL:HG23	1.95	0.48
5:E:339:ASN:OD1	5:E:340:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:345:ASN:HD21	6:F:345:SER:HA	1.78	0.48
21:U:681:ASN:ND2	21:U:725:MET:SD	2.86	0.48
28:b:146:GLU:HG2	28:b:147:GLU:H	1.79	0.48
1:A:101:ILE:N	1:A:114:ASN:O	2.45	0.48
1:A:217:PRO:HA	1:A:428:ARG:NE	2.29	0.48
3:C:43:ARG:HG2	4:D:61:ILE:HD12	1.94	0.48
4:D:241:GLY:O	4:D:245:ARG:NH2	2.46	0.48
5:E:65:THR:HG22	5:E:66:GLU:H	1.79	0.48
7:G:39:SER:H	7:G:172:GLN:HE21	1.59	0.48
8:H:118:MET:HE3	8:H:130:PHE:HB2	1.96	0.48
9:I:93:ILE:HA	9:I:96:ARG:HG2	1.94	0.48
12:L:205:LEU:HD22	12:L:239:ARG:HH22	1.78	0.48
15:O:51:ASP:OD2	16:P:99:ARG:NH2	2.46	0.48
22:V:47:SER:HA	22:V:50:GLU:HB2	1.94	0.48
23:W:136:ILE:H	23:W:141:GLU:HG2	1.78	0.48
26:Z:58:PHE:CZ	26:Z:68:TRP:HB2	2.49	0.48
27:a:319:LEU:HA	27:a:337:GLN:HE21	1.78	0.48
2:B:409:GLU:CD	2:B:413:LYS:HB3	2.39	0.48
4:D:218:ALA:O	4:D:222:HIS:ND1	2.39	0.48
4:D:261:ILE:HG12	4:D:306:LYS:HB2	1.95	0.48
5:E:235:ILE:HG22	5:E:279:THR:HB	1.95	0.48
12:L:195:LEU:O	12:L:198:THR:OG1	2.30	0.48
22:V:417:ILE:HG12	22:V:422:ILE:HD12	1.94	0.48
26:Z:69:PHE:HZ	28:b:92:VAL:HG22	1.79	0.48
29:c:30:GLN:HB3	29:c:66:THR:HG22	1.95	0.48
32:f:11:TRP:HB3	32:f:12:GLN:HB3	1.96	0.48
1:A:206:ILE:HG23	1:A:207:GLU:H	1.79	0.48
1:A:362:MET:HE3	2:B:210:TYR:HB3	1.96	0.48
9:I:86:LEU:HB3	9:I:114:LEU:HD11	1.96	0.48
11:K:69:GLU:HA	11:K:75:GLY:HA2	1.96	0.48
25:Y:145:LEU:HA	25:Y:157:ILE:HG22	1.95	0.48
25:Y:362:LYS:HZ3	25:Y:366:TYR:HE2	1.60	0.48
26:Z:74:TYR:HD1	29:c:101:GLN:HE21	1.61	0.48
27:a:24:ARG:O	27:a:28:LEU:HD13	2.13	0.48
28:b:68:THR:HA	28:b:71:ILE:HD13	1.95	0.48
2:B:103:ARG:HD2	2:B:107:MET:HE1	1.95	0.48
2:B:260:LEU:N	2:B:261:GLY:HA2	2.29	0.48
9:I:4:ARG:HH12	12:L:9:ASP:CG	2.21	0.48
10:J:115:LYS:HE3	10:J:127:PHE:HB2	1.95	0.48
12:L:117:GLN:NE2	13:M:83:ASP:OD1	2.45	0.48
13:M:22:GLN:HB3	13:M:130:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:42:ILE:HG12	16:P:52:GLY:HA2	1.96	0.48
18:R:157:ARG:HD3	18:R:195:LEU:HD13	1.95	0.48
22:V:81:GLN:HB3	22:V:83:GLU:N	2.27	0.48
22:V:306:ARG:HB3	22:V:339:LEU:HD21	1.95	0.48
23:W:91:SER:HB2	23:W:92:LYS:HA	1.94	0.48
30:d:125:LYS:HB3	30:d:129:THR:HG22	1.95	0.48
31:e:57:ARG:HB2	31:e:59:GLU:HB2	1.95	0.48
2:B:176:VAL:CG2	2:B:177:GLU:HA	2.38	0.48
20:T:142:GLY:HA2	20:T:176:LEU:HD21	1.96	0.48
24:X:360:ASP:OD1	24:X:361:VAL:N	2.45	0.48
25:Y:77:ASN:ND2	25:Y:114:ILE:HG21	2.29	0.48
25:Y:297:ARG:HD3	31:e:52:PHE:CE1	2.48	0.48
27:a:163:TYR:HE1	27:a:169:HIS:HA	1.78	0.48
1:A:164:MET:HG2	1:A:244:GLU:HG3	1.95	0.48
1:A:375:ARG:HG3	1:A:376:LEU:HD12	1.96	0.48
2:B:93:GLU:HG3	2:B:94:GLU:H	1.79	0.48
7:G:80:MET:HG3	7:G:87:SER:HB2	1.95	0.48
12:L:65:HIS:H	12:L:223:ILE:HD11	1.78	0.48
13:M:68:ASN:ND2	13:M:224:HIS:O	2.46	0.48
16:P:29:GLY:HA2	16:P:35:VAL:HG23	1.94	0.48
20:T:24:ALA:H	20:T:42:ILE:HD11	1.77	0.48
21:U:591:CYS:HA	21:U:625:ILE:HA	1.96	0.48
23:W:186:ILE:O	23:W:189:GLN:NE2	2.44	0.48
26:Z:222:ILE:N	26:Z:223:ASN:HA	2.28	0.48
26:Z:256:GLN:HG2	30:d:246:VAL:HG21	1.95	0.48
1:A:80:LEU:HD21	2:B:138:PHE:HB2	1.96	0.48
2:B:151:LEU:HD11	2:B:163:LEU:HD13	1.96	0.48
3:C:103:ILE:HG13	3:C:126:ILE:HG22	1.95	0.48
4:D:91:GLN:N	4:D:104:GLY:O	2.33	0.48
8:H:19:LEU:HD13	8:H:22:ILE:HD12	1.96	0.48
20:T:23:ALA:HB3	20:T:169:VAL:HG11	1.94	0.48
22:V:471:GLU:HB3	22:V:472:PRO:HD3	1.96	0.48
24:X:347:ILE:HG22	24:X:385:LEU:HB2	1.96	0.48
27:a:351:ASP:O	27:a:355:PHE:HB2	2.13	0.48
32:f:685:VAL:HG23	32:f:686:ARG:H	1.79	0.48
1:A:312:ARG:HA	1:A:313:GLY:HA2	1.58	0.47
11:K:178:GLN:NE2	11:K:181:LEU:HD22	2.29	0.47
12:L:229:VAL:HG12	12:L:233:LEU:HG	1.96	0.47
20:T:99:ARG:HG3	20:T:105:PRO:HA	1.95	0.47
23:W:231:ILE:HG21	23:W:250:ILE:HG22	1.96	0.47
32:f:523:GLY:HA3	32:f:527:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:LYS:HG2	22:V:495:ARG:HB3	1.95	0.47
3:C:295:THR:HG22	3:C:296:ASN:H	1.79	0.47
4:D:89:ILE:HD13	5:E:78:ARG:HB3	1.96	0.47
4:D:313:ARG:NH2	4:D:315:ASP:OD2	2.47	0.47
5:E:58:GLY:HA2	5:E:73:ALA:HA	1.96	0.47
12:L:123:TYR:N	13:M:127:ALA:O	2.47	0.47
14:N:176:LEU:HD12	14:N:187:GLN:HE21	1.78	0.47
17:Q:9:GLY:HA3	17:Q:12:TYR:CE2	2.49	0.47
24:X:417:LYS:HZ3	26:Z:283:ARG:HH22	1.60	0.47
26:Z:228:TYR:CE1	27:a:338:PRO:HB2	2.49	0.47
27:a:155:PHE:HE2	27:a:178:ARG:HD3	1.79	0.47
27:a:244:ASN:ND2	27:a:276:CYS:HB3	2.29	0.47
32:f:446:ASN:C	32:f:448:LEU:H	2.22	0.47
1:A:247:GLN:HB2	1:A:248:LYS:O	2.13	0.47
11:K:108:THR:HB	11:K:147:ASP:HA	1.97	0.47
22:V:273:LYS:HA	22:V:274:SER:HB2	1.94	0.47
26:Z:151:THR:OG1	27:a:146:PRO:O	2.23	0.47
3:C:56:VAL:HG21	4:D:75:ALA:HB1	1.96	0.47
3:C:203:VAL:O	3:C:207:THR:OG1	2.22	0.47
4:D:366:ARG:HB3	4:D:367:PRO:HD3	1.96	0.47
13:M:66:LEU:HD13	13:M:214:SER:HB2	1.96	0.47
19:S:142:SER:HA	19:S:145:LEU:HB2	1.96	0.47
21:U:437:TYR:HE2	29:c:25:VAL:HG21	1.80	0.47
21:U:443:LEU:HD21	21:U:464:GLN:HB2	1.97	0.47
21:U:571:CYS:HB2	21:U:601:ARG:HH21	1.78	0.47
23:W:428:TRP:HE1	29:c:244:VAL:C	2.23	0.47
25:Y:51:ALA:CB	25:Y:116:ASP:H	2.27	0.47
27:a:31:LYS:HG3	28:b:176:GLY:HA2	1.96	0.47
1:A:429:TYR:CD2	10:J:12:PRO:HD2	2.49	0.47
3:C:170:LYS:C	3:C:172:PRO:HD3	2.40	0.47
5:E:306:GLU:C	5:E:308:ALA:H	2.22	0.47
7:G:49:VAL:HG22	7:G:219:VAL:HG23	1.96	0.47
7:G:69:LEU:HD11	7:G:216:GLU:HB3	1.97	0.47
11:K:16:SER:OG	11:K:17:PRO:HD2	2.14	0.47
11:K:121:LEU:HD13	11:K:123:PHE:HE2	1.79	0.47
13:M:106:ILE:HD12	13:M:107:PRO:HD2	1.97	0.47
19:S:23:VAL:O	19:S:196:CYS:N	2.41	0.47
25:Y:101:ARG:HD3	25:Y:130:LYS:HD3	1.95	0.47
25:Y:356:THR:OG1	25:Y:357:ASN:O	2.28	0.47
26:Z:45:LYS:HG3	26:Z:46:LYS:H	1.80	0.47
27:a:54:ASP:HA	27:a:57:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PRO:N	1:A:312:ARG:HA	2.30	0.47
2:B:99:VAL:O	2:B:103:ARG:HG2	2.14	0.47
2:B:106:PRO:HB3	3:C:121:TYR:HB2	1.95	0.47
5:E:257:LEU:HA	5:E:260:LEU:HD12	1.96	0.47
5:E:341:ALA:HB1	6:F:345:SER:H	1.78	0.47
6:F:224:LEU:HB2	6:F:348:LEU:HD13	1.96	0.47
11:K:69:GLU:HG2	11:K:71:ASP:O	2.15	0.47
22:V:179:LYS:HD3	22:V:214:HIS:HA	1.97	0.47
23:W:52:LYS:HA	23:W:55:ARG:HB3	1.95	0.47
25:Y:316:LEU:HG	25:Y:352:GLU:HG3	1.97	0.47
29:c:223:LYS:NZ	29:c:230:THR:HG23	2.30	0.47
30:d:10:ASN:OD1	30:d:11:ARG:N	2.47	0.47
2:B:255:LEU:HD11	3:C:264:GLY:HA2	1.96	0.47
4:D:64:GLU:HG3	21:U:607:VAL:HG21	1.97	0.47
4:D:145:PRO:HB2	4:D:146:GLU:HB2	1.97	0.47
4:D:358:VAL:HG12	4:D:363:TYR:HE2	1.80	0.47
4:D:377:SER:CB	5:E:292:PRO:HB2	2.44	0.47
5:E:211:SER:HA	5:E:214:LEU:HB3	1.96	0.47
13:M:165:ILE:HG22	13:M:166:GLY:H	1.80	0.47
16:P:68:LYS:HD2	16:P:71:LEU:HD23	1.97	0.47
17:Q:85:ARG:O	17:Q:89:ALA:N	2.39	0.47
22:V:259:LEU:HD11	22:V:294:ARG:HD2	1.97	0.47
22:V:468:SER:HA	25:Y:363:ASN:HD21	1.79	0.47
24:X:206:LEU:O	24:X:210:LEU:N	2.41	0.47
24:X:377:ILE:HB	24:X:388:PHE:HE2	1.80	0.47
25:Y:63:TRP:HB3	25:Y:64:GLN:C	2.40	0.47
25:Y:138:LEU:HD22	25:Y:168:ILE:HD13	1.96	0.47
32:f:52:ILE:HG13	32:f:64:GLU:HG2	1.96	0.47
1:A:375:ARG:HH22	11:K:205:VAL:C	2.22	0.47
1:A:428:ARG:NH2	2:B:340:ALA:HB2	2.28	0.47
3:C:245:ILE:HG23	3:C:290:LYS:HB2	1.97	0.47
4:D:54:LEU:HA	4:D:57:GLN:HB2	1.97	0.47
5:E:119:VAL:HG21	6:F:147:PRO:HD2	1.97	0.47
9:I:122:THR:HG22	9:I:129:PRO:HB3	1.96	0.47
11:K:79:SER:HB2	11:K:140:ALA:H	1.80	0.47
11:K:155:HIS:CG	11:K:168:ARG:HG2	2.50	0.47
15:O:66:HIS:HD2	15:O:78:THR:HG23	1.80	0.47
17:Q:29:LYS:HD2	18:R:122:SER:O	2.15	0.47
20:T:32:SER:HA	20:T:182:ARG:HG2	1.97	0.47
21:U:336:GLU:HA	21:U:339:LEU:HB3	1.96	0.47
22:V:363:LEU:HA	22:V:378:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:273:GLN:HB3	27:a:310:LEU:HD11	1.97	0.47
29:c:181:LEU:O	29:c:185:ASN:N	2.43	0.47
32:f:69:LYS:HE3	32:f:114:ASN:HD21	1.79	0.47
32:f:481:LYS:NZ	32:f:505:GLU:OE1	2.37	0.47
32:f:610:THR:HG23	32:f:611:HIS:CD2	2.50	0.47
3:C:74:GLY:HA3	3:C:87:VAL:HG13	1.97	0.47
6:F:379:VAL:HG13	6:F:417:HIS:HD1	1.80	0.47
11:K:109:VAL:HB	11:K:147:ASP:HB3	1.97	0.47
14:N:7:GLN:HA	14:N:12:VAL:HA	1.97	0.47
14:N:103:TRP:HA	14:N:109:GLY:HA2	1.97	0.47
21:U:176:MET:HA	21:U:179:TYR:CE2	2.50	0.47
21:U:202:VAL:HG11	21:U:219:CYS:HB3	1.95	0.47
21:U:842:LYS:HB3	21:U:843:GLU:O	2.15	0.47
22:V:479:ARG:NH1	25:Y:370:ILE:HG21	2.29	0.47
3:C:86:LEU:HD21	3:C:94:LYS:HB3	1.97	0.47
4:D:95:ALA:HB2	4:D:124:LEU:HD21	1.97	0.47
9:I:99:LEU:HD11	16:P:66:ARG:HD3	1.96	0.47
21:U:510:GLU:HA	21:U:547:GLY:HA3	1.97	0.47
22:V:56:ALA:O	22:V:59:ALA:HB3	2.15	0.47
22:V:144:ASP:N	22:V:145:LEU:HA	2.29	0.47
25:Y:92:GLU:HA	25:Y:100:ILE:HD13	1.97	0.47
25:Y:349:LYS:C	25:Y:351:ASN:H	2.23	0.47
26:Z:109:ASN:ND2	26:Z:119:SER:O	2.43	0.47
26:Z:186:THR:HG23	26:Z:187:LEU:H	1.80	0.47
29:c:98:MET:O	29:c:102:THR:OG1	2.24	0.47
1:A:157:ILE:HG21	1:A:259:GLU:OE1	2.16	0.46
1:A:184:ILE:HD13	1:A:224:LEU:HD22	1.97	0.46
4:D:159:LYS:HD2	4:D:221:HIS:CE1	2.50	0.46
4:D:385:LEU:HD22	4:D:402:ALA:HB2	1.97	0.46
5:E:47:LEU:HA	5:E:50:LEU:HD12	1.96	0.46
5:E:100:LEU:HD23	5:E:107:ILE:HG13	1.97	0.46
6:F:438:TYR:CE2	11:K:20:ARG:HB3	2.43	0.46
15:O:7:VAL:HG22	15:O:12:ILE:HG12	1.97	0.46
16:P:99:ARG:O	16:P:99:ARG:NH1	2.42	0.46
18:R:59:LEU:HD22	18:R:83:LEU:HB2	1.96	0.46
22:V:239:THR:HA	22:V:240:LEU:HA	1.68	0.46
23:W:16:MET:HG3	23:W:54:THR:HB	1.96	0.46
24:X:396:THR:HG23	25:Y:366:TYR:CD1	2.50	0.46
32:f:297:ARG:HA	32:f:298:ASN:C	2.40	0.46
3:C:14:GLY:O	3:C:18:SER:N	2.25	0.46
4:D:377:SER:HB3	5:E:292:PRO:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:300:LYS:HE3	6:F:304:ARG:HB3	1.98	0.46
6:F:366:MET:HE1	6:F:384:LEU:HD22	1.97	0.46
7:G:43:ARG:HG3	7:G:48:ALA:HB2	1.97	0.46
7:G:88:ARG:HH12	13:M:156:VAL:HG13	1.81	0.46
10:J:120:GLN:OE1	11:K:134:SER:N	2.48	0.46
12:L:49:LEU:HD21	12:L:199:LEU:HD21	1.97	0.46
15:O:177:VAL:N	15:O:184:ASP:O	2.48	0.46
16:P:27:ARG:HB2	16:P:183:MET:HB2	1.97	0.46
26:Z:96:HIS:HE1	26:Z:121:LEU:HD13	1.80	0.46
29:c:295:ASN:HA	29:c:298:GLN:HG2	1.96	0.46
2:B:261:GLY:O	2:B:264:PRO:HD3	2.15	0.46
3:C:69:GLN:H	3:C:118:ASN:HD22	1.63	0.46
11:K:23:GLN:NE2	11:K:136:PRO:HD2	2.30	0.46
21:U:378:CYS:HB2	21:U:740:GLY:HA2	1.97	0.46
21:U:664:GLY:HA2	21:U:698:GLN:HE22	1.81	0.46
23:W:403:PHE:HB3	23:W:416:GLN:HG3	1.97	0.46
26:Z:14:LEU:HD23	29:c:43:LYS:HD3	1.96	0.46
27:a:161:LYS:HA	27:a:164:GLN:HG2	1.98	0.46
27:a:309:LEU:H	27:a:309:LEU:HD12	1.80	0.46
32:f:106:ALA:HB1	32:f:107:LEU:CA	2.46	0.46
1:A:279:ALA:HB2	2:B:310:LEU:HD23	1.97	0.46
1:A:290:GLY:HA2	1:A:291:GLY:HA3	1.56	0.46
1:A:368:ILE:HG23	1:A:406:GLU:HB3	1.97	0.46
3:C:232:ARG:NE	3:C:275:GLU:OE1	2.42	0.46
5:E:232:MET:HB2	5:E:277:MET:HG2	1.97	0.46
7:G:96:TYR:O	7:G:100:ASN:ND2	2.46	0.46
7:G:119:ALA:HA	7:G:122:SER:HB2	1.97	0.46
9:I:105:ILE:HD12	9:I:106:PRO:HD2	1.98	0.46
12:L:109:VAL:HG21	12:L:145:PHE:HD2	1.80	0.46
16:P:135:ASP:OD1	16:P:135:ASP:N	2.48	0.46
18:R:9:ARG:NH2	18:R:146:ASP:OD2	2.47	0.46
21:U:378:CYS:SG	21:U:783:TYR:HD1	2.39	0.46
21:U:388:ASP:OD1	21:U:389:ASN:N	2.46	0.46
22:V:173:ILE:O	22:V:177:ASN:N	2.42	0.46
23:W:445:LEU:HD12	23:W:448:LYS:HZ1	1.81	0.46
27:a:25:LEU:HA	27:a:28:LEU:HD22	1.96	0.46
29:c:28:ALA:HB1	29:c:180:ASN:HD21	1.80	0.46
2:B:239:VAL:HA	2:B:242:GLN:HG3	1.97	0.46
3:C:166:GLU:OE2	3:C:207:THR:OG1	2.33	0.46
4:D:322:LEU:HB3	4:D:330:LYS:HE2	1.97	0.46
4:D:376:ASN:HD21	33:D:501:ATP:H1'	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:116:LYS:HE3	8:H:84:ARG:HD2	1.97	0.46
9:I:164:ILE:HA	9:I:165:GLY:HA2	1.56	0.46
9:I:184:MET:HA	9:I:185:THR:C	2.41	0.46
11:K:11:GLY:O	11:K:12:VAL:HG22	2.15	0.46
23:W:45:GLU:HA	23:W:96:GLN:HB3	1.98	0.46
23:W:253:THR:HB	23:W:254:PRO:HD3	1.97	0.46
23:W:263:TRP:HH2	23:W:295:LYS:HG3	1.80	0.46
25:Y:25:LEU:O	25:Y:29:PRO:HG2	2.16	0.46
25:Y:286:TRP:O	25:Y:287:LEU:HG	2.16	0.46
25:Y:314:LEU:O	25:Y:354:VAL:N	2.48	0.46
25:Y:349:LYS:O	25:Y:350:VAL:HG22	2.16	0.46
25:Y:387:ILE:HA	25:Y:388:ASN:HA	1.54	0.46
27:a:62:ASN:OD1	27:a:103:LYS:NZ	2.46	0.46
27:a:232:TRP:HZ3	27:a:253:THR:HA	1.80	0.46
30:d:225:PHE:HA	30:d:226:ALA:HA	1.73	0.46
32:f:676:GLU:HA	32:f:679:ARG:HH11	1.80	0.46
4:D:153:MET:HB3	4:D:228:ILE:HD13	1.96	0.46
6:F:151:VAL:HG12	6:F:163:THR:HA	1.97	0.46
6:F:298:SER:HB2	6:F:299:GLU:HA	1.97	0.46
6:F:363:ALA:HB2	6:F:385:ALA:HB2	1.96	0.46
7:G:230:LEU:HD11	7:G:235:ILE:HG13	1.96	0.46
20:T:50:MET:N	20:T:113:GLY:O	2.49	0.46
21:U:735:GLY:O	21:U:739:ALA:N	2.48	0.46
23:W:451:MET:HE1	26:Z:156:GLU:HA	1.96	0.46
26:Z:59:ASP:HB2	28:b:95:LEU:HD11	1.98	0.46
26:Z:72:HIS:HB2	28:b:63:THR:OG1	2.16	0.46
27:a:100:THR:HA	27:a:103:LYS:HE2	1.98	0.46
27:a:287:ASN:HA	27:a:288:HIS:C	2.41	0.46
28:b:91:ARG:NH1	28:b:134:GLU:OE2	2.42	0.46
29:c:100:LYS:HA	29:c:105:PRO:HB3	1.97	0.46
32:f:228:GLN:HE22	32:f:250:SER:HA	1.80	0.46
2:B:155:LYS:HA	2:B:156:VAL:HA	1.62	0.46
2:B:182:GLU:HB2	2:B:239:VAL:HG21	1.96	0.46
3:C:251:ILE:HG23	3:C:262:GLY:HA2	1.97	0.46
4:D:49:GLN:O	4:D:53:PHE:N	2.40	0.46
11:K:67:ILE:HG12	11:K:218:ALA:HB2	1.97	0.46
11:K:79:SER:H	11:K:139:VAL:HG23	1.81	0.46
22:V:256:ARG:HG3	31:e:5:LYS:HD3	1.98	0.46
23:W:436:MET:HA	23:W:439:VAL:HG22	1.97	0.46
24:X:396:THR:HG21	25:Y:365:GLN:HB3	1.98	0.46
25:Y:89:GLU:HA	25:Y:92:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:34:ARG:HH12	26:Z:102:HIS:CE1	2.34	0.46
30:d:62:SER:HA	30:d:65:ARG:HG2	1.98	0.46
32:f:190:TYR:HD1	32:f:230:LYS:HE3	1.81	0.46
1:A:387:SER:HA	1:A:390:THR:HB	1.97	0.46
2:B:428:TYR:HA	2:B:431:GLN:HB2	1.98	0.46
6:F:145:LEU:HG	6:F:146:LYS:H	1.81	0.46
6:F:221:LYS:HA	6:F:327:LYS:HG3	1.97	0.46
9:I:95:GLN:HE22	9:I:98:LEU:HD23	1.80	0.46
10:J:9:VAL:HG22	11:K:23:GLN:HE21	1.81	0.46
11:K:23:GLN:NE2	11:K:135:ARG:HB2	2.30	0.46
11:K:50:VAL:HG22	11:K:51:GLU:H	1.81	0.46
12:L:186:GLU:HA	12:L:189:LYS:HE3	1.97	0.46
14:N:31:THR:HB	14:N:33:LYS:HZ1	1.80	0.46
16:P:158:MET:HE2	16:P:163:LEU:HA	1.96	0.46
23:W:135:LYS:CB	23:W:136:ILE:HB	2.46	0.46
26:Z:187:LEU:O	26:Z:191:ILE:HD12	2.16	0.46
2:B:409:GLU:OE1	2:B:413:LYS:HB3	2.16	0.46
7:G:139:ILE:HG13	7:G:153:LYS:HG3	1.97	0.46
9:I:167:ASN:O	9:I:168:SER:HB3	2.16	0.46
19:S:171:ALA:HA	19:S:174:LEU:HD12	1.98	0.46
21:U:328:ILE:HG13	21:U:329:LEU:N	2.31	0.46
21:U:586:VAL:HG11	21:U:601:ARG:HH12	1.81	0.46
21:U:764:LEU:O	21:U:767:THR:OG1	2.26	0.46
21:U:813:TYR:OH	21:U:883:ARG:NH1	2.49	0.46
23:W:326:MET:O	23:W:330:LYS:N	2.48	0.46
29:c:154:LYS:HG2	29:c:156:VAL:H	1.81	0.46
29:c:260:GLU:O	29:c:264:LYS:N	2.43	0.46
1:A:322:ASN:OD1	1:A:428:ARG:NH1	2.46	0.46
7:G:50:ILE:O	7:G:218:GLY:N	2.49	0.46
12:L:26:MET:HE1	12:L:148:CYS:HB2	1.98	0.46
21:U:20:LYS:HD2	21:U:48:LEU:HD11	1.98	0.46
21:U:469:SER:OG	21:U:472:ILE:HG13	2.16	0.46
23:W:155:GLN:NE2	23:W:161:GLU:HG3	2.31	0.46
25:Y:203:ASP:OD1	25:Y:203:ASP:N	2.46	0.46
25:Y:336:ARG:NH1	31:e:56:LEU:HB3	2.31	0.46
29:c:211:GLU:O	29:c:215:LYS:N	2.36	0.46
32:f:370:SER:HA	32:f:371:CYS:SG	2.55	0.46
1:A:427:PRO:HB2	1:A:429:TYR:CD2	2.50	0.45
3:C:77:VAL:HG22	3:C:86:LEU:HD22	1.97	0.45
7:G:67:THR:HG22	7:G:69:LEU:H	1.81	0.45
7:G:103:TYR:HE1	14:N:57:ASP:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:210:PHE:HE1	7:G:214:GLU:HB2	1.81	0.45
10:J:76:LEU:HD13	10:J:78:ALA:HB3	1.98	0.45
18:R:11:GLY:HA3	18:R:179:VAL:O	2.15	0.45
18:R:143:TYR:HA	18:R:155:LEU:HD21	1.98	0.45
22:V:282:ASN:OD1	25:Y:382:LYS:HG3	2.16	0.45
25:Y:170:GLU:CG	25:Y:171:GLY:HA3	2.44	0.45
1:A:206:ILE:HG12	6:F:401:VAL:HA	1.99	0.45
1:A:398:ARG:NH2	2:B:195:GLN:HB2	2.31	0.45
5:E:281:ARG:NH1	6:F:294:LYS:O	2.45	0.45
6:F:128:THR:HG23	6:F:130:GLN:H	1.81	0.45
14:N:40:ARG:NH1	14:N:180:ALA:O	2.48	0.45
16:P:141:THR:HG21	16:P:180:VAL:HG11	1.98	0.45
20:T:187:PHE:CE2	20:T:205:THR:HG23	2.51	0.45
21:U:337:LEU:HD12	21:U:338:HIS:N	2.30	0.45
21:U:485:ALA:HB3	21:U:519:VAL:HG12	1.97	0.45
21:U:794:ASP:OD1	21:U:795:LEU:N	2.49	0.45
22:V:153:LYS:O	22:V:157:THR:OG1	2.28	0.45
23:W:275:ILE:O	23:W:357:ARG:NE	2.49	0.45
29:c:249:LEU:HA	29:c:252:ALA:HB3	1.99	0.45
32:f:18:GLU:OE1	32:f:79:ASN:ND2	2.49	0.45
32:f:246:HIS:CE1	32:f:250:SER:HB3	2.51	0.45
1:A:420:TYR:CE1	2:B:350:LYS:HG2	2.51	0.45
2:B:201:VAL:HB	2:B:241:ASN:HD21	1.82	0.45
2:B:300:GLY:HA3	2:B:301:GLY:HA2	1.70	0.45
2:B:415:THR:HB	2:B:418:ASP:HB3	1.98	0.45
4:D:276:ASP:O	4:D:280:GLY:N	2.49	0.45
9:I:101:TYR:HD1	17:Q:79:ALA:HB1	1.81	0.45
13:M:171:ALA:HB3	13:M:200:VAL:HG21	1.99	0.45
21:U:16:GLU:OE1	21:U:18:GLN:HG2	2.15	0.45
21:U:550:VAL:O	21:U:554:LEU:N	2.49	0.45
22:V:99:ARG:NH2	22:V:147:PHE:H	2.08	0.45
23:W:70:VAL:HA	23:W:73:MET:HE3	1.99	0.45
24:X:406:ASN:ND2	29:c:264:LYS:HD2	2.31	0.45
25:Y:48:ASN:O	25:Y:114:ILE:HG13	2.15	0.45
29:c:33:ILE:HA	29:c:69:VAL:HG13	1.97	0.45
29:c:263:ASP:O	29:c:266:THR:OG1	2.34	0.45
1:A:318:LEU:HD23	1:A:319:MET:N	2.31	0.45
1:A:409:PHE:O	1:A:413:VAL:HG23	2.16	0.45
2:B:254:GLU:HB2	2:B:288:ASP:HB2	1.99	0.45
2:B:324:ASP:HB2	2:B:326:LYS:HG2	1.98	0.45
4:D:401:LYS:HA	4:D:404:LYS:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:193:ARG:HA	12:L:196:ARG:HD2	1.99	0.45
22:V:290:TYR:OH	22:V:294:ARG:NH2	2.49	0.45
23:W:431:LYS:HA	23:W:435:LEU:HD13	1.97	0.45
29:c:226:MET:O	29:c:228:GLY:N	2.50	0.45
32:f:371:CYS:O	32:f:372:ASN:HB2	2.16	0.45
1:A:160:THR:O	1:A:162:THR:N	2.49	0.45
1:A:292:ASP:OD1	2:B:303:ARG:NH1	2.49	0.45
4:D:279:THR:O	4:D:283:ARG:N	2.47	0.45
10:J:7:ILE:HG22	10:J:8:THR:HG23	1.98	0.45
11:K:73:HIS:CE1	11:K:108:THR:HG22	2.51	0.45
17:Q:42:ILE:HA	17:Q:106:GLY:HA2	1.97	0.45
21:U:106:ASP:HA	21:U:109:THR:HG22	1.98	0.45
21:U:173:VAL:N	21:U:174:PRO:HD3	2.32	0.45
23:W:142:ARG:NH2	23:W:178:GLU:HB2	2.30	0.45
23:W:259:GLU:HB3	23:W:263:TRP:HB2	1.99	0.45
32:f:269:GLN:HE21	32:f:272:LYS:H	1.64	0.45
32:f:391:LEU:HD13	32:f:424:VAL:HG11	1.99	0.45
32:f:525:PRO:O	32:f:526:THR:HG22	2.17	0.45
1:A:310:ASP:HA	1:A:311:PRO:HA	1.58	0.45
2:B:96:ARG:HH22	3:C:84:LYS:HG3	1.82	0.45
5:E:230:ILE:HB	5:E:275:MET:HA	1.98	0.45
9:I:148:TYR:HA	9:I:158:GLY:HA2	1.98	0.45
14:N:132:SER:HA	14:N:135:ILE:HG12	1.99	0.45
21:U:804:SER:HB3	21:U:839:ALA:HB3	1.99	0.45
22:V:137:GLU:HA	22:V:140:ASP:HB2	1.97	0.45
22:V:318:GLN:O	22:V:319:HIS:ND1	2.50	0.45
23:W:13:ILE:HG22	23:W:54:THR:HG21	1.99	0.45
25:Y:78:GLU:HA	25:Y:81:LEU:HB3	1.99	0.45
25:Y:110:TYR:O	25:Y:113:ARG:HB3	2.16	0.45
25:Y:283:LYS:HZ2	31:e:60:LEU:HD23	1.81	0.45
27:a:31:LYS:HG3	28:b:177:PRO:HD3	1.99	0.45
27:a:243:GLY:HA3	27:a:244:ASN:HA	1.61	0.45
28:b:164:ASP:H	28:b:165:GLY:HA2	1.79	0.45
30:d:201:ASN:OD1	30:d:201:ASN:N	2.49	0.45
32:f:223:ASN:OD1	32:f:224:ALA:N	2.49	0.45
32:f:376:THR:HG21	32:f:410:LYS:HE2	1.97	0.45
32:f:606:ALA:HA	32:f:609:LEU:HD13	1.98	0.45
5:E:236:ASP:N	5:E:236:ASP:OD1	2.50	0.45
13:M:110:HIS:NE2	14:N:70:LEU:HA	2.31	0.45
17:Q:25:ILE:HG13	17:Q:26:VAL:H	1.80	0.45
21:U:340:GLN:HG3	21:U:880:ASN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:327:GLU:HA	23:W:330:LYS:HB3	1.98	0.45
32:f:370:SER:HB3	32:f:372:ASN:HD22	1.82	0.45
32:f:400:PRO:HB2	32:f:440:ALA:HB3	1.98	0.45
7:G:68:HIS:HE2	7:G:80:MET:C	2.23	0.45
9:I:3:ARG:HH11	11:K:11:GLY:H	1.65	0.45
13:M:110:HIS:HE1	14:N:69:GLU:HG2	1.82	0.45
16:P:54:ALA:HB3	16:P:106:GLU:HB2	1.98	0.45
20:T:111:VAL:HG13	20:T:137:LEU:HD12	1.99	0.45
21:U:377:HIS:O	21:U:380:THR:HG22	2.17	0.45
21:U:500:ASN:HA	21:U:503:GLN:HG2	1.99	0.45
23:W:23:THR:HA	23:W:26:GLN:HB2	1.99	0.45
23:W:88:MET:SD	23:W:96:GLN:NE2	2.90	0.45
27:a:80:ILE:HD12	27:a:83:VAL:HB	1.99	0.45
27:a:342:ASP:HB2	27:a:345:GLN:HG2	1.99	0.45
29:c:256:ASN:OD1	29:c:291:LEU:HD22	2.17	0.45
32:f:73:TYR:HD2	32:f:74:LEU:HD12	1.82	0.45
1:A:206:ILE:HA	6:F:373:MET:SD	2.57	0.45
3:C:117:ARG:O	3:C:121:TYR:HA	2.17	0.45
6:F:228:PRO:O	6:F:231:THR:HG23	2.16	0.45
6:F:283:ILE:HG22	6:F:328:VAL:HG13	1.98	0.45
6:F:288:LEU:HD12	6:F:291:ILE:HD11	1.98	0.45
7:G:43:ARG:HA	7:G:48:ALA:HA	1.99	0.45
8:H:153:GLY:O	9:I:81:SER:OG	2.30	0.45
9:I:45:LEU:HD11	9:I:137:ILE:HG12	1.98	0.45
13:M:40:ARG:HH11	13:M:148:LEU:HB3	1.82	0.45
21:U:54:PHE:CZ	21:U:56:SER:HB2	2.52	0.45
21:U:751:ARG:HG3	21:U:908:ILE:HG21	1.97	0.45
24:X:200:ILE:HG22	24:X:201:TYR:H	1.81	0.45
24:X:244:SER:O	24:X:248:ILE:N	2.45	0.45
25:Y:251:HIS:HA	25:Y:257:ARG:HD3	1.97	0.45
27:a:116:THR:HA	27:a:158:LEU:HD21	1.98	0.45
29:c:144:VAL:HB	29:c:158:ASP:HB3	1.99	0.45
29:c:191:ALA:HA	29:c:194:HIS:CE1	2.52	0.45
31:e:46:ASP:HA	31:e:49:GLU:HB3	1.99	0.45
32:f:293:ASN:HD21	32:f:303:ALA:HB1	1.81	0.45
32:f:653:GLY:O	32:f:656:HIS:NE2	2.50	0.45
1:A:315:ILE:H	1:A:315:ILE:HG13	1.55	0.45
4:D:130:VAL:HA	4:D:142:VAL:HA	1.99	0.45
6:F:85:THR:HA	6:F:86:LEU:HA	1.59	0.45
9:I:95:GLN:HG2	16:P:73:LEU:HG	1.98	0.45
11:K:111:SER:HB3	19:S:79:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:160:SER:OG	12:L:165:SER:HB3	2.17	0.45
18:R:8:PHE:HE2	18:R:13:ILE:HG12	1.82	0.45
19:S:57:PHE:HD2	19:S:60:ASP:H	1.65	0.45
22:V:32:PRO:O	22:V:36:GLU:HB3	2.17	0.45
22:V:197:THR:C	22:V:199:ASN:H	2.24	0.45
22:V:455:LYS:HD2	22:V:457:TYR:CE2	2.52	0.45
26:Z:68:TRP:HH2	26:Z:111:LEU:HD22	1.81	0.45
28:b:156:PHE:O	28:b:160:LEU:HB2	2.17	0.45
29:c:40:LYS:O	29:c:44:HIS:HB3	2.17	0.45
1:A:250:VAL:O	6:F:259:MET:N	2.50	0.44
1:A:419:SER:HA	1:A:422:LYS:HE3	1.99	0.44
7:G:47:CYS:HB3	7:G:221:THR:HG23	1.99	0.44
10:J:9:VAL:HG22	11:K:23:GLN:NE2	2.32	0.44
13:M:236:GLU:O	13:M:240:LYS:NZ	2.45	0.44
14:N:99:ILE:HG23	14:N:113:SER:HA	2.00	0.44
15:O:50:ALA:HB2	16:P:129:CYS:HB2	1.99	0.44
22:V:280:ALA:HB1	22:V:281:ASN:ND2	2.32	0.44
22:V:439:ALA:HB1	30:d:181:CYS:O	2.17	0.44
24:X:289:CYS:O	24:X:293:ALA:N	2.49	0.44
24:X:417:LYS:HG2	26:Z:283:ARG:NH1	2.31	0.44
25:Y:215:ASP:O	25:Y:218:THR:OG1	2.27	0.44
29:c:161:ARG:NH1	29:c:162:LEU:O	2.50	0.44
30:d:65:ARG:HG3	30:d:67:ASP:H	1.82	0.44
30:d:147:SER:OG	30:d:150:LYS:N	2.51	0.44
2:B:392:GLY:O	2:B:395:ILE:HG22	2.16	0.44
3:C:41:ASN:HD21	22:V:495:ARG:HA	1.81	0.44
3:C:49:ARG:O	3:C:53:ASN:N	2.47	0.44
3:C:257:SER:O	3:C:258:ARG:HB2	2.17	0.44
4:D:105:SER:HB3	4:D:111:TYR:CE2	2.53	0.44
4:D:406:VAL:HA	4:D:407:ILE:HA	1.51	0.44
6:F:430:LYS:O	6:F:431:LYS:HG3	2.17	0.44
11:K:199:LEU:HD13	11:K:241:ILE:HD12	1.99	0.44
18:R:41:LEU:HD23	18:R:103:GLY:HA3	1.98	0.44
23:W:55:ARG:NH1	23:W:78:LYS:HG3	2.32	0.44
24:X:258:LYS:HD2	24:X:294:SER:OG	2.18	0.44
25:Y:300:ARG:HH12	31:e:63:HIS:CG	2.36	0.44
27:a:125:ILE:HG22	27:a:126:GLY:C	2.42	0.44
29:c:150:SER:OG	29:c:154:LYS:HB3	2.18	0.44
32:f:281:ILE:HG13	32:f:282:LYS:H	1.81	0.44
32:f:681:LEU:HB2	32:f:682:PRO:HD3	2.00	0.44
3:C:235:PHE:HD1	3:C:276:LEU:HG	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:33:LYS:O	15:O:45:GLY:N	2.42	0.44
16:P:101:GLY:O	17:Q:93:ARG:NH1	2.50	0.44
18:R:97:MET:H	18:R:116:SER:HB3	1.81	0.44
19:S:211:ARG:NE	19:S:213:ASP:O	2.51	0.44
21:U:561:GLU:HG2	21:U:562:GLU:H	1.82	0.44
21:U:773:PHE:HD1	21:U:773:PHE:HA	1.69	0.44
22:V:156:SER:HB2	22:V:160:LEU:HD12	1.99	0.44
22:V:244:ALA:C	22:V:246:GLY:H	2.25	0.44
22:V:275:VAL:HB	22:V:277:PRO:HD3	1.98	0.44
23:W:120:ILE:O	23:W:124:LEU:N	2.45	0.44
24:X:187:ARG:O	24:X:191:THR:N	2.45	0.44
32:f:617:LEU:HB3	32:f:618:THR:CB	2.38	0.44
32:f:663:VAL:HA	32:f:664:ALA:HA	1.65	0.44
1:A:328:ASP:HB3	1:A:329:PRO:HD3	1.98	0.44
3:C:154:LEU:O	3:C:157:GLN:N	2.51	0.44
4:D:46:LYS:HZ1	21:U:183:LEU:HD22	1.83	0.44
7:G:139:ILE:HG12	7:G:153:LYS:NZ	2.33	0.44
11:K:108:THR:C	11:K:110:GLU:H	2.24	0.44
12:L:31:GLN:O	12:L:51:ARG:NH1	2.49	0.44
14:N:73:PRO:HB3	14:N:105:PRO:HG2	2.00	0.44
20:T:89:HIS:CE1	20:T:131:ALA:HB1	2.52	0.44
20:T:136:SER:HB2	20:T:150:LEU:HD13	1.99	0.44
26:Z:242:LEU:C	26:Z:244:GLU:H	2.25	0.44
27:a:245:VAL:HA	27:a:246:GLU:C	2.43	0.44
31:e:4:LYS:HD2	31:e:4:LYS:HA	1.93	0.44
1:A:395:PHE:HA	1:A:398:ARG:HB2	1.99	0.44
3:C:167:LEU:HD22	3:C:175:PHE:CZ	2.52	0.44
4:D:96:VAL:HG23	4:D:97:ASP:OD1	2.18	0.44
5:E:349:GLU:HG2	5:E:374:VAL:HG21	2.00	0.44
6:F:81:LYS:O	6:F:85:THR:HG22	2.18	0.44
11:K:10:ARG:NH1	12:L:21:GLN:HE22	2.14	0.44
11:K:41:GLN:NE2	11:K:152:GLN:HA	2.32	0.44
17:Q:114:ALA:HB1	17:Q:126:LYS:HE2	1.99	0.44
18:R:19:ARG:NE	18:R:29:GLN:HE22	2.11	0.44
27:a:261:LEU:HD11	27:a:268:LEU:HD12	1.98	0.44
29:c:40:LYS:HE3	29:c:43:LYS:HZ1	1.82	0.44
32:f:298:ASN:HA	32:f:299:GLU:HA	1.77	0.44
1:A:105:ASP:N	1:A:105:ASP:OD1	2.50	0.44
1:A:261:PHE:O	1:A:265:ARG:HG3	2.18	0.44
1:A:375:ARG:HH12	11:K:205:VAL:HB	1.81	0.44
2:B:173:VAL:HG23	2:B:174:MET:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:412:GLN:NE2	4:D:415:GLU:H	2.16	0.44
5:E:281:ARG:NH2	6:F:296:PHE:HA	2.32	0.44
6:F:125:LYS:HD2	6:F:131:THR:HG23	2.00	0.44
7:G:141:ILE:HD13	7:G:220:VAL:HG11	1.99	0.44
10:J:96:LEU:HA	17:Q:62:LYS:HG2	1.99	0.44
21:U:446:LEU:O	21:U:450:HIS:ND1	2.34	0.44
21:U:470:ASN:OD1	21:U:471:ASP:HA	2.18	0.44
21:U:669:ILE:HG12	21:U:694:ILE:HG21	2.00	0.44
22:V:212:TYR:CG	31:e:4:LYS:NZ	2.85	0.44
23:W:247:TYR:HA	23:W:250:ILE:HG23	1.99	0.44
24:X:264:PRO:C	24:X:266:ASP:H	2.26	0.44
25:Y:301:ILE:O	25:Y:305:SER:N	2.44	0.44
29:c:226:MET:C	29:c:228:GLY:H	2.24	0.44
30:d:160:ALA:N	30:d:161:GLU:HA	2.32	0.44
30:d:215:TRP:CG	30:d:216:VAL:N	2.85	0.44
30:d:216:VAL:HG11	30:d:223:TYR:HB2	2.00	0.44
3:C:25:LEU:HD23	4:D:47:LEU:HB2	2.00	0.44
3:C:368:MET:HA	3:C:371:LEU:HB3	1.99	0.44
4:D:213:THR:OG1	33:D:501:ATP:O2A	2.26	0.44
5:E:76:GLY:N	5:E:77:PRO:HD2	2.32	0.44
5:E:129:ASN:H	5:E:190:GLN:HG2	1.82	0.44
6:F:268:VAL:HA	6:F:271:ALA:HB3	1.99	0.44
6:F:344:ARG:HB3	6:F:347:ARG:HB2	1.99	0.44
10:J:100:ASP:N	10:J:100:ASP:OD1	2.50	0.44
12:L:160:SER:O	12:L:169:ARG:NH2	2.51	0.44
21:U:242:LEU:HD13	21:U:324:LYS:HD2	1.99	0.44
22:V:212:TYR:CZ	31:e:4:LYS:CG	3.00	0.44
23:W:398:VAL:HA	24:X:341:PRO:HB3	1.98	0.44
23:W:403:PHE:HD2	23:W:416:GLN:HA	1.83	0.44
26:Z:208:ILE:HD12	27:a:353:LEU:HD23	2.00	0.44
32:f:444:SER:HB2	32:f:449:LYS:HD2	1.99	0.44
32:f:638:LEU:HA	32:f:639:THR:C	2.42	0.44
2:B:182:GLU:HB2	2:B:239:VAL:HG11	2.00	0.44
2:B:364:ILE:HG23	2:B:368:HIS:CE1	2.52	0.44
4:D:207:PRO:HG2	4:D:312:ASN:HA	1.99	0.44
6:F:189:GLY:HA3	6:F:364:ARG:HB3	2.00	0.44
6:F:356:MET:HG2	6:F:390:ASP:HA	1.99	0.44
7:G:24:GLN:OE1	13:M:14:PHE:N	2.49	0.44
7:G:152:TYR:CD1	7:G:162:GLY:HA3	2.52	0.44
12:L:20:HIS:HB3	12:L:24:TYR:CZ	2.53	0.44
12:L:120:THR:O	13:M:129:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:178:PHE:HB2	17:Q:194:ILE:HB	1.99	0.44
21:U:465:LEU:HA	21:U:473:VAL:HG11	1.99	0.44
21:U:563:ALA:O	21:U:567:ILE:HG12	2.18	0.44
26:Z:171:GLY:HA3	29:c:38:LEU:HD11	2.00	0.44
30:d:120:GLU:O	30:d:123:PRO:HD3	2.18	0.44
32:f:314:ASN:HD21	32:f:355:VAL:HG13	1.82	0.44
32:f:365:MET:HE3	32:f:672:VAL:HG11	1.99	0.44
1:A:363:SER:HB2	1:A:403:ILE:HG22	1.99	0.44
5:E:57:VAL:HG12	5:E:111:LEU:HD21	2.00	0.44
5:E:222:ALA:HB1	5:E:228:CYS:SG	2.58	0.44
5:E:374:VAL:O	5:E:378:LYS:HG2	2.18	0.44
11:K:10:ARG:O	11:K:14:THR:OG1	2.27	0.44
12:L:196:ARG:HB2	12:L:239:ARG:HH21	1.83	0.44
17:Q:108:ASP:OD2	17:Q:111:GLU:N	2.49	0.44
18:R:81:LYS:HD3	18:R:120:ARG:HD2	1.99	0.44
21:U:107:HIS:HA	21:U:110:LYS:HE3	2.00	0.44
21:U:428:PRO:HD2	21:U:464:GLN:NE2	2.32	0.44
22:V:323:GLY:HA2	22:V:326:GLN:HB2	1.99	0.44
23:W:343:SER:HB2	23:W:346:GLU:HB3	2.00	0.44
25:Y:311:TYR:HD2	25:Y:314:LEU:HD12	1.83	0.44
26:Z:205:LEU:HA	26:Z:208:ILE:HG22	1.99	0.44
29:c:75:MET:HE3	29:c:76:PRO:HD2	1.98	0.44
30:d:79:LYS:HA	30:d:121:ARG:HH21	1.83	0.44
3:C:285:ALA:HA	3:C:286:THR:HA	1.78	0.43
5:E:128:GLY:HA2	5:E:129:ASN:HB2	2.00	0.43
7:G:212:PRO:O	7:G:215:ILE:HG13	2.18	0.43
9:I:240:HIS:O	9:I:244:GLU:N	2.33	0.43
15:O:98:LEU:HB2	15:O:113:ILE:HB	2.00	0.43
21:U:26:LYS:O	21:U:30:VAL:HG22	2.18	0.43
21:U:161:ASP:OD1	21:U:162:VAL:N	2.47	0.43
22:V:174:PHE:HA	22:V:177:ASN:HB2	2.00	0.43
22:V:419:LEU:HD23	22:V:458:VAL:HG23	1.99	0.43
22:V:486:ILE:HG12	25:Y:381:GLN:HE21	1.83	0.43
23:W:306:LEU:O	23:W:310:THR:HG22	2.17	0.43
23:W:409:LEU:HD23	24:X:384:VAL:HG21	2.00	0.43
25:Y:357:ASN:OD1	25:Y:358:ARG:N	2.51	0.43
25:Y:387:ILE:HD13	26:Z:283:ARG:HD3	2.00	0.43
26:Z:199:LYS:HA	26:Z:202:ASN:HD21	1.83	0.43
26:Z:252:LYS:HE2	29:c:305:ASP:HB3	2.00	0.43
30:d:135:HIS:HB3	30:d:136:PRO:HD3	2.00	0.43
32:f:510:GLU:C	32:f:512:ALA:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG13	1:A:117:GLN:H	1.82	0.43
1:A:250:VAL:HG11	1:A:297:ARG:NH2	2.34	0.43
3:C:192:PRO:HA	3:C:193:GLY:HA3	1.68	0.43
5:E:149:ILE:O	5:E:152:PRO:HD2	2.17	0.43
17:Q:152:SER:HB3	17:Q:155:ARG:HB2	1.99	0.43
21:U:772:TRP:CD1	21:U:774:PRO:HD2	2.53	0.43
23:W:124:LEU:O	23:W:128:LEU:HG	2.19	0.43
26:Z:250:TYR:O	26:Z:254:ASN:HB2	2.18	0.43
27:a:308:GLU:HB3	27:a:312:MET:HE2	2.00	0.43
29:c:53:VAL:HG12	29:c:77:GLN:HG2	2.00	0.43
30:d:184:LYS:HA	30:d:185:ALA:HA	1.75	0.43
1:A:221:GLY:C	1:A:223:THR:H	2.26	0.43
2:B:226:GLY:C	2:B:230:THR:HB	2.44	0.43
2:B:313:LEU:HD13	2:B:341:LEU:HD22	2.01	0.43
2:B:319:PHE:HA	2:B:320:ASP:HA	1.49	0.43
4:D:83:GLN:HG3	4:D:133:HIS:CD2	2.54	0.43
4:D:147:ALA:O	5:E:62:LYS:HD2	2.18	0.43
4:D:388:ARG:HH12	5:E:143:ARG:HG2	1.83	0.43
5:E:112:PRO:O	5:E:113:ARG:HG3	2.18	0.43
11:K:116:VAL:HA	11:K:119:LEU:HG	2.00	0.43
16:P:53:LEU:HD13	16:P:60:VAL:HA	2.00	0.43
21:U:181:LEU:HB3	21:U:218:GLN:NE2	2.34	0.43
21:U:374:SER:HB2	21:U:410:VAL:HG11	2.00	0.43
22:V:89:LYS:HD3	22:V:92:ARG:HH11	1.82	0.43
22:V:99:ARG:NH1	22:V:150:ARG:HH21	2.16	0.43
22:V:182:LYS:NZ	22:V:210:CYS:HB2	2.33	0.43
22:V:215:ALA:HB1	22:V:256:ARG:NH2	2.34	0.43
22:V:480:ILE:HG22	22:V:484:LEU:HD23	2.00	0.43
23:W:370:TYR:OH	23:W:373:ILE:HD12	2.18	0.43
23:W:444:HIS:HD2	23:W:448:LYS:NZ	2.16	0.43
24:X:354:ILE:HG21	24:X:361:VAL:HG11	2.00	0.43
28:b:9:CYS:HB3	28:b:111:ALA:HA	2.01	0.43
28:b:52:ILE:HD13	28:b:60:VAL:HG23	2.00	0.43
1:A:139:ARG:HG3	1:A:156:LYS:HG3	2.01	0.43
3:C:73:VAL:HB	4:D:110:ASN:HB2	1.99	0.43
3:C:76:VAL:O	3:C:111:ASN:N	2.44	0.43
3:C:215:SER:HB3	3:C:216:GLY:HA2	2.01	0.43
4:D:82:ILE:HA	4:D:83:GLN:HA	1.64	0.43
4:D:413:GLU:HG2	7:G:157:ALA:HB2	2.01	0.43
5:E:171:LEU:N	5:E:297:ARG:O	2.49	0.43
6:F:421:MET:HA	6:F:424:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:152:THR:HG22	11:K:82:ILE:HB	2.00	0.43
16:P:159:ASP:OD1	16:P:159:ASP:N	2.52	0.43
21:U:338:HIS:CE1	21:U:787:CYS:HB3	2.54	0.43
25:Y:50:MET:SD	25:Y:74:LYS:HB3	2.58	0.43
25:Y:301:ILE:HA	25:Y:304:TYR:HB2	1.99	0.43
27:a:208:GLU:HG2	27:a:271:LYS:HD2	2.01	0.43
28:b:142:ASN:HD21	28:b:170:LEU:HD21	1.84	0.43
29:c:32:TYR:HB3	29:c:208:ARG:HD3	2.00	0.43
1:A:183:GLN:HG2	1:A:344:SER:OG	2.19	0.43
2:B:107:MET:HB2	2:B:153:ASN:HA	1.99	0.43
3:C:72:TYR:N	3:C:116:LEU:O	2.50	0.43
5:E:155:ASN:HB3	5:E:158:LEU:HG	1.99	0.43
5:E:168:LYS:O	5:E:275:MET:HG2	2.17	0.43
6:F:188:ILE:HG22	33:F:501:ATP:H2	1.83	0.43
8:H:118:MET:HE2	8:H:151:PRO:HA	2.01	0.43
11:K:225:ASN:HB2	11:K:226:PHE:CD1	2.53	0.43
15:O:6:VAL:HG11	15:O:154:LEU:HD23	1.99	0.43
16:P:149:MET:HE3	16:P:153:LEU:HD11	1.99	0.43
22:V:414:TYR:OH	25:Y:331:ASP:O	2.37	0.43
27:a:144:ASN:HA	27:a:145:LEU:HA	1.58	0.43
32:f:458:SER:O	32:f:459:GLU:HB2	2.18	0.43
1:A:97:ARG:HA	1:A:98:CYS:HA	1.52	0.43
1:A:100:LYS:HB3	1:A:115:VAL:HG23	2.01	0.43
2:B:139:VAL:HB	2:B:141:LYS:N	2.34	0.43
2:B:285:ASP:OD2	2:B:286:GLU:HG2	2.18	0.43
3:C:25:LEU:O	3:C:29:GLU:N	2.43	0.43
5:E:169:GLY:O	5:E:296:ASP:HB2	2.18	0.43
6:F:204:LEU:HB2	6:F:212:PHE:HZ	1.84	0.43
6:F:364:ARG:O	6:F:368:ILE:HG12	2.18	0.43
20:T:54:SER:N	20:T:109:THR:O	2.50	0.43
24:X:378:LEU:HG	24:X:385:LEU:HD13	2.01	0.43
25:Y:112:CYS:SG	25:Y:120:ALA:HB2	2.58	0.43
26:Z:26:ILE:HA	26:Z:29:VAL:HG12	1.99	0.43
29:c:287:HIS:O	29:c:291:LEU:HG	2.18	0.43
1:A:206:ILE:HG13	1:A:207:GLU:H	1.84	0.43
3:C:65:LEU:HA	29:c:190:GLN:NE2	2.34	0.43
3:C:161:ILE:HD13	3:C:186:VAL:HG21	2.00	0.43
4:D:218:ALA:HA	4:D:221:HIS:HD2	1.84	0.43
5:E:58:GLY:N	5:E:98:VAL:O	2.41	0.43
5:E:214:LEU:HA	5:E:217:GLU:HB3	2.00	0.43
5:E:327:ASP:C	5:E:364:GLN:HE22	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:383:LYS:HG3	5:E:384:LEU:HD12	2.00	0.43
7:G:123:GLN:HE21	7:G:158:GLY:HA3	1.82	0.43
9:I:4:ARG:NH2	13:M:9:LEU:HD13	2.33	0.43
10:J:173:GLU:HA	10:J:176:TYR:HD2	1.84	0.43
11:K:74:ILE:HG23	11:K:144:GLY:O	2.19	0.43
13:M:40:ARG:HA	13:M:45:VAL:HA	1.99	0.43
20:T:124:TYR:CE2	20:T:126:ASP:HB2	2.54	0.43
21:U:413:LYS:NZ	21:U:448:LEU:O	2.51	0.43
22:V:221:LEU:HD12	22:V:222:ASP:H	1.82	0.43
23:W:3:ASP:OD1	23:W:4:GLY:N	2.52	0.43
23:W:221:LYS:HG3	23:W:224:LEU:HB2	2.01	0.43
26:Z:128:PRO:HB2	29:c:219:ASN:HD22	1.82	0.43
29:c:58:LEU:HB2	29:c:73:PHE:HE2	1.84	0.43
32:f:350:LYS:HD2	32:f:390:GLU:HA	2.01	0.43
1:A:271:LEU:HA	1:A:315:ILE:HD13	2.00	0.43
5:E:182:LEU:HD11	33:E:401:ATP:H2'	1.99	0.43
6:F:120:LYS:HG2	6:F:136:VAL:HG21	2.00	0.43
9:I:98:LEU:HD12	9:I:102:GLN:HA	1.99	0.43
10:J:43:LEU:HD23	10:J:134:VAL:HG11	2.01	0.43
18:R:100:MET:HG2	18:R:113:TYR:HD1	1.84	0.43
22:V:167:LEU:HD11	22:V:171:VAL:HB	2.00	0.43
22:V:357:LEU:O	22:V:361:PHE:N	2.52	0.43
23:W:183:VAL:HA	23:W:186:ILE:HG22	2.00	0.43
25:Y:286:TRP:CD1	25:Y:287:LEU:HD23	2.53	0.43
28:b:16:MET:O	28:b:25:ARG:HB2	2.19	0.43
30:d:226:ALA:HA	30:d:227:SER:HA	1.69	0.43
3:C:154:LEU:O	3:C:158:ILE:HG23	2.19	0.43
5:E:55:GLN:HB3	5:E:100:LEU:O	2.19	0.43
9:I:8:ARG:HD3	10:J:7:ILE:HD11	2.01	0.43
10:J:34:GLY:HA2	10:J:43:LEU:HA	2.01	0.43
10:J:180:ALA:HA	10:J:181:ILE:HA	1.68	0.43
11:K:209:LYS:O	11:K:214:ASN:ND2	2.51	0.43
17:Q:103:LEU:HD23	17:Q:117:TYR:HD1	1.83	0.43
19:S:150:ASP:HB3	19:S:156:LYS:HD2	2.01	0.43
21:U:457:ILE:HG23	21:U:460:TYR:HB3	1.99	0.43
22:V:94:VAL:HG11	22:V:134:PHE:HB3	2.01	0.43
25:Y:104:MET:O	25:Y:108:ALA:HB3	2.19	0.43
25:Y:108:ALA:HA	25:Y:111:LEU:HG	2.00	0.43
26:Z:172:VAL:HG13	29:c:217:LEU:HD11	2.01	0.43
27:a:33:LEU:HD13	27:a:36:GLN:HB2	1.99	0.43
27:a:308:GLU:OE1	27:a:308:GLU:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PHE:HB2	1:A:271:LEU:HB2	2.01	0.43
3:C:215:SER:HB3	3:C:216:GLY:CA	2.49	0.43
3:C:285:ALA:HB1	3:C:286:THR:HB	2.00	0.43
4:D:53:PHE:O	4:D:57:GLN:HG2	2.19	0.43
5:E:240:GLY:HA2	6:F:299:GLU:HB2	2.01	0.43
22:V:175:MET:C	22:V:178:SER:HG	2.25	0.43
22:V:409:MET:HG3	25:Y:339:ALA:HB2	2.01	0.43
24:X:245:PRO:HA	24:X:248:ILE:HG22	2.00	0.43
26:Z:208:ILE:HD13	27:a:354:GLU:HB2	2.01	0.43
27:a:155:PHE:CE2	27:a:178:ARG:HD3	2.54	0.43
3:C:217:SER:N	3:C:218:GLU:HB3	2.34	0.42
4:D:325:GLY:N	4:D:328:ASP:OD1	2.52	0.42
5:E:205:ASP:OD2	5:E:211:SER:N	2.50	0.42
7:G:58:ASP:OD1	7:G:59:LYS:N	2.52	0.42
11:K:169:ALA:HB3	11:K:178:GLN:HG2	2.01	0.42
12:L:215:VAL:HB	12:L:221:PHE:CD1	2.52	0.42
13:M:120:HIS:NE2	13:M:124:LEU:HD21	2.34	0.42
15:O:45:GLY:HA2	15:O:98:LEU:HD22	2.00	0.42
21:U:699:THR:O	21:U:702:THR:OG1	2.30	0.42
23:W:49:SER:O	23:W:53:GLN:N	2.51	0.42
26:Z:121:LEU:HG	26:Z:138:TYR:HB2	2.01	0.42
26:Z:237:LEU:HB2	26:Z:239:ASP:OD1	2.19	0.42
26:Z:241:SER:HA	26:Z:242:LEU:HA	1.40	0.42
27:a:220:PRO:HA	27:a:223:GLU:HG2	2.00	0.42
27:a:253:THR:HG23	27:a:261:LEU:HD21	2.01	0.42
27:a:274:LEU:HB2	27:a:319:LEU:HD21	2.00	0.42
30:d:52:ARG:O	30:d:56:GLU:N	2.47	0.42
32:f:11:TRP:HA	32:f:12:GLN:HA	1.76	0.42
32:f:481:LYS:O	32:f:484:PRO:HD2	2.19	0.42
1:A:173:THR:HA	1:A:230:ALA:HB3	2.01	0.42
2:B:277:HIS:HB3	2:B:279:PRO:HD2	2.00	0.42
2:B:338:ASP:N	2:B:341:LEU:HG	2.34	0.42
4:D:315:ASP:OD1	4:D:315:ASP:N	2.50	0.42
4:D:392:TYR:CD2	4:D:393:ILE:HG13	2.53	0.42
5:E:141:GLN:HB3	5:E:183:LEU:HD11	2.02	0.42
5:E:254:GLN:O	5:E:258:MET:HG2	2.19	0.42
6:F:428:GLN:CG	6:F:429:ALA:HA	2.49	0.42
10:J:88:ARG:HB3	17:Q:66:LEU:HD11	2.01	0.42
13:M:230:ASP:OD1	13:M:230:ASP:N	2.52	0.42
21:U:470:ASN:HA	21:U:471:ASP:HA	1.84	0.42
23:W:86:ASN:HD22	23:W:88:MET:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:287:LYS:HE3	26:Z:287:LYS:HB2	1.79	0.42
32:f:462:ASP:C	32:f:464:LYS:H	2.26	0.42
2:B:120:HIS:ND1	2:B:134:SER:OG	2.52	0.42
3:C:65:LEU:HA	29:c:190:GLN:CD	2.43	0.42
5:E:126:ASP:OD2	5:E:185:ARG:HG2	2.19	0.42
10:J:78:ALA:HA	10:J:81:ARG:HH12	1.85	0.42
12:L:66:VAL:HG11	12:L:88:MET:HG3	2.01	0.42
14:N:44:CYS:SG	14:N:99:ILE:HB	2.59	0.42
15:O:8:TYR:CE2	15:O:13:VAL:HG23	2.51	0.42
22:V:350:GLN:O	22:V:354:LYS:N	2.53	0.42
22:V:394:LEU:O	22:V:398:LEU:N	2.50	0.42
25:Y:184:GLN:O	25:Y:188:CYS:N	2.45	0.42
27:a:55:GLY:O	27:a:58:LYS:HG2	2.19	0.42
28:b:16:MET:HA	28:b:25:ARG:HD2	2.01	0.42
1:A:164:MET:HE3	1:A:239:ARG:HH12	1.84	0.42
1:A:291:GLY:O	1:A:294:GLU:HG2	2.19	0.42
2:B:320:ASP:N	2:B:320:ASP:OD1	2.52	0.42
2:B:360:THR:O	2:B:364:ILE:N	2.52	0.42
3:C:259:LEU:H	3:C:259:LEU:HD13	1.85	0.42
5:E:54:GLY:H	6:F:158:TYR:HD2	1.67	0.42
6:F:144:LYS:HA	6:F:145:LEU:HA	1.71	0.42
13:M:45:VAL:HG11	13:M:138:GLY:HA3	2.01	0.42
16:P:107:PRO:HG2	16:P:124:LEU:HB2	2.01	0.42
19:S:64:LEU:HD21	19:S:92:LEU:HD11	2.00	0.42
21:U:607:VAL:O	21:U:615:ARG:NH1	2.52	0.42
21:U:713:TYR:HB2	21:U:734:GLN:HE21	1.83	0.42
21:U:780:SER:HA	21:U:783:TYR:CD2	2.54	0.42
22:V:59:ALA:HA	22:V:60:ALA:C	2.44	0.42
23:W:439:VAL:HG21	29:c:232:GLN:HA	2.02	0.42
25:Y:105:MET:HB3	25:Y:127:THR:HG21	2.01	0.42
26:Z:67:VAL:HG13	28:b:92:VAL:HG23	2.00	0.42
26:Z:191:ILE:HD11	27:a:375:LEU:HD11	2.00	0.42
27:a:325:ASP:OD1	27:a:327:VAL:HG12	2.19	0.42
30:d:49:ILE:HD12	30:d:52:ARG:HH11	1.85	0.42
30:d:52:ARG:O	30:d:56:GLU:HG3	2.19	0.42
30:d:68:ILE:HB	30:d:69:PRO:HD3	2.01	0.42
30:d:171:LEU:O	30:d:175:ARG:HG2	2.19	0.42
32:f:390:GLU:HB3	32:f:391:LEU:HA	2.01	0.42
2:B:227:PRO:HD3	2:B:332:ASN:O	2.19	0.42
2:B:283:PHE:CE2	2:B:285:ASP:HB2	2.55	0.42
2:B:294:ARG:HG2	2:B:295:TYR:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ARG:HB2	2:B:344:PRO:HD3	2.02	0.42
3:C:220:VAL:O	3:C:224:ILE:HB	2.19	0.42
5:E:113:ARG:HB3	5:E:221:TYR:OH	2.19	0.42
13:M:51:LYS:HB3	13:M:210:GLU:HB3	2.00	0.42
19:S:22:ILE:HG23	19:S:197:ILE:HG13	2.00	0.42
22:V:127:THR:HA	22:V:131:LEU:HG	2.01	0.42
29:c:116:PRO:HA	29:c:147:PRO:HD2	2.02	0.42
31:e:60:LEU:O	31:e:64:GLY:N	2.49	0.42
1:A:385:ILE:HA	1:A:388:VAL:HG23	2.00	0.42
5:E:180:LYS:HG3	5:E:181:THR:N	2.34	0.42
5:E:313:LEU:HD21	5:E:328:TYR:CD2	2.54	0.42
8:H:66:GLU:HG3	8:H:91:ARG:NH2	2.33	0.42
8:H:83:TYR:HB2	8:H:132:VAL:HG21	2.01	0.42
11:K:17:PRO:HA	12:L:24:TYR:CZ	2.55	0.42
16:P:25:ASP:HA	16:P:185:VAL:HA	2.00	0.42
16:P:44:PRO:HA	16:P:50:TYR:HD1	1.85	0.42
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	2.01	0.42
22:V:25:GLU:O	22:V:28:PRO:HD2	2.19	0.42
22:V:232:HIS:HA	22:V:235:LEU:HB3	2.02	0.42
23:W:66:ILE:HG23	23:W:67:LEU:HB2	2.01	0.42
23:W:428:TRP:CD1	29:c:245:VAL:HG23	2.54	0.42
24:X:356:LEU:HD11	24:X:360:ASP:OD1	2.19	0.42
29:c:272:ILE:HB	29:c:273:LYS:HA	2.01	0.42
30:d:40:GLY:HA3	30:d:41:THR:O	2.20	0.42
32:f:660:TYR:HA	32:f:661:GLY:C	2.45	0.42
2:B:153:ASN:HD21	2:B:160:ILE:HB	1.85	0.42
2:B:387:LYS:HD2	2:B:430:LYS:HZ2	1.84	0.42
3:C:235:PHE:CD1	3:C:275:GLU:HG3	2.55	0.42
4:D:228:ILE:HB	4:D:262:ILE:HG12	2.01	0.42
8:H:10:LEU:HD23	8:H:126:GLY:H	1.84	0.42
16:P:189:ILE:HG23	16:P:196:THR:HB	2.02	0.42
21:U:358:ASP:O	21:U:360:VAL:HG23	2.20	0.42
22:V:157:THR:OG1	22:V:158:PRO:HD3	2.19	0.42
22:V:197:THR:HG22	22:V:199:ASN:H	1.83	0.42
22:V:345:ARG:HG2	22:V:364:THR:HG21	2.01	0.42
22:V:403:ILE:HD11	22:V:428:LEU:HD11	2.02	0.42
22:V:475:ALA:O	22:V:479:ARG:HG2	2.19	0.42
23:W:80:TRP:CD1	23:W:84:ASN:HD21	2.37	0.42
25:Y:324:GLY:N	25:Y:325:VAL:HA	2.35	0.42
26:Z:262:LEU:O	26:Z:266:ILE:HD12	2.20	0.42
27:a:203:ALA:HA	27:a:206:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:32:TYR:HE1	29:c:206:ASN:HD21	1.68	0.42
32:f:23:GLU:HB3	32:f:24:PRO:HD3	2.01	0.42
32:f:83:GLU:HB3	32:f:84:PRO:HD3	2.02	0.42
2:B:108:SER:HA	3:C:95:PHE:HA	2.02	0.42
3:C:171:HIS:HD2	3:C:174:LEU:HD21	1.85	0.42
3:C:214:VAL:HG21	3:C:249:ASP:N	2.22	0.42
3:C:327:ASP:O	3:C:331:ILE:HG12	2.20	0.42
5:E:181:THR:O	5:E:185:ARG:HB2	2.20	0.42
5:E:240:GLY:HA2	6:F:299:GLU:CD	2.45	0.42
6:F:172:VAL:HG22	6:F:267:LEU:HD11	2.01	0.42
6:F:188:ILE:O	6:F:188:ILE:HG13	2.20	0.42
7:G:43:ARG:NH2	7:G:164:LYS:HG2	2.35	0.42
7:G:44:GLY:N	7:G:47:CYS:O	2.44	0.42
9:I:218:ARG:NH1	9:I:223:THR:OG1	2.53	0.42
11:K:21:LEU:HD13	11:K:123:PHE:HZ	1.85	0.42
12:L:44:ALA:N	12:L:137:TYR:OH	2.53	0.42
21:U:181:LEU:HB3	21:U:218:GLN:HE22	1.84	0.42
21:U:684:ARG:O	21:U:688:LEU:HG	2.19	0.42
22:V:31:ALA:HB3	22:V:32:PRO:HD3	2.01	0.42
25:Y:111:LEU:HD23	25:Y:114:ILE:HD13	2.01	0.42
25:Y:218:THR:O	25:Y:221:THR:OG1	2.29	0.42
27:a:25:LEU:HD22	27:a:44:PHE:HE2	1.84	0.42
27:a:35:HIS:CE1	28:b:17:ARG:HB2	2.54	0.42
27:a:320:VAL:HG21	27:a:333:MET:SD	2.60	0.42
30:d:175:ARG:NH2	30:d:205:LYS:HZ3	2.17	0.42
32:f:350:LYS:HA	32:f:356:ALA:HB3	2.02	0.42
1:A:90:GLU:O	1:A:94:GLN:HB2	2.19	0.42
1:A:212:VAL:O	1:A:319:MET:HB2	2.20	0.42
3:C:54:ALA:O	3:C:58:LEU:N	2.53	0.42
4:D:205:TYR:CG	4:D:206:GLY:N	2.88	0.42
5:E:90:SER:O	5:E:93:LYS:NZ	2.40	0.42
7:G:87:SER:O	7:G:91:VAL:HG23	2.20	0.42
10:J:9:VAL:HB	10:J:10:PHE:HB3	2.01	0.42
10:J:120:GLN:O	11:K:134:SER:OG	2.37	0.42
11:K:206:MET:HE1	11:K:210:LEU:HD13	2.00	0.42
13:M:108:LEU:HD11	13:M:137:LEU:HB3	2.02	0.42
18:R:19:ARG:CZ	18:R:171:GLY:HA3	2.50	0.42
21:U:517:GLY:HA3	21:U:554:LEU:HB3	2.01	0.42
21:U:810:THR:O	21:U:883:ARG:NH1	2.52	0.42
22:V:372:LEU:H	22:V:427:GLN:HE22	1.67	0.42
23:W:200:ILE:O	23:W:204:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:243:ILE:HA	23:W:246:HIS:HB3	2.02	0.42
27:a:374:ILE:HD12	30:d:254:GLU:HG2	2.01	0.42
28:b:16:MET:HE3	28:b:25:ARG:HB3	2.02	0.42
29:c:285:GLU:HB3	29:c:286:GLU:HA	2.01	0.42
32:f:281:ILE:HG23	32:f:282:LYS:N	2.35	0.42
32:f:391:LEU:CD1	32:f:392:LYS:H	2.28	0.42
2:B:164:MET:HE2	2:B:164:MET:HA	2.02	0.42
2:B:191:ASP:OD1	2:B:191:ASP:N	2.52	0.42
2:B:226:GLY:HA2	2:B:227:PRO:HD3	1.90	0.42
4:D:385:LEU:O	4:D:388:ARG:HB3	2.20	0.42
10:J:137:ASP:CG	10:J:143:ARG:HB3	2.45	0.42
19:S:20:PHE:HB2	19:S:198:VAL:O	2.20	0.42
21:U:654:MET:O	21:U:658:ILE:HG12	2.19	0.42
22:V:259:LEU:HD12	22:V:295:ILE:HG12	2.02	0.42
22:V:497:PRO:HG3	26:Z:286:GLU:HG3	2.02	0.42
23:W:135:LYS:HB3	23:W:136:ILE:CA	2.48	0.42
23:W:136:ILE:N	23:W:141:GLU:OE2	2.53	0.42
24:X:261:LEU:C	24:X:263:THR:H	2.28	0.42
25:Y:356:THR:HA	25:Y:357:ASN:OD1	2.18	0.42
26:Z:176:LEU:C	26:Z:178:ASP:H	2.27	0.42
27:a:148:VAL:C	27:a:150:SER:H	2.28	0.42
30:d:114:GLU:HA	30:d:117:THR:HG22	2.02	0.42
32:f:61:ASP:C	32:f:63:ASP:H	2.28	0.42
32:f:291:ILE:HG23	32:f:651:ILE:HD12	2.02	0.42
3:C:39:SER:O	3:C:43:ARG:N	2.48	0.41
3:C:310:ARG:HA	3:C:311:ILE:HA	1.68	0.41
4:D:93:LEU:HD23	4:D:102:ILE:HD12	2.02	0.41
5:E:194:ASN:ND2	5:E:227:PRO:O	2.53	0.41
6:F:191:LEU:HG	6:F:194:GLN:HE21	1.84	0.41
6:F:321:GLN:HG3	6:F:322:PRO:HD3	2.01	0.41
8:H:43:GLY:HA2	8:H:144:PRO:HG3	2.02	0.41
10:J:36:ARG:HA	10:J:41:VAL:HG12	2.02	0.41
11:K:36:THR:OG1	11:K:170:ILE:O	2.24	0.41
11:K:200:ILE:HA	11:K:203:LYS:NZ	2.34	0.41
12:L:137:TYR:CZ	12:L:216:GLY:HA2	2.55	0.41
14:N:1:THR:H1	14:N:33:LYS:HE2	1.85	0.41
15:O:19:ARG:CZ	15:O:170:GLY:HA3	2.50	0.41
20:T:192:VAL:HG12	20:T:197:VAL:HG22	2.01	0.41
21:U:789:ILE:HB	21:U:911:ILE:HB	2.02	0.41
22:V:48:THR:HG23	22:V:147:PHE:HE2	1.84	0.41
23:W:107:GLN:HB3	23:W:111:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:286:TRP:C	25:Y:288:PHE:H	2.27	0.41
26:Z:182:THR:N	26:Z:183:THR:HA	2.30	0.41
27:a:4:VAL:HB	27:a:5:PRO:HD3	2.02	0.41
28:b:140:ILE:HD13	28:b:157:VAL:HG22	2.01	0.41
29:c:272:ILE:HB	29:c:274:ASN:HA	2.01	0.41
31:e:6:GLN:N	31:e:7:PRO:HD2	2.35	0.41
32:f:600:LEU:HD11	32:f:641:LEU:HD13	2.02	0.41
3:C:141:GLU:OE2	4:D:326:ARG:NH2	2.52	0.41
3:C:149:GLU:O	3:C:331:ILE:HD12	2.20	0.41
4:D:157:ASP:O	4:D:159:LYS:HG2	2.19	0.41
5:E:119:VAL:HG11	6:F:146:LYS:HD2	2.02	0.41
6:F:150:LEU:HB3	6:F:164:LEU:O	2.20	0.41
7:G:56:VAL:HA	7:G:61:LEU:HD13	2.02	0.41
7:G:174:GLU:HB2	7:G:205:VAL:HG22	2.02	0.41
9:I:33:THR:OG1	9:I:50:ARG:NH2	2.53	0.41
9:I:88:ASN:HA	9:I:91:ARG:HB3	2.02	0.41
10:J:154:HIS:CE1	11:K:60:GLU:H	2.32	0.41
22:V:313:LEU:HD22	22:V:329:HIS:CE1	2.54	0.41
23:W:90:LEU:HD22	23:W:135:LYS:HE2	2.02	0.41
23:W:150:ALA:O	23:W:154:GLU:HG3	2.20	0.41
25:Y:198:ALA:HB2	25:Y:226:VAL:HG13	2.03	0.41
26:Z:121:LEU:HD11	26:Z:138:TYR:HD2	1.85	0.41
26:Z:201:LEU:HD22	27:a:357:CYS:HA	2.03	0.41
26:Z:262:LEU:HD12	29:c:249:LEU:HD22	2.03	0.41
28:b:35:ILE:HD13	28:b:184:ILE:HD13	2.01	0.41
29:c:229:LEU:C	29:c:231:LEU:H	2.27	0.41
31:e:3:GLU:HG2	31:e:4:LYS:HD3	2.02	0.41
32:f:382:THR:HG22	32:f:386:LYS:NZ	2.35	0.41
1:A:83:ASP:HB2	2:B:102:LEU:HD23	2.01	0.41
1:A:106:SER:HB2	6:F:165:PRO:O	2.20	0.41
1:A:210:LYS:O	1:A:336:ARG:NH2	2.53	0.41
1:A:406:GLU:HG3	1:A:407:LYS:H	1.86	0.41
2:B:376:ASP:O	2:B:378:VAL:N	2.53	0.41
2:B:437:GLY:HA3	2:B:438:LEU:C	2.46	0.41
3:C:183:PRO:HA	3:C:311:ILE:HG13	2.02	0.41
4:D:289:LEU:HD12	4:D:292:LEU:HD11	2.02	0.41
7:G:231:THR:O	7:G:233:ALA:N	2.52	0.41
9:I:180:LYS:HE3	9:I:180:LYS:HB3	1.91	0.41
12:L:116:THR:HG22	12:L:128:TYR:HD2	1.84	0.41
13:M:169:ARG:HG3	13:M:170:GLN:N	2.35	0.41
14:N:67:SER:HA	14:N:70:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:49:THR:HA	20:T:114:GLY:HA3	2.02	0.41
21:U:576:PRO:HA	21:U:579:ARG:HE	1.85	0.41
23:W:59:ASP:HA	23:W:63:THR:HG23	2.02	0.41
25:Y:307:LEU:HD11	25:Y:319:MET:SD	2.59	0.41
29:c:113:HIS:NE2	29:c:126:ASP:OD2	2.53	0.41
30:d:139:LEU:HD11	30:d:151:VAL:HG13	2.01	0.41
1:A:102:ILE:HG22	1:A:113:ILE:HG12	2.02	0.41
3:C:210:THR:HG23	3:C:244:SER:HB3	2.01	0.41
3:C:214:VAL:HG22	3:C:215:SER:N	2.33	0.41
3:C:283:PHE:HD1	3:C:284:GLU:HG2	1.85	0.41
4:D:99:ASN:C	4:D:115:ILE:HG12	2.45	0.41
4:D:358:VAL:HG12	4:D:363:TYR:CE2	2.55	0.41
4:D:375:ILE:HG23	4:D:376:ASN:H	1.84	0.41
5:E:232:MET:N	5:E:276:ILE:O	2.53	0.41
6:F:166:THR:O	6:F:166:THR:OG1	2.39	0.41
6:F:311:LEU:HD23	6:F:314:LEU:HD22	2.01	0.41
9:I:38:LEU:HD11	9:I:160:LYS:HB3	2.01	0.41
21:U:770:TRP:CG	29:c:179:SER:HB2	2.55	0.41
21:U:788:VAL:HG12	21:U:910:GLY:H	1.84	0.41
22:V:288:TYR:HA	22:V:291:TYR:HD2	1.85	0.41
23:W:45:GLU:HB2	23:W:93:ARG:HA	2.02	0.41
23:W:72:LYS:HD2	23:W:123:ARG:HD3	2.02	0.41
23:W:455:LEU:HD12	23:W:456:GLN:N	2.34	0.41
24:X:268:GLN:O	24:X:272:SER:HB2	2.20	0.41
25:Y:292:TYR:O	25:Y:296:VAL:HG23	2.21	0.41
26:Z:109:ASN:OD1	26:Z:119:SER:HB2	2.20	0.41
26:Z:148:GLY:HA2	27:a:181:GLY:C	2.44	0.41
28:b:48:ASN:OD1	28:b:48:ASN:N	2.53	0.41
29:c:157:ILE:HG23	29:c:158:ASP:N	2.35	0.41
32:f:567:ILE:HB	32:f:602:MET:SD	2.60	0.41
2:B:313:LEU:HD22	2:B:341:LEU:HD22	2.03	0.41
2:B:431:GLN:HA	2:B:434:THR:OG1	2.21	0.41
5:E:268:ASP:OD1	5:E:269:THR:N	2.49	0.41
7:G:39:SER:H	7:G:172:GLN:NE2	2.18	0.41
7:G:61:LEU:HG	7:G:66:VAL:HG21	2.02	0.41
8:H:59:GLU:N	8:H:59:GLU:OE1	2.52	0.41
8:H:67:PRO:O	8:H:91:ARG:NH2	2.54	0.41
8:H:174:LEU:HD21	8:H:194:THR:HG21	2.02	0.41
14:N:144:ARG:NH2	14:N:151:GLU:OE1	2.54	0.41
18:R:161:TYR:CE1	18:R:196:HIS:HA	2.56	0.41
22:V:137:GLU:N	22:V:138:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:234:ARG:HA	22:V:237:THR:HG22	2.02	0.41
25:Y:16:ASP:OD2	25:Y:113:ARG:HG3	2.21	0.41
25:Y:145:LEU:HD23	25:Y:157:ILE:HB	2.02	0.41
26:Z:67:VAL:HG12	28:b:95:LEU:HD23	2.02	0.41
27:a:175:ASP:HA	27:a:178:ARG:HH11	1.85	0.41
28:b:184:ILE:H	28:b:184:ILE:HG13	1.73	0.41
28:b:184:ILE:C	28:b:187:PRO:HD2	2.45	0.41
1:A:350:GLY:HA2	1:A:353:HIS:HD1	1.86	0.41
3:C:186:VAL:HG23	3:C:313:ARG:HB3	2.03	0.41
3:C:339:THR:HG23	3:C:341:GLY:H	1.85	0.41
6:F:431:LYS:HG2	6:F:432:LYS:HD2	2.02	0.41
7:G:14:THR:O	7:G:15:ILE:HG23	2.21	0.41
7:G:132:ARG:HD3	7:G:133:PRO:HD2	2.01	0.41
7:G:184:LYS:HA	7:G:185:LYS:C	2.45	0.41
11:K:178:GLN:HB3	11:K:182:GLN:NE2	2.36	0.41
14:N:36:PRO:HA	14:N:42:PHE:CE1	2.56	0.41
21:U:495:ASP:HA	21:U:498:LYS:NZ	2.36	0.41
21:U:581:SER:O	21:U:585:THR:OG1	2.34	0.41
27:a:12:GLN:HG2	27:a:13:ASN:OD1	2.21	0.41
27:a:34:TRP:CE3	27:a:37:LEU:HD23	2.55	0.41
29:c:168:MET:HA	29:c:172:HIS:ND1	2.36	0.41
29:c:250:GLU:O	29:c:253:LYS:HG2	2.21	0.41
32:f:436:VAL:HG21	32:f:675:ASP:OD1	2.20	0.41
1:A:212:VAL:HG12	1:A:339:ARG:HB3	2.02	0.41
2:B:436:GLU:HG2	2:B:439:TYR:CD1	2.56	0.41
3:C:163:GLU:O	3:C:167:LEU:HB2	2.21	0.41
7:G:101:TRP:CD1	7:G:109:ILE:HA	2.56	0.41
9:I:57:ASP:HB3	9:I:59:VAL:HG13	2.03	0.41
9:I:119:GLN:HB2	9:I:154:GLY:HA3	2.01	0.41
9:I:140:ASP:OD1	9:I:144:GLY:N	2.54	0.41
19:S:13:LEU:HD13	19:S:137:ALA:HB2	2.02	0.41
22:V:496:PHE:HB2	22:V:497:PRO:HD3	2.03	0.41
23:W:128:LEU:HD23	23:W:147:LYS:HZ2	1.86	0.41
23:W:373:ILE:HG23	23:W:413:ILE:HG13	2.03	0.41
23:W:406:VAL:HA	23:W:413:ILE:HG22	2.03	0.41
24:X:390:GLU:O	24:X:392:PRO:HD3	2.20	0.41
26:Z:84:LYS:HE3	29:c:76:PRO:HB3	2.03	0.41
31:e:64:GLY:HA2	31:e:67:MET:HE3	2.03	0.41
3:C:84:LYS:HG2	3:C:98:ASP:HA	2.02	0.41
4:D:412:GLN:OE1	4:D:415:GLU:HB2	2.21	0.41
6:F:192:ASP:HA	6:F:195:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:221:LYS:HG3	6:F:346:GLY:HA2	2.02	0.41
10:J:221:ASN:O	10:J:223:GLU:N	2.47	0.41
11:K:60:GLU:OE1	11:K:63:SER:N	2.54	0.41
13:M:110:HIS:CD2	14:N:70:LEU:HD23	2.55	0.41
21:U:566:LEU:O	21:U:570:LEU:HG	2.19	0.41
21:U:800:VAL:HG22	21:U:898:CYS:SG	2.60	0.41
22:V:104:THR:HA	22:V:107:ARG:HG2	2.02	0.41
22:V:235:LEU:HD12	22:V:247:GLN:HG3	2.02	0.41
22:V:349:ARG:HD2	22:V:354:LYS:HG3	2.03	0.41
22:V:417:ILE:HD11	22:V:422:ILE:HB	2.03	0.41
23:W:359:VAL:O	23:W:363:ILE:HG12	2.21	0.41
25:Y:227:SER:O	25:Y:231:LEU:HB3	2.21	0.41
25:Y:268:TYR:CZ	25:Y:307:LEU:HD12	2.56	0.41
26:Z:96:HIS:NE2	26:Z:123:ILE:HG12	2.36	0.41
29:c:246:LYS:O	29:c:250:GLU:N	2.52	0.41
30:d:175:ARG:HD2	30:d:205:LYS:NZ	2.35	0.41
32:f:39:HIS:CG	32:f:40:ASN:H	2.39	0.41
1:A:206:ILE:HG23	1:A:207:GLU:N	2.35	0.41
1:A:309:PHE:CZ	6:F:235:LEU:HD12	2.56	0.41
2:B:150:VAL:HG12	2:B:162:VAL:HG12	2.03	0.41
2:B:153:ASN:N	2:B:158:ALA:O	2.31	0.41
2:B:180:PRO:HG3	2:B:243:THR:HG22	2.03	0.41
3:C:62:GLU:HG2	4:D:114:ARG:NH2	2.36	0.41
4:D:150:SER:HB3	5:E:61:LEU:HD22	2.03	0.41
4:D:200:ARG:NH1	4:D:300:ASP:OD1	2.39	0.41
5:E:72:LYS:HB2	5:E:78:ARG:HG2	2.02	0.41
5:E:125:GLU:N	5:E:125:GLU:OE1	2.54	0.41
5:E:352:MET:HE1	6:F:220:PRO:HG3	2.02	0.41
6:F:88:TYR:HB2	6:F:154:ASN:HA	2.03	0.41
7:G:37:LEU:HD11	7:G:53:GLN:O	2.21	0.41
7:G:179:LEU:HB2	8:H:56:LEU:HD11	2.02	0.41
9:I:97:TYR:O	9:I:101:TYR:HB2	2.21	0.41
10:J:105:GLU:CD	10:J:109:ARG:HE	2.28	0.41
11:K:10:ARG:C	11:K:12:VAL:H	2.29	0.41
12:L:171:TYR:O	12:L:175:HIS:ND1	2.48	0.41
17:Q:8:GLN:HB2	17:Q:115:LEU:HD22	2.02	0.41
21:U:356:THR:HG21	21:U:731:ILE:HD13	2.02	0.41
21:U:427:LEU:HG	21:U:464:GLN:HE21	1.85	0.41
22:V:194:LYS:HG2	22:V:200:ARG:HH22	1.86	0.41
22:V:224:LEU:HB2	22:V:227:VAL:HB	2.01	0.41
22:V:295:ILE:O	22:V:298:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:392:TYR:O	22:V:395:ILE:HG22	2.21	0.41
22:V:455:LYS:H	22:V:456:GLY:HA2	1.83	0.41
23:W:56:THR:HG21	23:W:103:LYS:HE3	2.02	0.41
23:W:310:THR:C	23:W:312:MET:H	2.29	0.41
23:W:445:LEU:HD12	23:W:448:LYS:NZ	2.36	0.41
24:X:367:GLN:HA	24:X:370:LEU:HD12	2.02	0.41
24:X:377:ILE:HG12	25:Y:312:ARG:HB3	2.01	0.41
25:Y:48:ASN:ND2	25:Y:77:ASN:HB2	2.35	0.41
25:Y:191:ILE:HD12	25:Y:191:ILE:HA	1.91	0.41
26:Z:33:LYS:HD3	26:Z:60:GLU:H	1.85	0.41
26:Z:120:VAL:HG23	26:Z:138:TYR:O	2.21	0.41
27:a:100:THR:HG22	27:a:103:LYS:HE2	2.03	0.41
27:a:307:VAL:O	27:a:311:VAL:HG22	2.20	0.41
29:c:229:LEU:HB3	29:c:231:LEU:HB2	2.03	0.41
30:d:108:SER:HB3	30:d:169:ILE:HG22	2.02	0.41
32:f:297:ARG:HA	32:f:298:ASN:O	2.21	0.41
1:A:344:SER:CA	1:A:345:LEU:HB3	2.51	0.41
2:B:106:PRO:HB2	2:B:154:HIS:CD2	2.55	0.41
2:B:178:LYS:NZ	3:C:278:ASN:HB3	2.36	0.41
3:C:249:ASP:HA	3:C:250:GLU:HA	1.72	0.41
3:C:313:ARG:HH11	3:C:314:LYS:H	1.69	0.41
4:D:249:ASP:HA	4:D:252:ARG:HG2	2.03	0.41
5:E:266:GLY:C	5:E:268:ASP:H	2.28	0.41
6:F:225:MET:HG2	6:F:233:LYS:HD2	2.02	0.41
7:G:184:LYS:HB2	7:G:185:LYS:O	2.21	0.41
13:M:188:ASP:O	13:M:192:GLU:HG2	2.21	0.41
15:O:110:LEU:HB3	15:O:122:LEU:O	2.21	0.41
19:S:11:THR:HG21	19:S:141:ALA:HB3	2.01	0.41
21:U:347:ASN:HB3	21:U:813:TYR:HB2	2.01	0.41
22:V:64:GLN:N	22:V:64:GLN:OE1	2.54	0.41
22:V:283:ASN:ND2	22:V:317:PRO:O	2.54	0.41
22:V:455:LYS:HD2	22:V:457:TYR:HE2	1.86	0.41
25:Y:39:ASP:HA	25:Y:42:MET:HB3	2.03	0.41
25:Y:186:LEU:HA	25:Y:189:VAL:HG12	2.03	0.41
1:A:187:LEU:O	1:A:190:VAL:HG12	2.21	0.40
2:B:224:LEU:HD22	2:B:351:ILE:HG12	2.03	0.40
3:C:49:ARG:NH2	4:D:69:LYS:HG3	2.35	0.40
3:C:157:GLN:NE2	3:C:318:PRO:HD3	2.34	0.40
5:E:44:GLU:OE1	6:F:76:ASN:ND2	2.53	0.40
9:I:159:TRP:HB3	10:J:54:GLN:HB3	2.03	0.40
11:K:73:HIS:ND1	11:K:74:ILE:HG13	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:182:CYS:SG	12:L:187:LEU:HD13	2.61	0.40
13:M:8:ASP:OD1	13:M:8:ASP:N	2.54	0.40
13:M:80:LEU:HD23	13:M:82:ALA:H	1.86	0.40
13:M:215:TRP:HH2	13:M:219:LEU:H	1.69	0.40
15:O:202:TYR:HD2	16:P:152:SER:HB3	1.86	0.40
22:V:106:ARG:HA	22:V:109:ASN:HB2	2.02	0.40
22:V:176:MET:HA	22:V:179:LYS:HE2	2.03	0.40
23:W:172:GLU:N	23:W:172:GLU:OE1	2.54	0.40
23:W:449:GLU:HG2	23:W:453:HIS:CE1	2.55	0.40
25:Y:300:ARG:O	25:Y:304:TYR:N	2.51	0.40
26:Z:36:VAL:HG22	26:Z:96:HIS:HB3	2.02	0.40
26:Z:257:MET:HE3	26:Z:261:TYR:HE2	1.87	0.40
27:a:166:ILE:N	27:a:167:GLY:HA3	2.36	0.40
30:d:101:LEU:HD21	30:d:162:SER:HB2	2.03	0.40
31:e:40:GLU:N	31:e:41:ASP:HA	2.36	0.40
32:f:604:ARG:NH2	32:f:607:GLN:HG3	2.36	0.40
1:A:377:CYS:HB2	1:A:380:SER:OG	2.21	0.40
2:B:198:LYS:N	2:B:237:LYS:HZ3	2.19	0.40
4:D:43:ARG:HA	4:D:46:LYS:HD2	2.02	0.40
5:E:309:ARG:HD3	5:E:332:VAL:HB	2.04	0.40
6:F:102:ASN:HA	6:F:103:ASP:HA	1.51	0.40
9:I:90:LEU:HD12	9:I:114:LEU:HB2	2.03	0.40
9:I:243:GLU:O	9:I:247:ALA:N	2.53	0.40
14:N:91:ARG:NH1	20:T:59:ASP:OD1	2.54	0.40
15:O:13:VAL:HG22	15:O:177:VAL:HA	2.03	0.40
21:U:93:ASN:OD1	21:U:94:SER:N	2.54	0.40
22:V:91:PRO:HA	22:V:94:VAL:HG12	2.02	0.40
22:V:97:ALA:N	22:V:98:LEU:HA	2.35	0.40
25:Y:63:TRP:HB3	25:Y:65:ILE:N	2.37	0.40
25:Y:101:ARG:HG3	25:Y:104:MET:SD	2.62	0.40
27:a:13:ASN:OD1	27:a:19:PRO:HG2	2.06	0.40
30:d:47:GLN:O	30:d:51:ALA:N	2.53	0.40
1:A:190:VAL:HG11	1:A:212:VAL:HG11	2.03	0.40
1:A:292:ASP:O	1:A:296:GLN:HG2	2.21	0.40
1:A:351:ARG:HH11	1:A:379:ASN:H	1.69	0.40
2:B:109:VAL:HB	3:C:94:LYS:HB2	2.03	0.40
2:B:174:MET:HE3	2:B:272:ARG:NH2	2.36	0.40
2:B:345:GLY:HA2	2:B:346:ARG:HA	1.74	0.40
4:D:45:LYS:O	4:D:48:GLN:NE2	2.54	0.40
5:E:86:GLN:NE2	5:E:108:MET:HG3	2.36	0.40
5:E:233:ASP:OD2	6:F:315:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:228:PRO:HA	6:F:229:PRO:HD3	1.84	0.40
7:G:23:TYR:O	7:G:26:GLU:HG2	2.21	0.40
11:K:146:VAL:HG22	11:K:151:PRO:HA	2.03	0.40
17:Q:20:VAL:HG21	17:Q:175:LEU:HA	2.03	0.40
19:S:40:SER:O	19:S:42:LYS:HD2	2.21	0.40
19:S:125:ASP:N	19:S:125:ASP:OD1	2.55	0.40
21:U:420:LEU:HB2	21:U:457:ILE:HD11	2.03	0.40
25:Y:98:SER:O	25:Y:102:ASP:HB2	2.22	0.40
26:Z:62:ASP:OD1	26:Z:62:ASP:N	2.55	0.40
27:a:50:PHE:N	27:a:51:ALA:HA	2.35	0.40
27:a:57:ILE:HG13	27:a:61:GLU:HG2	2.04	0.40
29:c:42:LEU:HD12	29:c:43:LYS:N	2.36	0.40
29:c:113:HIS:CE1	29:c:144:VAL:HG22	2.56	0.40
29:c:159:ALA:HB3	29:c:205:ILE:HD11	2.03	0.40
32:f:320:LEU:HA	32:f:358:VAL:HG13	2.03	0.40
32:f:529:ARG:HA	32:f:562:VAL:HG12	2.04	0.40
1:A:95:VAL:HG12	1:A:144:ARG:HG2	2.03	0.40
1:A:354:ILE:HB	1:A:385:ILE:HD11	2.04	0.40
2:B:187:ILE:O	2:B:367:ILE:HG21	2.22	0.40
2:B:365:PHE:HE2	2:B:378:VAL:HG11	1.87	0.40
3:C:148:TYR:HA	3:C:151:ILE:HG22	2.04	0.40
5:E:364:GLN:HA	5:E:367:PHE:HB2	2.02	0.40
6:F:219:PRO:HA	6:F:220:PRO:HD3	1.99	0.40
9:I:160:LYS:HG3	10:J:55:ASP:HB2	2.03	0.40
19:S:58:HIS:HB3	20:T:130:VAL:HG22	2.03	0.40
20:T:25:ASP:HA	20:T:187:PHE:HA	2.04	0.40
22:V:149:PRO:HG3	22:V:203:LEU:HG	2.03	0.40
22:V:416:ARG:HE	22:V:459:GLN:HB3	1.86	0.40
24:X:291:ALA:O	24:X:294:SER:OG	2.38	0.40
25:Y:183:TYR:OH	25:Y:212:GLU:OE1	2.39	0.40
25:Y:360:ASP:O	25:Y:365:GLN:HB2	2.21	0.40
26:Z:62:ASP:OD1	26:Z:63:LYS:HG2	2.22	0.40
26:Z:148:GLY:HA2	27:a:181:GLY:O	2.21	0.40
26:Z:201:LEU:HB3	27:a:357:CYS:SG	2.62	0.40
27:a:229:ASP:HB3	27:a:234:ILE:HD11	2.02	0.40
32:f:22:ARG:HA	32:f:25:LEU:HD12	2.03	0.40
32:f:69:LYS:HE3	32:f:114:ASN:ND2	2.36	0.40
1:A:115:VAL:HG12	1:A:119:ALA:O	2.21	0.40
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.52	0.40
11:K:10:ARG:HH11	12:L:21:GLN:HE22	1.68	0.40
11:K:97:GLN:NE2	18:R:64:ARG:HG2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:137:TYR:CZ	12:L:142:PRO:HB3	2.56	0.40
19:S:149:LEU:O	19:S:153:VAL:N	2.54	0.40
21:U:397:THR:HA	21:U:401:LYS:NZ	2.36	0.40
21:U:842:LYS:HA	21:U:843:GLU:CB	2.48	0.40
22:V:208:ALA:O	31:e:4:LYS:NZ	2.50	0.40
22:V:237:THR:OG1	22:V:241:ARG:NH2	2.54	0.40
23:W:62:SER:HB2	23:W:71:VAL:HG11	2.03	0.40
23:W:155:GLN:HG2	23:W:157:GLY:H	1.86	0.40
25:Y:110:TYR:CE1	25:Y:113:ARG:HD3	2.57	0.40
25:Y:145:LEU:HD13	25:Y:183:TYR:CD1	2.56	0.40
25:Y:300:ARG:HH12	31:e:63:HIS:CD2	2.39	0.40
25:Y:357:ASN:CB	25:Y:358:ARG:HA	2.51	0.40
26:Z:39:LEU:HB2	26:Z:95:TYR:HD2	1.86	0.40
27:a:291:LEU:O	27:a:331:VAL:N	2.54	0.40
28:b:163:LYS:HA	28:b:164:ASP:HA	1.95	0.40
29:c:157:ILE:O	29:c:158:ASP:HB2	2.22	0.40
30:d:103:LEU:HD22	30:d:119:LEU:HD21	2.02	0.40
30:d:105:PHE:HB2	30:d:166:PHE:CE1	2.56	0.40
32:f:220:GLY:HA2	32:f:223:ASN:HD21	1.87	0.40
32:f:397:ARG:HB3	32:f:679:ARG:NH2	2.36	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	A	359/433 (83%)	311 (87%)	44 (12%)	4 (1%)	11	46
2	B	346/440 (79%)	297 (86%)	46 (13%)	3 (1%)	14	51
3	C	382/398 (96%)	339 (89%)	41 (11%)	2 (0%)	24	63
4	D	378/418 (90%)	333 (88%)	44 (12%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	351/403 (87%)	322 (92%)	28 (8%)	1 (0%)	36	72
6	F	362/439 (82%)	322 (89%)	38 (10%)	2 (1%)	21	59
7	G	238/245 (97%)	213 (90%)	23 (10%)	2 (1%)	16	54
8	H	229/233 (98%)	211 (92%)	18 (8%)	0	100	100
9	I	248/260 (95%)	220 (89%)	28 (11%)	0	100	100
10	J	237/247 (96%)	214 (90%)	20 (8%)	3 (1%)	9	42
11	K	224/240 (93%)	204 (91%)	18 (8%)	2 (1%)	14	51
12	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
13	M	238/254 (94%)	216 (91%)	22 (9%)	0	100	100
14	N	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
15	O	216/276 (78%)	197 (91%)	19 (9%)	0	100	100
16	P	200/204 (98%)	185 (92%)	15 (8%)	0	100	100
17	Q	197/201 (98%)	180 (91%)	17 (9%)	0	100	100
18	R	199/262 (76%)	184 (92%)	15 (8%)	0	100	100
19	S	211/240 (88%)	200 (95%)	11 (5%)	0	100	100
20	T	213/263 (81%)	208 (98%)	5 (2%)	0	100	100
21	U	798/953 (84%)	735 (92%)	62 (8%)	1 (0%)	48	83
22	V	478/533 (90%)	413 (86%)	63 (13%)	2 (0%)	30	67
23	W	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	18	56
24	X	239/422 (57%)	213 (89%)	26 (11%)	0	100	100
25	Y	376/389 (97%)	335 (89%)	39 (10%)	2 (0%)	24	63
26	Z	284/324 (88%)	253 (89%)	30 (11%)	1 (0%)	30	67
27	a	371/376 (99%)	331 (89%)	38 (10%)	2 (0%)	24	63
28	b	189/377 (50%)	174 (92%)	15 (8%)	0	100	100
29	c	274/309 (89%)	242 (88%)	28 (10%)	4 (2%)	8	40
30	d	255/349 (73%)	227 (89%)	27 (11%)	1 (0%)	30	67
31	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
32	f	686/749 (92%)	573 (84%)	109 (16%)	4 (1%)	21	59
All	All	9693/11269 (86%)	8692 (90%)	961 (10%)	40 (0%)	31	67

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	VAL
10	J	104	VAL
11	K	12	VAL
11	K	109	VAL
21	U	364	VAL
23	W	68	VAL
23	W	136	ILE
25	Y	350	VAL
32	f	62	ILE
32	f	447	VAL
2	B	176	VAL
3	C	214	VAL
29	c	157	ILE
29	c	227	GLU
32	f	131	VAL
1	A	206	ILE
1	A	317	VAL
2	B	218	PRO
4	D	151	ILE
10	J	199	VAL
27	a	340	VAL
32	f	281	ILE
3	C	298	ILE
6	F	282	ILE
7	G	15	ILE
23	W	138	VAL
25	Y	67	VAL
29	c	156	VAL
22	V	241	ARG
26	Z	144	VAL
30	d	213	ARG
22	V	101	LEU
27	a	336	VAL
2	B	325	VAL
29	c	189	ILE
1	A	172	VAL
6	F	326	VAL
7	G	170	VAL
10	J	98	VAL
5	E	175	PRO

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	A	308/372 (83%)	300 (97%)	8 (3%)	40	62
2	B	304/385 (79%)	294 (97%)	10 (3%)	33	55
3	C	332/346 (96%)	319 (96%)	13 (4%)	28	49
4	D	333/366 (91%)	323 (97%)	10 (3%)	36	57
5	E	308/353 (87%)	304 (99%)	4 (1%)	61	74
6	F	312/379 (82%)	306 (98%)	6 (2%)	50	67
7	G	193/209 (92%)	188 (97%)	5 (3%)	40	62
8	H	164/190 (86%)	164 (100%)	0	100	100
9	I	193/220 (88%)	190 (98%)	3 (2%)	55	70
10	J	152/210 (72%)	151 (99%)	1 (1%)	76	81
11	K	186/202 (92%)	182 (98%)	4 (2%)	45	64
12	L	198/229 (86%)	194 (98%)	4 (2%)	48	66
13	M	192/211 (91%)	189 (98%)	3 (2%)	55	70
14	N	148/180 (82%)	146 (99%)	2 (1%)	59	72
15	O	177/227 (78%)	175 (99%)	2 (1%)	65	76
16	P	172/173 (99%)	171 (99%)	1 (1%)	78	83
17	Q	164/171 (96%)	163 (99%)	1 (1%)	78	83
18	R	153/201 (76%)	153 (100%)	0	100	100
19	S	174/198 (88%)	172 (99%)	2 (1%)	65	76
20	T	175/214 (82%)	175 (100%)	0	100	100
21	U	685/816 (84%)	678 (99%)	7 (1%)	68	78
22	V	414/459 (90%)	407 (98%)	7 (2%)	53	69
23	W	416/416 (100%)	409 (98%)	7 (2%)	53	69
24	X	208/362 (58%)	204 (98%)	4 (2%)	50	67
25	Y	334/344 (97%)	331 (99%)	3 (1%)	70	79
26	Z	257/295 (87%)	251 (98%)	6 (2%)	44	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	333/336 (99%)	325 (98%)	8 (2%)	43	64
28	b	167/312 (54%)	164 (98%)	3 (2%)	51	68
29	c	243/267 (91%)	233 (96%)	10 (4%)	27	49
30	d	231/293 (79%)	228 (99%)	3 (1%)	61	74
31	e	38/63 (60%)	38 (100%)	0	100	100
32	f	582/628 (93%)	569 (98%)	13 (2%)	45	64
All	All	8246/9627 (86%)	8096 (98%)	150 (2%)	51	68

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LEU
1	A	153	LEU
1	A	157	ILE
1	A	161	VAL
1	A	191	VAL
1	A	220	THR
1	A	250	VAL
1	A	315	ILE
2	B	105	THR
2	B	135	ILE
2	B	136	LEU
2	B	159	VAL
2	B	164	MET
2	B	173	VAL
2	B	190	LEU
2	B	256	ILE
2	B	281	ILE
2	B	334	ILE
3	C	11	LEU
3	C	66	LEU
3	C	99	VAL
3	C	131	VAL
3	C	148	TYR
3	C	167	LEU
3	C	235	PHE
3	C	249	ASP
3	C	259	LEU
3	C	286	THR
3	C	295	THR

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Mol	Chain	Res	Type
3	C	298	ILE
3	C	315	ILE
4	D	61	ILE
4	D	89	ILE
4	D	103	VAL
4	D	116	LEU
4	D	186	THR
4	D	234	GLU
4	D	303	VAL
4	D	344	ILE
4	D	358	VAL
4	D	406	VAL
5	E	80	VAL
5	E	204	VAL
5	E	315	ILE
5	E	326	ILE
6	F	85	THR
6	F	124	ILE
6	F	169	ASP
6	F	231	THR
6	F	282	ILE
6	F	283	ILE
7	G	15	ILE
7	G	22	LEU
7	G	109	ILE
7	G	140	LEU
7	G	230	LEU
9	I	55	LEU
9	I	123	GLN
9	I	206	LEU
10	J	104	VAL
11	K	12	VAL
11	K	20	ARG
11	K	111	SER
11	K	139	VAL
12	L	38	LEU
12	L	46	LEU
12	L	173	GLU
12	L	212	ILE
13	M	106	ILE
13	M	165	ILE
13	M	233	GLU

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Mol	Chain	Res	Type
14	N	30	VAL
14	N	75	LEU
15	O	66	HIS
15	O	94	ILE
16	P	137	VAL
17	Q	151	ILE
19	S	164	VAL
19	S	168	LEU
21	U	67	VAL
21	U	473	VAL
21	U	554	LEU
21	U	603	LEU
21	U	629	THR
21	U	746	ILE
21	U	773	PHE
22	V	221	LEU
22	V	224	LEU
22	V	255	LEU
22	V	299	GLN
22	V	320	THR
22	V	322	VAL
22	V	453	HIS
23	W	250	ILE
23	W	297	GLU
23	W	371	THR
23	W	384	LEU
23	W	402	ILE
23	W	432	LEU
23	W	455	LEU
24	X	200	ILE
24	X	331	LEU
24	X	356	LEU
24	X	387	ILE
25	Y	350	VAL
25	Y	356	THR
25	Y	377	LEU
26	Z	91	ILE
26	Z	176	LEU
26	Z	186	THR
26	Z	196	HIS
26	Z	237	LEU
26	Z	266	ILE

Continued on next page...

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Mol	Chain	Res	Type
27	a	28	LEU
27	a	33	LEU
27	a	125	ILE
27	a	185	ILE
27	a	217	LEU
27	a	234	ILE
27	a	245	VAL
27	a	340	VAL
28	b	53	THR
28	b	92	VAL
28	b	97	LEU
29	c	25	VAL
29	c	33	ILE
29	c	42	LEU
29	c	62	VAL
29	c	69	VAL
29	c	144	VAL
29	c	172	HIS
29	c	229	LEU
29	c	244	VAL
29	c	275	VAL
30	d	122	LEU
30	d	158	ILE
30	d	189	ILE
32	f	62	ILE
32	f	107	LEU
32	f	129	VAL
32	f	301	ASP
32	f	317	THR
32	f	334	ASN
32	f	339	LEU
32	f	391	LEU
32	f	507	ILE
32	f	526	THR
32	f	600	LEU
32	f	663	VAL
32	f	685	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN

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Mol	Chain	Res	Type
1	A	314	ASN
2	B	153	ASN
2	B	154	HIS
2	B	241	ASN
3	C	50	ASN
3	C	206	HIS
4	D	187	HIS
4	D	221	HIS
4	D	302	ASN
4	D	376	ASN
4	D	412	GLN
5	E	86	GLN
5	E	190	GLN
5	E	220	ASN
5	E	307	GLN
5	E	364	GLN
6	F	76	ASN
6	F	116	GLN
6	F	255	GLN
6	F	325	GLN
7	G	75	ASN
7	G	128	ASN
8	H	119	GLN
9	I	95	GLN
9	I	109	GLN
9	I	119	GLN
10	J	92	GLN
10	J	146	GLN
11	K	23	GLN
11	K	41	GLN
11	K	97	GLN
11	K	178	GLN
11	K	214	ASN
12	L	20	HIS
12	L	21	GLN
12	L	68	ASN
13	M	180	GLN
14	N	154	GLN
14	N	187	GLN
15	O	66	HIS
16	P	162	HIS
16	P	169	GLN

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Mol	Chain	Res	Type
17	Q	8	GLN
17	Q	99	HIS
18	R	10	HIS
18	R	29	GLN
18	R	119	ASN
18	R	178	HIS
19	S	151	ASN
20	T	65	GLN
21	U	70	HIS
21	U	107	HIS
21	U	111	GLN
21	U	267	ASN
21	U	345	ASN
21	U	438	GLN
21	U	453	HIS
21	U	464	GLN
21	U	467	ASN
21	U	475	HIS
21	U	491	GLN
21	U	500	ASN
21	U	698	GLN
21	U	777	HIS
21	U	805	ASN
22	V	281	ASN
22	V	299	GLN
22	V	400	HIS
22	V	427	GLN
22	V	459	GLN
22	V	487	HIS
23	W	106	GLN
23	W	235	GLN
23	W	246	HIS
24	X	207	GLN
24	X	262	ASN
24	X	406	ASN
25	Y	251	HIS
25	Y	363	ASN
25	Y	367	GLN
25	Y	378	ASN
26	Z	77	ASN
26	Z	96	HIS
26	Z	102	HIS

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Mol	Chain	Res	Type
26	Z	194	GLN
26	Z	224	HIS
26	Z	231	GLN
26	Z	256	GLN
27	a	23	HIS
27	a	46	GLN
27	a	152	HIS
27	a	164	GLN
27	a	227	ASN
27	a	257	GLN
27	a	290	GLN
27	a	337	GLN
28	b	47	ASN
28	b	76	HIS
28	b	105	HIS
28	b	149	ASN
29	c	30	GLN
29	c	92	GLN
29	c	115	HIS
29	c	190	GLN
29	c	199	HIS
29	c	219	ASN
29	c	283	HIS
29	c	287	HIS
30	d	102	ASN
30	d	109	GLN
31	e	6	GLN
32	f	65	ASN
32	f	114	ASN
32	f	228	GLN
32	f	246	HIS
32	f	269	GLN
32	f	406	ASN
32	f	433	ASN
32	f	565	ASN
32	f	611	HIS

5.3.3 RNA ⓘ

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	1.41	4 (12%)	48,52,52	1.75	9 (18%)
33	ATP	F	501	-	32,33,33	1.39	4 (12%)	48,52,52	1.78	8 (16%)
33	ATP	A	501	-	32,33,33	1.41	4 (12%)	48,52,52	1.76	11 (22%)
33	ATP	D	501	-	32,33,33	1.43	5 (15%)	48,52,52	1.78	9 (18%)

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	-	-	3/22/38/38	0/3/3/3
33	ATP	F	501	-	-	4/22/38/38	0/3/3/3
33	ATP	A	501	-	-	3/22/38/38	0/3/3/3
33	ATP	D	501	-	-	7/22/38/38	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	4.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	401	ATP	C5-C4	4.73	1.47	1.39
33	D	501	ATP	C5-C4	4.73	1.47	1.39
33	A	501	ATP	C5-C4	4.68	1.47	1.39
33	D	501	ATP	C5-C6	2.77	1.48	1.41
33	F	501	ATP	C5-C6	2.74	1.48	1.41
33	A	501	ATP	C5-C6	2.74	1.48	1.41
33	E	401	ATP	C5-C6	2.72	1.48	1.41
33	A	501	ATP	C8-N7	2.43	1.36	1.31
33	D	501	ATP	C8-N7	2.34	1.36	1.31
33	F	501	ATP	C8-N7	2.31	1.36	1.31
33	E	401	ATP	C8-N7	2.30	1.36	1.31
33	F	501	ATP	C5-N7	-2.30	1.34	1.39
33	E	401	ATP	C5-N7	-2.30	1.34	1.39
33	D	501	ATP	C5-N7	-2.23	1.35	1.39
33	A	501	ATP	C5-N7	-2.16	1.35	1.39
33	D	501	ATP	PA-O3A	2.05	1.61	1.59

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	F	501	ATP	C5-C4-N3	-6.14	118.26	126.72
33	D	501	ATP	C5-C4-N3	-5.77	118.77	126.72
33	E	401	ATP	C5-C4-N3	-5.70	118.86	126.72
33	A	501	ATP	C5-C4-N3	-5.70	118.87	126.72
33	F	501	ATP	N3-C4-N9	4.85	135.42	127.17
33	E	401	ATP	N3-C4-N9	4.59	134.97	127.17
33	D	501	ATP	N3-C4-N9	4.53	134.87	127.17
33	A	501	ATP	N3-C4-N9	4.46	134.76	127.17
33	F	501	ATP	C2-N3-C4	3.73	120.95	111.83
33	A	501	ATP	C2-N3-C4	3.69	120.83	111.83
33	E	401	ATP	C2-N3-C4	3.64	120.72	111.83
33	D	501	ATP	C2-N3-C4	3.63	120.69	111.83
33	A	501	ATP	C4-C5-N7	-3.55	106.53	110.58
33	D	501	ATP	C4-C5-N7	-3.49	106.59	110.58
33	F	501	ATP	C4-C5-N7	-3.49	106.59	110.58
33	D	501	ATP	O4'-C1'-N9	3.44	114.69	108.09
33	E	401	ATP	C4-C5-N7	-3.38	106.71	110.58
33	A	501	ATP	N3-C2-N1	-3.37	123.49	128.58
33	E	401	ATP	N3-C2-N1	-3.26	123.64	128.58
33	D	501	ATP	N3-C2-N1	-3.12	123.85	128.58
33	F	501	ATP	N3-C2-N1	-3.09	123.91	128.58
33	E	401	ATP	C4-N9-C8	2.71	108.58	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	501	ATP	C4-N9-C8	2.70	108.58	105.74
33	D	501	ATP	C4-N9-C8	2.58	108.44	105.74
33	F	501	ATP	C5-N7-C8	2.57	107.49	103.45
33	A	501	ATP	C5-N7-C8	2.55	107.45	103.45
33	E	401	ATP	C5-N7-C8	2.53	107.43	103.45
33	D	501	ATP	C5-N7-C8	2.53	107.42	103.45
33	E	401	ATP	C3'-C2'-C1'	2.49	106.17	101.46
33	F	501	ATP	C4-N9-C8	2.45	108.31	105.74
33	F	501	ATP	C3'-C2'-C1'	2.42	106.04	101.46
33	A	501	ATP	C3'-C2'-C1'	2.20	105.63	101.46
33	A	501	ATP	C6-C5-N7	2.17	136.27	132.09
33	D	501	ATP	C6-C5-N7	2.06	136.07	132.09
33	A	501	ATP	C2-N1-C6	2.03	122.06	118.73
33	E	401	ATP	C6-C5-N7	2.03	135.99	132.09
33	A	501	ATP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (17) torsion outliers are listed below:

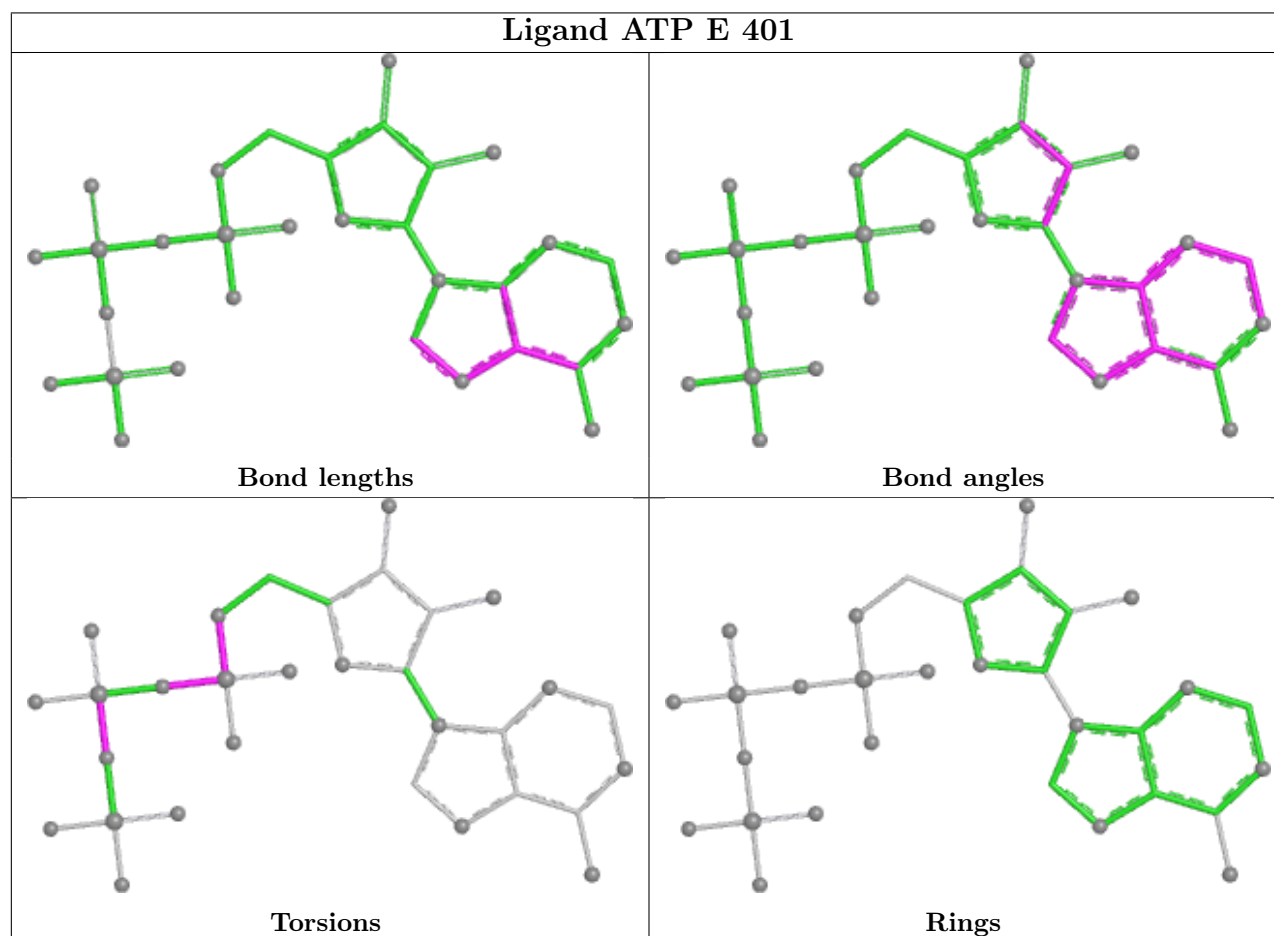
Mol	Chain	Res	Type	Atoms
33	D	501	ATP	C5'-O5'-PA-O1A
33	F	501	ATP	C5'-O5'-PA-O3A
33	F	501	ATP	O4'-C4'-C5'-O5'
33	F	501	ATP	C3'-C4'-C5'-O5'
33	D	501	ATP	PB-O3A-PA-O5'
33	D	501	ATP	C2'-C1'-N9-C8
33	E	401	ATP	PB-O3A-PA-O1A
33	A	501	ATP	O4'-C4'-C5'-O5'
33	A	501	ATP	C5'-O5'-PA-O1A
33	D	501	ATP	C5'-O5'-PA-O2A
33	D	501	ATP	C5'-O5'-PA-O3A
33	E	401	ATP	C5'-O5'-PA-O1A
33	F	501	ATP	C5'-O5'-PA-O1A
33	A	501	ATP	C3'-C4'-C5'-O5'
33	D	501	ATP	O4'-C1'-N9-C8
33	E	401	ATP	PG-O3B-PB-O1B
33	D	501	ATP	C2'-C1'-N9-C4

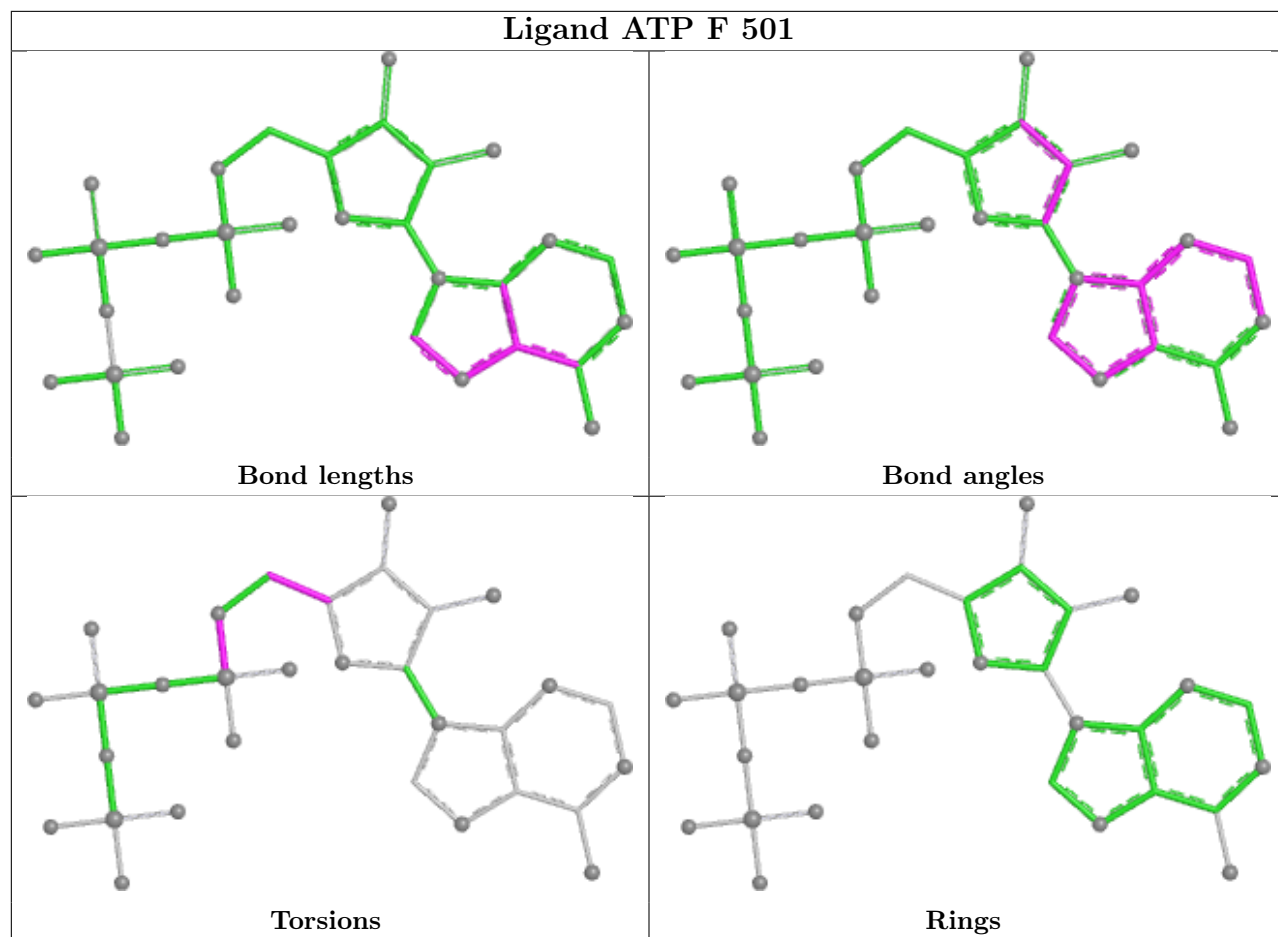
There are no ring outliers.

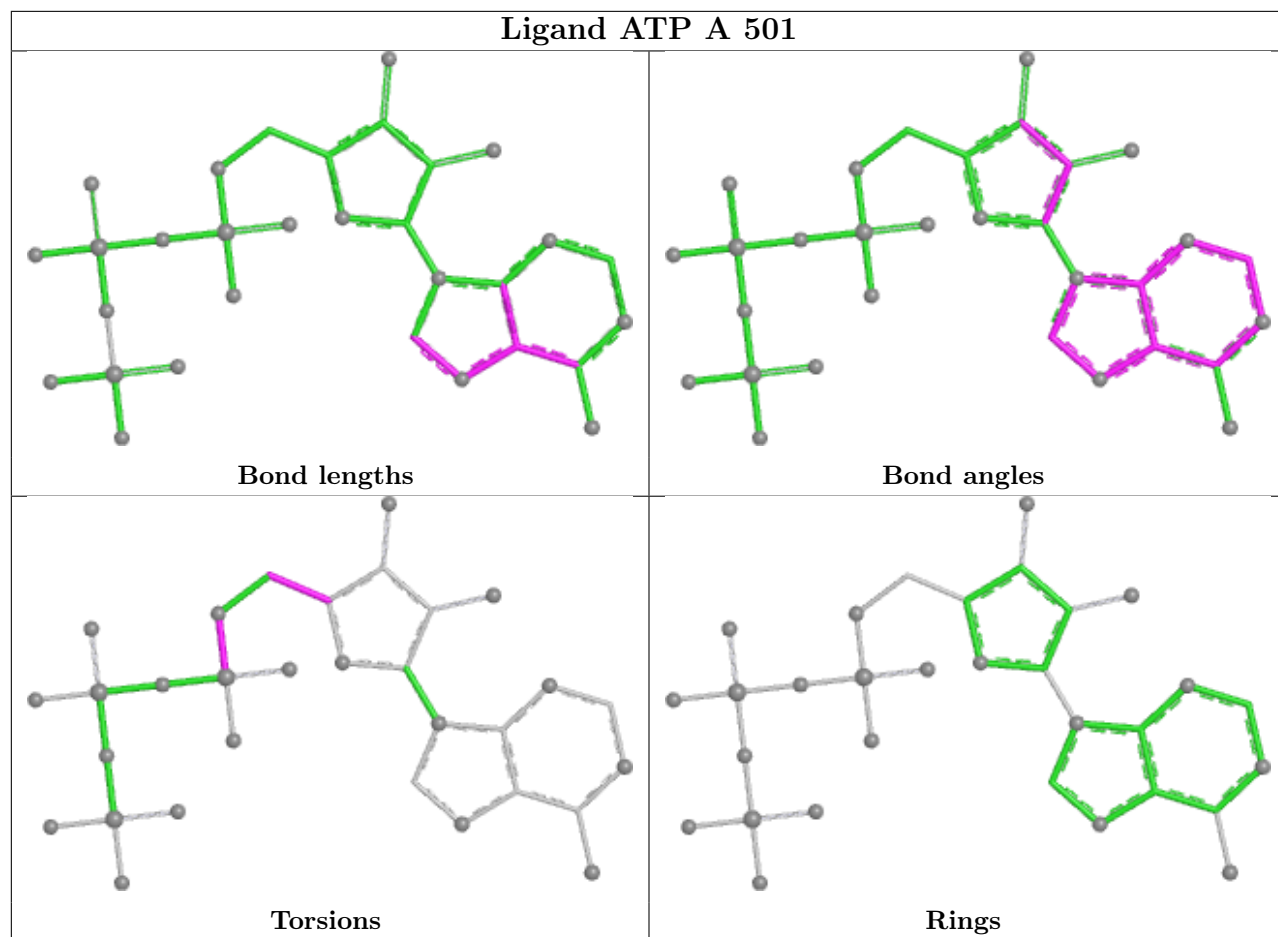
4 monomers are involved in 7 short contacts:

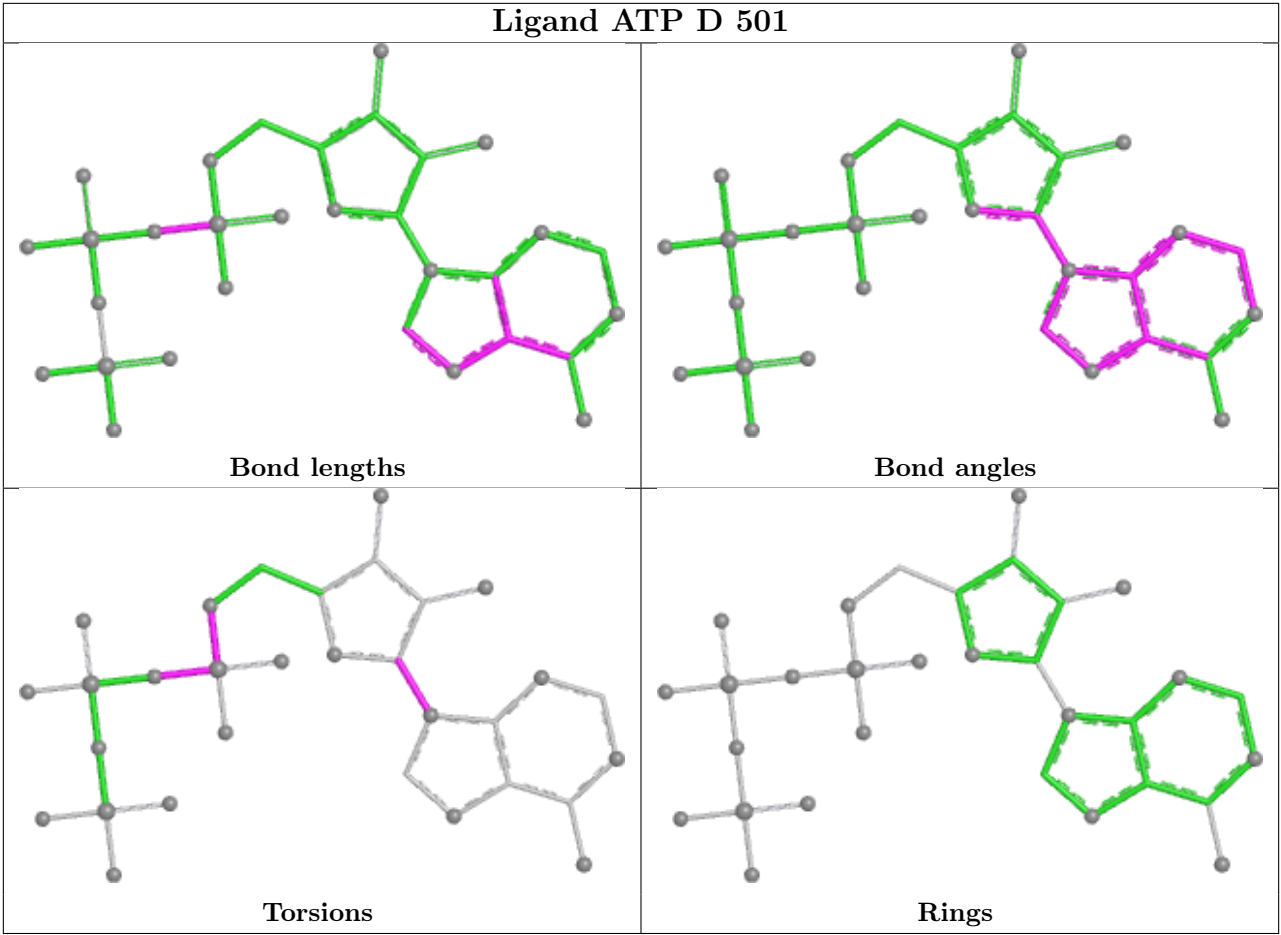
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	E	401	ATP	2	0
33	F	501	ATP	2	0
33	A	501	ATP	1	0
33	D	501	ATP	2	0

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
32	f	4
16	P	1
15	O	1
8	H	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	9.37
1	f	79:ASN	C	80:TYR	N	8.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	348:ASP	C	349:SER	N	6.07
1	P	81:GLN	C	82:ILE	N	4.19
1	O	74:PRO	C	75:ARG	N	3.14
1	H	79:MET	C	80:GLY	N	3.08
1	f	681:LEU	C	682:PRO	N	1.68

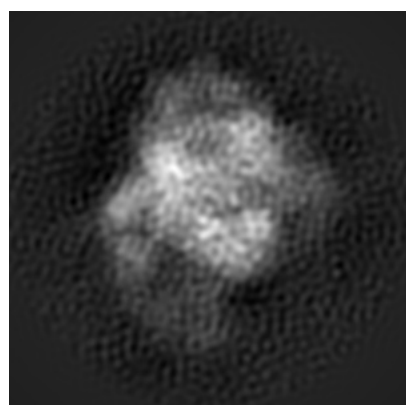
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8336. These allow visual inspection of the internal detail of the map and identification of artifacts.

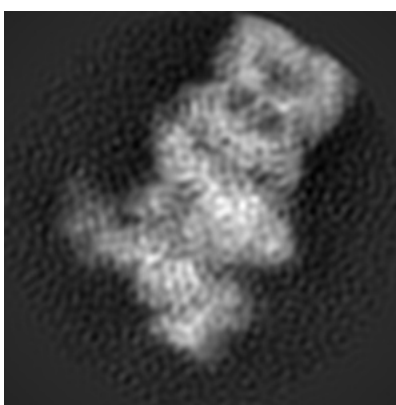
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

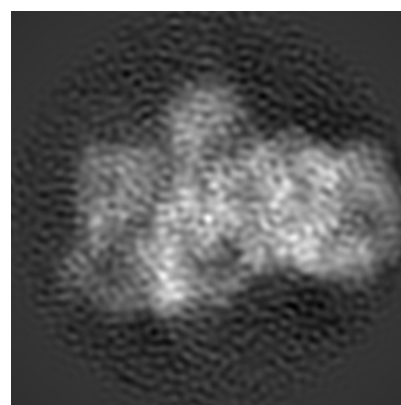
6.1.1 Primary map



X



Y

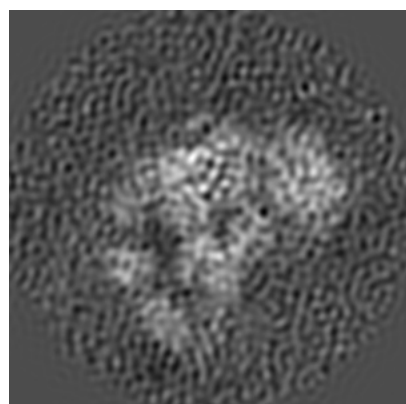


Z

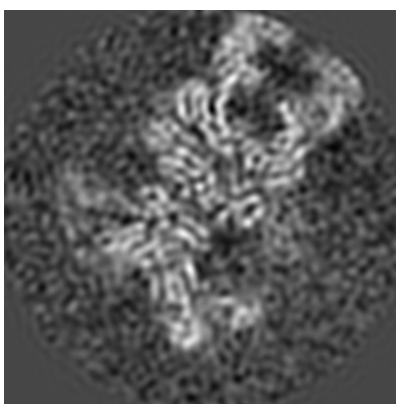
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

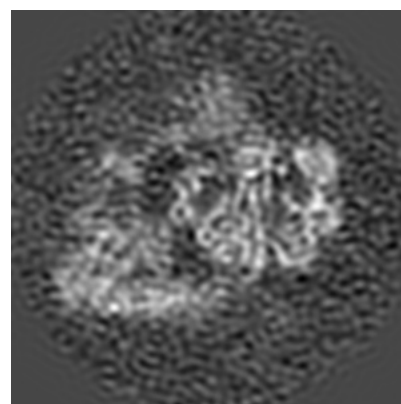
6.2.1 Primary map



X Index: 180



Y Index: 180

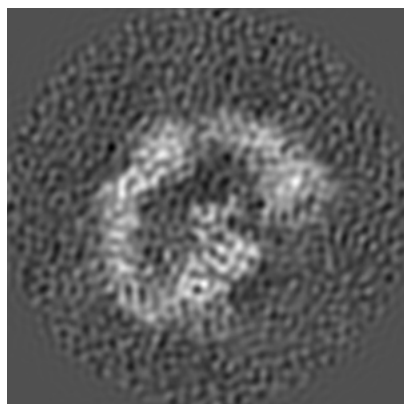


Z Index: 180

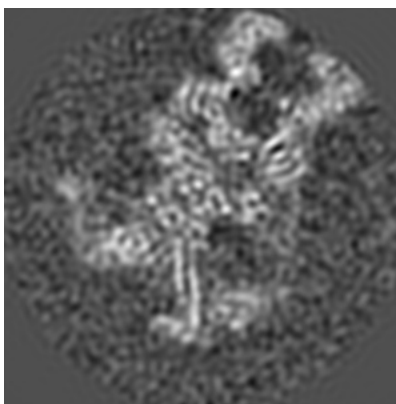
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

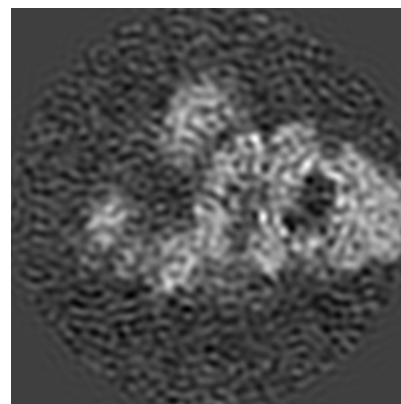
6.3.1 Primary map



X Index: 150



Y Index: 174

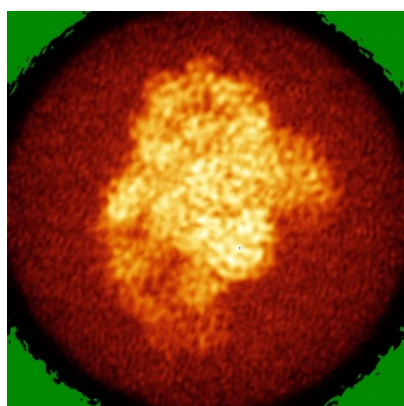


Z Index: 216

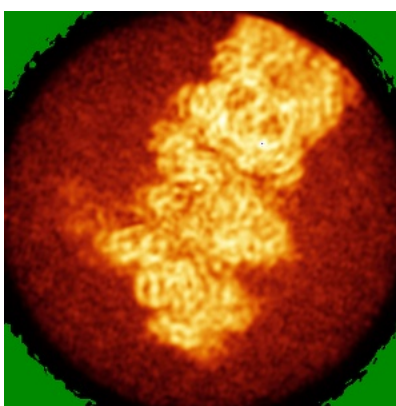
The images above show the largest variance slices of the map in three orthogonal directions.

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

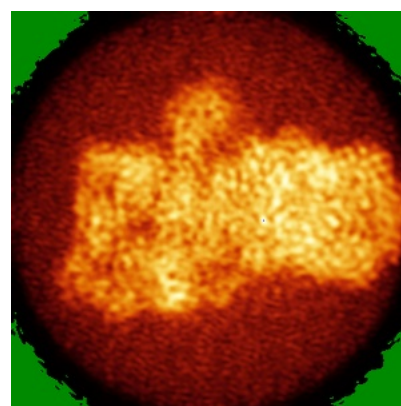
6.4.1 Primary map



X



Y

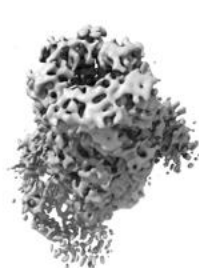


Z

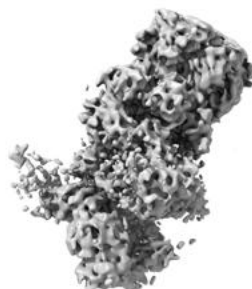
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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.

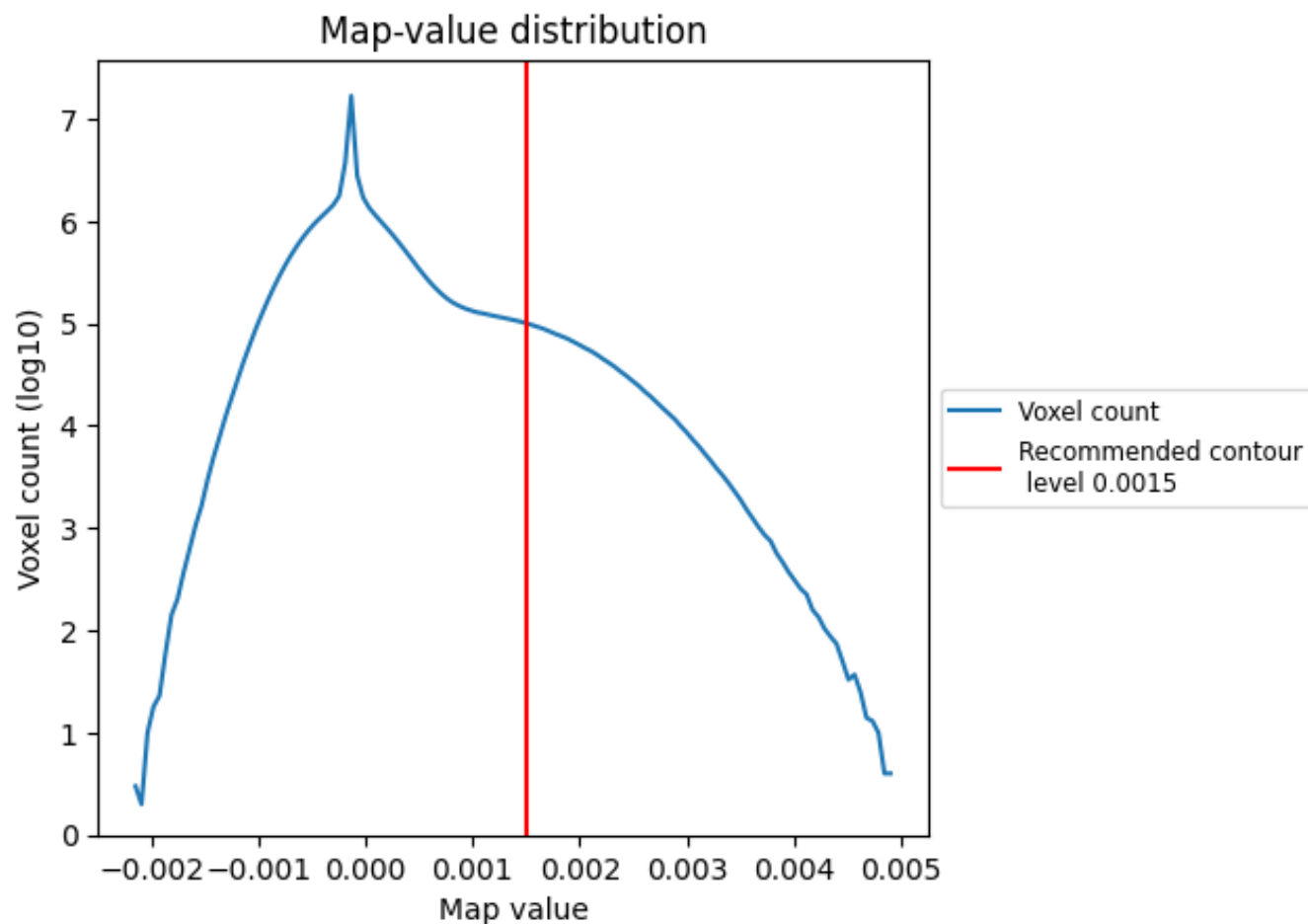
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

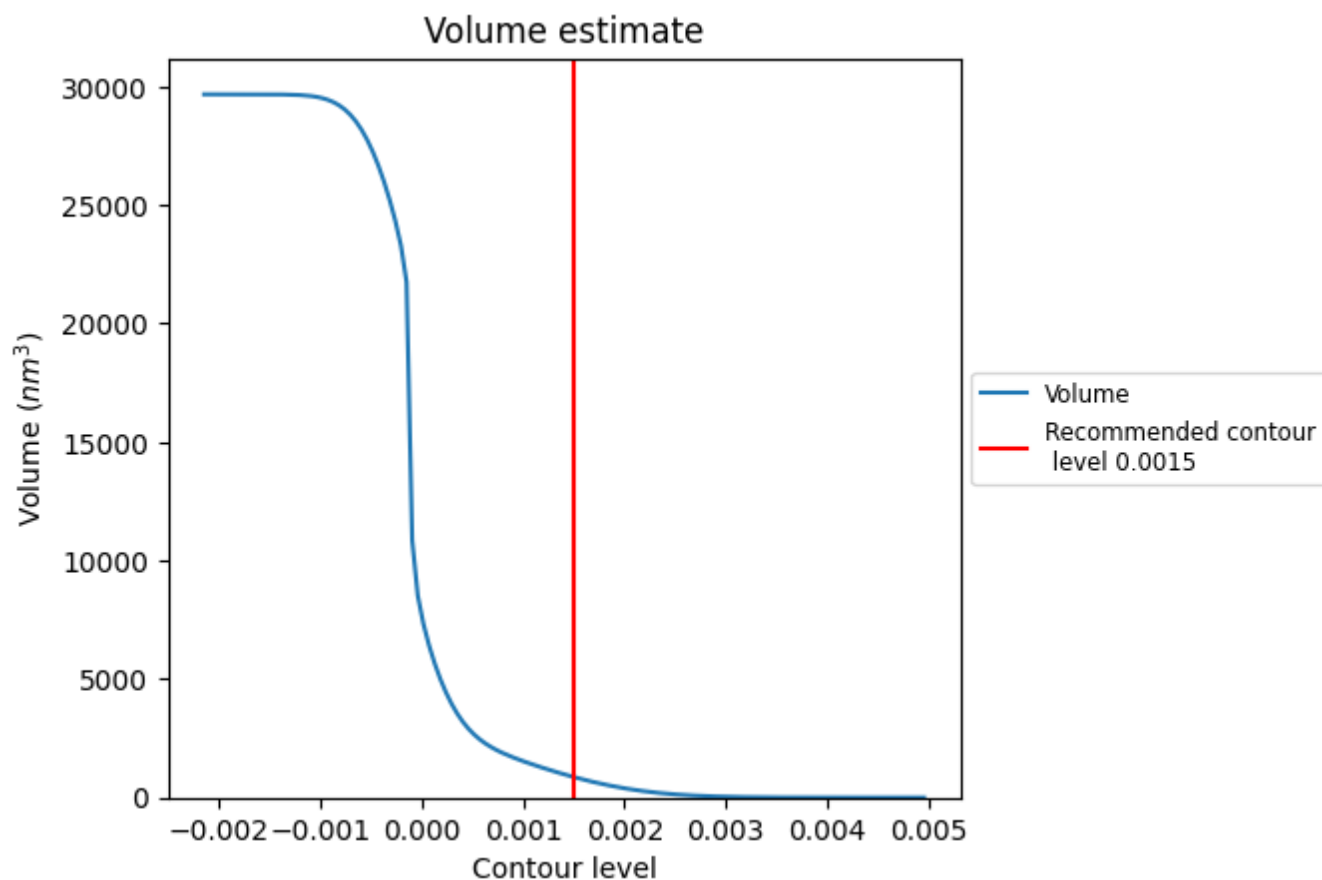
This section contains the results of statistical analysis of the map.

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.

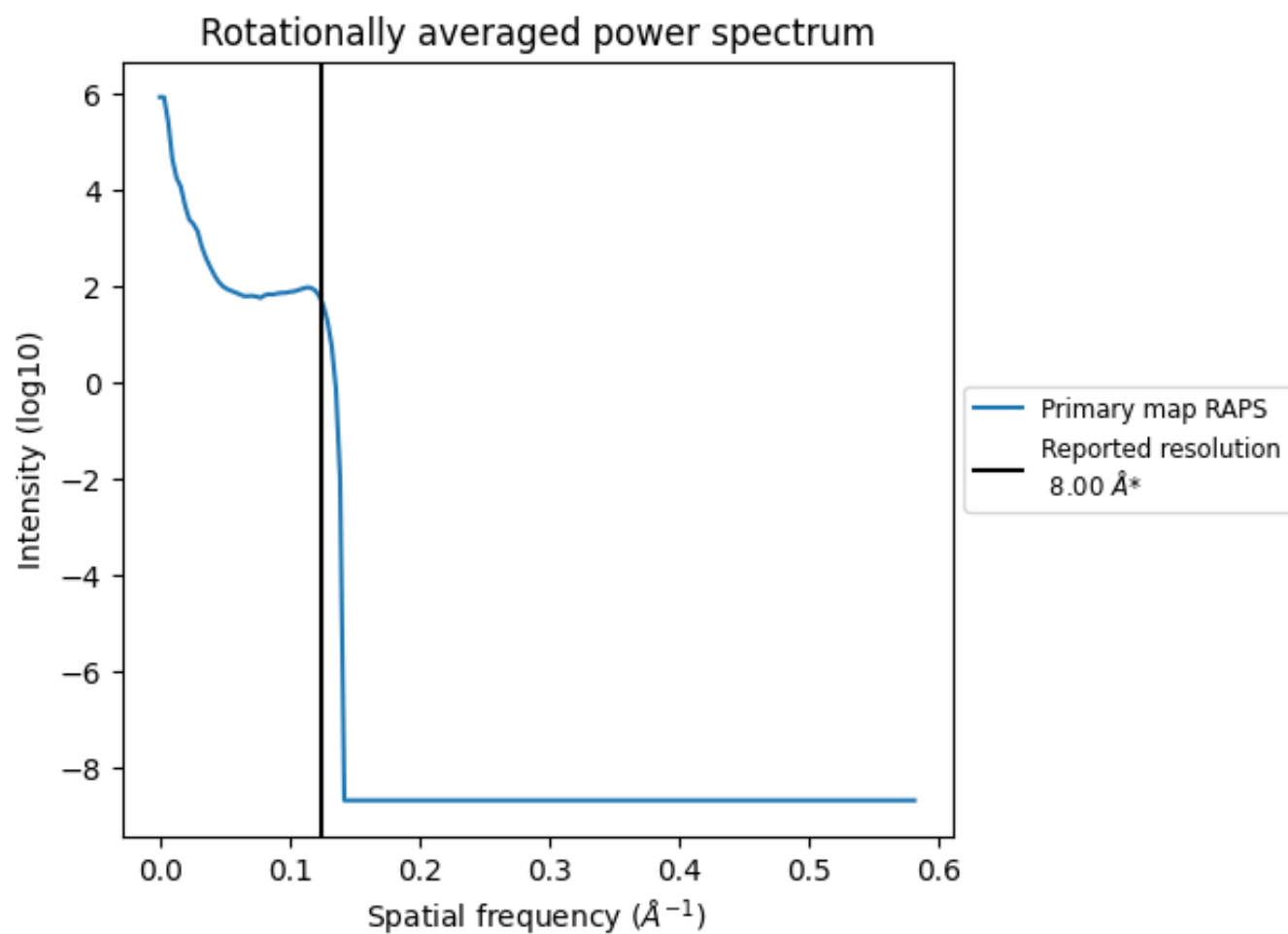
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 868 nm³; this corresponds to an approximate mass of 784 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

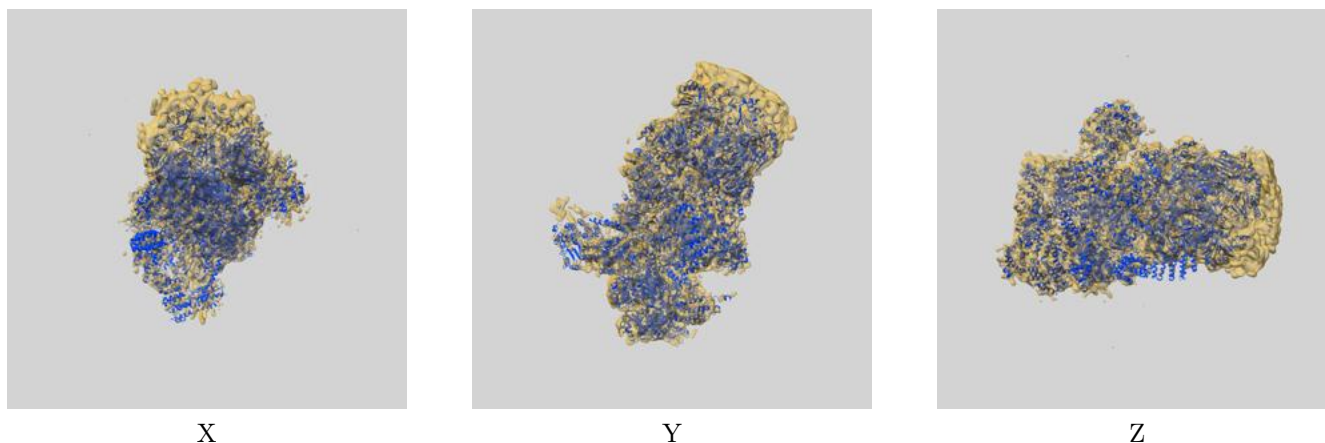
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

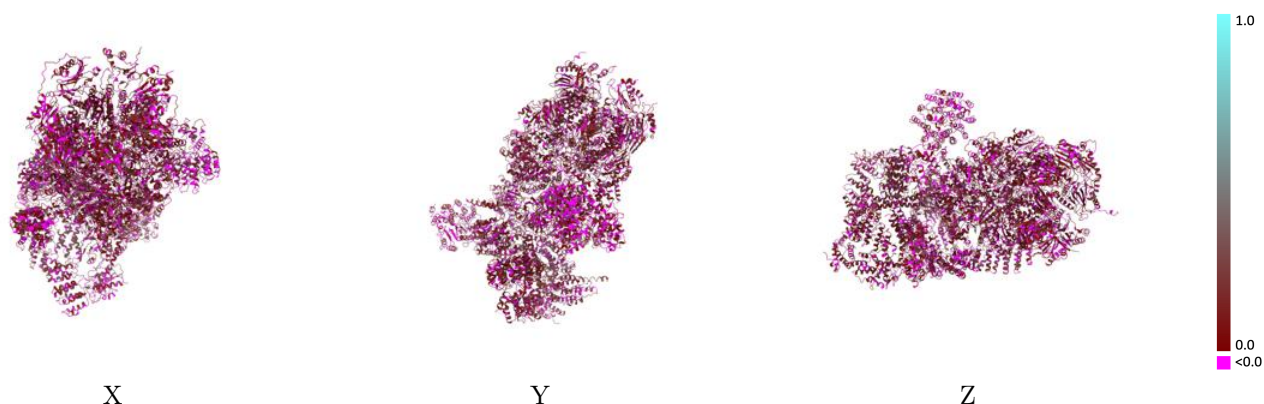
This section contains information regarding the fit between EMDB map EMD-8336 and PDB model 5T0I. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



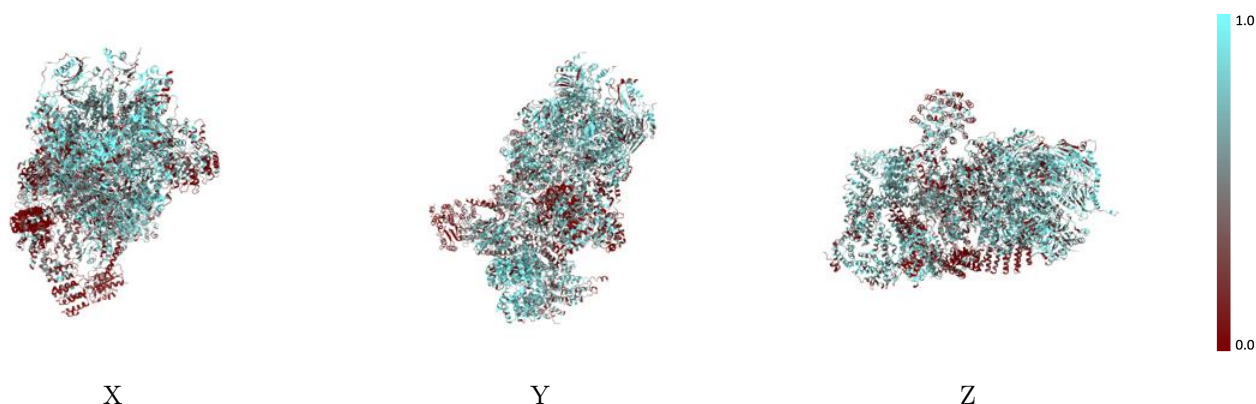
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



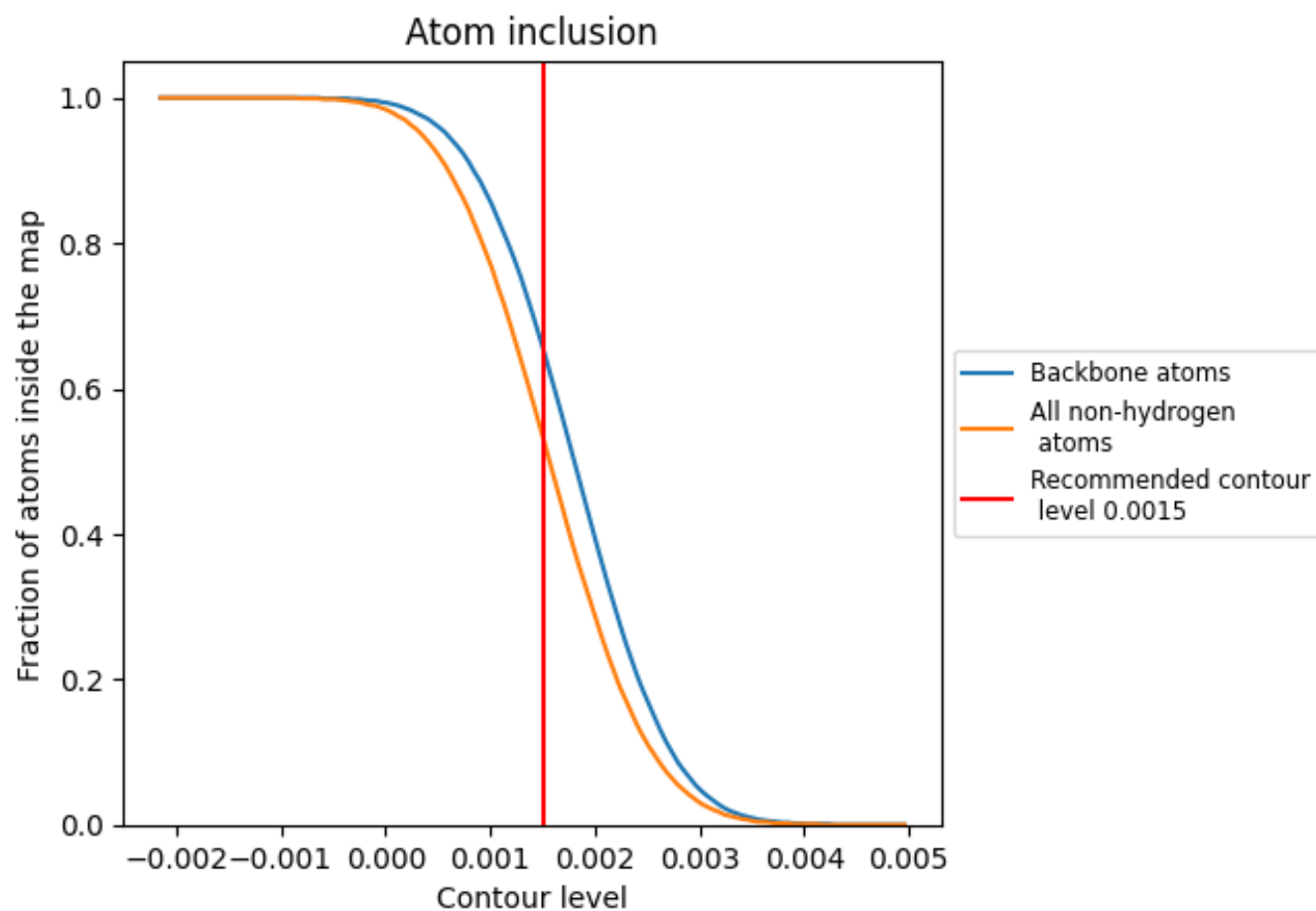
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 54% 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	 0.5360	 0.0930
A	 0.5950	 0.1120
B	 0.4740	 0.1100
C	 0.5090	 0.1010
D	 0.5380	 0.1100
E	 0.5180	 0.1120
F	 0.5610	 0.1080
G	 0.6320	 0.1080
H	 0.6790	 0.1010
I	 0.6170	 0.1140
J	 0.5880	 0.1120
K	 0.6520	 0.0980
L	 0.7030	 0.1200
M	 0.5990	 0.1010
N	 0.5820	 0.0900
O	 0.6750	 0.1000
P	 0.6570	 0.0950
Q	 0.5970	 0.0910
R	 0.6080	 0.0760
S	 0.6940	 0.1000
T	 0.7150	 0.1020
U	 0.7090	 0.1140
V	 0.5630	 0.1080
W	 0.2230	 0.0720
X	 0.2170	 0.0470
Y	 0.6030	 0.0880
Z	 0.5070	 0.0810
a	 0.2840	 0.0690
b	 0.1120	 0.0440
c	 0.5220	 0.1080
d	 0.5140	 0.0820
e	 0.6000	 0.0890
f	 0.4160	 0.0390

