



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:14 AM UTC

PDB ID : 9SZT / pdb_00009szt
EMDB ID : EMD-52193
Title : Co-chaperone Bag1-bound human 26S proteasome in SBAG1.2 state
Authors : Cheng, T.C.; Sakata, E.; Muntaner, J.; Maestro-Lopez, M.; Cuellar, J.; Valpuesta, J.M.
Deposited on : 2025-10-15
Resolution : 3.50 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

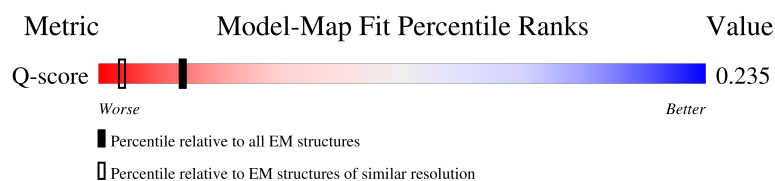
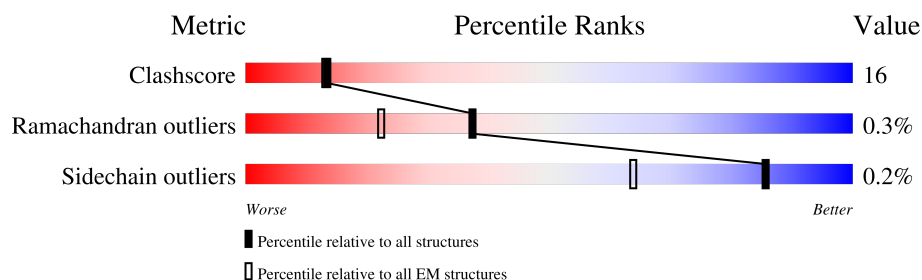
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

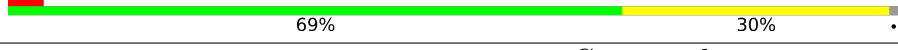
The reported resolution of this entry is 3.50 Å.

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.



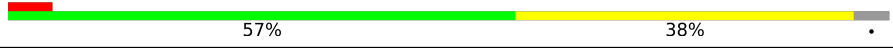
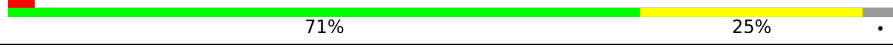
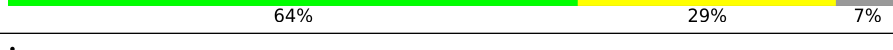
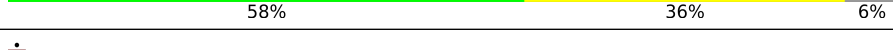
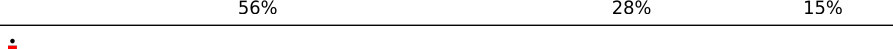
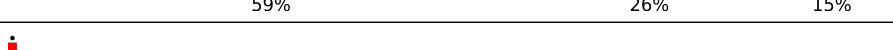
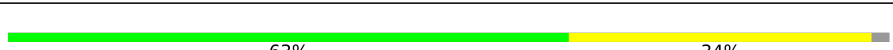
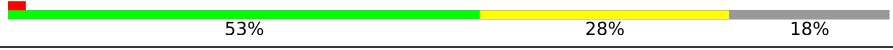
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	G	246	
1	g	246	
2	H	234	
2	h	234	

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Mol	Chain	Length	Quality of chain
3	I	261	
3	i	261	
4	J	248	
4	j	248	
5	L	269	
5	l	269	
6	M	255	
6	m	255	
7	N	239	
7	n	239	
8	O	277	
8	o	277	
9	P	205	
9	p	205	
10	Q	201	
10	q	201	
11	R	263	
11	r	263	
12	S	241	
12	s	241	
13	T	264	
13	t	264	
14	K	241	
14	k	241	
15	f	908	

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Mol	Chain	Length	Quality of chain
16	x	230	
17	a	376	
18	b	377	
19	c	310	
20	d	350	
21	e	70	
22	U	953	
23	V	534	
24	X	422	
25	Y	389	
26	Z	324	
27	W	456	
28	A	433	
29	B	440	
30	C	398	
31	D	418	
32	E	403	
33	F	439	

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 104201 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	237	Total	C	N	O	S	0	0
			1841	1168	307	353	13		
1	g	243	Total	C	N	O	S	0	0
			1885	1194	316	362	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	226	Total	C	N	O	S	0	0
			1749	1116	297	330	6		
2	h	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	247	Total	C	N	O	S	0	0
			1933	1222	330	372	9		
3	i	250	Total	C	N	O	S	0	0
			1971	1245	339	377	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	237	Total	C	N	O	S	0	0
			1869	1171	332	361	5		
4	j	238	Total	C	N	O	S	0	0
			1878	1178	333	362	5		

- Molecule 5 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		
5	l	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	238	Total	C	N	O	S	0	0
			1862	1180	318	353	11		
6	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
7	n	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
8	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
9	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
11	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
12	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		
13	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 14 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	k	234	Total	C	N	O	S	0	0
			1789	1125	295	358	11		
14	K	222	Total	C	N	O	S	0	0
			1694	1066	280	338	10		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	823	Total	C	N	O	S	0	0
			6292	3963	1077	1208	44		

- Molecule 16 is a protein called BAG family molecular chaperone regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	x	85	Total	C	N	O	S	0	0
			635	397	110	125	3		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	373	Total	C	N	O	S	0	0
			2969	1887	510	557	15		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	287	Total	C	N	O	S	0	0
			2224	1398	388	419	19		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	252	Total	C	N	O	S	0	0
			2063	1338	335	382	8		

- Molecule 21 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	e	50	Total	C	N	O	0	0
			407	244	63	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	859	Total	C	N	O	S	0	0
			6648	4199	1136	1269	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	444	Total	C	N	O	S	0	0
			3600	2289	645	653	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total	C	N	O	S	0	0
			3002	1912	509	569	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	380	Total	C	N	O	S	0	0
			3021	1904	530	570	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
			2248	1427	392	424	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	444	Total	C	N	O	S	0	0
			3570	2250	616	680	24		

- Molecule 28 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	403	Total	C	N	O	S	0	0
			3119	1958	548	596	17		

- Molecule 29 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	400	Total	C	N	O	S	0	0
			3060	1918	527	601	14		

- Molecule 30 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	368	Total	C	N	O	S	0	0
			2839	1766	518	537	18		

- Molecule 31 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D	372	Total	C	N	O	S	0	0
			2893	1818	504	560	11		

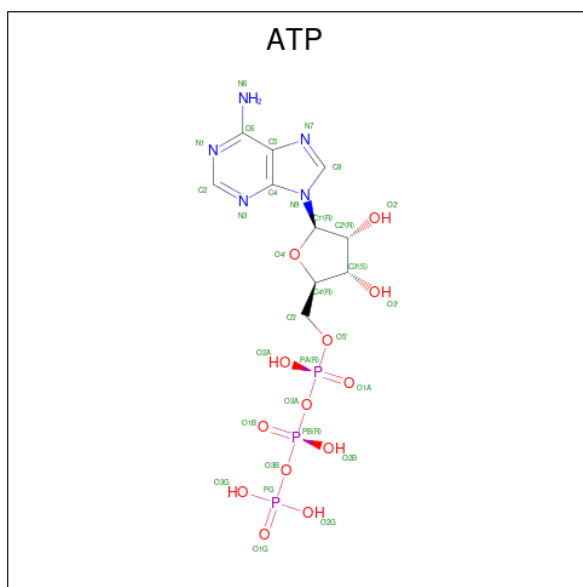
- Molecule 32 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	E	370	Total	C	N	O	S	0	0
			2929	1843	518	552	16		

- Molecule 33 is a protein called 26S protease regulatory subunit 6A.

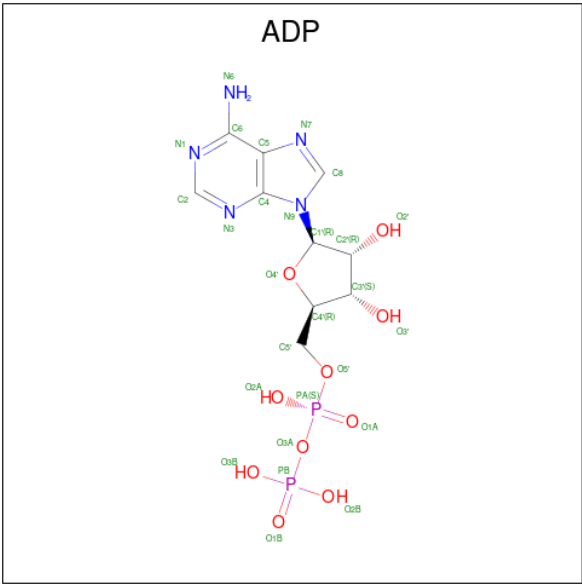
Mol	Chain	Residues	Atoms					AltConf	Trace
33	F	355	Total	C	N	O	S	0	0
			2699	1700	464	518	17		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

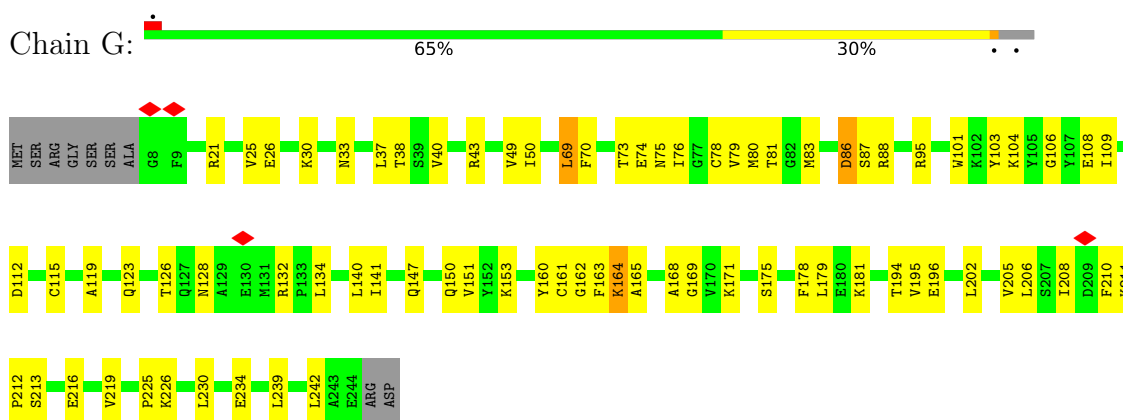


Mol	Chain	Residues	Atoms					AltConf
35	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

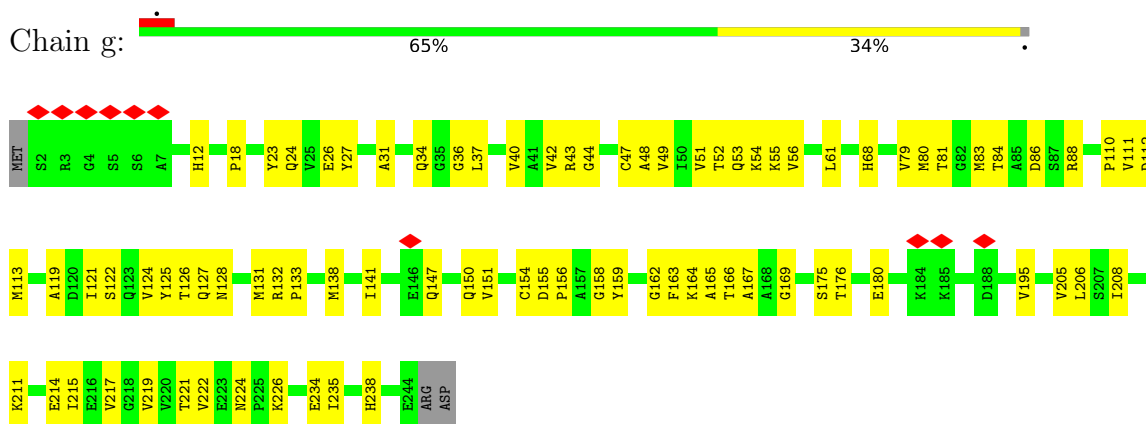
3 Residue-property plots

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

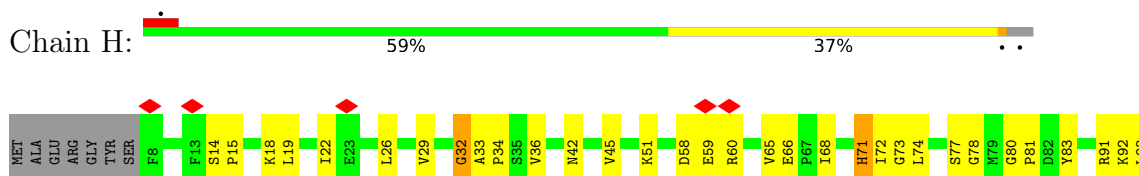
• Molecule 1: Proteasome subunit alpha type-6

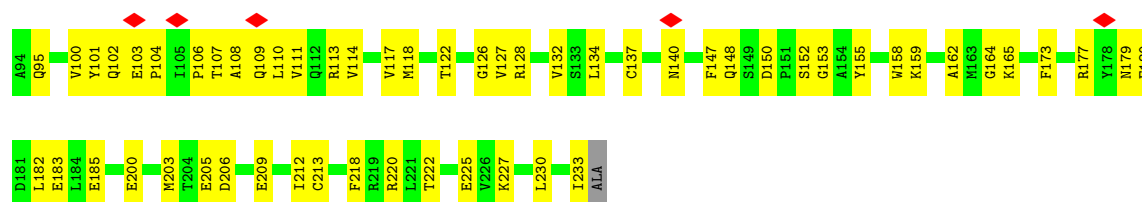


• Molecule 1: Proteasome subunit alpha type-6

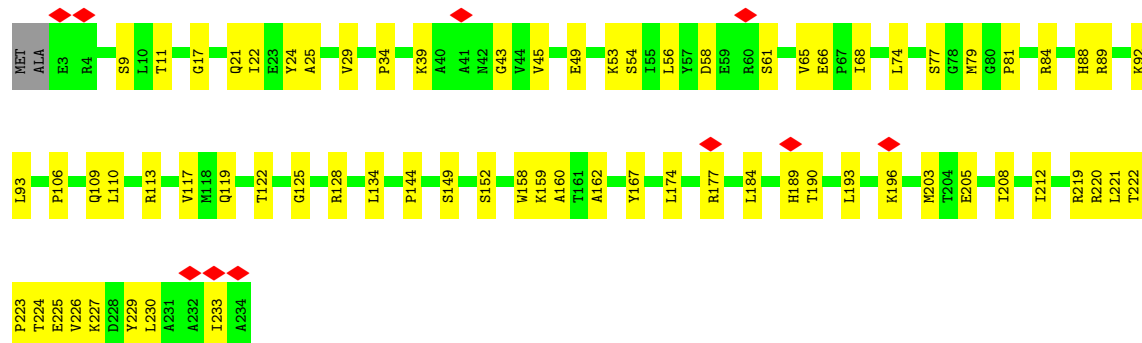


• Molecule 2: Proteasome subunit alpha type-2

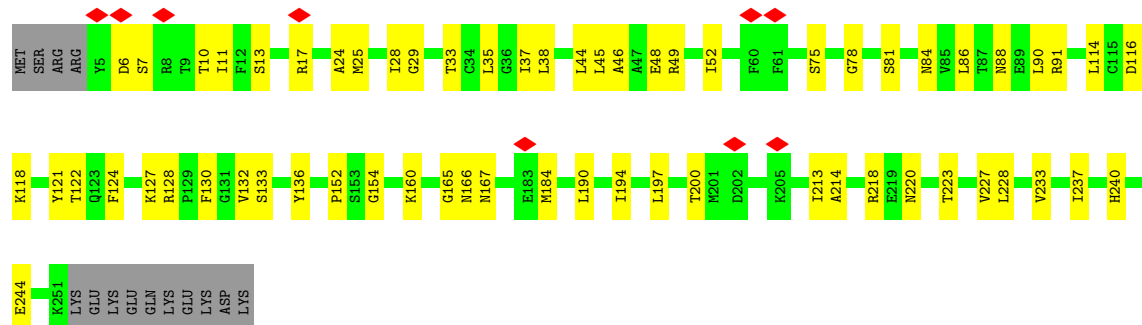




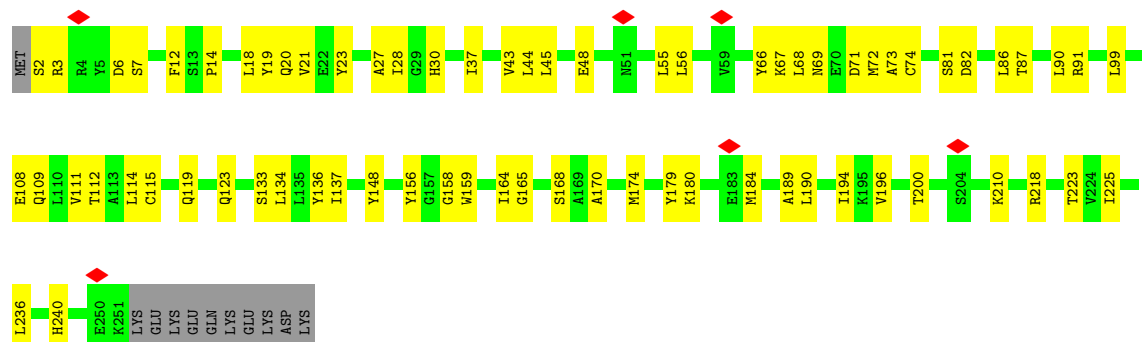
• Molecule 2: Proteasome subunit alpha type-2



• Molecule 3: Proteasome subunit alpha type-4



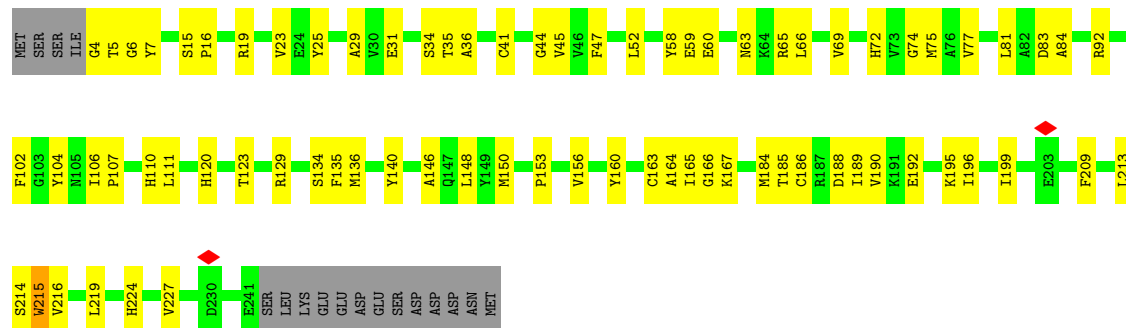
• Molecule 3: Proteasome subunit alpha type-4



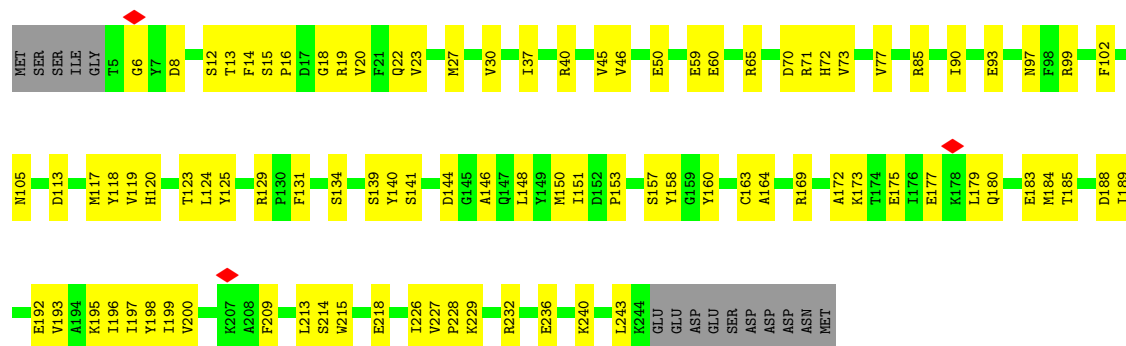
Chain J: 5% 57% 38% .



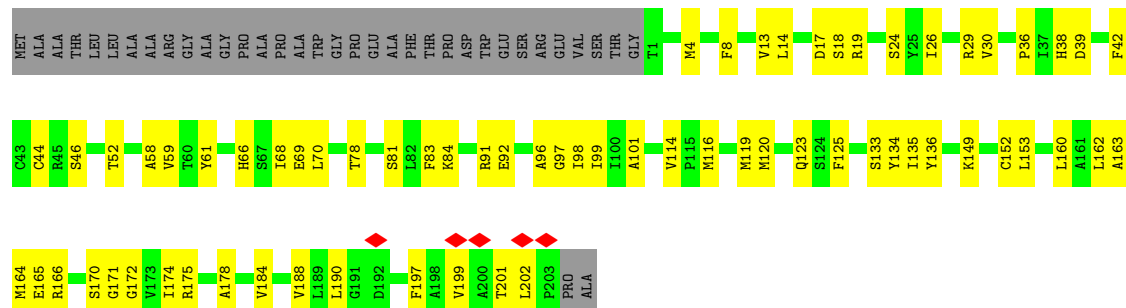
- Molecule 6: Proteasome subunit alpha type-3



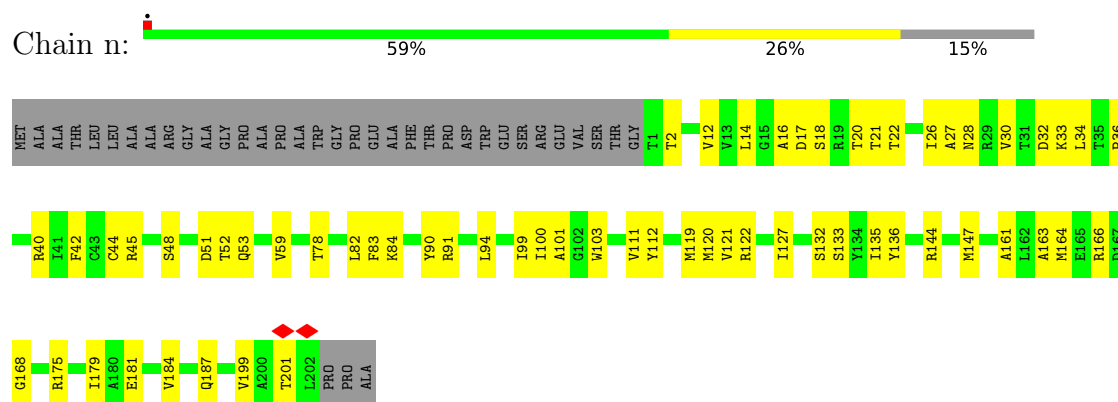
- Molecule 6: Proteasome subunit alpha type-3



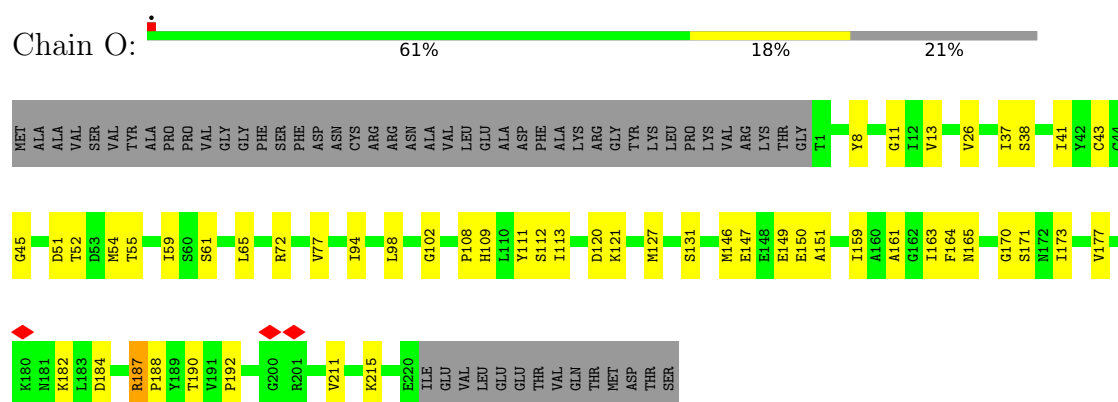
- Molecule 7: Proteasome subunit beta type-6



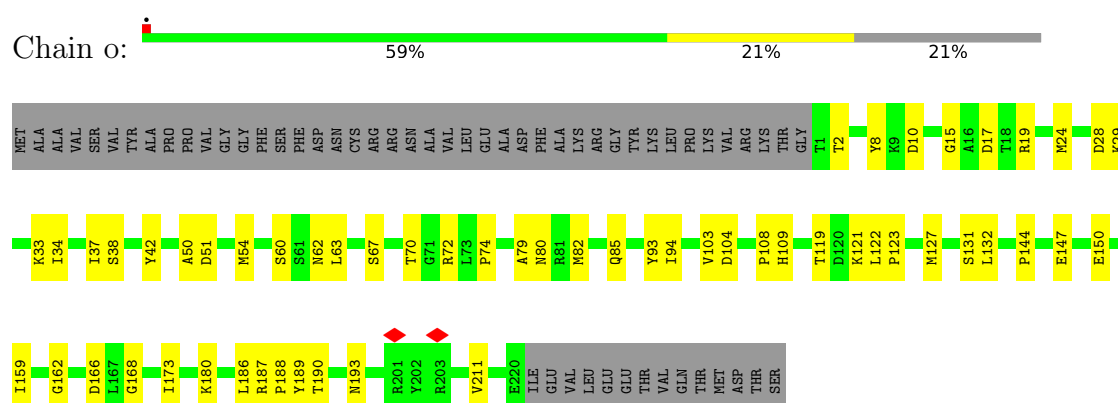
- Molecule 7: Proteasome subunit beta type-6



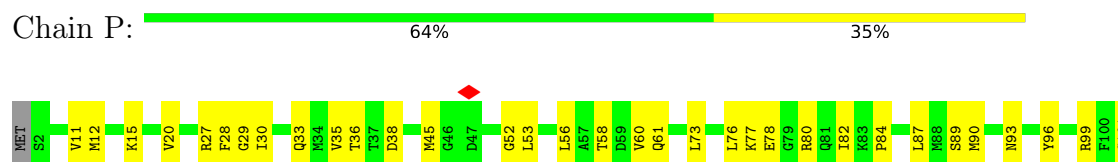
- Molecule 8: Proteasome subunit beta type-7

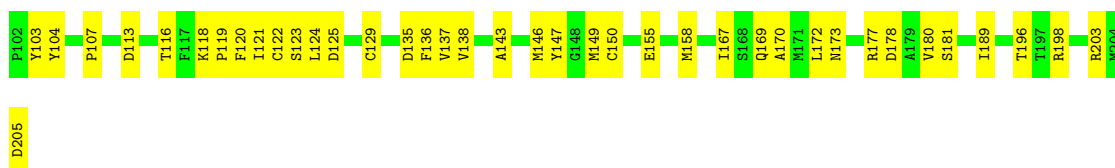


- Molecule 8: Proteasome subunit beta type-7

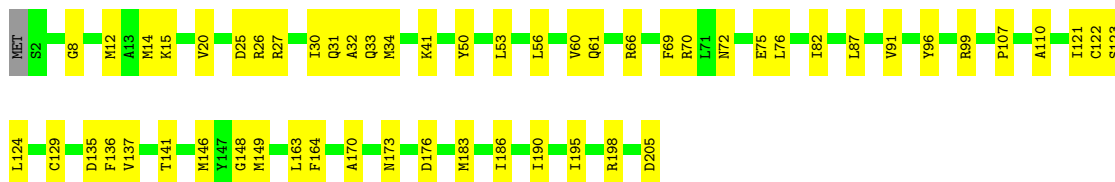


- Molecule 9: Proteasome subunit beta type-3

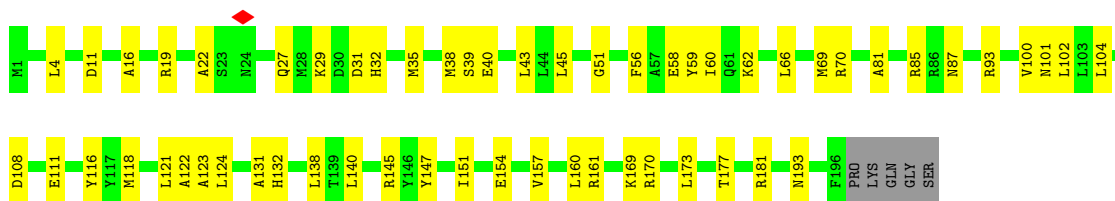




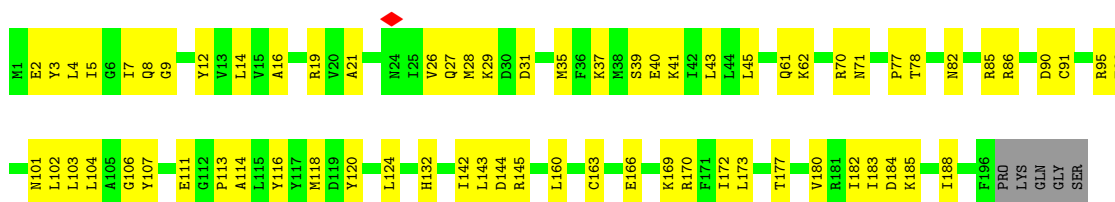
• Molecule 9: Proteasome subunit beta type-3



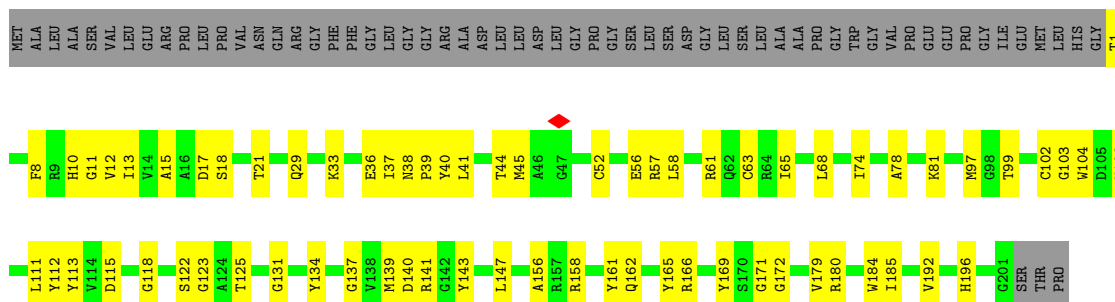
• Molecule 10: Proteasome subunit beta type-2



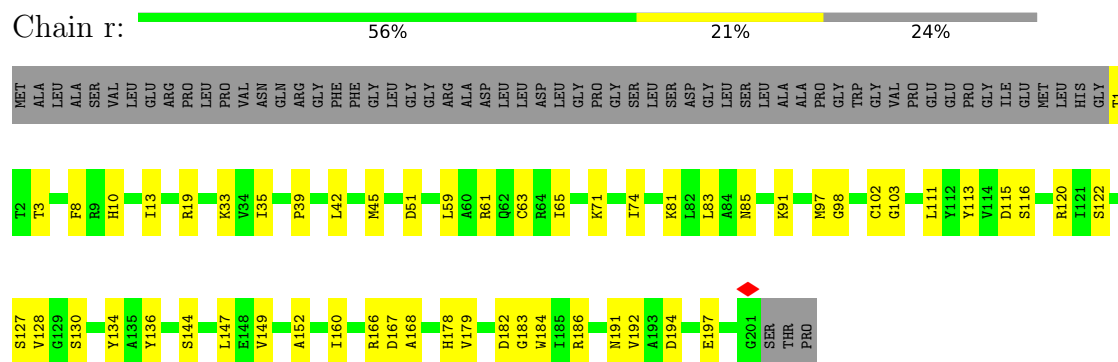
• Molecule 10: Proteasome subunit beta type-2



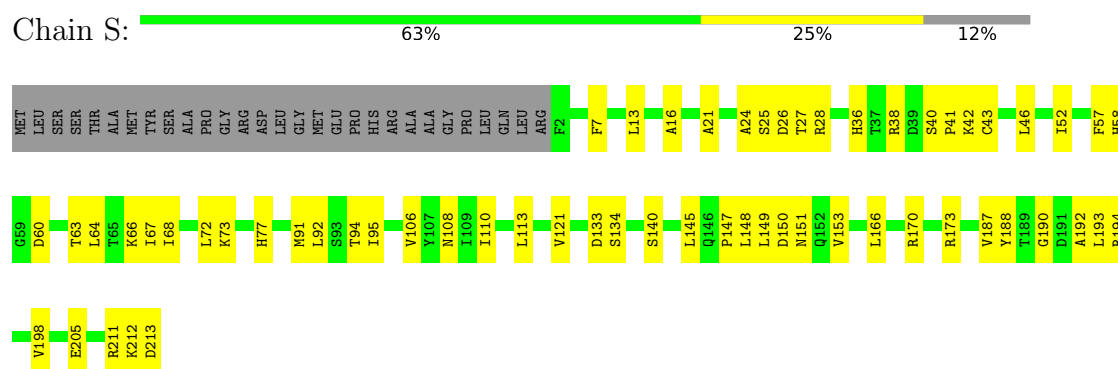
• Molecule 11: Proteasome subunit beta type-5



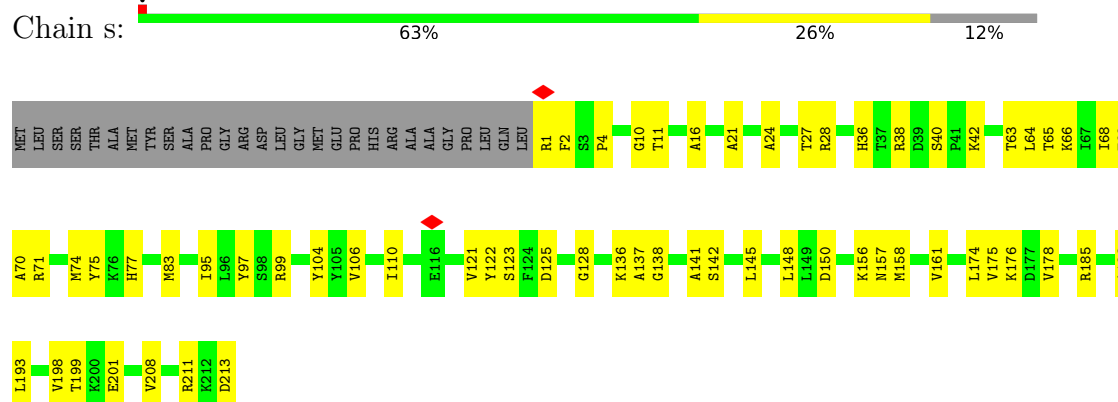
- Molecule 11: Proteasome subunit beta type-5



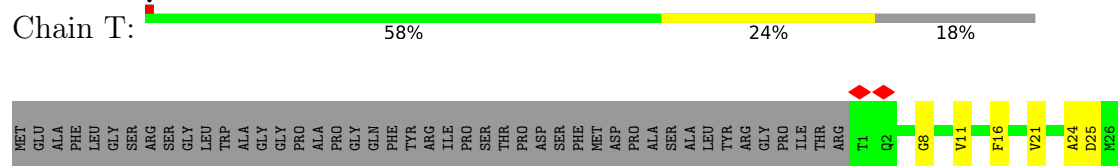
- Molecule 12: Proteasome subunit beta type-1

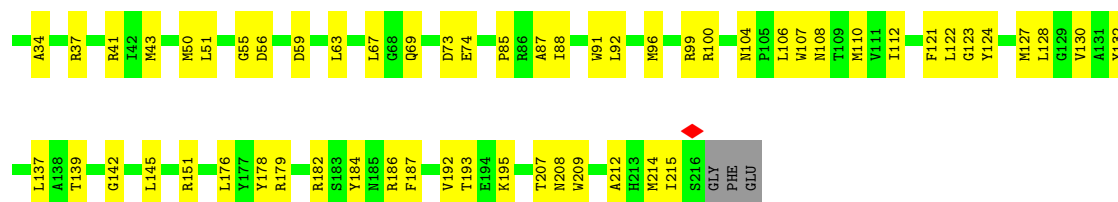


- Molecule 12: Proteasome subunit beta type-1

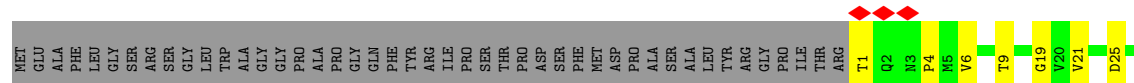


- Molecule 13: Proteasome subunit beta type-4





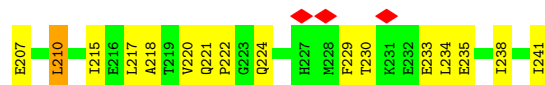
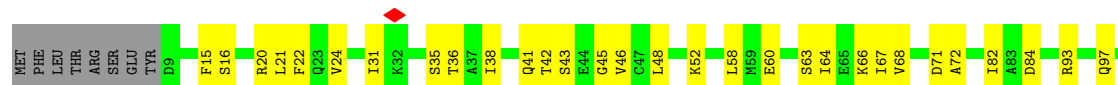
• Molecule 13: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit alpha type-5

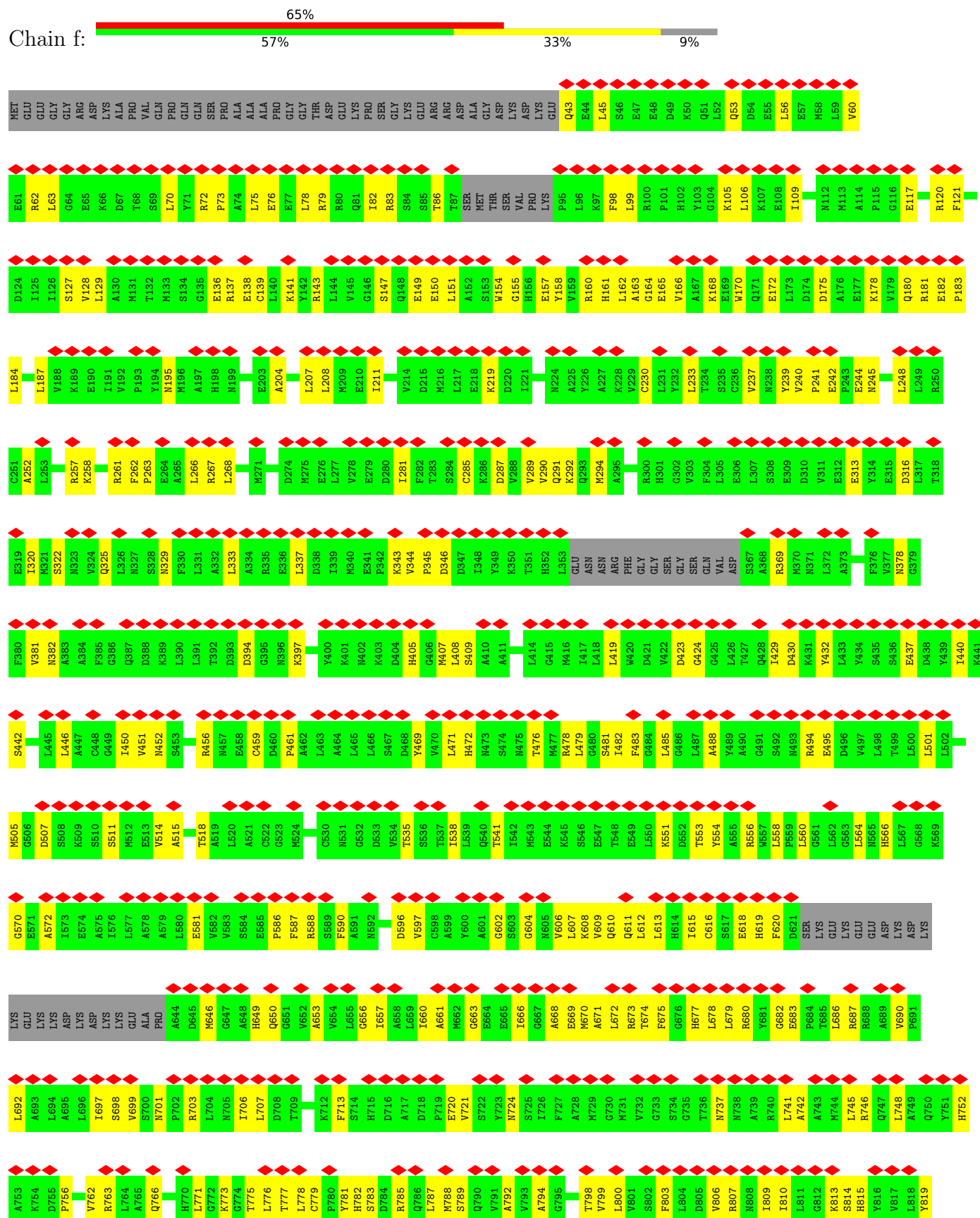


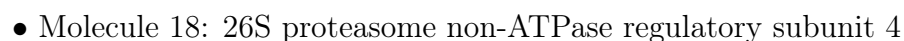
• Molecule 14: Proteasome subunit alpha type-5

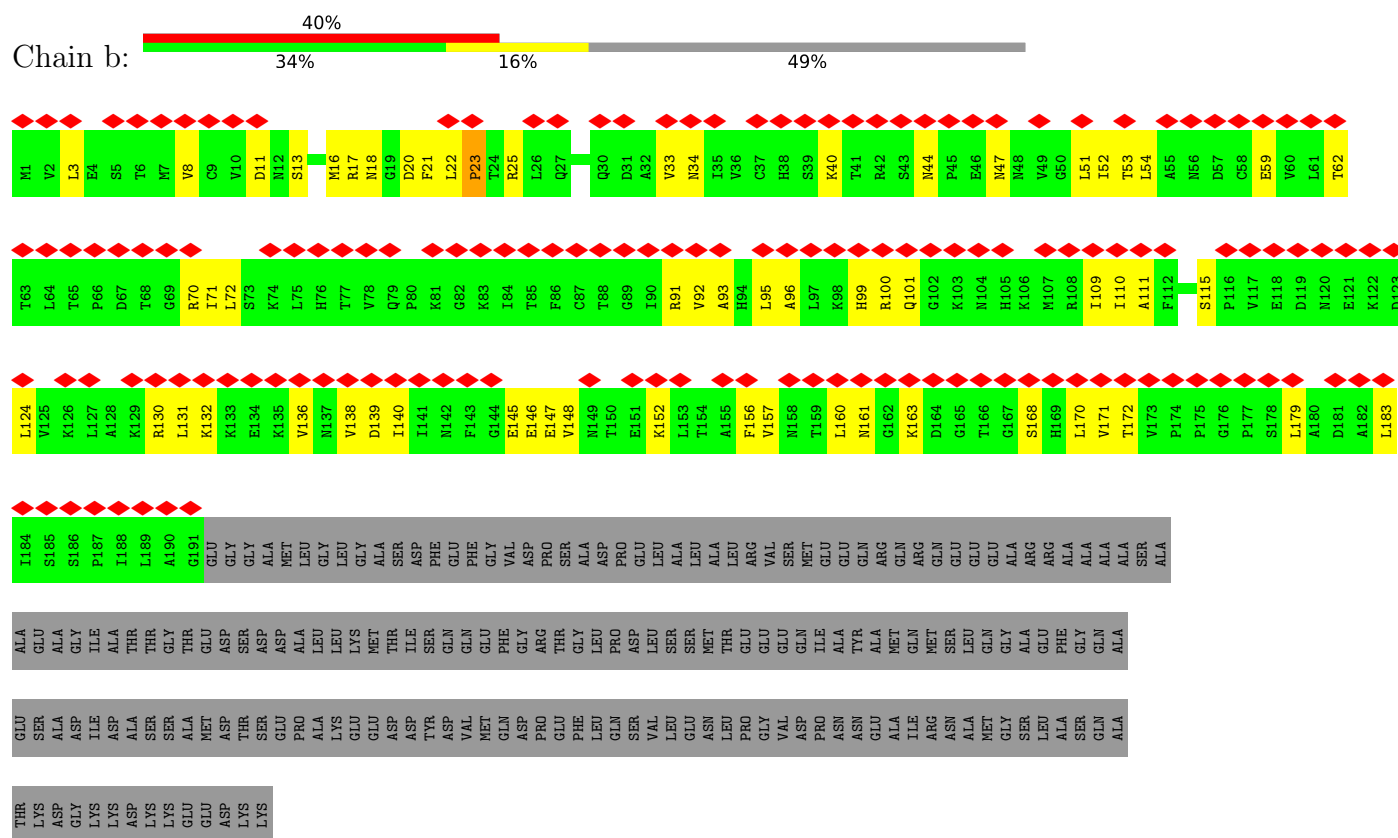


• Molecule 15: 26S proteasome non-ATPase regulatory subunit 2

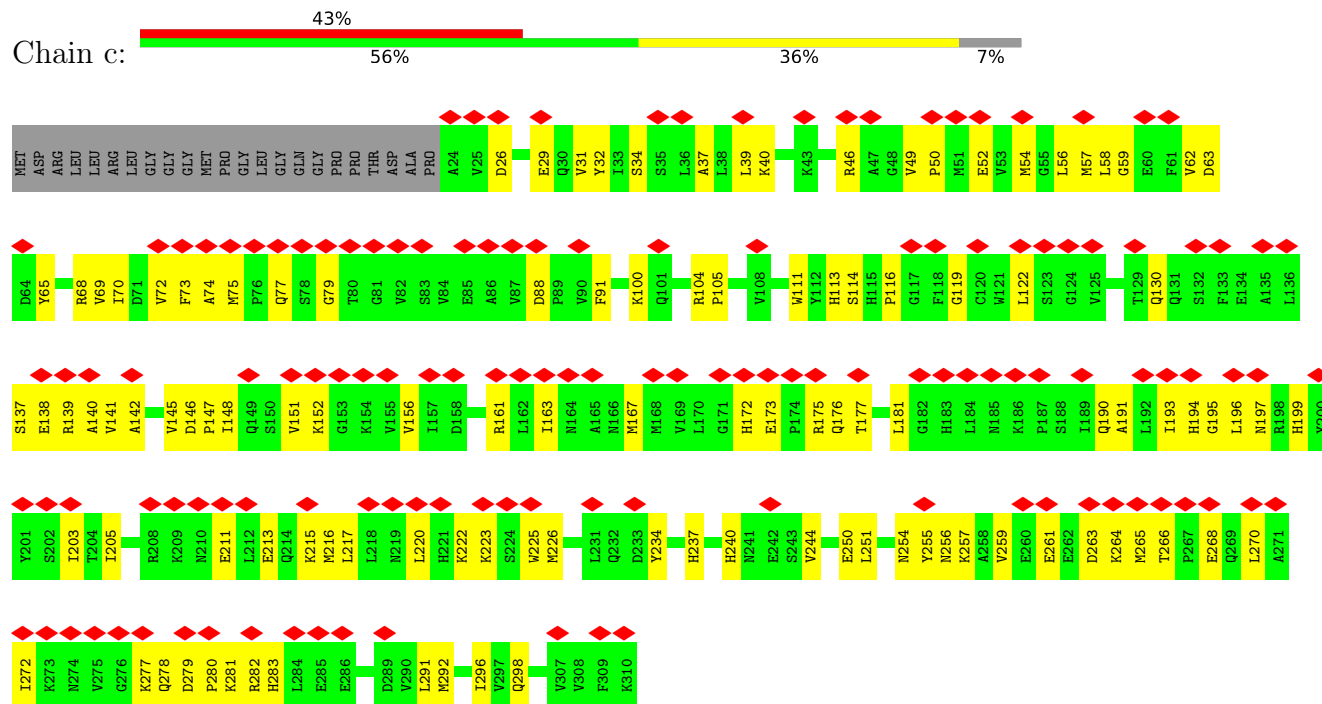
Chain f:





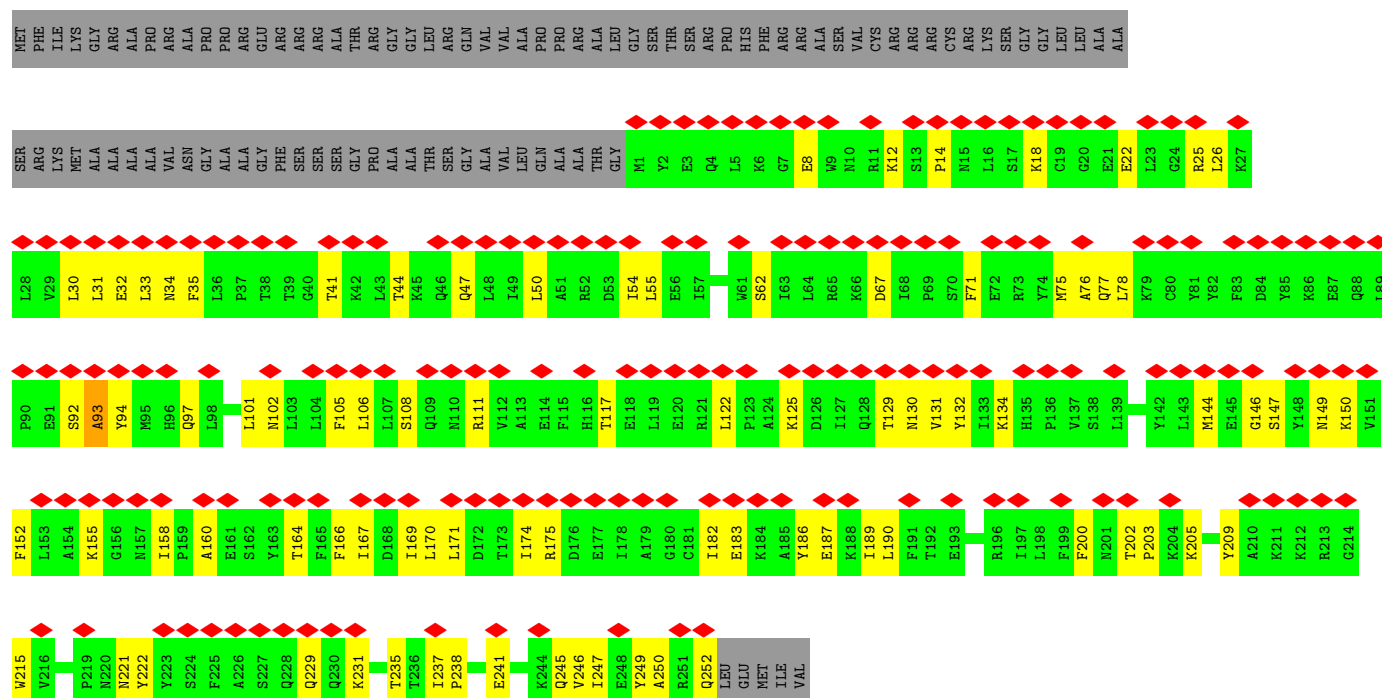


- Molecule 19: 26S proteasome non-ATPase regulatory subunit 14

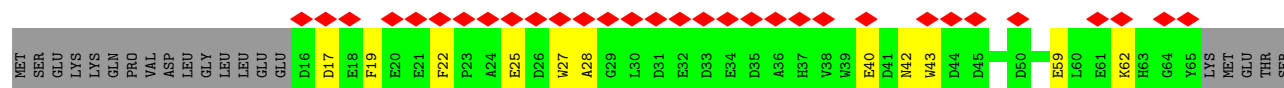
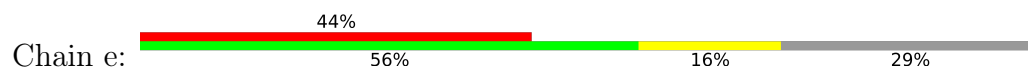


- Molecule 20: 26S proteasome non-ATPase regulatory subunit 8

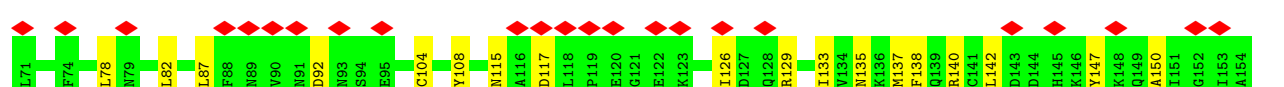
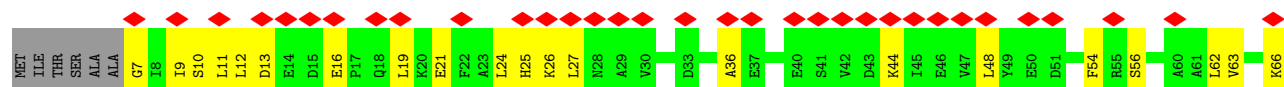


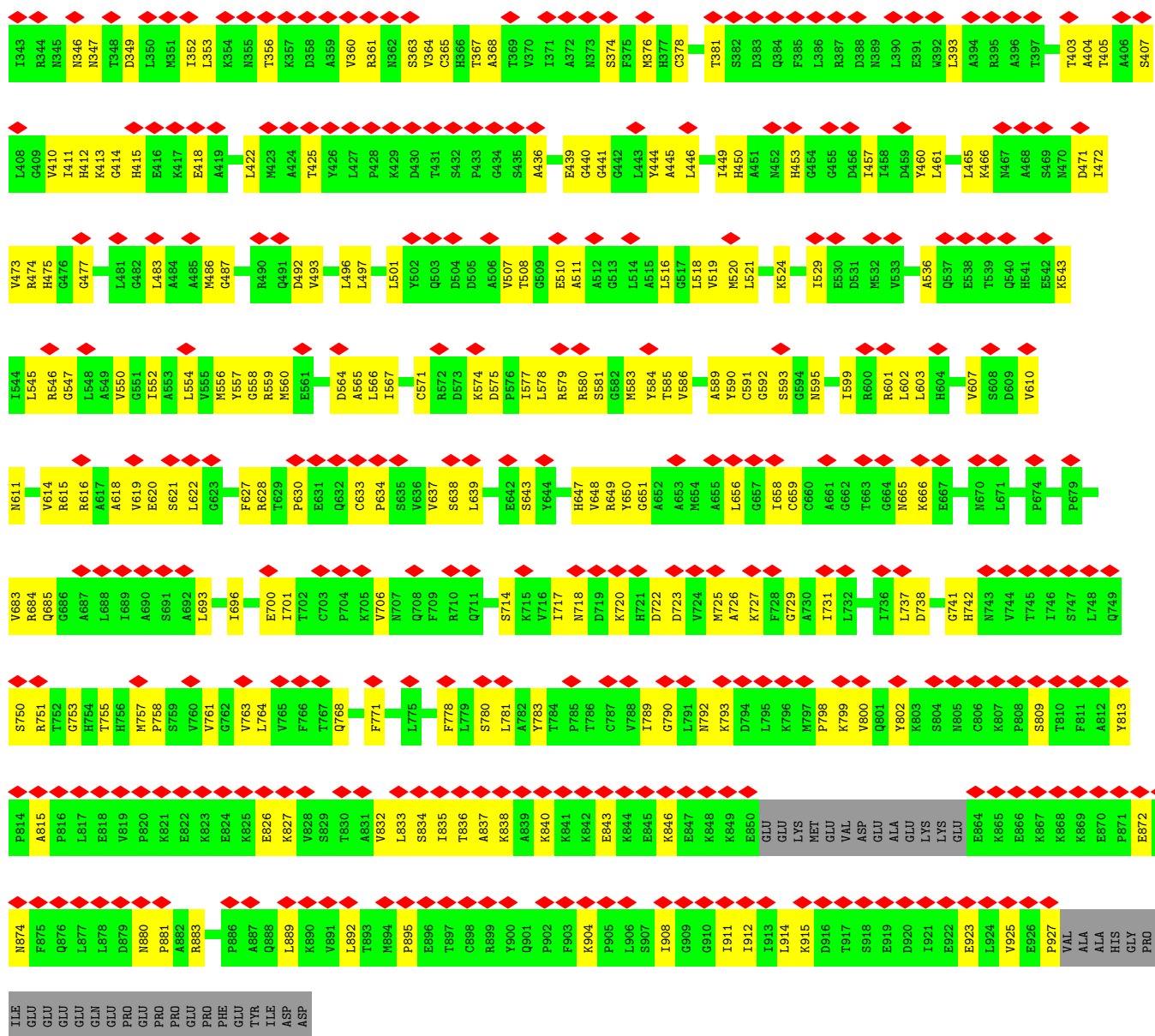


• Molecule 21: 26S proteasome complex subunit SEM1

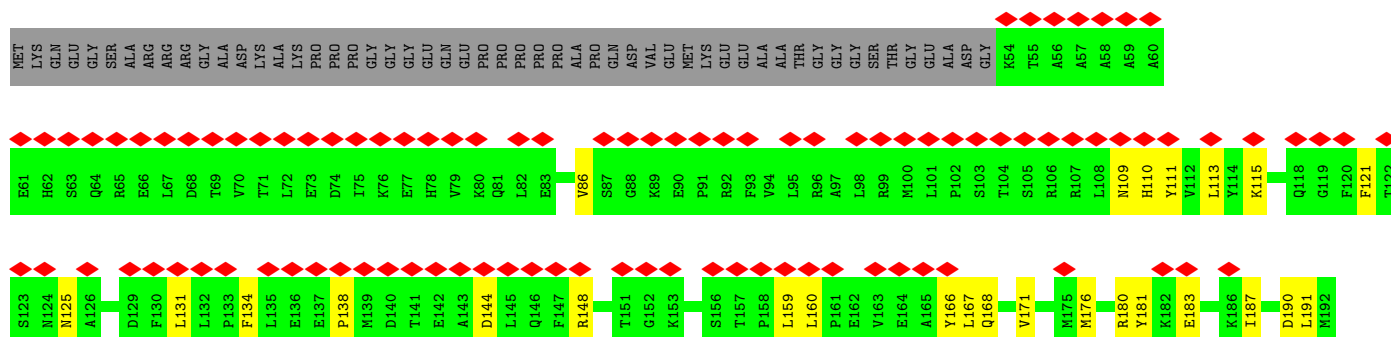
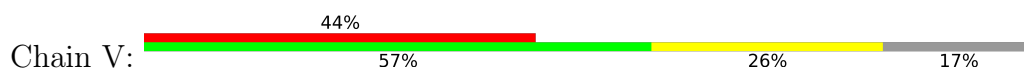


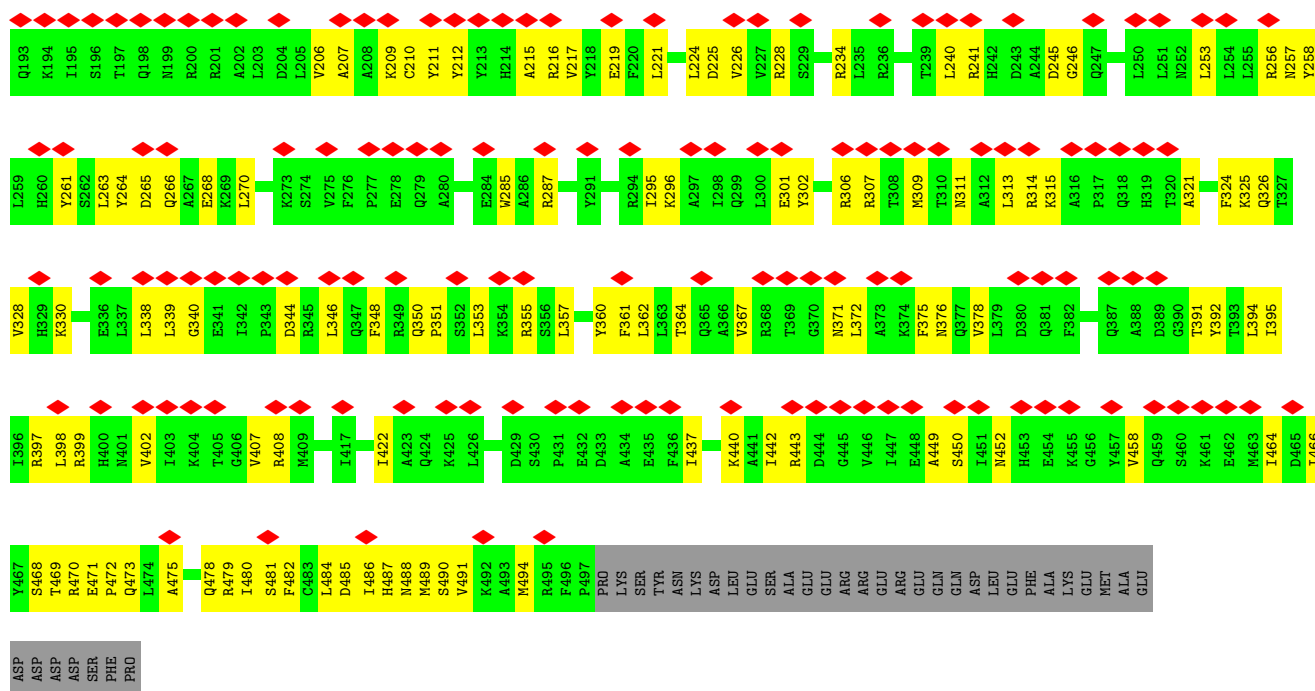
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1



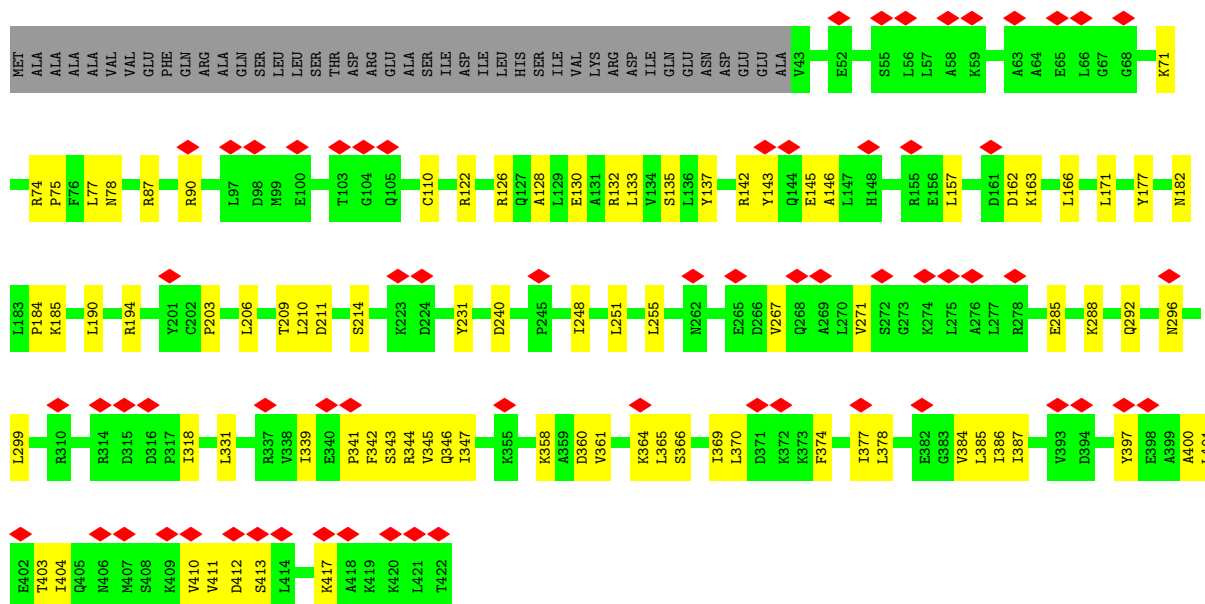


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 3

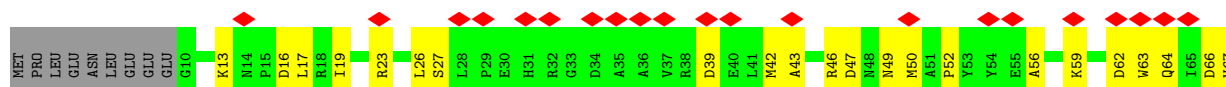


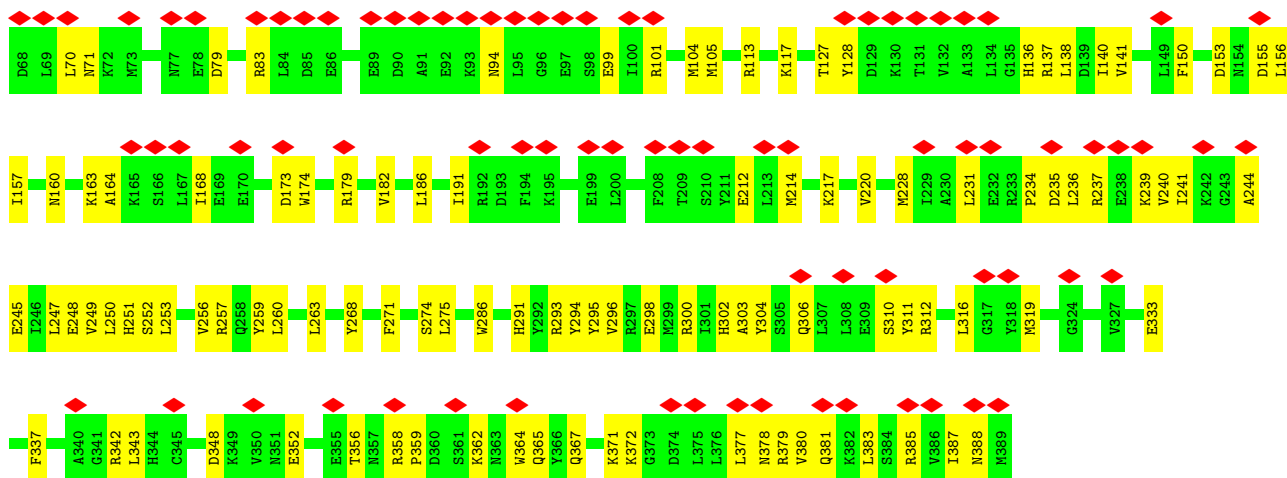


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

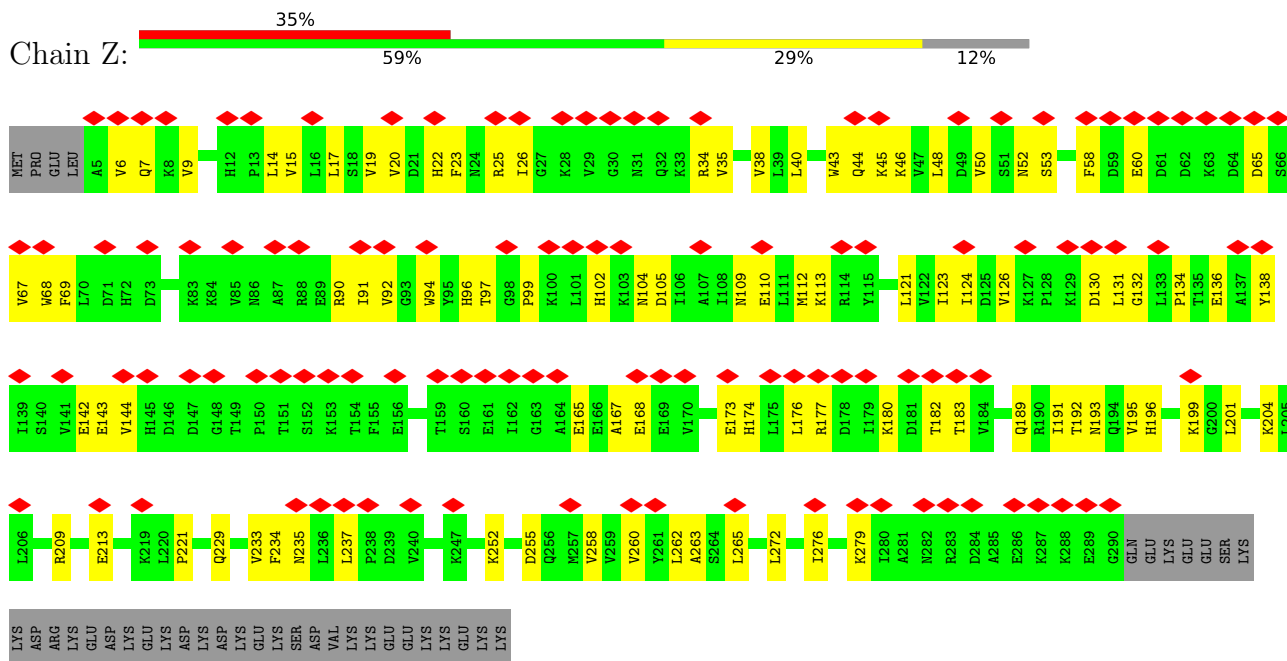


• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

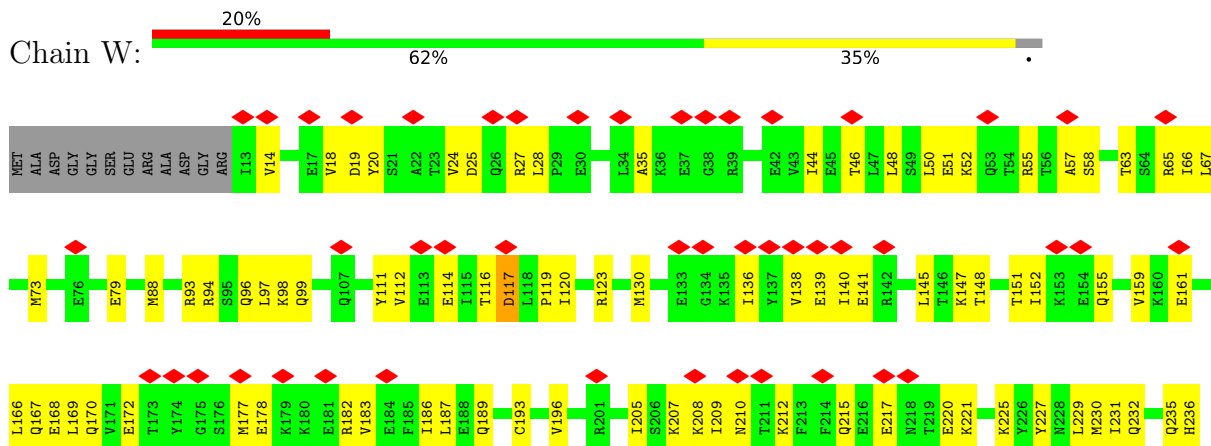


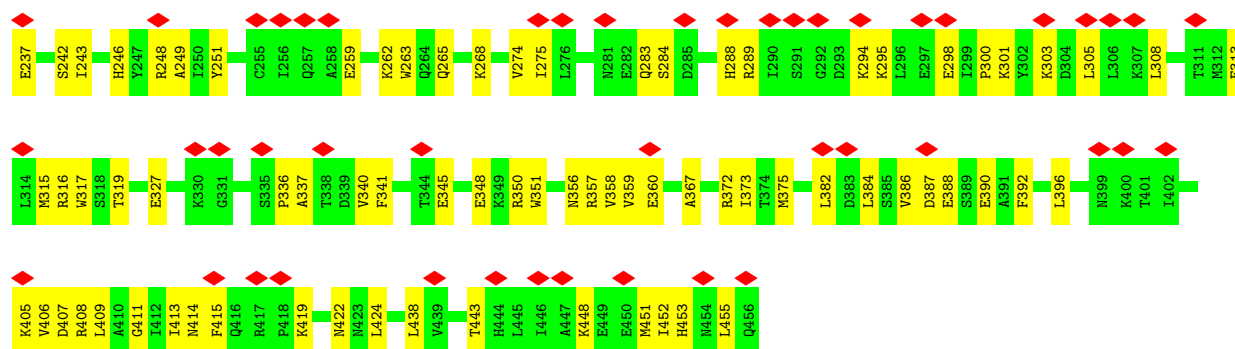


• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7



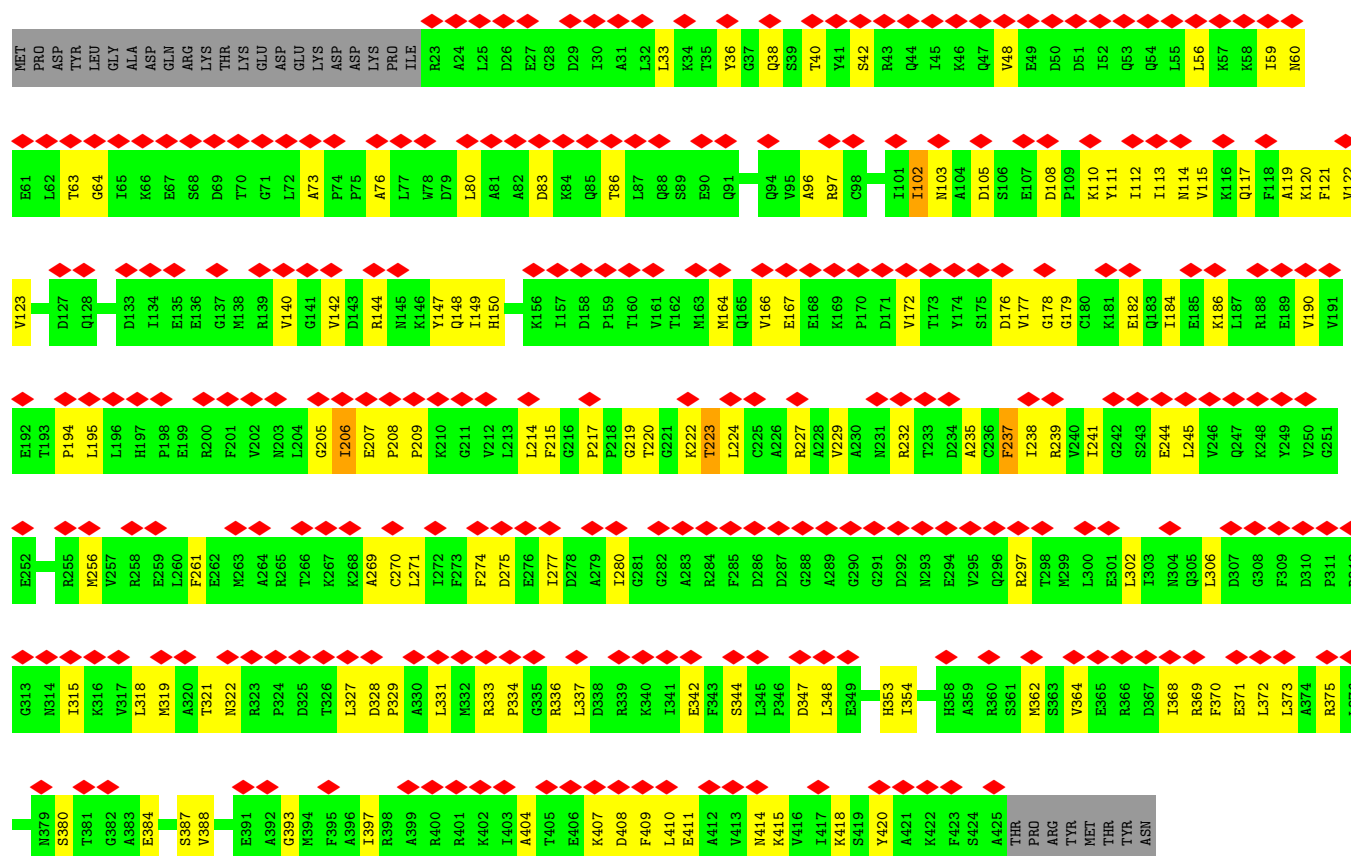
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 12





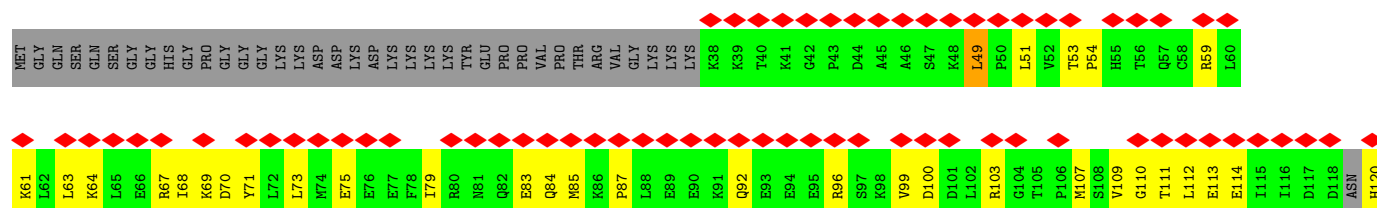
• Molecule 28: 26S protease regulatory subunit 7

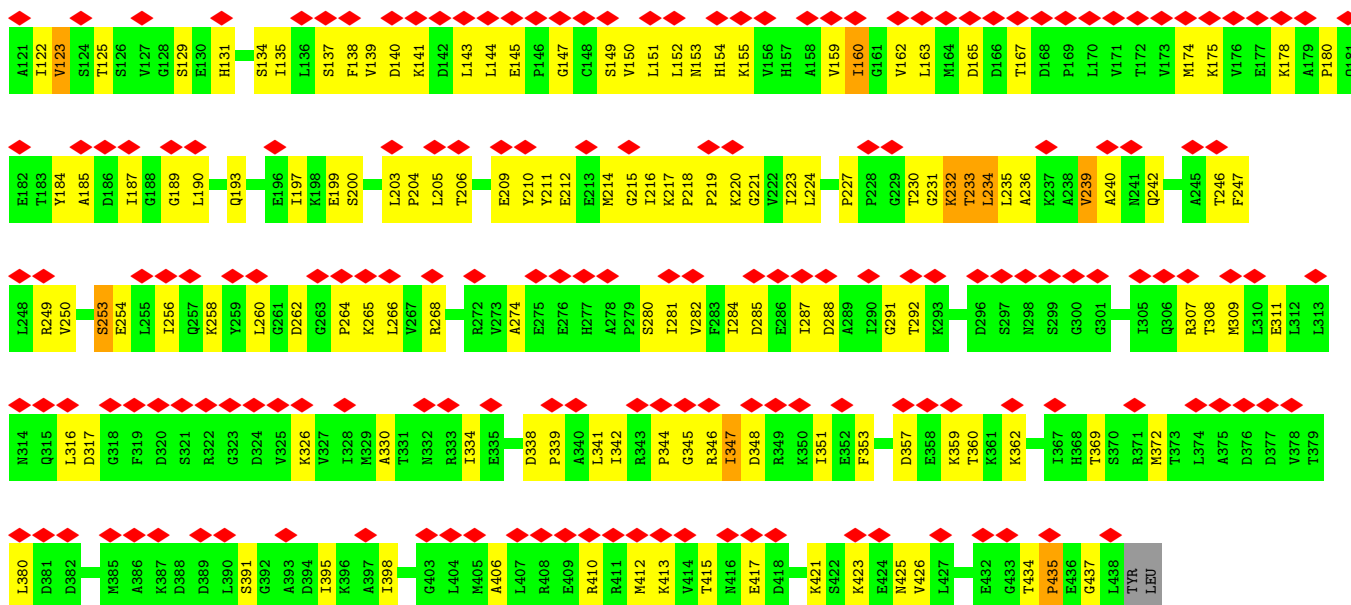
Chain A: 62% 62% 30% 7%



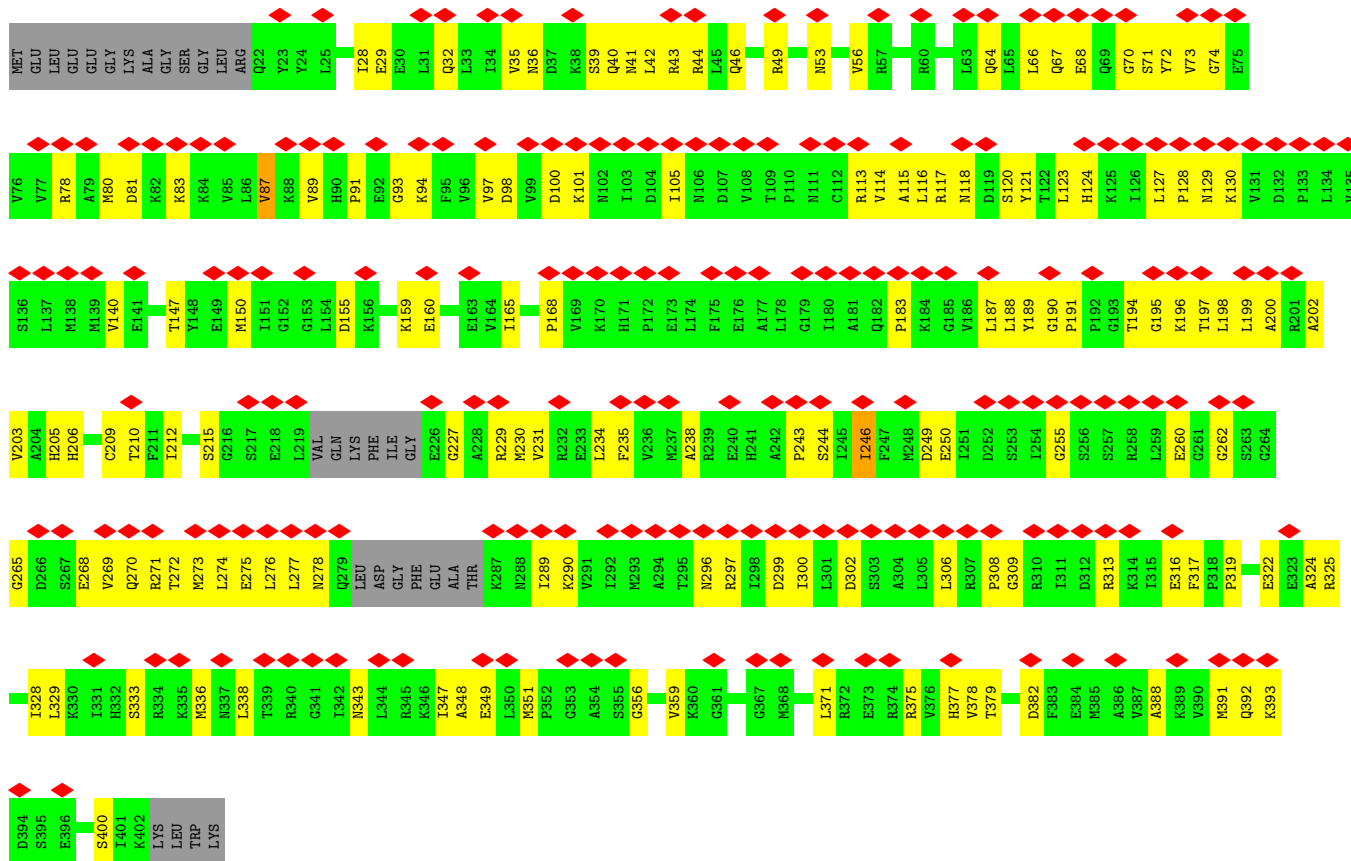
• Molecule 29: 26S protease regulatory subunit 4

Chain B: 55% 52% 37% 9%

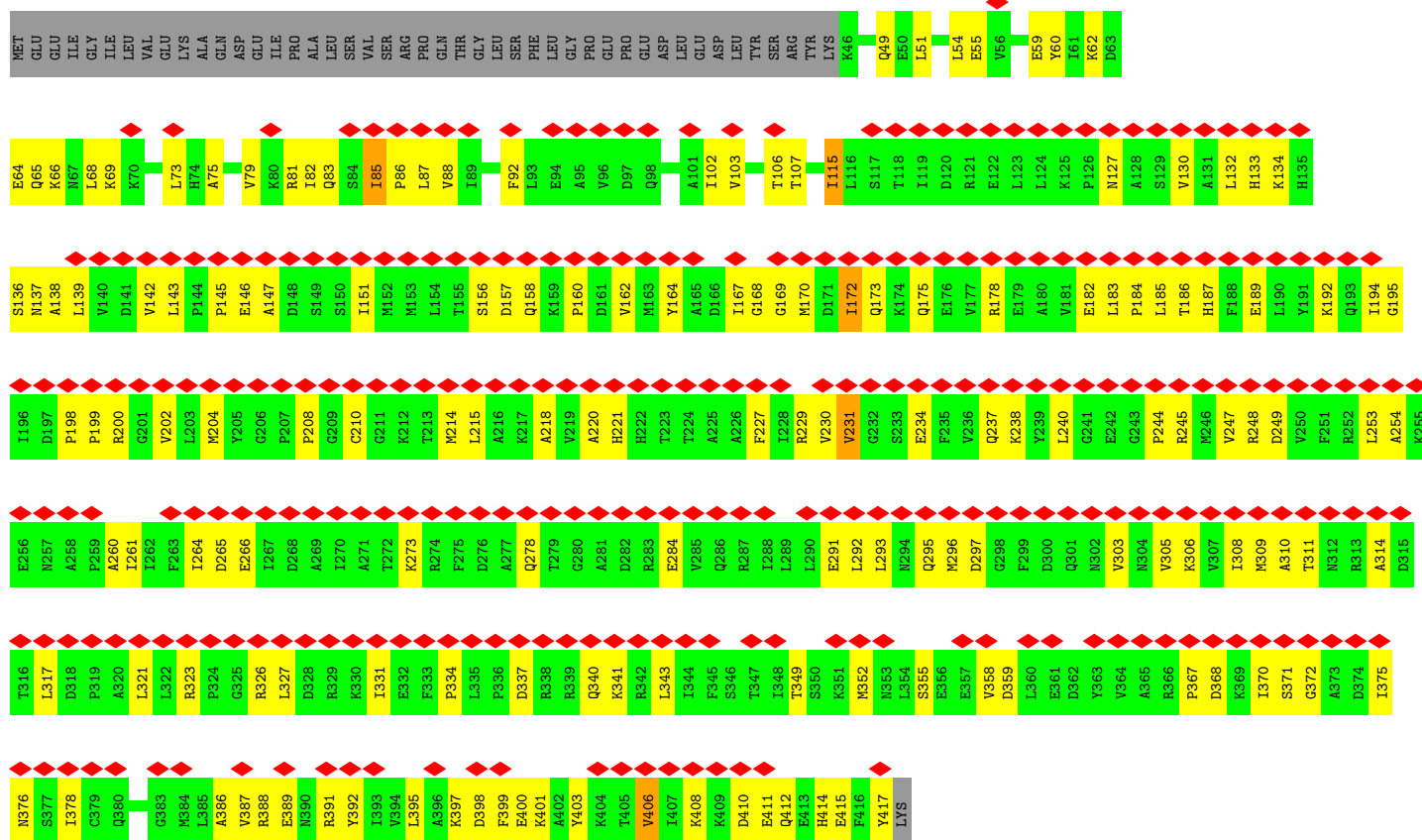




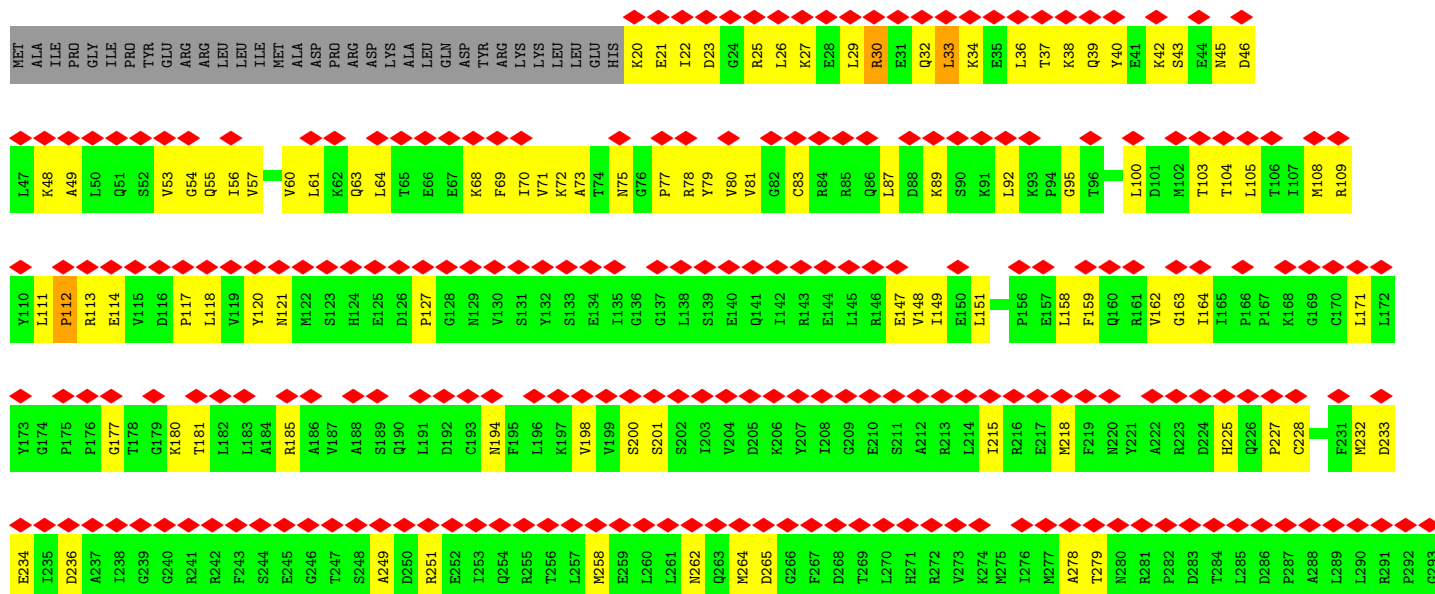
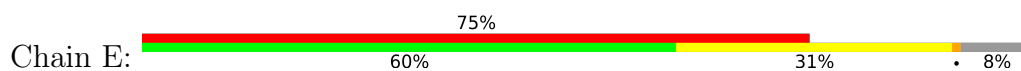
- Molecule 30: Isoform 2 of 26S proteasome regulatory subunit 8



- Molecule 31: 26S protease regulatory subunit 6B

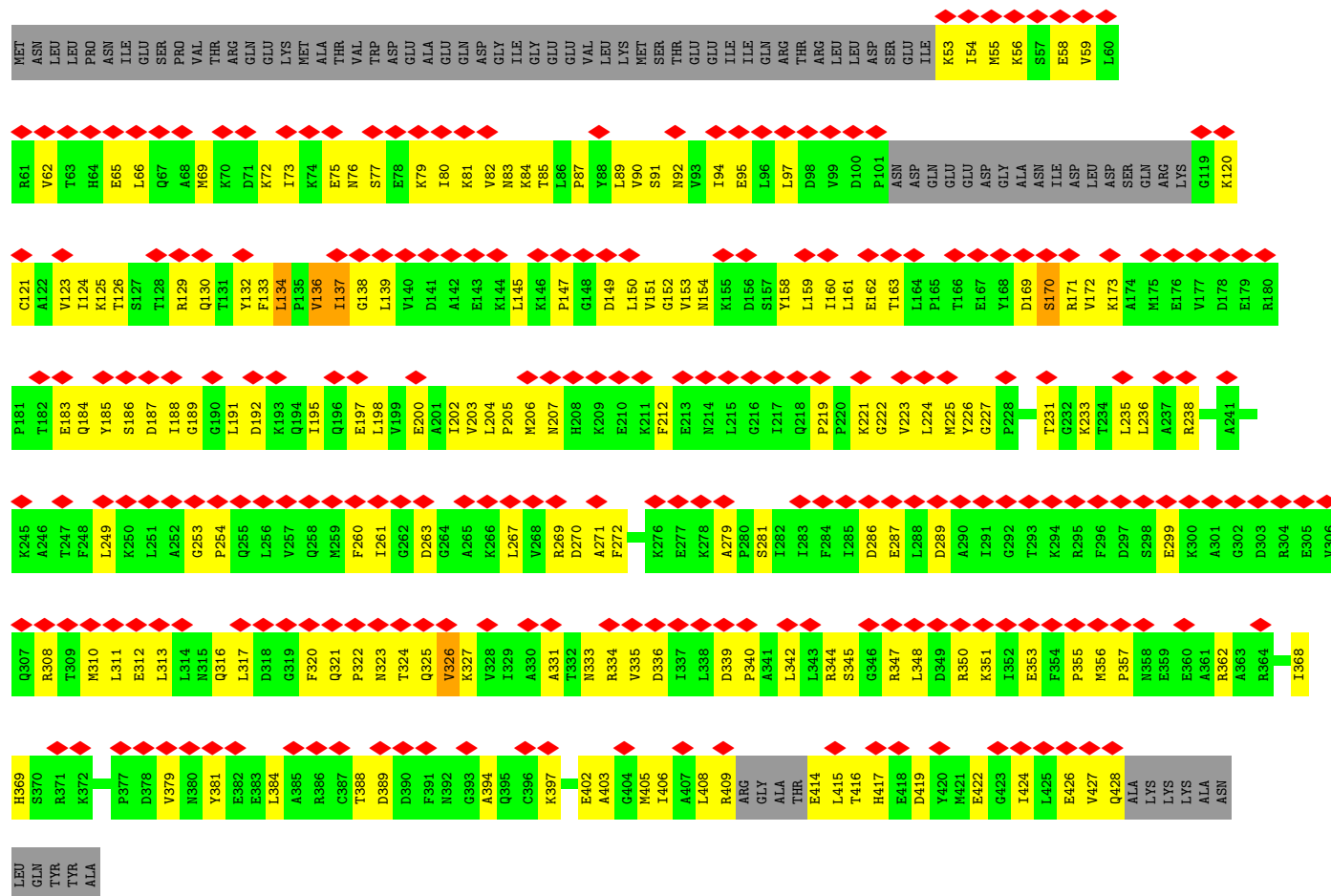
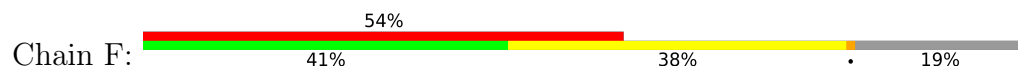


• Molecule 32: 26S proteasome regulatory subunit 10B





• Molecule 33: 26S protease regulatory subunit 6A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16466	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.168	Depositor
Minimum map value	-1.072	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	423.99002, 423.99002, 423.99002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4133, 1.4133, 1.4133	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.10	0/1873	0.31	0/2533
1	g	0.11	0/1918	0.33	0/2592
2	H	0.13	0/1784	0.36	0/2416
2	h	0.10	0/1852	0.30	0/2507
3	I	0.10	0/1962	0.29	0/2644
3	i	0.11	0/2001	0.32	0/2694
4	J	0.12	0/1894	0.37	0/2555
4	j	0.10	0/1904	0.28	0/2569
5	L	0.11	0/1899	0.29	0/2567
5	l	0.10	0/1899	0.29	0/2567
6	M	0.12	0/1897	0.32	0/2555
6	m	0.12	0/1916	0.32	0/2580
7	N	0.10	0/1548	0.26	0/2097
7	n	0.10	0/1540	0.29	0/2085
8	O	0.11	0/1686	0.30	0/2282
8	o	0.11	0/1686	0.28	0/2282
9	P	0.10	0/1620	0.29	0/2184
9	p	0.11	0/1620	0.28	0/2184
10	Q	0.12	0/1603	0.33	0/2168
10	q	0.11	0/1603	0.30	0/2168
11	R	0.09	0/1590	0.26	0/2147
11	r	0.10	0/1590	0.25	0/2147
12	S	0.12	0/1673	0.34	0/2254
12	s	0.11	0/1684	0.30	0/2268
13	T	0.09	0/1720	0.25	0/2328
13	t	0.10	0/1720	0.28	0/2328
14	K	0.10	0/1718	0.31	0/2319
14	k	0.09	0/1817	0.26	0/2455
15	f	0.11	0/6385	0.32	0/8637
16	x	0.07	0/643	0.26	0/868
17	a	0.10	0/3023	0.30	0/4093
18	b	0.10	0/1478	0.34	0/2001

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	c	0.11	0/2260	0.37	0/3052
20	d	0.10	0/2109	0.32	0/2851
21	e	0.08	0/415	0.31	0/563
22	U	0.10	0/6750	0.30	0/9116
23	V	0.10	0/3667	0.27	0/4951
24	X	0.09	0/3045	0.26	0/4104
25	Y	0.11	0/3063	0.31	0/4123
26	Z	0.10	0/2286	0.31	0/3099
27	W	0.11	0/3610	0.33	0/4853
28	A	0.12	0/3165	0.34	0/4273
29	B	0.15	0/3100	0.47	2/4189 (0.0%)
30	C	0.12	0/2865	0.37	0/3851
31	D	0.16	0/2932	0.43	1/3962 (0.0%)
32	E	0.16	0/2974	0.41	1/4006 (0.0%)
33	F	0.15	0/2731	0.40	0/3688
All	All	0.11	0/105718	0.32	4/142755 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	233	THR	N-CA-C	-13.79	95.88	113.12
29	B	234	LEU	N-CA-C	-9.59	100.68	112.38
32	E	344	ARG	CB-CG-CD	5.67	124.34	111.30
31	D	186	THR	CB-CA-C	-5.53	110.18	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1841	0	1848	56	0
1	g	1885	0	1891	66	0
2	H	1749	0	1750	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	1813	0	1806	56	0
3	I	1933	0	1947	49	0
3	i	1971	0	1992	66	0
4	J	1869	0	1891	76	0
4	j	1878	0	1899	52	0
5	L	1864	0	1852	48	0
5	l	1864	0	1852	66	0
6	M	1862	0	1842	59	0
6	m	1881	0	1868	71	0
7	N	1521	0	1494	53	0
7	n	1514	0	1487	55	0
8	O	1659	0	1681	39	0
8	o	1659	0	1681	41	0
9	P	1591	0	1609	72	0
9	p	1591	0	1609	46	0
10	Q	1571	0	1573	70	0
10	q	1571	0	1573	60	0
11	R	1559	0	1523	53	0
11	r	1559	0	1523	46	0
12	S	1643	0	1640	49	0
12	s	1654	0	1656	47	0
13	T	1687	0	1666	48	0
13	t	1687	0	1666	67	0
14	K	1694	0	1691	57	0
14	k	1789	0	1773	53	0
15	f	6292	0	6314	236	0
16	x	635	0	652	16	0
17	a	2969	0	2984	88	0
18	b	1458	0	1505	52	0
19	c	2224	0	2240	103	0
20	d	2063	0	2078	71	0
21	e	407	0	312	15	0
22	U	6648	0	6715	256	0
23	V	3600	0	3668	121	0
24	X	3002	0	3106	68	0
25	Y	3021	0	3022	104	0
26	Z	2248	0	2277	96	0
27	W	3570	0	3696	128	0
28	A	3119	0	3162	105	0
29	B	3060	0	3090	156	0
30	C	2839	0	2942	153	0
31	D	2893	0	2913	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	E	2929	0	2994	168	0
33	F	2699	0	2743	208	0
34	A	31	0	12	1	0
35	B	27	0	12	5	0
35	C	27	0	12	6	0
35	D	27	0	12	4	0
35	E	27	0	12	1	0
35	F	27	0	12	4	0
All	All	104201	0	104768	3369	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 (3369) 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)
22:U:607:VAL:HB	31:D:68:LEU:CD2	1.37	1.50
22:U:607:VAL:CB	31:D:68:LEU:HD21	1.40	1.48
30:C:56:VAL:CG2	31:D:79:VAL:HG21	1.51	1.40
30:C:56:VAL:HG21	31:D:79:VAL:CG2	1.57	1.30
6:M:41:CYS:SG	6:M:189:ILE:CB	2.32	1.18
22:U:599:ILE:HG22	31:D:60:TYR:OH	1.48	1.14
6:M:41:CYS:SG	6:M:189:ILE:HG13	1.89	1.10
10:Q:85:ARG:HD2	10:Q:124:LEU:HB2	1.37	1.07
6:M:41:CYS:SG	6:M:189:ILE:HG21	1.96	1.06
6:M:41:CYS:SG	6:M:189:ILE:CG1	2.43	1.05
9:P:58:THR:HA	10:Q:85:ARG:HH21	1.20	1.04
22:U:607:VAL:HB	31:D:68:LEU:CG	1.88	1.03
6:M:41:CYS:SG	6:M:189:ILE:HB	1.97	1.03
6:M:186:CYS:SG	6:M:219:LEU:HD13	1.99	1.02
30:C:42:LEU:HD13	31:D:62:LYS:HG3	1.44	0.99
6:M:41:CYS:SG	6:M:189:ILE:CG2	2.51	0.98
30:C:42:LEU:HD11	31:D:62:LYS:NZ	1.78	0.98
22:U:633:CYS:SG	22:U:634:PRO:HD3	2.03	0.97
30:C:42:LEU:HD11	31:D:62:LYS:HZ3	1.30	0.96
32:E:33:LEU:HA	32:E:36:LEU:HB3	1.45	0.96
22:U:607:VAL:CG1	31:D:68:LEU:HD11	1.97	0.94
32:E:118:LEU:HD22	33:F:147:PRO:HB2	1.51	0.91
32:E:114:GLU:HG2	33:F:94:ILE:HG22	1.53	0.91
15:f:803:PHE:HA	15:f:806:VAL:HG13	1.53	0.90
22:U:607:VAL:CA	31:D:68:LEU:HD21	2.01	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:85:ILE:HG21	32:E:105:LEU:HD11	1.56	0.88
2:H:71:HIS:HB2	2:H:107:THR:HG21	1.56	0.87
31:D:85:ILE:HG12	31:D:86:PRO:HD2	1.57	0.86
31:D:391:ARG:HG2	31:D:392:TYR:H	1.39	0.86
32:E:26:LEU:HD12	33:F:55:MET:HA	1.57	0.86
10:Q:140:LEU:HD13	11:r:166:ARG:HH21	1.41	0.85
11:R:158:ARG:HE	10:q:145:ARG:HG2	1.42	0.84
33:F:408:LEU:HD12	33:F:409:ARG:H	1.42	0.84
29:B:59:ARG:HH12	29:B:63:LEU:HB2	1.40	0.84
22:U:630:PRO:O	22:U:633:CYS:SG	2.35	0.83
1:G:88:ARG:HG3	6:M:156:VAL:HG21	1.59	0.83
22:U:521:LEU:HD13	22:U:554:LEU:HD12	1.61	0.83
32:E:341:ALA:HB1	33:F:344:ARG:HG3	1.60	0.83
32:E:341:ALA:HB2	33:F:344:ARG:CZ	2.09	0.82
31:D:264:ILE:HB	31:D:309:MET:HG3	1.60	0.82
20:d:122:LEU:HB3	20:d:125:LYS:HB3	1.62	0.82
28:A:140:VAL:HG11	28:A:149:ILE:HG23	1.61	0.82
10:Q:85:ARG:HD2	10:Q:124:LEU:CB	2.10	0.82
13:T:63:LEU:HD21	13:T:106:LEU:HD13	1.61	0.81
26:Z:252:LYS:HG3	26:Z:255:ASP:HB2	1.62	0.81
16:x:82:LEU:HD11	16:x:89:LEU:HD21	1.61	0.81
33:F:381:TYR:HA	33:F:384:LEU:HD13	1.62	0.81
22:U:554:LEU:HD13	22:U:761:VAL:HG21	1.63	0.80
32:E:54:GLY:HA3	33:F:158:TYR:HD2	1.45	0.80
26:Z:173:GLU:O	26:Z:177:ARG:HG3	1.81	0.80
32:E:112:PRO:O	32:E:113:ARG:HG3	1.81	0.80
4:J:88:ARG:HH11	10:Q:70:ARG:HA	1.46	0.80
14:k:13:ASN:HB3	5:l:126:ARG:HB3	1.64	0.80
32:E:177:GLY:HA3	33:F:344:ARG:HH22	1.45	0.80
28:A:373:LEU:HG	28:A:415:LYS:HE3	1.64	0.80
22:U:583:MET:HE3	22:U:618:ALA:HA	1.63	0.80
22:U:685:GLN:HB2	22:U:729:GLY:HA3	1.62	0.79
30:C:46:GLN:HG3	31:D:65:GLN:O	1.82	0.79
9:P:58:THR:HA	10:Q:85:ARG:NH2	1.96	0.79
19:c:141:VAL:HG12	19:c:161:ARG:HE	1.47	0.79
33:F:154:ASN:HB2	33:F:159:LEU:H	1.47	0.79
32:E:303:LEU:HD21	32:E:337:GLY:HA2	1.65	0.79
23:V:353:LEU:HB3	23:V:357:LEU:HD23	1.65	0.79
32:E:25:ARG:HG2	33:F:55:MET:HE3	1.65	0.78
28:A:33:LEU:HA	28:A:36:TYR:HB2	1.63	0.78
32:E:46:ASP:HB2	33:F:76:ASN:HD21	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:s:27:THR:HB	12:s:40:SER:H	1.47	0.78
19:c:211:GLU:HB3	19:c:215:LYS:HE3	1.66	0.78
5:L:13:TRP:HA	5:L:19:ILE:HG22	1.65	0.78
23:V:302:TYR:HB3	23:V:339:LEU:HD21	1.65	0.78
31:D:143:LEU:HG	31:D:145:PRO:HD2	1.65	0.78
4:J:81:ARG:HA	4:J:84:ILE:HD12	1.66	0.77
3:i:2:SER:N	5:l:123:TYR:HH	1.82	0.77
29:B:234:LEU:HD13	29:B:330:ALA:HB1	1.66	0.77
25:Y:101:ARG:NH1	25:Y:105:MET:SD	2.56	0.77
15:f:43:GLN:HE22	15:f:45:LEU:HD21	1.47	0.77
30:C:42:LEU:CD1	31:D:62:LYS:HG3	2.15	0.77
4:J:40:ILE:HD11	4:J:210:VAL:HG13	1.67	0.77
1:g:52:THR:HG21	1:g:79:VAL:HG21	1.65	0.77
31:D:376:ASN:ND2	35:D:501:ADP:N3	2.32	0.77
32:E:33:LEU:HD12	32:E:34:LYS:H	1.48	0.77
6:M:186:CYS:SG	6:M:219:LEU:CD1	2.73	0.77
32:E:177:GLY:CA	33:F:344:ARG:HH22	1.97	0.77
33:F:134:LEU:HB2	33:F:159:LEU:HD12	1.65	0.77
19:c:62:VAL:O	19:c:63:ASP:OD1	2.02	0.76
22:U:880:ASN:OD1	22:U:881:PRO:HD3	1.86	0.76
30:C:56:VAL:HG23	31:D:79:VAL:HG11	1.66	0.76
12:S:211:ARG:HB3	8:o:193:ASN:HD21	1.49	0.76
28:A:110:LYS:HE3	33:F:85:THR:OG1	1.85	0.76
28:A:102:ILE:HA	28:A:113:ILE:HG23	1.68	0.76
33:F:59:VAL:HA	33:F:62:VAL:HB	1.67	0.76
33:F:81:LYS:HA	33:F:84:LYS:HB3	1.67	0.76
6:M:41:CYS:SG	6:M:186:CYS:HA	2.26	0.76
6:M:47:PHE:HB2	6:M:214:SER:HB3	1.68	0.76
24:X:182:ASN:HD21	25:Y:248:GLU:HB2	1.51	0.75
5:l:125:ARG:HH21	5:l:126:ARG:HG2	1.51	0.75
26:Z:174:HIS:HA	26:Z:177:ARG:HD2	1.68	0.75
22:U:610:VAL:HA	22:U:615:ARG:HE	1.49	0.75
23:V:399:ARG:HH21	23:V:402:VAL:HG11	1.52	0.75
30:C:39:SER:HB3	31:D:62:LYS:HB2	1.68	0.75
14:K:230:THR:HG22	14:K:233:GLU:HB2	1.69	0.75
32:E:27:LYS:HA	32:E:30:ARG:HE	1.50	0.75
23:V:215:ALA:HB3	23:V:253:LEU:HD22	1.68	0.75
27:W:51:GLU:OE1	27:W:55:ARG:NH1	2.20	0.75
26:Z:99:PRO:HA	26:Z:123:ILE:HD13	1.67	0.75
32:E:177:GLY:CA	33:F:344:ARG:NH2	2.50	0.75
15:f:408:LEU:HB3	15:f:815:HIS:HE1	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:203:PRO:HG2	20:d:205:LYS:HB3	1.68	0.74
33:F:81:LYS:O	33:F:85:THR:N	2.20	0.74
19:c:88:ASP:HB3	19:c:91:PHE:HB3	1.69	0.74
31:D:244:PRO:HB3	31:D:291:GLU:HG3	1.70	0.74
26:Z:34:ARG:NH1	26:Z:97:THR:O	2.21	0.74
5:l:81:ALA:HB2	5:l:130:VAL:HG21	1.70	0.74
20:d:117:THR:HG21	23:V:265:ASP:HB3	1.69	0.74
33:F:353:GLU:HG3	33:F:355:PRO:HD3	1.69	0.74
11:R:161:TYR:HH	11:R:196:HIS:HD1	1.32	0.73
32:E:37:THR:HG22	33:F:66:LEU:HA	1.69	0.73
33:F:92:ASN:HB3	33:F:125:LYS:HB3	1.70	0.73
15:f:680:ARG:HG2	28:A:64:GLY:HA3	1.68	0.73
19:c:152:LYS:HG3	31:D:83:GLN:HA	1.68	0.73
22:U:583:MET:HE1	22:U:621:SER:HB2	1.70	0.73
31:D:254:ALA:HB1	31:D:305:VAL:HG11	1.70	0.73
32:E:61:LEU:HD11	32:E:78:ARG:HE	1.51	0.73
4:J:108:THR:HG21	4:J:145:TYR:HB2	1.71	0.73
29:B:211:TYR:HA	29:B:214:MET:HB2	1.71	0.73
7:n:121:VAL:HG21	13:t:39:ILE:HG22	1.71	0.73
30:C:56:VAL:CG2	31:D:79:VAL:CG2	2.37	0.73
30:C:35:VAL:HG11	31:D:59:GLU:HA	1.70	0.73
31:D:341:LYS:NZ	31:D:368:ASP:O	2.22	0.73
28:A:48:VAL:HG22	29:B:69:LYS:HZ3	1.54	0.72
12:S:57:PHE:HD1	12:S:60:ASP:H	1.37	0.72
4:J:73:PHE:HE1	4:J:84:ILE:HD11	1.53	0.72
7:N:202:LEU:HB2	7:n:122:ARG:HH22	1.52	0.72
9:P:61:GLN:HB2	10:Q:85:ARG:NH2	2.04	0.72
9:P:147:TYR:HB3	12:s:185:ARG:HG3	1.70	0.72
25:Y:237:ARG:HA	25:Y:241:ILE:HB	1.71	0.72
28:A:56:LEU:O	28:A:60:ASN:ND2	2.22	0.72
32:E:43:SER:OG	33:F:76:ASN:HB2	1.90	0.72
9:P:169:GLN:NE2	12:s:158:MET:SD	2.63	0.72
13:T:122:LEU:HG	13:T:137:LEU:HD12	1.71	0.72
4:j:92:GLN:HB3	10:q:62:LYS:HD2	1.72	0.72
12:s:110:ILE:HB	12:s:122:TYR:HB2	1.71	0.72
22:U:619:VAL:HG23	22:U:651:GLY:HA3	1.71	0.72
24:X:142:ARG:NH2	24:X:145:GLU:OE1	2.22	0.72
31:D:411:GLU:HG2	31:D:412:GLN:H	1.53	0.72
11:R:125:THR:OG1	11:R:139:MET:SD	2.46	0.72
22:U:202:VAL:HG21	22:U:223:LEU:HD22	1.71	0.72
28:A:96:ALA:HB1	29:B:131:HIS:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:116:ASP:OD1	4:J:81:ARG:NH1	2.23	0.72
3:I:133:SER:HB2	3:I:152:PRO:HD3	1.71	0.72
6:M:35:THR:HA	6:M:166:GLY:HA3	1.70	0.72
31:D:106:THR:HG21	32:E:78:ARG:HD2	1.70	0.72
32:E:57:VAL:HG21	33:F:133:PHE:HB2	1.71	0.72
5:L:40:SER:HB3	5:L:187:LEU:HD22	1.72	0.72
9:p:15:LYS:HE3	9:p:121:ILE:HG12	1.70	0.72
22:U:12:LEU:HB3	22:U:48:LEU:HD21	1.71	0.72
6:m:198:TYR:HB3	6:m:243:LEU:HD21	1.72	0.72
23:V:340:GLY:HA3	23:V:408:ARG:HH12	1.54	0.72
12:S:28:ARG:NH1	12:S:187:VAL:O	2.23	0.72
21:e:27:TRP:HA	23:V:355:ARG:HE	1.54	0.72
27:W:178:GLU:H	27:W:182:ARG:HB2	1.55	0.72
26:Z:102:HIS:HE1	26:Z:104:ASN:HB3	1.55	0.71
8:O:41:ILE:HG22	8:O:102:GLY:HA3	1.70	0.71
21:e:27:TRP:NE1	23:V:351:PRO:O	2.23	0.71
6:M:77:VAL:HG23	6:M:135:PHE:HB3	1.73	0.71
26:Z:90:ARG:HE	26:Z:91:ILE:H	1.36	0.71
20:d:155:LYS:HD3	20:d:170:LEU:HD22	1.73	0.71
22:U:607:VAL:CB	31:D:68:LEU:CD2	2.26	0.71
17:a:352:ARG:HH12	26:Z:235:ASN:HB3	1.55	0.71
19:c:216:MET:HG2	19:c:220:LEU:HD12	1.73	0.71
33:F:84:LYS:HA	33:F:161:LEU:HD13	1.71	0.71
6:m:214:SER:HB3	6:m:226:ILE:HD12	1.72	0.71
22:U:599:ILE:HG22	31:D:60:TYR:CZ	2.24	0.71
11:r:8:PHE:HE1	11:r:13:ILE:HG12	1.55	0.71
29:B:421:LYS:O	29:B:425:ASN:ND2	2.24	0.71
5:L:225:ASP:O	5:L:229:VAL:N	2.22	0.70
13:T:43:MET:HE1	13:T:67:LEU:HD23	1.74	0.70
7:n:12:VAL:HG11	7:n:101:ALA:HB1	1.73	0.70
29:B:220:LYS:NZ	29:B:345:GLY:O	2.22	0.70
30:C:42:LEU:CD1	31:D:62:LYS:HZ3	2.03	0.70
1:G:43:ARG:HB3	1:G:164:LYS:HA	1.73	0.70
16:x:74:LYS:HB2	16:x:103:ILE:HB	1.73	0.70
18:b:3:LEU:HD11	18:b:44:ASN:HD22	1.57	0.70
31:D:391:ARG:HG2	31:D:392:TYR:N	2.04	0.70
17:a:205:LEU:HB3	17:a:268:LEU:HD11	1.71	0.70
20:d:131:VAL:HA	20:d:134:LYS:HG2	1.73	0.70
10:q:26:VAL:HG11	11:r:136:TYR:HE2	1.55	0.70
15:f:461:PRO:HA	16:x:76:ILE:HG21	1.72	0.70
12:S:27:THR:HB	12:S:40:SER:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:s:24:ALA:HB1	12:s:193:LEU:HD11	1.74	0.70
22:U:237:VAL:HG13	22:U:321:GLN:H	1.55	0.70
26:Z:20:VAL:HG13	26:Z:126:VAL:HG13	1.74	0.70
5:L:129:GLY:HA2	5:L:149:PRO:HB3	1.73	0.70
4:J:28:LYS:NZ	29:B:437:GLY:O	2.24	0.70
22:U:633:CYS:SG	22:U:634:PRO:CD	2.78	0.70
30:C:198:LEU:HD13	35:C:501:ADP:H5'1	1.73	0.70
13:t:43:MET:HE1	13:t:67:LEU:HD23	1.72	0.70
15:f:538:ILE:HG23	15:f:558:LEU:HD12	1.72	0.70
6:M:34:SER:OG	6:M:65:ARG:NH1	2.25	0.69
5:L:226:ASP:OD1	5:L:227:ASP:N	2.22	0.69
31:D:168:GLY:H	35:D:501:ADP:HN62	1.40	0.69
33:F:55:MET:HE2	33:F:59:VAL:HG11	1.74	0.69
19:c:220:LEU:HB3	26:Z:134:PRO:HB3	1.74	0.69
32:E:38:LYS:N	32:E:39:GLN:OE1	2.25	0.69
11:r:63:CYS:HB2	11:r:74:ILE:HG21	1.74	0.69
15:f:456:ARG:NH2	15:f:488:ALA:O	2.25	0.69
15:f:677:HIS:ND1	29:B:75:GLU:OE2	2.25	0.69
15:f:720:GLU:HB2	15:f:807:ARG:HD3	1.74	0.69
31:D:185:LEU:O	31:D:187:HIS:ND1	2.24	0.69
27:W:360:GLU:HG3	27:W:396:LEU:HD21	1.75	0.69
29:B:233:THR:N	35:B:501:ADP:O1A	2.25	0.69
32:E:117:PRO:HB3	33:F:95:GLU:HB3	1.73	0.69
14:k:146:VAL:HG11	14:k:222:PRO:HA	1.73	0.69
15:f:369:ARG:HH12	15:f:756:PRO:HB2	1.56	0.69
22:U:571:CYS:SG	22:U:601:ARG:NH1	2.66	0.69
3:i:180:LYS:H	3:i:184:MET:HE2	1.57	0.69
19:c:254:ASN:O	19:c:278:GLN:NE2	2.26	0.69
19:c:54:MET:HG2	19:c:113:HIS:HD2	1.58	0.69
23:V:315:LYS:HA	25:Y:385:ARG:HG3	1.74	0.69
26:Z:121:LEU:HB2	26:Z:138:TYR:HB2	1.73	0.69
27:W:117:ASP:HB3	27:W:120:ILE:HG12	1.75	0.69
29:B:114:GLU:HB3	29:B:122:ILE:HB	1.75	0.69
30:C:322:GLU:HB2	30:C:349:GLU:HG2	1.74	0.69
31:D:400:GLU:HA	31:D:403:TYR:HB3	1.74	0.69
7:n:119:MET:HE3	13:t:58:ALA:HB2	1.75	0.69
15:f:344:VAL:HG12	15:f:346:ASP:H	1.58	0.69
32:E:177:GLY:HA3	32:E:339:ASN:HD22	1.58	0.69
19:c:58:LEU:HD13	19:c:73:PHE:HE2	1.57	0.68
22:U:205:TYR:HB3	22:U:215:ASN:HB2	1.74	0.68
10:Q:138:LEU:HD21	10:Q:170:ARG:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:18:LEU:HD12	3:i:20:GLN:HE22	1.58	0.68
14:K:35:SER:HB2	14:K:66:LYS:HE2	1.75	0.68
26:Z:94:TRP:HB3	26:Z:112:MET:HE3	1.74	0.68
24:X:203:PRO:HB2	24:X:206:LEU:HB3	1.75	0.68
30:C:46:GLN:OE1	31:D:69:LYS:HB3	1.94	0.68
4:J:73:PHE:CE1	4:J:84:ILE:HD11	2.29	0.68
11:R:44:THR:H	11:R:99:THR:HG23	1.58	0.68
29:B:125:THR:HG21	29:B:152:LEU:HD22	1.76	0.68
30:C:73:VAL:HG21	31:D:102:ILE:HD13	1.75	0.68
13:t:122:LEU:HG	13:t:137:LEU:HD12	1.74	0.68
18:b:109:ILE:HB	18:b:138:VAL:HG22	1.74	0.68
27:W:284:SER:O	27:W:288:HIS:ND1	2.26	0.68
2:h:68:ILE:HG21	2:h:110:LEU:HD11	1.76	0.68
8:o:62:ASN:ND2	8:o:82:MET:SD	2.66	0.68
8:o:104:ASP:O	8:o:180:LYS:NZ	2.26	0.68
15:f:836:GLU:HG3	15:f:838:ARG:HG2	1.74	0.68
27:W:186:ILE:HG21	27:W:209:ILE:HG21	1.74	0.68
28:A:333:ARG:O	28:A:337:LEU:N	2.26	0.68
33:F:145:LEU:HD13	33:F:151:VAL:HG11	1.75	0.68
2:H:92:LYS:HG2	8:O:65:LEU:HD11	1.74	0.68
2:H:159:LYS:NZ	2:H:180:GLU:O	2.25	0.68
14:k:50:VAL:HG11	14:k:66:LYS:HB2	1.76	0.68
27:W:390:GLU:OE1	27:W:408:ARG:NH1	2.27	0.68
22:U:607:VAL:HG11	31:D:68:LEU:HD11	1.75	0.68
29:B:99:VAL:HG23	29:B:137:SER:HB2	1.75	0.68
4:J:92:GLN:HG3	10:Q:66:LEU:HB2	1.77	0.67
9:P:78:GLU:HG2	9:P:80:ARG:H	1.59	0.67
15:f:852:VAL:HG22	29:B:185:ALA:HB1	1.76	0.67
17:a:72:ASN:HA	18:b:17:ARG:HH22	1.58	0.67
25:Y:157:ILE:HG22	25:Y:186:LEU:HD12	1.76	0.67
22:U:616:ARG:HB3	22:U:647:HIS:HB2	1.75	0.67
24:X:74:ARG:O	24:X:78:ASN:ND2	2.27	0.67
31:D:143:LEU:HD13	32:E:64:LEU:HD12	1.75	0.67
32:E:36:LEU:HG	32:E:37:THR:H	1.57	0.67
19:c:152:LYS:HD3	31:D:85:ILE:HD12	1.76	0.67
13:t:91:TRP:HE3	13:t:92:LEU:HD22	1.60	0.67
33:F:77:SER:O	33:F:81:LYS:N	2.27	0.67
1:G:49:VAL:HG12	1:G:219:VAL:HG22	1.77	0.67
13:T:25:ASP:HA	13:T:187:PHE:HA	1.75	0.67
22:U:347:ASN:ND2	22:U:741:GLY:O	2.26	0.67
5:l:52:ALA:HB1	5:l:57:ALA:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:33:LEU:HD21	18:b:145:GLU:HG3	1.77	0.67
29:B:135:ILE:HD12	29:B:159:VAL:HG12	1.77	0.67
31:D:273:LYS:NZ	32:E:251:ARG:HD3	2.09	0.67
20:d:129:THR:HG22	20:d:130:ASN:H	1.60	0.67
23:V:191:LEU:HD21	23:V:210:CYS:HB3	1.76	0.67
23:V:219:GLU:OE1	23:V:256:ARG:NH1	2.28	0.67
29:B:253:SER:OG	29:B:254:GLU:N	2.25	0.67
14:k:52:LYS:NZ	14:k:64:ILE:O	2.27	0.67
22:U:62:LEU:HD12	22:U:87:LEU:HB3	1.76	0.67
28:A:232:ARG:HH22	28:A:271:LEU:HB3	1.59	0.67
4:J:158:ALA:HB3	14:K:58:LEU:HD13	1.77	0.67
32:E:177:GLY:HA3	33:F:344:ARG:NH2	2.08	0.67
33:F:342:LEU:HB3	33:F:348:LEU:HD12	1.76	0.67
4:J:134:VAL:HG12	4:J:144:LEU:HD13	1.77	0.66
6:M:63:ASN:HB2	6:M:81:LEU:HD21	1.78	0.66
4:J:87:ALA:HB1	4:J:107:ILE:HD11	1.77	0.66
14:K:235:GLU:HA	14:K:238:ILE:HG12	1.77	0.66
19:c:119:GLY:HA3	19:c:190:GLN:HE21	1.59	0.66
22:U:599:ILE:CG2	31:D:60:TYR:OH	2.37	0.66
23:V:367:VAL:HA	23:V:402:VAL:HG23	1.77	0.66
24:X:182:ASN:HA	25:Y:244:ALA:HB1	1.76	0.66
6:M:59:GLU:HG2	6:M:60:GLU:H	1.59	0.66
11:R:103:GLY:HA2	11:R:179:VAL:HG11	1.77	0.66
12:S:68:ILE:HD11	12:S:92:LEU:HD13	1.77	0.66
2:h:11:THR:HB	2:h:21:GLN:HE21	1.60	0.66
15:f:809:ILE:HG12	15:f:814:SER:HB3	1.77	0.66
3:I:84:ASN:O	3:I:88:ASN:ND2	2.25	0.66
4:J:67:ASP:HB3	10:Q:69:MET:HE1	1.76	0.66
13:T:212:ALA:HA	7:n:30:VAL:HG21	1.77	0.66
8:o:63:LEU:HD11	8:o:79:ALA:HB2	1.78	0.66
24:X:255:LEU:HD11	24:X:267:VAL:HG13	1.77	0.66
5:l:85:CYS:SG	5:l:89:ARG:NH2	2.69	0.66
26:Z:173:GLU:O	26:Z:177:ARG:CG	2.43	0.66
27:W:248:ARG:HH12	27:W:289:ARG:HD2	1.61	0.66
30:C:202:ALA:O	30:C:205:HIS:ND1	2.28	0.66
27:W:183:VAL:HG11	27:W:215:GLN:HE22	1.58	0.66
29:B:232:LYS:HE3	29:B:235:LEU:HD22	1.78	0.66
31:D:391:ARG:HH12	31:D:398:ASP:CG	2.04	0.66
2:H:205:GLU:HB3	2:H:227:LYS:HB2	1.78	0.66
15:f:151:LEU:HD12	15:f:158:TYR:HE2	1.60	0.66
17:a:71:VAL:HG21	17:a:76:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:177:LEU:HD11	17:a:216:LEU:HD23	1.77	0.66
25:Y:23:ARG:NH2	25:Y:52:PRO:O	2.28	0.66
25:Y:247:LEU:O	25:Y:251:HIS:ND1	2.28	0.66
33:F:225:MET:SD	33:F:233:LYS:HB3	2.36	0.66
2:h:160:ALA:HB3	3:i:55:LEU:HD22	1.77	0.66
19:c:114:SER:HB2	19:c:147:PRO:HG3	1.78	0.66
23:V:372:LEU:O	23:V:376:ASN:ND2	2.27	0.66
24:X:343:SER:HB2	27:W:405:LYS:HB3	1.76	0.66
26:Z:102:HIS:CE1	26:Z:104:ASN:HB3	2.31	0.66
1:G:153:LYS:HZ1	1:G:168:ALA:HB2	1.61	0.66
9:P:61:GLN:OE1	10:Q:85:ARG:NE	2.28	0.66
15:f:505:MET:SD	15:f:518:THR:OG1	2.51	0.66
22:U:603:LEU:HB3	31:D:64:GLU:CD	2.21	0.66
22:U:639:LEU:HD11	31:D:68:LEU:HD12	1.78	0.66
2:H:148:GLN:OE1	2:H:158:TRP:NE1	2.29	0.65
10:Q:101:ASN:HB3	10:Q:132:HIS:CE1	2.31	0.65
23:V:338:LEU:HD11	23:V:397:ARG:HD2	1.78	0.65
10:Q:169:LYS:O	10:q:27:GLN:NE2	2.29	0.65
13:T:25:ASP:O	13:T:41:ARG:NH1	2.29	0.65
5:l:200:PRO:O	5:l:239:ARG:NH1	2.28	0.65
1:G:50:ILE:HD13	1:G:79:VAL:HB	1.78	0.65
4:J:45:VAL:HG11	4:J:61:LYS:HG2	1.79	0.65
10:Q:19:ARG:NH2	10:Q:31:ASP:OD1	2.29	0.65
3:i:48:GLU:OE2	3:i:210:LYS:NZ	2.29	0.65
22:U:376:MET:HE2	22:U:738:ASP:HB3	1.79	0.65
23:V:464:ILE:HG23	23:V:468:SER:HB3	1.78	0.65
33:F:200:GLU:HA	33:F:204:LEU:HD23	1.78	0.65
9:P:15:LYS:HB2	9:P:121:ILE:HD13	1.78	0.65
1:g:176:THR:HG23	2:h:56:LEU:HD21	1.78	0.65
11:r:97:MET:H	11:r:116:SER:HB3	1.60	0.65
24:X:413:SER:HB3	25:Y:379:ARG:HH22	1.61	0.65
25:Y:117:LYS:NZ	25:Y:153:ASP:OD2	2.30	0.65
2:H:110:LEU:HD12	2:H:113:ARG:HB2	1.77	0.65
32:E:40:TYR:N	33:F:69:MET:SD	2.62	0.65
32:E:117:PRO:HB2	33:F:147:PRO:HG3	1.78	0.65
5:L:67:ASP:OD1	5:L:68:ASN:N	2.28	0.65
12:s:36:HIS:O	13:t:151:ARG:NH1	2.29	0.65
26:Z:60:GLU:OE2	26:Z:102:HIS:NE2	2.29	0.65
32:E:112:PRO:O	32:E:113:ARG:CG	2.45	0.65
4:j:116:GLN:OE1	14:k:135:ARG:NH2	2.29	0.65
9:p:149:MET:HG2	9:p:170:ALA:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:707:LEU:HD22	15:f:741:LEU:HD13	1.79	0.65
22:U:643:SER:O	22:U:649:ARG:NE	2.26	0.65
22:U:837:ALA:HA	22:U:840:LYS:HB3	1.79	0.65
2:H:74:LEU:HD11	2:H:134:LEU:HD12	1.78	0.65
2:H:180:GLU:OE1	2:H:182:LEU:N	2.30	0.65
8:O:187:ARG:HB3	8:O:188:PRO:HD2	1.78	0.65
13:T:215:ILE:O	8:o:121:LYS:NZ	2.30	0.65
28:A:166:VAL:HA	28:A:238:ILE:HB	1.77	0.65
10:Q:27:GLN:NE2	10:q:169:LYS:O	2.30	0.65
15:f:160:ARG:HH12	29:B:413:LYS:HE3	1.62	0.65
22:U:792:ASN:HB3	22:U:914:LEU:HB3	1.77	0.65
30:C:89:VAL:HG12	30:C:91:PRO:HD2	1.77	0.65
7:N:190:LEU:HD12	13:t:209:TRP:HB2	1.78	0.65
33:F:231:THR:OG1	33:F:233:LYS:NZ	2.25	0.65
2:H:104:PRO:HD2	2:H:106:PRO:HD3	1.78	0.64
10:Q:35:MET:HG3	10:Q:181:ARG:HH11	1.62	0.64
8:o:70:THR:HG23	8:o:72:ARG:H	1.62	0.64
11:r:167:ASP:OD1	11:r:168:ALA:N	2.30	0.64
28:A:190:VAL:HG13	28:A:209:PRO:HB2	1.78	0.64
33:F:269:ARG:HA	33:F:316:GLN:HE22	1.62	0.64
22:U:529:ILE:HG12	22:U:566:LEU:HD21	1.79	0.64
32:E:117:PRO:HG3	33:F:95:GLU:H	1.62	0.64
4:J:132:LEU:HD22	4:J:159:ASN:HD22	1.62	0.64
30:C:235:PHE:HD2	30:C:276:LEU:HD13	1.62	0.64
30:C:270:GLN:NE2	30:C:273:MET:SD	2.70	0.64
32:E:75:ASN:HD22	33:F:129:ARG:C	2.04	0.64
28:A:167:GLU:HG3	28:A:239:ARG:HB3	1.79	0.64
1:g:163:PHE:HA	2:h:58:ASP:H	1.62	0.64
6:m:236:GLU:OE2	6:m:240:LYS:NZ	2.26	0.64
27:W:243:ILE:HA	27:W:246:HIS:CE1	2.32	0.64
19:c:163:ILE:HD12	19:c:167:MET:HB2	1.79	0.64
19:c:234:TYR:HA	19:c:237:HIS:HB2	1.79	0.64
22:U:637:VAL:HG21	22:U:656:LEU:HD11	1.78	0.64
32:E:33:LEU:CD2	33:F:62:VAL:HG13	2.28	0.64
14:k:40:ILE:HD11	14:k:181:LEU:HD11	1.79	0.64
22:U:446:LEU:O	22:U:450:HIS:ND1	2.21	0.64
4:j:36:ARG:HH21	4:j:157:LYS:HG2	1.63	0.64
10:q:172:ILE:HG23	10:q:173:LEU:HD12	1.79	0.64
11:r:42:LEU:HD21	11:r:184:TRP:HB3	1.80	0.64
11:r:81:LYS:NZ	11:r:85:ASN:OD1	2.30	0.64
15:f:482:ILE:HD13	15:f:518:THR:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:c:46:ARG:HH21	26:Z:167:ALA:HB2	1.61	0.64
22:U:367:THR:HB	22:U:403:THR:HG21	1.80	0.64
10:Q:173:LEU:HA	10:q:173:LEU:HA	1.79	0.64
14:k:85:ALA:HB2	14:k:139:VAL:HG21	1.79	0.64
18:b:171:VAL:HG11	18:b:183:LEU:HD22	1.80	0.64
22:U:510:GLU:HA	22:U:547:GLY:HA3	1.80	0.64
22:U:607:VAL:HB	31:D:68:LEU:HD21	0.69	0.64
26:Z:105:ASP:O	26:Z:109:ASN:ND2	2.30	0.64
26:Z:252:LYS:O	26:Z:255:ASP:N	2.30	0.64
31:D:87:LEU:O	32:E:80:VAL:HB	1.98	0.64
2:H:95:GLN:HG3	8:O:61:SER:HB3	1.79	0.63
29:B:51:LEU:O	29:B:64:LYS:NZ	2.29	0.63
32:E:22:ILE:HD12	33:F:55:MET:HB3	1.79	0.63
32:E:75:ASN:ND2	33:F:129:ARG:C	2.56	0.63
4:J:118:TYR:HA	4:J:124:ARG:HE	1.64	0.63
1:g:61:LEU:HA	6:m:160:TYR:HA	1.79	0.63
15:f:673:ARG:HH12	28:A:59:ILE:HD12	1.64	0.63
15:f:120:ARG:HD3	15:f:147:SER:HB3	1.80	0.63
15:f:157:GLU:O	15:f:161:HIS:ND1	2.23	0.63
15:f:668:ALA:HB1	15:f:697:ILE:HG23	1.80	0.63
22:U:159:ARG:HB3	22:U:162:VAL:HB	1.79	0.63
28:A:112:ILE:HA	28:A:122:VAL:HG22	1.80	0.63
33:F:134:LEU:HD12	33:F:137:ILE:HA	1.80	0.63
4:J:95:ARG:HG3	10:Q:62:LYS:NZ	2.14	0.63
6:m:183:GLU:OE1	6:m:183:GLU:N	2.32	0.63
15:f:856:ALA:HB3	15:f:858:LYS:HE3	1.79	0.63
23:V:212:TYR:HA	23:V:253:LEU:HD11	1.79	0.63
18:b:40:LYS:O	18:b:47:ASN:ND2	2.31	0.63
19:c:244:VAL:HG13	19:c:291:LEU:HD13	1.81	0.63
33:F:206:MET:HE2	33:F:327:LYS:HG2	1.81	0.63
1:g:88:ARG:NH2	6:m:157:SER:O	2.32	0.63
27:W:236:HIS:ND1	27:W:237:GLU:OE2	2.30	0.63
4:J:34:GLY:N	4:J:159:ASN:OD1	2.32	0.63
3:i:109:GLN:OE1	10:q:71:ASN:ND2	2.31	0.63
22:U:619:VAL:HG11	22:U:648:VAL:HG13	1.79	0.63
27:W:152:ILE:HD13	27:W:161:GLU:HB3	1.81	0.63
32:E:177:GLY:HA3	33:F:344:ARG:HH12	1.64	0.63
5:L:82:ARG:O	5:L:86:ASN:ND2	2.32	0.63
6:m:40:ARG:HD2	6:m:148:LEU:HB3	1.80	0.63
6:m:93:GLU:OE2	6:m:97:ASN:ND2	2.32	0.63
17:a:34:TRP:HB3	17:a:71:VAL:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:371:ASN:O	23:V:399:ARG:NH2	2.31	0.63
27:W:52:LYS:HD3	27:W:55:ARG:HH21	1.64	0.63
32:E:45:ASN:HA	32:E:48:LYS:HD3	1.81	0.63
31:D:202:VAL:HB	31:D:308:ILE:HG12	1.81	0.62
2:H:102:GLN:N	9:P:89:SER:OG	2.28	0.62
9:P:143:ALA:HA	9:P:146:MET:HE2	1.80	0.62
22:U:802:TYR:HA	22:U:895:PRO:HG3	1.81	0.62
25:Y:104:MET:HE2	25:Y:127:THR:HB	1.81	0.62
30:C:306:LEU:HG	30:C:308:PRO:HD2	1.80	0.62
8:O:13:VAL:HG22	8:O:177:VAL:HG12	1.80	0.62
12:S:36:HIS:HB3	13:T:132:TYR:CZ	2.35	0.62
12:s:66:LYS:HG3	13:t:94:ARG:NH2	2.15	0.62
28:A:269:ALA:HB1	28:A:315:ILE:HG12	1.81	0.62
31:D:147:ALA:HB2	31:D:253:LEU:HD22	1.79	0.62
33:F:235:LEU:HD11	35:F:501:ADP:H2'	1.81	0.62
2:H:65:VAL:O	2:H:220:ARG:NH1	2.31	0.62
12:S:26:ASP:OD1	12:S:27:THR:N	2.32	0.62
10:q:78:THR:O	10:q:82:ASN:ND2	2.32	0.62
14:K:201:ILE:O	14:K:205:VAL:HG23	1.99	0.62
15:f:469:TYR:HA	15:f:472:HIS:HB2	1.80	0.62
27:W:265:GLN:HB2	27:W:336:PRO:HD3	1.81	0.62
30:C:56:VAL:CG2	31:D:79:VAL:CB	2.78	0.62
31:D:314:ALA:HA	31:D:317:LEU:HD13	1.81	0.62
31:D:337:ASP:O	31:D:340:GLN:N	2.32	0.62
1:G:49:VAL:HG11	1:G:195:VAL:HG22	1.80	0.62
7:N:202:LEU:O	7:n:122:ARG:NH1	2.32	0.62
11:R:29:GLN:NE2	9:p:176:ASP:O	2.33	0.62
1:g:12:HIS:O	1:g:24:GLN:NE2	2.32	0.62
22:U:607:VAL:HB	31:D:68:LEU:CD1	2.28	0.62
32:E:83:CYS:HB3	32:E:87:LEU:HB2	1.80	0.62
15:f:672:LEU:HD11	15:f:706:ILE:HG12	1.81	0.62
15:f:781:TYR:O	15:f:785:ARG:NH1	2.26	0.62
20:d:241:GLU:OE1	20:d:245:GLN:NE2	2.32	0.62
23:V:296:LYS:HB3	23:V:301:GLU:HB2	1.82	0.62
25:Y:137:ARG:HD2	25:Y:168:ILE:HD12	1.81	0.62
14:k:121:LEU:HD23	5:l:79:ALA:HB3	1.81	0.62
27:W:172:GLU:HB2	27:W:182:ARG:HH21	1.65	0.62
31:D:146:GLU:HB3	31:D:249:ASP:HB3	1.81	0.62
32:E:378:LYS:NZ	33:F:340:PRO:HB3	2.14	0.62
1:g:68:HIS:NE2	1:g:80:MET:O	2.32	0.62
15:f:494:ARG:HH21	15:f:495:GLU:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:218:GLN:HG3	22:U:222:PHE:HE2	1.65	0.62
22:U:453:HIS:HB3	22:U:457:ILE:HG13	1.82	0.62
22:U:475:HIS:NE2	22:U:507:VAL:O	2.33	0.62
25:Y:250:LEU:HB3	25:Y:257:ARG:HB2	1.80	0.62
31:D:204:MET:HG3	31:D:310:ALA:HA	1.82	0.62
4:J:6:ALA:O	4:J:18:GLN:NE2	2.33	0.62
4:J:104:VAL:HG21	4:J:143:ARG:HB2	1.82	0.62
6:m:46:VAL:HG12	6:m:215:TRP:HB3	1.81	0.62
15:f:720:GLU:O	15:f:724:ASN:ND2	2.33	0.62
22:U:21:GLU:HG3	22:U:25:HIS:CE1	2.35	0.62
3:i:159:TRP:HA	4:j:54:GLN:HA	1.82	0.62
6:m:70:ASP:OD1	6:m:99:ARG:NH2	2.32	0.62
26:Z:193:ASN:HA	26:Z:196:HIS:CE1	2.35	0.62
28:A:115:VAL:HB	28:A:119:ALA:HB3	1.82	0.62
1:g:86:ASP:OD1	6:m:120:HIS:NE2	2.33	0.61
3:i:190:LEU:HD11	3:i:236:LEU:HD21	1.81	0.61
10:q:26:VAL:HG11	11:r:136:TYR:CE2	2.35	0.61
12:s:123:SER:HB3	12:s:136:LYS:HG2	1.82	0.61
15:f:230:CYS:HA	15:f:233:LEU:HD12	1.81	0.61
16:x:35:HIS:HB3	16:x:102:LEU:HB3	1.82	0.61
16:x:89:LEU:HB3	16:x:94:ILE:HD12	1.82	0.61
22:U:607:VAL:HG12	31:D:68:LEU:HD11	1.81	0.61
27:W:55:ARG:HH11	27:W:96:GLN:HG3	1.64	0.61
30:C:209:CYS:HA	30:C:243:PRO:HB2	1.82	0.61
33:F:222:GLY:HA3	33:F:348:LEU:HA	1.82	0.61
1:G:49:VAL:HG22	1:G:194:THR:HG22	1.82	0.61
1:G:95:ARG:NH2	7:N:68:ILE:O	2.30	0.61
15:f:679:LEU:HG	15:f:690:VAL:HG11	1.82	0.61
22:U:583:MET:HA	22:U:586:VAL:HG12	1.82	0.61
25:Y:245:GLU:OE1	25:Y:245:GLU:N	2.31	0.61
1:g:24:GLN:NE2	6:m:13:THR:OG1	2.33	0.61
13:t:99:ARG:HG2	13:t:106:LEU:HG	1.82	0.61
31:D:156:SER:HB3	31:D:227:PHE:HB3	1.81	0.61
7:N:17:ASP:OD1	7:N:18:SER:N	2.32	0.61
2:h:119:GLN:NE2	3:i:82:ASP:OD1	2.33	0.61
6:m:15:SER:HB3	6:m:19:ARG:H	1.64	0.61
19:c:29:GLU:OE1	19:c:161:ARG:NH2	2.33	0.61
25:Y:164:ALA:HA	25:Y:168:ILE:HB	1.82	0.61
26:Z:204:LYS:HD2	27:W:443:THR:HG21	1.82	0.61
28:A:102:ILE:HB	28:A:113:ILE:HG12	1.81	0.61
4:J:40:ILE:HD12	4:J:212:ARG:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:42:VAL:HG23	4:J:191:VAL:HG21	1.82	0.61
11:R:166:ARG:NH1	9:p:34:MET:O	2.31	0.61
6:m:164:ALA:O	6:m:173:LYS:NZ	2.33	0.61
6:m:214:SER:HA	6:m:227:VAL:HG23	1.81	0.61
15:f:452:ASN:ND2	15:f:452:ASN:O	2.34	0.61
19:c:130:GLN:HG3	19:c:142:ALA:HB2	1.82	0.61
30:C:190:GLY:HA3	30:C:317:PHE:HB2	1.82	0.61
31:D:412:GLN:HE22	31:D:415:GLU:HB3	1.65	0.61
4:J:64:ALA:HB2	4:J:217:LEU:HD12	1.83	0.61
13:T:16:PHE:HE2	13:T:21:VAL:HG23	1.65	0.61
31:D:127:ASN:HB3	31:D:248:ARG:HD3	1.81	0.61
12:s:28:ARG:NH2	12:s:213:ASP:O	2.34	0.61
12:s:158:MET:HE3	12:s:161:VAL:HG21	1.82	0.61
33:F:416:THR:HG22	33:F:417:HIS:CD2	2.36	0.61
33:F:134:LEU:HD13	33:F:160:ILE:H	1.66	0.61
12:S:13:LEU:HD22	12:S:145:LEU:HD21	1.83	0.61
1:g:132:ARG:NH2	6:m:123:THR:O	2.34	0.61
22:U:342:LEU:O	22:U:346:ASN:HB2	2.01	0.61
23:V:314:ARG:NH1	25:Y:378:ASN:OD1	2.34	0.61
23:V:491:VAL:HG13	30:C:41:ASN:HB3	1.83	0.61
5:L:103:LEU:HD12	5:L:104:PRO:HD2	1.83	0.61
7:n:91:ARG:NH1	13:t:59:ASP:OD1	2.33	0.61
15:f:596:ASP:OD1	15:f:608:LYS:NZ	2.32	0.61
29:B:412:MET:HB2	29:B:415:THR:HA	1.83	0.61
30:C:56:VAL:CG2	31:D:79:VAL:HG11	2.31	0.61
30:C:379:THR:HG23	30:C:382:ASP:H	1.66	0.61
2:H:93:LEU:HD13	2:H:117:VAL:HG12	1.83	0.60
8:o:122:LEU:HD12	8:o:123:PRO:HD2	1.82	0.60
15:f:419:LEU:HA	15:f:451:VAL:HA	1.83	0.60
18:b:16:MET:SD	18:b:115:SER:OG	2.57	0.60
22:U:347:ASN:HB2	22:U:741:GLY:HA3	1.83	0.60
31:D:237:GLN:HG2	31:D:238:LYS:H	1.65	0.60
7:N:98:ILE:HB	7:N:114:VAL:HG23	1.83	0.60
13:T:69:GLN:NE2	13:T:73:ASP:OD1	2.34	0.60
2:h:79:MET:HG3	2:h:81:PRO:HD2	1.83	0.60
7:n:22:THR:HG23	7:n:27:ALA:HB2	1.83	0.60
30:C:255:GLY:N	30:C:302:ASP:O	2.33	0.60
33:F:184:GLN:OE1	33:F:186:SER:N	2.32	0.60
33:F:357:PRO:O	33:F:362:ARG:NE	2.33	0.60
6:M:214:SER:OG	6:M:224:HIS:NE2	2.32	0.60
12:S:27:THR:HG22	12:S:41:PRO:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:88:VAL:N	31:D:132:LEU:O	2.27	0.60
32:E:117:PRO:HB2	33:F:147:PRO:HB3	1.83	0.60
6:M:5:THR:OG1	6:M:6:GLY:N	2.35	0.60
12:S:60:ASP:OD1	13:T:100:ARG:NH2	2.34	0.60
22:U:619:VAL:HG21	22:U:648:VAL:HA	1.83	0.60
11:R:33:LYS:HG3	11:R:45:MET:HB2	1.82	0.60
22:U:36:ALA:HB2	23:V:270:LEU:HB2	1.83	0.60
22:U:524:LYS:HA	22:U:556:MET:HE2	1.84	0.60
25:Y:256:VAL:HA	25:Y:259:TYR:CE2	2.35	0.60
26:Z:90:ARG:HH21	26:Z:91:ILE:HG13	1.66	0.60
5:l:107:ARG:HH12	13:t:83:TYR:HE1	1.48	0.60
15:f:886:GLU:HB3	15:f:906:TYR:HD2	1.66	0.60
20:d:12:LYS:HG2	20:d:14:PRO:HD3	1.83	0.60
10:Q:154:GLU:OE1	10:Q:154:GLU:N	2.35	0.60
3:i:111:VAL:HG22	3:i:136:TYR:HD2	1.65	0.60
30:C:150:MET:N	30:C:150:MET:SD	2.75	0.60
33:F:379:VAL:HG22	33:F:416:THR:HG23	1.82	0.60
14:K:42:THR:HG23	14:K:45:GLY:H	1.65	0.60
22:U:13:ASP:OD2	22:U:44:LYS:NZ	2.33	0.60
27:W:24:VAL:HG12	27:W:50:LEU:HD21	1.83	0.60
28:A:418:LYS:NZ	29:B:348:ASP:OD1	2.34	0.60
30:C:140:VAL:HG12	30:C:212:ILE:HG23	1.84	0.60
33:F:89:LEU:HD22	33:F:126:THR:HB	1.83	0.60
9:P:135:ASP:OD1	9:P:136:PHE:N	2.34	0.60
23:V:307:ARG:O	23:V:311:ASN:ND2	2.31	0.60
29:B:221:GLY:H	29:B:326:LYS:HE2	1.66	0.60
30:C:325:ARG:NH2	30:C:351:MET:O	2.34	0.60
32:E:117:PRO:HB3	33:F:95:GLU:CB	2.30	0.60
33:F:269:ARG:HA	33:F:316:GLN:NE2	2.16	0.60
5:L:100:ASP:OD2	12:S:66:LYS:NZ	2.29	0.60
2:h:159:LYS:N	3:i:55:LEU:O	2.30	0.60
18:b:18:ASN:HD21	18:b:25:ARG:HH12	1.50	0.60
22:U:265:ILE:HD11	22:U:326:ILE:HA	1.84	0.60
22:U:607:VAL:CB	31:D:68:LEU:CG	2.71	0.60
29:B:362:LYS:HG3	29:B:380:LEU:HD21	1.82	0.60
30:C:375:ARG:HG2	30:C:377:HIS:H	1.67	0.60
32:E:60:VAL:HA	32:E:71:VAL:HA	1.84	0.60
3:I:37:ILE:HD11	3:I:184:MET:HE1	1.84	0.59
9:P:113:ASP:OD2	9:P:116:THR:N	2.32	0.59
1:g:31:ALA:HA	1:g:34:GLN:HG2	1.83	0.59
25:Y:94:ASN:ND2	25:Y:99:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:54:PRO:HG2	29:B:61:LYS:HB2	1.83	0.59
29:B:216:ILE:HG13	29:B:218:PRO:HD3	1.81	0.59
29:B:415:THR:HG22	29:B:417:GLU:H	1.66	0.59
13:T:124:TYR:HB2	13:T:137:LEU:HD13	1.84	0.59
5:l:196:ARG:NH1	5:l:237:GLU:O	2.35	0.59
6:m:213:LEU:HG	6:m:227:VAL:HG21	1.84	0.59
7:n:14:LEU:HD21	7:n:101:ALA:HB3	1.84	0.59
13:t:166:ARG:NH1	13:t:200:GLU:OE1	2.34	0.59
14:K:168:ARG:NH1	14:K:169:ALA:O	2.35	0.59
18:b:132:LYS:HD2	18:b:163:LYS:HD3	1.83	0.59
19:c:175:ARG:HB3	19:c:181:LEU:HD11	1.83	0.59
25:Y:291:HIS:HA	25:Y:295:TYR:CZ	2.37	0.59
30:C:32:GLN:OE1	31:D:55:GLU:HA	2.02	0.59
30:C:338:LEU:HA	30:C:378:VAL:H	1.67	0.59
5:L:132:LEU:HB2	5:L:147:THR:HB	1.83	0.59
7:n:127:ILE:HG22	7:n:132:SER:HB2	1.83	0.59
20:d:32:GLU:HG3	20:d:33:LEU:H	1.66	0.59
22:U:607:VAL:C	31:D:68:LEU:HD21	2.26	0.59
28:A:97:ARG:HG3	28:A:144:ARG:H	1.65	0.59
32:E:127:PRO:HG2	32:E:185:ARG:HD2	1.83	0.59
32:E:295:LEU:O	32:E:298:LYS:NZ	2.36	0.59
6:m:141:SER:HB2	6:m:144:ASP:HB3	1.84	0.59
13:t:41:ARG:NH1	13:t:53:ALA:O	2.34	0.59
20:d:249:TYR:HB3	23:V:480:ILE:HG12	1.84	0.59
22:U:360:VAL:O	22:U:361:ARG:NH1	2.35	0.59
22:U:471:ASP:HB2	22:U:472:ILE:HD12	1.84	0.59
28:A:120:LYS:NZ	33:F:151:VAL:O	2.30	0.59
28:A:277:ILE:HG13	28:A:280:ILE:HD11	1.84	0.59
3:I:28:ILE:HG21	3:I:133:SER:HB3	1.84	0.59
11:R:17:ASP:OD2	11:R:171:GLY:N	2.35	0.59
19:c:172:HIS:CG	19:c:173:GLU:H	2.20	0.59
23:V:228:ARG:NH1	23:V:258:TYR:OH	2.36	0.59
32:E:352:MET:HE2	33:F:350:ARG:NH1	2.17	0.59
5:L:193:ARG:HG2	5:L:196:ARG:HH21	1.68	0.59
14:k:155:HIS:N	14:k:163:VAL:O	2.35	0.59
13:t:54:SER:O	13:t:108:ASN:ND2	2.34	0.59
19:c:250:GLU:OE2	19:c:254:ASN:ND2	2.35	0.59
26:Z:15:VAL:HG11	26:Z:50:VAL:HG12	1.85	0.59
27:W:242:SER:O	27:W:246:HIS:ND1	2.33	0.59
30:C:56:VAL:HG23	31:D:79:VAL:CG1	2.33	0.59
32:E:112:PRO:C	32:E:113:ARG:HG3	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:E:341:ALA:CB	33:F:344:ARG:HG3	2.32	0.59
5:l:44:ALA:HB1	5:l:144:ILE:HD11	1.84	0.59
11:r:113:TYR:CE1	11:r:128:VAL:HG21	2.37	0.59
15:f:616:CYS:HA	15:f:650:GLN:HG2	1.84	0.59
19:c:217:LEU:HD21	26:Z:17:LEU:HD13	1.84	0.59
22:U:177:LEU:O	22:U:205:TYR:OH	2.21	0.59
27:W:18:VAL:H	27:W:57:ALA:HB1	1.67	0.59
33:F:145:LEU:HD22	33:F:160:ILE:HG21	1.84	0.59
2:H:26:LEU:HA	2:H:29:VAL:HG12	1.85	0.59
19:c:56:LEU:HA	19:c:111:TRP:HA	1.82	0.59
19:c:255:TYR:HD1	19:c:280:PRO:HG3	1.67	0.59
20:d:235:THR:HG23	20:d:238:PRO:HG2	1.83	0.59
22:U:628:ARG:NH1	22:U:753:GLY:O	2.30	0.59
25:Y:67:VAL:O	25:Y:71:ASN:ND2	2.30	0.59
8:O:38:SER:HB3	8:O:41:ILE:HG12	1.85	0.59
8:O:182:LYS:HD2	8:O:184:ASP:HB2	1.85	0.59
2:h:193:LEU:HA	2:h:196:LYS:HE3	1.85	0.59
8:o:211:VAL:HG21	9:p:198:ARG:HD3	1.85	0.59
19:c:254:ASN:HB3	19:c:278:GLN:HB3	1.83	0.59
22:U:575:ASP:HB2	22:U:578:LEU:HD23	1.85	0.59
27:W:359:VAL:HG13	27:W:382:LEU:HD22	1.84	0.59
9:p:135:ASP:OD1	9:p:136:PHE:N	2.33	0.59
15:f:378:ASN:OD1	15:f:382:ASN:ND2	2.36	0.59
15:f:485:LEU:HD13	15:f:501:LEU:HD21	1.85	0.59
22:U:21:GLU:HB2	22:U:54:PHE:HZ	1.67	0.59
22:U:247:GLN:NE2	22:U:911:ILE:O	2.33	0.59
27:W:167:GLN:O	27:W:170:GLN:NE2	2.27	0.59
30:C:53:ASN:OD1	31:D:75:ALA:CB	2.51	0.59
32:E:27:LYS:HG2	32:E:30:ARG:HH21	1.68	0.59
33:F:169:ASP:O	33:F:171:ARG:N	2.36	0.59
3:i:73:ALA:HB2	3:i:225:ILE:HD13	1.85	0.58
15:f:771:LEU:HD22	15:f:778:LEU:HD21	1.84	0.58
15:f:845:ARG:NH2	15:f:882:LEU:O	2.36	0.58
29:B:190:LEU:HG	29:B:193:GLN:HB2	1.84	0.58
11:R:17:ASP:OD1	11:R:18:SER:N	2.35	0.58
4:j:87:ALA:HA	4:j:90:GLU:HG2	1.83	0.58
9:p:20:VAL:HG11	9:p:110:ALA:HB1	1.85	0.58
9:p:66:ARG:HH12	9:p:70:ARG:HB3	1.67	0.58
14:K:42:THR:OG1	14:K:189:MET:O	2.21	0.58
14:K:146:VAL:HG21	14:K:222:PRO:HA	1.83	0.58
18:b:11:ASP:HA	18:b:54:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:20:ASP:OD1	18:b:21:PHE:N	2.34	0.58
33:F:79:LYS:O	33:F:83:ASN:ND2	2.36	0.58
33:F:312:GLU:O	33:F:316:GLN:HG3	2.03	0.58
6:M:120:HIS:HA	6:M:123:THR:HG22	1.86	0.58
3:i:158:GLY:O	4:j:55:ASP:N	2.35	0.58
22:U:360:VAL:HG11	22:U:393:LEU:HD21	1.85	0.58
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.84	0.58
30:C:195:GLY:N	35:C:501:ADP:O2A	2.36	0.58
6:M:69:VAL:HA	6:M:92:ARG:HG2	1.85	0.58
15:f:581:GLU:HA	15:f:588:ARG:HD2	1.84	0.58
20:d:189:ILE:O	20:d:222:TYR:N	2.31	0.58
31:D:88:VAL:HG13	31:D:134:LYS:HA	1.84	0.58
31:D:355:SER:HB3	31:D:358:VAL:HB	1.84	0.58
10:Q:85:ARG:HA	10:Q:118:MET:HE1	1.85	0.58
19:c:54:MET:HG2	19:c:113:HIS:CD2	2.37	0.58
22:U:215:ASN:OD1	22:U:216:VAL:N	2.37	0.58
22:U:789:ILE:HB	22:U:911:ILE:HG13	1.85	0.58
30:C:42:LEU:CD1	31:D:62:LYS:NZ	2.59	0.58
3:i:218:ARG:NH1	3:i:223:THR:OG1	2.36	0.58
15:f:289:VAL:HA	15:f:292:LYS:HE2	1.83	0.58
22:U:352:ILE:HG21	22:U:376:MET:HE1	1.84	0.58
25:Y:231:LEU:HD11	25:Y:236:LEU:HD13	1.84	0.58
32:E:56:ILE:N	32:E:100:LEU:O	2.36	0.58
13:T:99:ARG:NH2	13:T:104:ASN:OD1	2.33	0.58
9:p:14:MET:HG3	9:p:163:LEU:HD11	1.84	0.58
19:c:57:MET:H	19:c:111:TRP:HA	1.68	0.58
22:U:78:LEU:HD11	22:U:104:CYS:HB2	1.86	0.58
33:F:91:SER:HA	33:F:124:ILE:HG23	1.85	0.58
11:r:35:ILE:HD11	11:r:45:MET:HE3	1.86	0.58
15:f:138:GLU:HA	15:f:141:LYS:HG2	1.85	0.58
24:X:157:LEU:HB3	24:X:166:LEU:HD21	1.86	0.58
31:D:85:ILE:CG2	32:E:105:LEU:HD11	2.33	0.58
6:m:179:LEU:HD21	6:m:189:ILE:HD12	1.85	0.58
15:f:806:VAL:HA	15:f:809:ILE:HG22	1.85	0.58
17:a:258:GLN:CD	17:a:258:GLN:H	2.12	0.58
28:A:115:VAL:HG12	28:A:117:GLN:H	1.69	0.58
33:F:153:VAL:HG22	33:F:160:ILE:HD13	1.85	0.58
33:F:394:ALA:HA	33:F:397:LYS:HE3	1.86	0.58
9:P:125:ASP:OD1	9:P:129:CYS:N	2.31	0.58
10:q:19:ARG:HB2	10:q:177:THR:HG23	1.85	0.58
13:t:89:HIS:HA	13:t:112:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:409:SER:HB2	15:f:815:HIS:ND1	2.18	0.58
22:U:229:VAL:HA	22:U:232:ILE:HG12	1.86	0.58
22:U:440:GLY:HA3	22:U:472:ILE:HG22	1.84	0.58
27:W:356:ASN:OD1	27:W:357:ARG:N	2.37	0.58
30:C:234:LEU:HD23	30:C:238:ALA:HB3	1.86	0.58
9:P:36:THR:OG1	9:P:38:ASP:OD1	2.22	0.57
1:g:36:GLY:O	1:g:55:LYS:NZ	2.37	0.57
4:j:90:GLU:OE1	4:j:110:TYR:HD2	1.87	0.57
5:l:153:TYR:H	6:m:85:ARG:HH12	1.50	0.57
19:c:193:ILE:HG23	29:B:155:LYS:NZ	2.19	0.57
20:d:30:LEU:HA	20:d:47:GLN:HE22	1.69	0.57
28:A:245:LEU:HA	28:A:256:MET:HE3	1.86	0.57
3:I:154:GLY:O	4:J:81:ARG:NH2	2.37	0.57
9:P:61:GLN:OE1	10:Q:85:ARG:CZ	2.52	0.57
3:i:37:ILE:HD12	3:i:189:ALA:HB1	1.85	0.57
14:K:121:LEU:HD23	14:K:136:PRO:HB3	1.86	0.57
15:f:535:THR:HG21	15:f:566:HIS:HE1	1.69	0.57
19:c:39:LEU:HD13	26:Z:14:LEU:HD12	1.85	0.57
22:U:799:LYS:HB2	22:U:923:GLU:HB3	1.85	0.57
25:Y:250:LEU:HD21	25:Y:260:LEU:HD13	1.85	0.57
27:W:96:GLN:HG2	27:W:97:LEU:H	1.69	0.57
7:n:53:GLN:NE2	8:o:119:THR:O	2.38	0.57
15:f:670:MET:HE1	15:f:673:ARG:HD3	1.86	0.57
22:U:564:ASP:OD1	22:U:565:ALA:N	2.36	0.57
29:B:53:THR:H	29:B:64:LYS:HZ3	1.52	0.57
33:F:235:LEU:HD23	33:F:238:ARG:HH21	1.68	0.57
1:g:12:HIS:C	1:g:24:GLN:HE21	2.11	0.57
1:g:141:ILE:HG22	1:g:151:VAL:HG22	1.85	0.57
7:n:144:ARG:H	7:n:147:MET:HE3	1.68	0.57
14:K:181:LEU:HA	14:K:184:VAL:HG22	1.86	0.57
22:U:799:LYS:HG2	22:U:925:VAL:HB	1.87	0.57
26:Z:182:THR:HG22	26:Z:183:THR:H	1.69	0.57
2:H:122:THR:OG1	2:H:152:SER:HA	2.05	0.57
3:I:38:LEU:HD23	3:I:160:LYS:HG2	1.85	0.57
13:T:51:LEU:HD11	13:T:110:MET:HE2	1.84	0.57
10:q:35:MET:HE2	10:q:43:LEU:HD21	1.85	0.57
14:K:221:GLN:HB2	14:K:224:GLN:HB2	1.85	0.57
18:b:139:ASP:HB3	18:b:168:SER:HB3	1.86	0.57
22:U:483:LEU:HD11	22:U:781:LEU:HD13	1.87	0.57
33:F:171:ARG:HH11	33:F:267:LEU:HD11	1.70	0.57
9:P:56:LEU:HD13	9:P:104:TYR:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:59:VAL:HG13	7:n:82:LEU:HD22	1.87	0.57
15:f:846:VAL:HG11	15:f:872:VAL:HG11	1.86	0.57
21:e:25:GLU:N	23:V:326:GLN:OE1	2.38	0.57
33:F:260:PHE:HB3	33:F:263:ASP:HB2	1.87	0.57
1:g:40:VAL:HG23	1:g:167:ALA:HB2	1.87	0.57
3:i:45:LEU:HG	3:i:137:ILE:HD13	1.86	0.57
22:U:790:GLY:HA3	22:U:800:VAL:HG21	1.85	0.57
29:B:233:THR:C	29:B:235:LEU:N	2.59	0.57
32:E:33:LEU:CD1	32:E:34:LYS:H	2.16	0.57
13:T:8:GLY:N	13:T:55:GLY:O	2.27	0.57
1:g:111:VAL:HG21	1:g:150:GLN:HB2	1.87	0.57
12:s:16:ALA:HB2	12:s:121:VAL:HG23	1.86	0.57
24:X:184:PRO:HD2	25:Y:244:ALA:HB2	1.87	0.57
33:F:53:LYS:HD3	33:F:54:ILE:HG22	1.85	0.57
2:H:14:SER:OG	3:I:128:ARG:NH2	2.38	0.57
20:d:105:PHE:O	20:d:108:SER:OG	2.20	0.57
12:S:213:ASP:OD1	8:o:193:ASN:ND2	2.37	0.57
6:m:72:HIS:ND1	6:m:139:SER:OG	2.31	0.57
12:s:75:TYR:CD1	12:s:83:MET:HG2	2.39	0.57
2:h:106:PRO:HB2	2:h:109:GLN:HG2	1.87	0.56
14:k:73:HIS:CE1	14:k:106:THR:HB	2.40	0.56
14:k:98:ASN:OD1	11:r:61:ARG:NH1	2.38	0.56
7:n:101:ALA:HB2	7:n:111:VAL:HG13	1.87	0.56
18:b:124:LEU:HD21	18:b:156:PHE:HB2	1.86	0.56
19:c:256:ASN:O	19:c:259:VAL:HG12	2.05	0.56
20:d:158:ILE:HD11	20:d:167:ILE:HG23	1.87	0.56
22:U:620:GLU:HB3	22:U:651:GLY:HA2	1.87	0.56
23:V:321:ALA:HB1	23:V:324:PHE:HB3	1.87	0.56
23:V:357:LEU:HA	23:V:360:TYR:HB2	1.87	0.56
27:W:340:VAL:HA	27:W:350:ARG:HH11	1.68	0.56
9:P:155:GLU:HB2	9:P:158:MET:HE3	1.85	0.56
1:g:49:VAL:HG21	1:g:195:VAL:HG12	1.86	0.56
2:h:208:ILE:HD12	2:h:230:LEU:HD21	1.85	0.56
15:f:692:LEU:HB3	15:f:800:LEU:HD12	1.87	0.56
21:e:40:GLU:O	25:Y:293:ARG:NH1	2.38	0.56
28:A:306:LEU:O	28:A:336:ARG:NE	2.38	0.56
29:B:309:MET:N	29:B:309:MET:SD	2.78	0.56
32:E:46:ASP:HB2	33:F:76:ASN:ND2	2.19	0.56
32:E:201:SER:HB3	33:F:269:ARG:NH2	2.20	0.56
4:J:64:ALA:O	4:J:88:ARG:NH2	2.37	0.56
12:S:13:LEU:HD11	12:S:149:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:65:VAL:O	2:h:220:ARG:NH2	2.38	0.56
5:l:14:SER:OG	5:l:16:GLN:OE1	2.23	0.56
5:l:180:MET:HG3	5:l:181:GLU:HG3	1.87	0.56
11:r:127:SER:HB3	11:r:136:TYR:CE1	2.40	0.56
24:X:412:ASP:OD1	24:X:413:SER:N	2.38	0.56
25:Y:155:ASP:OD1	25:Y:156:LEU:N	2.38	0.56
26:Z:165:GLU:HB3	26:Z:168:GLU:HG2	1.87	0.56
29:B:398:ILE:HD12	29:B:426:VAL:HG23	1.88	0.56
8:O:146:MET:HE2	8:O:151:ALA:HA	1.86	0.56
11:R:38:ASN:HB2	11:R:39:PRO:HD2	1.86	0.56
13:T:112:ILE:O	13:T:123:GLY:N	2.35	0.56
14:k:52:LYS:HE3	14:k:54:ILE:HD11	1.87	0.56
5:l:82:ARG:O	5:l:86:ASN:ND2	2.34	0.56
15:f:560:LEU:HD21	15:f:798:THR:HA	1.87	0.56
15:f:775:THR:HA	15:f:873:LEU:HD11	1.86	0.56
26:Z:209:ARG:NH1	26:Z:213:GLU:OE1	2.38	0.56
30:C:198:LEU:HB2	35:C:501:ADP:H5'2	1.86	0.56
32:E:72:LYS:NZ	32:E:73:ALA:O	2.30	0.56
13:T:88:ILE:HG22	13:T:112:ILE:HD13	1.86	0.56
3:i:86:LEU:O	3:i:90:LEU:HD23	2.06	0.56
8:o:15:GLY:HA3	8:o:159:ILE:HD11	1.87	0.56
10:q:14:LEU:HD13	10:q:182:ILE:HG12	1.87	0.56
22:U:546:ARG:HE	22:U:771:PHE:HB3	1.70	0.56
25:Y:173:ASP:OD1	25:Y:174:TRP:N	2.32	0.56
30:C:229:ARG:O	30:C:231:VAL:N	2.39	0.56
30:C:260:GLU:HG2	30:C:262:GLY:H	1.70	0.56
31:D:88:VAL:HG12	32:E:80:VAL:H	1.70	0.56
2:H:15:PRO:HG2	2:H:18:LYS:HB2	1.86	0.56
9:P:138:VAL:HG21	9:P:146:MET:HB2	1.87	0.56
3:i:12:PHE:HE2	4:j:126:PRO:HD2	1.69	0.56
14:k:121:LEU:HD11	5:l:126:ARG:HH12	1.71	0.56
9:p:30:ILE:HG23	9:p:32:ALA:H	1.71	0.56
15:f:237:VAL:O	15:f:245:ASN:ND2	2.39	0.56
19:c:52:GLU:HG2	19:c:116:PRO:HD2	1.86	0.56
3:I:44:LEU:HD22	3:I:190:LEU:HD23	1.88	0.56
7:N:166:ARG:NH1	13:t:34:ALA:O	2.38	0.56
12:s:176:LYS:HE2	12:s:208:VAL:HG21	1.87	0.56
15:f:849:ALA:HB3	15:f:879:ARG:HD3	1.88	0.56
18:b:138:VAL:HB	18:b:160:LEU:HD13	1.88	0.56
31:D:370:ILE:HD12	31:D:408:LYS:HG3	1.88	0.56
33:F:123:VAL:HG22	33:F:133:PHE:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:148:CYS:SG	5:L:150:SER:OG	2.54	0.56
8:O:43:CYS:SG	8:O:98:LEU:HD12	2.45	0.56
5:l:34:ALA:O	5:l:62:LYS:NZ	2.39	0.56
17:a:51:ALA:O	17:a:86:GLN:NE2	2.36	0.56
25:Y:259:TYR:HB3	25:Y:274:SER:HB2	1.87	0.56
30:C:250:GLU:HG3	30:C:296:ASN:H	1.71	0.56
3:I:213:ILE:HG13	3:I:228:LEU:HB2	1.88	0.56
7:N:135:ILE:HD13	7:N:163:ALA:HB2	1.87	0.56
10:Q:4:LEU:HB2	10:Q:132:HIS:HB3	1.88	0.56
24:X:370:LEU:HD21	25:Y:306:GLN:HE21	1.71	0.56
30:C:71:SER:HB2	30:C:115:ALA:HB1	1.88	0.56
31:D:192:LYS:O	31:D:194:ILE:N	2.39	0.56
31:D:229:ARG:O	31:D:231:VAL:N	2.39	0.56
13:T:91:TRP:HE3	13:T:92:LEU:HD22	1.71	0.56
6:m:99:ARG:NH1	13:t:69:GLN:OE1	2.38	0.56
21:e:19:PHE:HB2	23:V:321:ALA:HA	1.87	0.56
22:U:405:THR:HG21	22:U:441:GLY:HA2	1.87	0.56
22:U:524:LYS:HD3	22:U:559:ARG:HE	1.71	0.56
29:B:107:MET:HG2	29:B:151:LEU:HD13	1.86	0.56
31:D:273:LYS:HZ2	32:E:251:ARG:HD3	1.70	0.56
31:D:303:VAL:HG23	31:D:305:VAL:HG23	1.88	0.56
2:H:100:VAL:HG13	9:P:93:ASN:HD22	1.71	0.55
9:P:27:ARG:NH1	9:P:180:VAL:O	2.39	0.55
11:R:141:ARG:HG3	10:q:142:ILE:HD12	1.88	0.55
7:n:59:VAL:HG11	7:n:83:PHE:CZ	2.41	0.55
15:f:60:VAL:O	15:f:105:LYS:NZ	2.34	0.55
17:a:33:LEU:HD13	18:b:18:ASN:HD22	1.69	0.55
30:C:231:VAL:HG21	30:C:269:VAL:HG22	1.88	0.55
30:C:274:LEU:O	30:C:278:ASN:ND2	2.34	0.55
33:F:85:THR:HG22	33:F:85:THR:O	2.05	0.55
33:F:197:GLU:OE2	33:F:350:ARG:NH2	2.39	0.55
4:J:173:GLU:HA	14:K:58:LEU:HD21	1.87	0.55
14:k:182:GLN:HB2	5:l:56:LEU:HD21	1.89	0.55
15:f:252:ALA:HB1	15:f:268:LEU:HD13	1.86	0.55
22:U:466:LYS:HZ2	22:U:496:LEU:HD22	1.71	0.55
22:U:545:LEU:HB3	22:U:577:ILE:HG21	1.88	0.55
22:U:833:LEU:HB2	29:B:73:LEU:HD12	1.88	0.55
29:B:112:LEU:O	29:B:147:GLY:N	2.31	0.55
30:C:78:ARG:HE	30:C:80:MET:HE3	1.71	0.55
33:F:226:TYR:HE1	33:F:351:LYS:HB2	1.71	0.55
1:G:196:GLU:HB3	1:G:242:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:177:ARG:NE	12:s:150:ASP:OD2	2.36	0.55
15:f:806:VAL:O	15:f:810:ILE:HG22	2.06	0.55
17:a:91:ASN:OD1	17:a:92:VAL:N	2.39	0.55
17:a:374:ILE:HD13	20:d:250:ALA:HB1	1.89	0.55
28:A:369:ARG:HB3	28:A:372:LEU:HD13	1.88	0.55
31:D:130:VAL:HG12	31:D:142:VAL:HG13	1.87	0.55
31:D:208:PRO:HB2	31:D:375:ILE:HD12	1.88	0.55
31:D:399:PHE:O	31:D:403:TYR:N	2.39	0.55
32:E:181:THR:N	35:E:501:ADP:O1B	2.31	0.55
14:K:200:ILE:HG22	14:K:241:ILE:HG23	1.89	0.55
19:c:57:MET:HA	19:c:72:VAL:HG23	1.88	0.55
22:U:536:ALA:HB1	22:U:578:LEU:HD21	1.88	0.55
23:V:125:ASN:HD22	23:V:159:LEU:HG	1.72	0.55
25:Y:79:ASP:HB3	25:Y:83:ARG:HH21	1.72	0.55
25:Y:286:TRP:CD1	25:Y:286:TRP:H	2.23	0.55
28:A:120:LYS:HE3	33:F:152:GLY:HA2	1.88	0.55
6:M:45:VAL:HG23	6:M:146:ALA:HB1	1.89	0.55
14:K:38:ILE:HD11	14:K:177:ALA:HB1	1.88	0.55
15:f:407:MET:HB3	15:f:440:ILE:HG12	1.87	0.55
20:d:132:TYR:HD1	20:d:160:ALA:HA	1.72	0.55
21:e:42:ASN:OD1	21:e:43:TRP:N	2.39	0.55
23:V:86:VAL:HG21	23:V:160:LEU:HD13	1.87	0.55
27:W:308:LEU:HD22	27:W:315:MET:HE3	1.89	0.55
2:H:34:PRO:HA	2:H:164:GLY:HA3	1.89	0.55
5:L:107:ARG:NH2	13:T:74:GLU:OE2	2.39	0.55
1:g:54:LYS:N	1:g:214:GLU:O	2.33	0.55
9:p:30:ILE:HG22	9:p:33:GLN:HG2	1.89	0.55
18:b:96:ALA:O	18:b:99:HIS:ND1	2.40	0.55
20:d:105:PHE:HE1	20:d:169:ILE:HG12	1.71	0.55
22:U:611:ASN:HB3	22:U:614:VAL:HG12	1.88	0.55
24:X:404:ILE:HG12	26:Z:262:LEU:HD21	1.89	0.55
29:B:338:ASP:HB3	29:B:341:LEU:HD23	1.88	0.55
32:E:376:ASP:HA	32:E:379:LYS:HD3	1.89	0.55
12:S:153:VAL:HG22	12:S:166:LEU:HD21	1.86	0.55
1:g:42:VAL:HG23	1:g:165:ALA:HB2	1.89	0.55
8:o:70:THR:O	8:o:72:ARG:NH1	2.39	0.55
19:c:26:ASP:H	19:c:176:GLN:HE21	1.53	0.55
25:Y:156:LEU:O	25:Y:160:ASN:ND2	2.40	0.55
27:W:94:ARG:HD2	27:W:94:ARG:O	2.07	0.55
27:W:98:LYS:H	27:W:98:LYS:HD2	1.72	0.55
27:W:99:GLN:NE2	27:W:139:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:113:ARG:HE	30:C:130:LYS:H	1.55	0.55
31:D:247:VAL:HG12	31:D:295:GLN:HG3	1.89	0.55
32:E:25:ARG:HE	33:F:55:MET:HE3	1.72	0.55
32:E:121:ASN:ND2	33:F:147:PRO:HD2	2.22	0.55
32:E:177:GLY:HA3	33:F:344:ARG:NH1	2.21	0.55
32:E:380:LEU:HB3	33:F:336:ASP:HB3	1.88	0.55
4:J:140:GLY:HA2	4:J:213:ARG:HH12	1.71	0.55
3:i:6:ASP:OD1	3:i:7:SER:N	2.39	0.55
5:l:72:ILE:HG21	5:l:88:MET:HE1	1.89	0.55
5:l:95:SER:HB2	5:l:103:LEU:HD12	1.87	0.55
5:l:157:ARG:HG3	6:m:59:GLU:OE2	2.05	0.55
17:a:251:LEU:HG	17:a:255:TRP:HE1	1.71	0.55
19:c:263:ASP:OD1	19:c:264:LYS:N	2.37	0.55
30:C:194:THR:HG1	30:C:356:GLY:H	1.52	0.55
31:D:261:ILE:HG22	31:D:306:LYS:HB3	1.89	0.55
6:M:15:SER:OG	6:M:19:ARG:N	2.40	0.55
8:O:45:GLY:HA2	8:O:98:LEU:HD13	1.89	0.55
14:k:203:LYS:HG3	14:k:210:LEU:HD21	1.89	0.55
15:f:669:GLU:HG2	29:B:49:LEU:HD23	1.89	0.55
15:f:675:PHE:HB3	15:f:690:VAL:HG13	1.89	0.55
25:Y:298:GLU:OE2	25:Y:302:HIS:NE2	2.40	0.55
28:A:410:LEU:O	28:A:414:ASN:ND2	2.39	0.55
30:C:272:THR:O	30:C:276:LEU:HD12	2.07	0.55
7:N:92:GLU:OE1	7:N:92:GLU:N	2.32	0.55
11:R:36:GLU:OE1	11:R:36:GLU:N	2.40	0.55
11:R:57:ARG:NH2	14:K:104:ASN:OD1	2.39	0.55
12:S:52:ILE:HG22	12:S:110:ILE:HG12	1.89	0.55
5:l:203:GLN:O	5:l:239:ARG:NH1	2.40	0.55
18:b:34:ASN:HB3	18:b:72:LEU:HD11	1.89	0.55
22:U:607:VAL:CB	31:D:68:LEU:HD11	2.37	0.55
24:X:410:VAL:HG23	24:X:411:VAL:HG13	1.89	0.55
26:Z:130:ASP:OD1	26:Z:131:LEU:N	2.36	0.55
30:C:46:GLN:OE1	31:D:69:LYS:N	2.40	0.55
31:D:162:VAL:HG21	31:D:214:MET:HE1	1.89	0.55
32:E:33:LEU:HD21	33:F:62:VAL:HG13	1.89	0.55
32:E:344:ARG:HD2	32:E:348:THR:OG1	2.06	0.55
2:H:66:GLU:OE1	2:H:91:ARG:NH2	2.41	0.54
12:S:170:ARG:HA	12:S:173:ARG:HE	1.71	0.54
7:n:20:THR:O	7:n:27:ALA:N	2.40	0.54
11:r:59:LEU:HD22	11:r:83:LEU:HD22	1.88	0.54
18:b:111:ALA:HB3	18:b:140:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:34:ASN:OD1	20:d:35:PHE:N	2.39	0.54
24:X:71:LYS:O	24:X:74:ARG:NH1	2.40	0.54
32:E:43:SER:OG	33:F:72:LYS:HG3	2.07	0.54
1:G:175:SER:HB3	1:G:205:VAL:HG21	1.88	0.54
8:O:37:ILE:HB	8:O:41:ILE:HG13	1.89	0.54
8:O:111:TYR:CE2	8:O:121:LYS:HB2	2.42	0.54
13:T:11:VAL:HG23	13:T:24:ALA:HB2	1.89	0.54
3:i:99:LEU:HD12	9:p:69:PHE:HB2	1.89	0.54
13:t:44:ARG:HG3	13:t:197:VAL:HG21	1.89	0.54
23:V:265:ASP:OD1	23:V:266:GLN:N	2.40	0.54
23:V:313:LEU:HD13	23:V:328:VAL:HG11	1.88	0.54
30:C:195:GLY:HA2	35:C:501:ADP:O3B	2.07	0.54
4:J:155:ALA:HB3	14:K:63:SER:HB2	1.89	0.54
5:L:44:ALA:HB1	5:L:144:ILE:HD11	1.88	0.54
11:r:144:SER:HB3	11:r:147:LEU:HG	1.88	0.54
22:U:108:TYR:OH	22:U:159:ARG:NH1	2.40	0.54
22:U:925:VAL:HG13	22:U:927:PRO:HD3	1.90	0.54
31:D:386:ALA:HB1	31:D:399:PHE:CE1	2.42	0.54
33:F:189:GLY:H	35:F:501:ADP:HN62	1.55	0.54
7:N:165:GLU:OE1	13:t:37:ARG:NH1	2.40	0.54
5:l:146:GLN:HG3	5:l:159:MET:HG2	1.89	0.54
7:n:90:TYR:HB3	7:n:94:LEU:HD23	1.89	0.54
14:K:68:VAL:HG11	14:K:93:ARG:HH22	1.72	0.54
15:f:56:LEU:HD12	15:f:98:PHE:HD2	1.73	0.54
15:f:607:LEU:O	15:f:610:GLN:HG3	2.08	0.54
15:f:720:GLU:HG2	15:f:724:ASN:HD21	1.73	0.54
22:U:633:CYS:HB3	22:U:659:CYS:SG	2.47	0.54
25:Y:27:SER:HB3	25:Y:59:LYS:HD3	1.88	0.54
28:A:209:PRO:HG3	33:F:405:MET:HG2	1.89	0.54
29:B:239:VAL:HA	29:B:242:GLN:HB2	1.89	0.54
29:B:282:VAL:HG12	29:B:284:ILE:HG23	1.90	0.54
32:E:201:SER:HB3	33:F:269:ARG:HH22	1.72	0.54
32:E:341:ALA:HB2	33:F:344:ARG:NE	2.22	0.54
4:j:173:GLU:HA	14:k:58:LEU:HD21	1.90	0.54
7:n:28:ASN:HD21	8:o:122:LEU:HD13	1.71	0.54
22:U:465:LEU:HD21	22:U:477:GLY:HA3	1.89	0.54
25:Y:236:LEU:HG	25:Y:240:VAL:HG22	1.89	0.54
31:D:172:ILE:HD12	31:D:334:PRO:HD2	1.89	0.54
32:E:60:VAL:O	32:E:95:GLY:N	2.30	0.54
32:E:258:MET:SD	32:E:262:ASN:ND2	2.81	0.54
9:P:33:GLN:OE1	11:r:134:TYR:OH	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:84:PRO:HB2	9:P:120:PHE:CD2	2.42	0.54
4:j:116:GLN:OE1	4:j:119:THR:OG1	2.26	0.54
7:n:40:ARG:HG2	7:n:103:TRP:HE3	1.72	0.54
24:X:360:ASP:OD1	24:X:361:VAL:N	2.40	0.54
29:B:316:LEU:HD13	29:B:347:ILE:HD12	1.90	0.54
5:L:46:LEU:HD21	5:L:135:ALA:HB2	1.90	0.54
1:g:53:GLN:HA	1:g:215:ILE:HG22	1.89	0.54
13:t:192:VAL:HG22	13:t:197:VAL:HG12	1.89	0.54
20:d:30:LEU:HD13	20:d:54:ILE:HD11	1.90	0.54
25:Y:294:TYR:HD1	25:Y:298:GLU:HB2	1.73	0.54
27:W:212:LYS:NZ	27:W:215:GLN:OE1	2.40	0.54
27:W:248:ARG:HA	27:W:251:TYR:HB3	1.90	0.54
29:B:232:LYS:N	35:B:501:ADP:O1A	2.41	0.54
30:C:289:ILE:C	30:C:290:LYS:HD3	2.33	0.54
31:D:240:LEU:HD13	31:D:284:GLU:HB3	1.90	0.54
32:E:33:LEU:HD23	33:F:62:VAL:HG13	1.90	0.54
33:F:138:GLY:H	33:F:159:LEU:HD11	1.72	0.54
1:G:69:LEU:HD11	1:G:216:GLU:HG2	1.89	0.54
2:H:22:ILE:HD12	2:H:152:SER:HB2	1.90	0.54
8:O:109:HIS:HB3	8:O:111:TYR:HE1	1.73	0.54
2:h:22:ILE:HD13	2:h:152:SER:HA	1.89	0.54
11:r:13:ILE:HG13	11:r:152:ALA:HB1	1.89	0.54
14:K:141:LEU:HD23	14:K:156:MET:HE3	1.90	0.54
15:f:325:GLN:O	15:f:329:ASN:ND2	2.37	0.54
22:U:843:GLU:HA	22:U:846:LYS:HG2	1.88	0.54
25:Y:46:ARG:NH1	25:Y:46:ARG:HA	2.23	0.54
2:H:147:PHE:HD2	2:H:155:TYR:HB2	1.72	0.54
12:s:4:PRO:O	13:t:100:ARG:NH2	2.40	0.54
17:a:138:VAL:O	17:a:142:LEU:HG	2.08	0.54
22:U:835:ILE:N	29:B:70:ASP:OD2	2.24	0.54
24:X:285:GLU:HA	24:X:288:LYS:HD2	1.89	0.54
25:Y:387:ILE:HD13	26:Z:276:ILE:HG22	1.89	0.54
26:Z:94:TRP:CZ3	26:Z:96:HIS:HB3	2.43	0.54
27:W:27:ARG:NH2	27:W:46:THR:OG1	2.40	0.54
27:W:112:VAL:HG21	27:W:147:LYS:HE2	1.89	0.54
30:C:87:VAL:HG11	30:C:116:LEU:HD11	1.90	0.54
4:J:160:ALA:HB1	4:J:168:VAL:HG13	1.90	0.54
8:O:112:SER:OG	8:O:120:ASP:OD1	2.23	0.54
5:l:50:LYS:HB2	5:l:59:HIS:HB3	1.88	0.54
6:m:119:VAL:HG13	6:m:131:PHE:HD2	1.73	0.54
8:o:37:ILE:HG23	8:o:60:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:782:HIS:CD2	15:f:789:SER:HB3	2.43	0.54
17:a:368:GLU:O	17:a:372:HIS:ND1	2.38	0.54
19:c:195:GLY:O	19:c:199:HIS:N	2.41	0.54
23:V:473:GLN:HB2	26:Z:260:VAL:HG21	1.88	0.54
31:D:218:ALA:O	31:D:220:ALA:N	2.34	0.54
33:F:310:MET:HE1	33:F:339:ASP:OD1	2.08	0.54
1:G:73:THR:HG22	1:G:76:ILE:HB	1.90	0.53
1:G:208:ILE:HG23	1:G:210:PHE:H	1.72	0.53
9:P:103:TYR:HA	10:Q:93:ARG:HH22	1.74	0.53
11:R:15:ALA:HB2	11:R:156:ALA:HB1	1.91	0.53
13:T:37:ARG:HD3	7:n:166:ARG:HH11	1.72	0.53
10:q:16:ALA:HB2	10:q:160:LEU:HD11	1.90	0.53
15:f:105:LYS:HZ3	15:f:109:ILE:HD11	1.73	0.53
20:d:146:GLY:N	23:V:440:LYS:HZ3	2.06	0.53
22:U:82:LEU:HG	22:U:129:ARG:HG3	1.90	0.53
22:U:519:VAL:HG23	22:U:520:MET:SD	2.48	0.53
23:V:207:ALA:HB1	23:V:211:TYR:CZ	2.43	0.53
23:V:245:ASP:OD1	23:V:246:GLY:N	2.40	0.53
25:Y:234:PRO:O	25:Y:236:LEU:N	2.38	0.53
26:Z:109:ASN:HD21	26:Z:121:LEU:HD21	1.73	0.53
28:A:123:VAL:HA	33:F:85:THR:O	2.08	0.53
32:E:69:PHE:HZ	32:E:89:LYS:HD2	1.72	0.53
1:G:37:LEU:HD11	1:G:81:THR:HA	1.90	0.53
6:m:164:ALA:HB3	6:m:173:LYS:HZ2	1.72	0.53
27:W:25:ASP:HA	27:W:65:ARG:HH22	1.72	0.53
28:A:205:GLY:O	28:A:207:GLU:N	2.41	0.53
30:C:160:GLU:OE1	30:C:313:ARG:NH2	2.41	0.53
30:C:196:LYS:N	35:C:501:ADP:O1B	2.42	0.53
31:D:388:ARG:O	31:D:398:ASP:HB3	2.08	0.53
32:E:64:LEU:HD23	32:E:68:LYS:HB3	1.90	0.53
32:E:234:GLU:OE1	33:F:311:LEU:HD13	2.07	0.53
4:J:204:LYS:HD2	4:J:222:PRO:HB3	1.89	0.53
9:P:138:VAL:HG11	9:P:146:MET:HB3	1.90	0.53
23:V:131:LEU:HD11	23:V:171:VAL:HG21	1.90	0.53
29:B:265:LYS:HE3	29:B:311:GLU:HG3	1.90	0.53
30:C:100:ASP:OD1	30:C:101:LYS:N	2.39	0.53
31:D:375:ILE:HG12	31:D:378:ILE:HG12	1.88	0.53
33:F:281:SER:H	33:F:326:VAL:HG22	1.73	0.53
8:O:173:ILE:HD12	8:O:190:THR:HB	1.90	0.53
12:s:1:ARG:HH11	12:s:2:PHE:H	1.57	0.53
12:s:174:LEU:O	12:s:178:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:472:HIS:O	15:f:478:ARG:NE	2.40	0.53
18:b:124:LEU:HD13	18:b:152:LYS:HB3	1.90	0.53
22:U:265:ILE:HD11	22:U:326:ILE:HG12	1.88	0.53
25:Y:16:ASP:HB3	25:Y:150:PHE:CE1	2.44	0.53
25:Y:300:ARG:NH1	25:Y:333:GLU:OE2	2.41	0.53
33:F:192:ASP:HA	33:F:195:ILE:HG12	1.89	0.53
33:F:226:TYR:CE1	33:F:351:LYS:HB2	2.43	0.53
1:G:50:ILE:HG23	1:G:141:ILE:HD13	1.90	0.53
2:H:113:ARG:O	2:H:117:VAL:HG23	2.08	0.53
3:I:7:SER:HB2	3:I:11:ILE:HD13	1.91	0.53
4:J:125:ARG:HG2	4:J:126:PRO:HD2	1.89	0.53
5:L:126:ARG:HD2	14:K:15:PHE:HE1	1.73	0.53
13:T:85:PRO:HB2	13:T:121:PHE:HD2	1.73	0.53
1:g:110:PRO:HG2	1:g:113:MET:HB2	1.91	0.53
1:g:131:MET:HE2	6:m:125:TYR:HE1	1.72	0.53
15:f:777:THR:HB	15:f:828:ARG:HD3	1.89	0.53
23:V:110:HIS:HB2	23:V:138:PRO:HD3	1.91	0.53
29:B:220:LYS:HB3	29:B:348:ASP:H	1.74	0.53
32:E:177:GLY:HA2	33:F:344:ARG:NH2	2.24	0.53
33:F:408:LEU:HD12	33:F:409:ARG:N	2.19	0.53
10:q:29:LYS:HG2	10:q:31:ASP:H	1.74	0.53
15:f:553:THR:HG23	15:f:554:TYR:CD1	2.44	0.53
17:a:205:LEU:O	17:a:271:LYS:NZ	2.40	0.53
20:d:171:LEU:HA	20:d:174:ILE:HG22	1.91	0.53
20:d:190:LEU:HA	20:d:221:ASN:HA	1.89	0.53
21:e:27:TRP:HB2	23:V:355:ARG:HB3	1.91	0.53
27:W:367:ALA:HA	27:W:415:PHE:CD2	2.44	0.53
29:B:96:ARG:HA	29:B:100:ASP:HB3	1.89	0.53
30:C:39:SER:HA	30:C:42:LEU:HD12	1.91	0.53
30:C:187:LEU:HD22	30:C:189:TYR:HD1	1.73	0.53
31:D:220:ALA:HB2	31:D:261:ILE:HD11	1.90	0.53
1:G:161:CYS:SG	1:G:162:GLY:N	2.82	0.53
1:g:44:GLY:N	1:g:47:CYS:O	2.33	0.53
3:i:112:THR:HG23	4:j:81:ARG:HD2	1.91	0.53
3:i:123:GLN:NE2	4:j:125:ARG:O	2.42	0.53
7:n:83:PHE:CD2	7:n:100:ILE:HG12	2.44	0.53
22:U:557:TYR:HA	22:U:589:ALA:HA	1.91	0.53
22:U:567:ILE:HG13	22:U:586:VAL:HB	1.90	0.53
23:V:376:ASN:ND2	23:V:399:ARG:HD3	2.24	0.53
27:W:51:GLU:OE2	27:W:93:ARG:NH1	2.42	0.53
29:B:123:VAL:HG11	29:B:159:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:258:LYS:O	29:B:307:ARG:NH1	2.42	0.53
29:B:317:ASP:OD1	29:B:346:ARG:NH1	2.42	0.53
31:D:359:ASP:HB3	31:D:395:LEU:HD23	1.89	0.53
1:G:80:MET:HE2	1:G:87:SER:HA	1.91	0.53
9:P:12:MET:HA	9:P:138:VAL:HG12	1.90	0.53
3:i:66:TYR:HB2	3:i:74:CYS:SG	2.49	0.53
8:o:93:TYR:O	9:p:99:ARG:NH2	2.41	0.53
8:o:173:ILE:HD11	8:o:190:THR:HB	1.89	0.53
12:s:175:VAL:HA	12:s:178:VAL:HG22	1.89	0.53
28:A:120:LYS:HD3	33:F:150:LEU:HA	1.91	0.53
5:L:156:CYS:HA	6:M:58:TYR:HA	1.89	0.53
6:M:136:MET:HB3	6:M:148:LEU:HD11	1.91	0.53
8:O:51:ASP:OD2	9:P:99:ARG:NH2	2.37	0.53
10:Q:147:TYR:HA	10:Q:151:ILE:HD11	1.89	0.53
13:T:193:THR:HG23	13:T:195:LYS:H	1.73	0.53
4:j:83:VAL:HG21	4:j:129:ILE:HD11	1.91	0.53
5:l:157:ARG:NE	5:l:176:MET:SD	2.81	0.53
6:m:169:ARG:HB2	6:m:173:LYS:HZ3	1.74	0.53
15:f:803:PHE:HA	15:f:806:VAL:CG1	2.33	0.53
17:a:103:LYS:HG3	17:a:104:VAL:HG23	1.91	0.53
19:c:237:HIS:HA	19:c:240:HIS:HB3	1.90	0.53
23:V:225:ASP:HB3	23:V:261:TYR:HE2	1.73	0.53
29:B:224:LEU:HB2	29:B:330:ALA:HA	1.90	0.53
29:B:262:ASP:HA	29:B:265:LYS:HD2	1.91	0.53
31:D:133:HIS:CB	31:D:136:SER:HB2	2.39	0.53
33:F:224:LEU:O	33:F:351:LYS:HA	2.09	0.53
6:M:192:GLU:O	6:M:196:ILE:HG12	2.09	0.53
4:j:56:GLU:OE2	4:j:60:ARG:NH2	2.42	0.53
15:f:313:GLU:HG3	15:f:316:ASP:HB2	1.90	0.53
15:f:337:LEU:HD21	15:f:871:PRO:HB2	1.91	0.53
18:b:13:SER:OG	18:b:16:MET:SD	2.59	0.53
29:B:231:GLY:O	29:B:234:LEU:HB2	2.09	0.53
8:O:215:LYS:HE2	8:O:215:LYS:HA	1.92	0.52
10:Q:58:GLU:O	10:Q:62:LYS:HG2	2.09	0.52
12:S:27:THR:OG1	12:S:192:ALA:HB3	2.09	0.52
3:i:69:ASN:ND2	3:i:71:ASP:OD1	2.37	0.52
14:k:83:ALA:HA	14:k:86:LYS:HE3	1.90	0.52
9:p:190:ILE:HA	9:p:195:ILE:HG22	1.91	0.52
15:f:430:ASP:OD1	16:x:74:LYS:NZ	2.38	0.52
15:f:610:GLN:HG2	22:U:832:VAL:HG11	1.90	0.52
23:V:339:LEU:O	23:V:408:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:171:LEU:HD13	24:X:210:LEU:HD13	1.90	0.52
32:E:64:LEU:HD13	32:E:70:ILE:HD11	1.91	0.52
33:F:73:ILE:HA	33:F:76:ASN:HB3	1.90	0.52
33:F:419:ASP:OD1	33:F:419:ASP:N	2.42	0.52
3:I:24:ALA:O	3:I:28:ILE:HG12	2.09	0.52
4:J:96:LEU:HA	10:Q:62:LYS:HE3	1.91	0.52
6:m:8:ASP:O	6:m:22:GLN:NE2	2.38	0.52
6:m:50:GLU:OE2	6:m:209:PHE:HB2	2.08	0.52
13:t:19:GLY:HA3	13:t:193:THR:HG22	1.90	0.52
15:f:674:THR:O	15:f:678:LEU:HG	2.09	0.52
22:U:16:GLU:HB2	22:U:19:LEU:HB2	1.92	0.52
22:U:183:LEU:HD22	22:U:187:LEU:HD22	1.91	0.52
22:U:378:CYS:HG	22:U:783:TYR:HH	1.52	0.52
22:U:378:CYS:SG	22:U:783:TYR:OH	2.66	0.52
22:U:607:VAL:CG2	31:D:68:LEU:HD21	2.31	0.52
25:Y:141:VAL:HG21	25:Y:168:ILE:HG21	1.91	0.52
26:Z:174:HIS:O	26:Z:177:ARG:CD	2.57	0.52
31:D:311:THR:HG21	31:D:317:LEU:HD11	1.91	0.52
32:E:33:LEU:HB2	32:E:37:THR:OG1	2.09	0.52
5:L:34:ALA:HA	5:L:162:GLY:HA3	1.91	0.52
6:M:140:TYR:HB3	6:M:216:VAL:HG22	1.91	0.52
12:S:25:SER:HB2	12:S:42:LYS:HB2	1.91	0.52
13:t:25:ASP:OD1	13:t:41:ARG:NH2	2.39	0.52
15:f:570:GLY:O	15:f:572:ALA:N	2.42	0.52
24:X:401:LEU:HB2	25:Y:365:GLN:HE22	1.73	0.52
29:B:232:LYS:C	29:B:235:LEU:H	2.17	0.52
30:C:199:LEU:HA	30:C:202:ALA:HB3	1.91	0.52
1:G:123:GLN:HA	1:G:126:THR:HG22	1.90	0.52
5:L:36:VAL:HG22	5:L:47:VAL:HB	1.90	0.52
8:O:54:MET:HG2	9:P:96:TYR:CE1	2.44	0.52
15:f:450:ILE:HG23	15:f:822:VAL:HG11	1.92	0.52
17:a:61:GLU:OE2	17:a:65:SER:OG	2.26	0.52
17:a:290:GLN:HG2	17:a:290:GLN:O	2.10	0.52
27:W:217:GLU:N	27:W:217:GLU:OE1	2.42	0.52
28:A:235:ALA:HB1	28:A:270:CYS:HA	1.90	0.52
2:H:222:THR:N	2:H:225:GLU:OE1	2.42	0.52
11:R:102:CYS:HB3	11:R:111:LEU:HG	1.89	0.52
2:h:93:LEU:HD13	2:h:113:ARG:HB3	1.92	0.52
10:q:4:LEU:HD11	10:q:45:LEU:HB3	1.90	0.52
19:c:148:ILE:HA	32:E:103:THR:HG23	1.91	0.52
28:A:80:LEU:HD21	29:B:99:VAL:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:370:ILE:HG23	31:D:408:LYS:HG3	1.91	0.52
32:E:117:PRO:HB2	33:F:147:PRO:CB	2.39	0.52
2:H:32:GLY:N	31:D:417:TYR:OH	2.42	0.52
3:I:35:LEU:HG	3:I:46:ALA:HB3	1.92	0.52
9:P:149:MET:HG2	9:P:170:ALA:HA	1.92	0.52
13:T:27:LEU:HD22	13:T:184:TYR:HB2	1.89	0.52
15:f:619:HIS:HA	29:B:87:PRO:HA	1.92	0.52
16:x:70:GLN:HA	16:x:73:GLN:HG2	1.92	0.52
20:d:25:ARG:HH21	20:d:50:LEU:HB2	1.75	0.52
22:U:685:GLN:HG2	22:U:725:MET:HG3	1.91	0.52
28:A:327:LEU:HB3	28:A:329:PRO:HD2	1.92	0.52
33:F:416:THR:HG22	33:F:417:HIS:HD2	1.74	0.52
1:G:205:VAL:HG12	1:G:206:LEU:HG	1.92	0.52
4:J:115:LYS:HD3	4:J:149:PRO:HA	1.91	0.52
9:P:189:ILE:HB	9:P:196:THR:HB	1.92	0.52
12:S:26:ASP:OD2	12:S:190:GLY:N	2.33	0.52
3:i:108:GLU:HA	3:i:148:TYR:HE2	1.75	0.52
14:k:121:LEU:HG	5:l:126:ARG:HH22	1.75	0.52
10:q:5:ILE:HD11	10:q:143:LEU:HD11	1.92	0.52
10:q:103:LEU:HG	10:q:132:HIS:CD2	2.45	0.52
23:V:168:GLN:NE2	23:V:190:ASP:OD2	2.37	0.52
23:V:212:TYR:O	23:V:216:ARG:HG2	2.10	0.52
24:X:137:TYR:HB3	24:X:146:ALA:HB2	1.92	0.52
30:C:32:GLN:CD	31:D:54:LEU:HG	2.35	0.52
31:D:391:ARG:HH22	31:D:397:LYS:HD2	1.75	0.52
1:G:106:GLY:HA3	8:O:77:VAL:HG12	1.92	0.52
2:H:106:PRO:HB2	2:H:110:LEU:HB2	1.91	0.52
9:P:122:CYS:SG	9:P:123:SER:N	2.82	0.52
13:T:67:LEU:HD11	13:T:88:ILE:HD12	1.90	0.52
1:g:163:PHE:HA	2:h:58:ASP:N	2.25	0.52
9:p:91:VAL:HG13	9:p:124:LEU:HD11	1.91	0.52
14:K:135:ARG:HG2	14:K:136:PRO:HD2	1.91	0.52
16:x:56:GLN:HE22	16:x:86:GLU:HA	1.75	0.52
19:c:225:TRP:CZ3	19:c:226:MET:HE3	2.45	0.52
23:V:225:ASP:OD1	23:V:226:VAL:N	2.43	0.52
27:W:227:TYR:O	27:W:231:ILE:HG23	2.10	0.52
32:E:381:GLU:HG3	33:F:336:ASP:HA	1.92	0.52
6:M:59:GLU:HG2	6:M:60:GLU:N	2.22	0.52
6:M:184:MET:HB3	6:M:188:ASP:OD1	2.10	0.52
2:h:160:ALA:HB1	2:h:174:LEU:HD13	1.92	0.52
14:k:117:SER:HB2	14:k:156:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:k:141:LEU:HB2	14:k:156:MET:HB3	1.92	0.52
11:r:33:LYS:HG3	11:r:45:MET:HG3	1.91	0.52
17:a:193:GLN:HB3	17:a:225:LEU:HD13	1.92	0.52
22:U:742:HIS:O	22:U:883:ARG:NE	2.43	0.52
29:B:274:ALA:HB1	29:B:280:SER:HB3	1.92	0.52
7:N:66:HIS:CE1	7:N:70:LEU:HD11	2.45	0.52
12:S:36:HIS:O	13:T:151:ARG:NH2	2.43	0.52
10:q:183:ILE:HD12	10:q:188:ILE:HG12	1.92	0.52
14:K:71:ASP:OD1	14:K:72:ALA:N	2.37	0.52
15:f:43:GLN:HE22	15:f:45:LEU:CD2	2.21	0.52
15:f:846:VAL:HG21	15:f:872:VAL:HG21	1.92	0.52
17:a:77:VAL:HA	17:a:80:ILE:HG12	1.92	0.52
30:C:42:LEU:HD11	31:D:62:LYS:HZ2	1.66	0.52
30:C:56:VAL:HG23	31:D:79:VAL:CB	2.39	0.52
33:F:75:GLU:O	33:F:79:LYS:HG2	2.09	0.52
4:J:192:ILE:C	4:J:194:ALA:H	2.18	0.51
4:j:212:ARG:HB2	4:j:215:GLN:HB2	1.92	0.51
17:a:350:LYS:HE2	26:Z:213:GLU:HA	1.92	0.51
27:W:52:LYS:HD3	27:W:55:ARG:NH2	2.24	0.51
32:E:33:LEU:HB3	32:E:37:THR:HG23	1.92	0.51
33:F:334:ARG:HB3	33:F:336:ASP:OD1	2.10	0.51
15:f:479:LEU:HD21	15:f:514:VAL:HA	1.90	0.51
15:f:844:VAL:HG12	15:f:882:LEU:HD13	1.92	0.51
22:U:593:SER:OG	22:U:595:ASN:OD1	2.28	0.51
23:V:167:LEU:O	23:V:171:VAL:HG23	2.10	0.51
23:V:225:ASP:HB3	23:V:261:TYR:CE2	2.45	0.51
28:A:274:PHE:HB2	28:A:319:MET:HG2	1.93	0.51
30:C:46:GLN:HE22	31:D:68:LEU:C	2.19	0.51
1:G:165:ALA:HB1	1:G:179:LEU:HD13	1.90	0.51
5:L:11:THR:HG23	6:M:129:ARG:HB3	1.91	0.51
9:P:12:MET:SD	9:P:167:ILE:HG13	2.51	0.51
13:T:50:MET:HE3	13:T:192:VAL:HB	1.92	0.51
1:g:224:ASN:O	1:g:226:LYS:N	2.43	0.51
2:h:222:THR:N	2:h:225:GLU:OE2	2.42	0.51
5:l:167:SER:HB2	5:l:197:GLU:HG2	1.93	0.51
8:o:38:SER:HB2	8:o:74:PRO:HG2	1.92	0.51
9:p:82:ILE:HG12	9:p:87:LEU:HB2	1.93	0.51
18:b:95:LEU:HB3	26:Z:69:PHE:CD1	2.45	0.51
23:V:490:SER:O	23:V:494:MET:HG2	2.09	0.51
11:R:57:ARG:HG2	14:K:101:PHE:HD1	1.75	0.51
14:k:235:GLU:HA	14:k:238:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:79:ASP:OD2	13:t:81:HIS:ND1	2.43	0.51
24:X:346:GLN:HA	24:X:384:VAL:HA	1.92	0.51
7:N:201:THR:OG1	13:t:38:ASN:ND2	2.43	0.51
9:P:203:ARG:NH2	9:P:205:ASP:OD2	2.43	0.51
13:T:142:GLY:HA2	13:T:176:LEU:HD21	1.93	0.51
4:j:37:GLY:HA2	4:j:181:ILE:HD12	1.93	0.51
14:k:210:LEU:HD23	14:k:210:LEU:H	1.75	0.51
22:U:218:GLN:HG3	22:U:222:PHE:CE2	2.45	0.51
22:U:492:ASP:OD1	22:U:493:VAL:N	2.43	0.51
25:Y:62:ASP:OD1	25:Y:63:TRP:N	2.43	0.51
26:Z:138:TYR:HE1	27:W:448:LYS:HD3	1.74	0.51
28:A:347:ASP:OD1	28:A:348:LEU:N	2.37	0.51
29:B:180:PRO:HD2	29:B:242:GLN:HB3	1.93	0.51
1:G:178:PHE:HA	1:G:181:LYS:HE2	1.92	0.51
4:J:150:SER:OG	4:J:151:GLY:N	2.44	0.51
15:f:551:LYS:HD2	15:f:586:PRO:HB2	1.92	0.51
15:f:597:VAL:HG11	15:f:612:LEU:HD11	1.93	0.51
15:f:670:MET:CG	29:B:71:TYR:HB3	2.40	0.51
19:c:163:ILE:HG23	19:c:199:HIS:HB3	1.91	0.51
21:e:59:GLU:HA	21:e:62:LYS:NZ	2.26	0.51
22:U:571:CYS:HA	22:U:579:ARG:HA	1.91	0.51
24:X:299:LEU:HD22	24:X:331:LEU:HD12	1.92	0.51
30:C:329:LEU:HD11	30:C:348:ALA:HB2	1.92	0.51
30:C:333:SER:HA	30:C:336:MET:HG2	1.91	0.51
32:E:117:PRO:HB2	33:F:147:PRO:CG	2.40	0.51
33:F:308:ARG:O	33:F:312:GLU:HG2	2.10	0.51
33:F:362:ARG:HD2	33:F:388:THR:HG22	1.92	0.51
4:J:98:VAL:HG13	11:R:78:ALA:HB1	1.92	0.51
10:Q:102:LEU:HD12	10:Q:118:MET:HE2	1.93	0.51
13:t:43:MET:HE2	13:t:64:LYS:HA	1.92	0.51
16:x:58:LEU:HD12	16:x:89:LEU:HD12	1.93	0.51
20:d:8:GLU:HB3	20:d:18:LYS:NZ	2.26	0.51
20:d:26:LEU:HD22	20:d:30:LEU:HD22	1.93	0.51
24:X:271:VAL:HB	24:X:288:LYS:HE2	1.92	0.51
25:Y:296:VAL:HB	25:Y:300:ARG:HH21	1.75	0.51
29:B:262:ASP:O	29:B:266:LEU:HG	2.11	0.51
31:D:397:LYS:HA	31:D:400:GLU:HG3	1.91	0.51
32:E:75:ASN:HD22	33:F:130:GLN:CA	2.23	0.51
33:F:389:ASP:N	33:F:389:ASP:OD1	2.40	0.51
4:J:158:ALA:HB1	4:J:172:LEU:HD13	1.92	0.51
7:n:199:VAL:HG13	7:n:201:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:52:LYS:NZ	14:K:64:ILE:O	2.43	0.51
15:f:612:LEU:HD22	15:f:653:ALA:HA	1.92	0.51
15:f:862:ILE:HG23	15:f:865:PHE:HE1	1.76	0.51
19:c:261:GLU:HB3	19:c:270:LEU:HD21	1.91	0.51
22:U:580:ARG:HD3	22:U:771:PHE:CZ	2.46	0.51
27:W:316:ARG:HG2	27:W:319:THR:HG23	1.93	0.51
33:F:187:ASP:HA	33:F:368:ILE:HG21	1.93	0.51
9:P:61:GLN:HB2	10:Q:85:ARG:CZ	2.41	0.51
12:S:188:TYR:CZ	8:o:24:MET:HE2	2.45	0.51
13:T:124:TYR:HE1	13:T:139:THR:HG22	1.76	0.51
1:g:37:LEU:HG	1:g:53:GLN:HE21	1.75	0.51
2:h:39:LYS:HD3	2:h:159:LYS:HA	1.92	0.51
6:m:14:PHE:HB3	6:m:18:GLY:HA2	1.93	0.51
15:f:405:HIS:CE1	15:f:813:LYS:HE2	2.46	0.51
20:d:105:PHE:HD1	20:d:169:ILE:HG21	1.76	0.51
22:U:717:ILE:HG13	22:U:731:ILE:HG12	1.92	0.51
23:V:440:LYS:HE3	23:V:443:ARG:HH21	1.75	0.51
25:Y:191:ILE:HD12	25:Y:293:ARG:HD2	1.92	0.51
26:Z:52:ASN:OD1	26:Z:53:SER:N	2.43	0.51
28:A:195:LEU:HD13	28:A:232:ARG:HD2	1.92	0.51
29:B:140:ASP:OD2	29:B:143:LEU:HB2	2.11	0.51
29:B:292:THR:HA	29:B:309:MET:HE3	1.92	0.51
31:D:323:ARG:HD3	31:D:326:ARG:HH21	1.76	0.51
7:N:81:SER:HA	7:N:84:LYS:HG2	1.92	0.51
9:P:101:GLY:O	10:Q:93:ARG:NH1	2.44	0.51
15:f:423:ASP:OD1	15:f:424:GLY:N	2.44	0.51
17:a:188:LEU:HD11	17:a:193:GLN:HG3	1.91	0.51
22:U:9:ILE:HB	22:U:44:LYS:HE3	1.93	0.51
23:V:219:GLU:HA	23:V:224:LEU:HB3	1.91	0.51
23:V:268:GLU:HB3	23:V:295:ILE:HD11	1.93	0.51
27:W:138:VAL:HG12	27:W:139:GLU:HG2	1.94	0.51
31:D:398:ASP:HA	31:D:401:LYS:HE3	1.91	0.51
6:M:52:LEU:HG	6:M:209:PHE:CE1	2.46	0.50
7:N:8:PHE:HE2	7:N:13:VAL:HG23	1.77	0.50
10:Q:16:ALA:HB2	10:Q:160:LEU:HD11	1.92	0.50
7:n:119:MET:HE2	13:t:6:VAL:HG22	1.93	0.50
15:f:698:SER:HB2	15:f:703:ARG:HH21	1.75	0.50
27:W:79:GLU:O	27:W:79:GLU:HG2	2.11	0.50
28:A:176:ASP:HA	28:A:227:ARG:HG2	1.93	0.50
29:B:249:ARG:NH1	30:C:275:GLU:OE2	2.44	0.50
31:D:245:ARG:HA	31:D:248:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:88:HIS:CD2	2:h:92:LYS:HE2	2.46	0.50
2:h:119:GLN:HB2	3:i:81:SER:OG	2.10	0.50
3:i:90:LEU:HD21	3:i:114:LEU:HD22	1.93	0.50
4:j:69:VAL:HG22	4:j:104:VAL:HG22	1.92	0.50
8:o:50:ALA:HB2	9:p:129:CYS:HB2	1.93	0.50
14:K:36:THR:HA	14:K:171:GLY:HA3	1.93	0.50
15:f:208:LEU:HD23	15:f:211:ILE:HD11	1.94	0.50
17:a:293:PHE:HB2	17:a:329:LYS:HG2	1.93	0.50
18:b:91:ARG:NH1	18:b:130:ARG:HD3	2.25	0.50
20:d:252:GLN:OE1	23:V:484:LEU:HB2	2.11	0.50
22:U:82:LEU:O	22:U:129:ARG:HD2	2.11	0.50
23:V:264:TYR:HD2	23:V:295:ILE:HG13	1.77	0.50
25:Y:128:TYR:HB2	25:Y:140:ILE:HD13	1.93	0.50
32:E:29:LEU:O	32:E:32:GLN:HG2	2.11	0.50
1:G:30:LYS:HA	1:G:33:ASN:HD22	1.77	0.50
9:P:82:ILE:HG12	9:P:87:LEU:HB2	1.94	0.50
1:g:175:SER:HA	1:g:205:VAL:HG21	1.93	0.50
2:h:177:ARG:HG3	2:h:190:THR:HG22	1.93	0.50
13:t:56:ASP:N	13:t:107:TRP:O	2.40	0.50
17:a:236:THR:HG21	17:a:253:THR:HG21	1.94	0.50
17:a:291:LEU:HB2	17:a:331:VAL:HB	1.93	0.50
22:U:457:ILE:HA	22:U:460:TYR:HE1	1.76	0.50
22:U:650:TYR:HB2	22:U:683:VAL:HA	1.93	0.50
23:V:482:PHE:O	23:V:486:ILE:HG12	2.11	0.50
27:W:98:LYS:HB3	27:W:139:GLU:HG3	1.94	0.50
30:C:329:LEU:HD23	30:C:359:VAL:HG13	1.92	0.50
32:E:360:ASP:N	32:E:360:ASP:OD1	2.45	0.50
12:S:24:ALA:HB1	12:S:193:LEU:HD11	1.93	0.50
1:g:88:ARG:NH1	6:m:113:ASP:OD1	2.45	0.50
14:K:210:LEU:HD21	14:K:241:ILE:HG21	1.93	0.50
15:f:471:LEU:O	15:f:471:LEU:HD23	2.11	0.50
15:f:653:ALA:O	15:f:657:ILE:HG12	2.11	0.50
17:a:41:VAL:HG12	17:a:79:ILE:HG21	1.92	0.50
27:W:205:ILE:HA	27:W:208:LYS:HG2	1.92	0.50
31:D:66:LYS:O	31:D:69:LYS:HG2	2.11	0.50
1:g:83:MET:HE3	1:g:84:THR:H	1.76	0.50
7:n:32:ASP:O	7:n:45:ARG:NH2	2.41	0.50
15:f:83:ARG:HD2	15:f:83:ARG:O	2.12	0.50
30:C:36:ASN:O	30:C:40:GLN:HG2	2.12	0.50
33:F:254:PRO:HD3	33:F:287:GLU:HB2	1.92	0.50
7:N:44:CYS:HB2	7:N:99:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:53:LEU:HB2	9:P:60:VAL:HG13	1.93	0.50
13:T:182:ARG:HH21	7:n:168:GLY:HA3	1.76	0.50
14:k:70:ILE:HD11	14:k:89:ILE:HD12	1.92	0.50
14:k:117:SER:OG	5:l:82:ARG:NH1	2.44	0.50
7:n:44:CYS:HB2	7:n:99:ILE:HB	1.94	0.50
8:o:166:ASP:OD1	8:o:168:GLY:N	2.44	0.50
11:r:182:ASP:OD1	11:r:183:GLY:N	2.43	0.50
28:A:217:PRO:HD2	28:A:344:SER:HB2	1.93	0.50
5:L:109:VAL:HA	5:L:112:ILE:HD12	1.94	0.50
8:O:161:ALA:O	8:O:165:ASN:ND2	2.45	0.50
10:Q:140:LEU:HB2	11:r:134:TYR:HE1	1.76	0.50
2:h:134:LEU:HB2	2:h:149:SER:OG	2.12	0.50
8:o:104:ASP:OD2	8:o:109:HIS:ND1	2.44	0.50
11:r:19:ARG:NH1	11:r:168:ALA:O	2.44	0.50
15:f:170:TRP:O	15:f:181:ARG:NH1	2.44	0.50
17:a:134:THR:O	17:a:138:VAL:HG23	2.11	0.50
22:U:580:ARG:NE	22:U:584:TYR:OH	2.44	0.50
22:U:700:GLU:HA	22:U:706:VAL:HB	1.94	0.50
23:V:486:ILE:HG21	26:Z:272:LEU:HA	1.94	0.50
29:B:189:GLY:HA3	29:B:360:THR:HG23	1.93	0.50
30:C:72:TYR:O	30:C:116:LEU:N	2.40	0.50
30:C:336:MET:HB2	31:D:194:ILE:O	2.11	0.50
32:E:39:GLN:HB3	33:F:73:ILE:HD12	1.94	0.50
1:G:70:PHE:HB3	1:G:95:ARG:HH12	1.76	0.50
3:I:90:LEU:HD13	3:I:114:LEU:HD22	1.94	0.50
7:N:116:MET:SD	7:N:116:MET:N	2.83	0.50
8:O:159:ILE:HG21	8:O:173:ILE:HG23	1.94	0.50
15:f:564:LEU:HD13	15:f:794:ALA:HB1	1.94	0.50
15:f:670:MET:HG3	29:B:71:TYR:HD2	1.76	0.50
17:a:338:PRO:HG3	26:Z:233:VAL:HG23	1.94	0.50
19:c:194:HIS:HD2	29:B:155:LYS:HD3	1.77	0.50
27:W:35:ALA:HB3	27:W:73:MET:HE1	1.93	0.50
31:D:107:THR:H	32:E:77:PRO:HB3	1.76	0.50
4:J:95:ARG:HG3	10:Q:62:LYS:HZ2	1.75	0.50
10:q:37:LYS:O	10:q:61:GLN:NE2	2.32	0.50
10:q:101:ASN:OD1	10:q:120:TYR:N	2.45	0.50
14:K:82:ILE:H	14:K:82:ILE:HD12	1.76	0.50
20:d:55:LEU:HD13	20:d:78:LEU:HA	1.93	0.50
25:Y:13:LYS:HA	25:Y:16:ASP:HB2	1.93	0.50
27:W:448:LYS:O	27:W:452:ILE:HG12	2.12	0.50
28:A:215:PHE:CE1	28:A:342:GLU:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:262:ASP:HA	29:B:265:LYS:HB2	1.94	0.50
32:E:198:VAL:O	32:E:232:MET:HA	2.12	0.50
8:O:8:TYR:CD1	8:O:13:VAL:HG23	2.47	0.49
9:P:123:SER:HB2	9:P:137:VAL:HB	1.94	0.49
1:g:163:PHE:CE2	1:g:166:THR:HG22	2.46	0.49
8:o:147:GLU:HG3	8:o:150:GLU:H	1.77	0.49
18:b:145:GLU:H	18:b:145:GLU:CD	2.20	0.49
23:V:392:TYR:HA	23:V:395:ILE:HB	1.94	0.49
24:X:132:ARG:NH1	24:X:135:SER:OG	2.44	0.49
27:W:152:ILE:HA	27:W:155:GLN:HE21	1.77	0.49
27:W:220:GLU:OE1	27:W:220:GLU:N	2.45	0.49
28:A:122:VAL:HB	33:F:87:PRO:HD2	1.94	0.49
31:D:352:MET:O	31:D:355:SER:N	2.45	0.49
33:F:224:LEU:HD21	33:F:335:VAL:HG23	1.94	0.49
7:N:4:MET:HB3	7:N:160:LEU:HD21	1.94	0.49
7:N:91:ARG:NH2	13:T:56:ASP:OD2	2.36	0.49
6:m:185:THR:O	6:m:189:ILE:HG12	2.12	0.49
6:m:195:LYS:O	6:m:199:ILE:HD12	2.12	0.49
12:s:64:LEU:O	12:s:68:ILE:HG12	2.13	0.49
22:U:457:ILE:HA	22:U:460:TYR:CE1	2.47	0.49
24:X:78:ASN:HB3	24:X:122:ARG:HH22	1.76	0.49
25:Y:236:LEU:HD12	25:Y:239:LYS:HB2	1.94	0.49
28:A:219:GLY:N	34:A:501:ATP:O2G	2.45	0.49
29:B:103:ARG:HG2	29:B:160:ILE:HB	1.94	0.49
29:B:223:ILE:HD11	29:B:347:ILE:HB	1.94	0.49
31:D:297:ASP:OD2	31:D:326:ARG:NH1	2.45	0.49
32:E:25:ARG:CG	33:F:55:MET:HE3	2.38	0.49
32:E:40:TYR:HB2	33:F:69:MET:SD	2.52	0.49
32:E:63:GLN:NE2	32:E:92:LEU:O	2.45	0.49
4:J:66:ASP:HB3	4:J:95:ARG:NH2	2.27	0.49
4:J:196:LEU:HD12	4:J:201:SER:HB2	1.94	0.49
8:O:147:GLU:OE1	8:O:149:GLU:N	2.44	0.49
6:m:173:LYS:O	6:m:177:GLU:HG2	2.12	0.49
13:t:136:SER:HB3	13:t:154:LEU:HD12	1.93	0.49
15:f:117:GLU:OE1	15:f:120:ARG:NH2	2.44	0.49
15:f:241:PRO:HG2	22:U:838:LYS:HG3	1.95	0.49
15:f:618:GLU:HB2	15:f:620:PHE:CD2	2.48	0.49
15:f:670:MET:HG2	29:B:71:TYR:HB3	1.94	0.49
15:f:682:GLY:HA3	15:f:686:LEU:HD23	1.94	0.49
29:B:154:HIS:CG	29:B:155:LYS:H	2.30	0.49
30:C:115:ALA:O	30:C:124:HIS:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:234:GLU:O	1:g:238:HIS:ND1	2.45	0.49
6:m:105:ASN:OD1	6:m:105:ASN:N	2.45	0.49
13:t:46:ASN:OD1	13:t:49:THR:N	2.43	0.49
15:f:608:LYS:O	15:f:612:LEU:HG	2.11	0.49
22:U:607:VAL:CG2	31:D:68:LEU:CD2	2.89	0.49
22:U:832:VAL:HB	22:U:836:THR:CB	2.42	0.49
23:V:348:PHE:HE1	23:V:357:LEU:HD12	1.76	0.49
27:W:55:ARG:NH1	27:W:96:GLN:HG3	2.28	0.49
29:B:110:GLY:HA3	29:B:125:THR:HA	1.94	0.49
8:O:163:ILE:HG12	8:O:170:GLY:HA2	1.95	0.49
10:Q:59:TYR:HE2	10:Q:87:ASN:HD21	1.60	0.49
16:x:56:GLN:NE2	16:x:85:MET:O	2.46	0.49
19:c:281:LYS:HZ2	19:c:282:ARG:HD3	1.78	0.49
26:Z:189:GLN:NE2	26:Z:193:ASN:OD1	2.46	0.49
29:B:232:LYS:HA	29:B:235:LEU:HB3	1.94	0.49
30:C:87:VAL:O	30:C:94:LYS:HA	2.13	0.49
32:E:43:SER:HA	33:F:76:ASN:ND2	2.27	0.49
32:E:159:PHE:O	32:E:163:GLY:N	2.41	0.49
33:F:357:PRO:HB2	33:F:362:ARG:HG3	1.93	0.49
9:P:149:MET:HE2	9:P:173:ASN:ND2	2.27	0.49
11:R:8:PHE:HE1	11:R:13:ILE:HG12	1.77	0.49
10:q:8:GLN:NE2	10:q:113:PRO:O	2.46	0.49
15:f:151:LEU:HD12	15:f:158:TYR:CE2	2.45	0.49
15:f:887:PHE:HB3	15:f:900:LEU:HB3	1.94	0.49
17:a:26:GLU:HA	17:a:29:TYR:CE2	2.48	0.49
20:d:78:LEU:HD22	20:d:102:ASN:ND2	2.27	0.49
27:W:14:VAL:HG23	27:W:58:SER:HB3	1.94	0.49
29:B:150:VAL:HG12	29:B:162:VAL:HG23	1.95	0.49
30:C:191:PRO:HG3	30:C:319:PRO:HG3	1.93	0.49
31:D:230:VAL:HG11	31:D:264:ILE:HG12	1.94	0.49
2:H:213:CYS:HB2	2:H:218:PHE:HD1	1.77	0.49
3:I:121:TYR:HA	3:I:127:LYS:HD2	1.94	0.49
1:g:43:ARG:HA	1:g:48:ALA:HA	1.94	0.49
20:d:76:ALA:O	22:U:7:GLY:N	2.45	0.49
22:U:696:ILE:HG22	22:U:737:LEU:HA	1.94	0.49
27:W:123:ARG:NH1	27:W:123:ARG:O	2.46	0.49
30:C:147:THR:OG1	30:C:150:MET:SD	2.68	0.49
31:D:370:ILE:CG2	31:D:408:LYS:HG3	2.43	0.49
32:E:77:PRO:HG2	32:E:79:TYR:CE1	2.48	0.49
5:L:238:GLU:HG2	5:L:240:PRO:HD3	1.94	0.49
10:Q:56:PHE:HE2	10:Q:102:LEU:HD11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:l:159:MET:SD	5:l:169:ARG:NH1	2.84	0.49
13:t:133:GLU:OE1	13:t:133:GLU:N	2.46	0.49
15:f:792:ALA:HB1	15:f:824:ALA:HA	1.95	0.49
18:b:70:ARG:HG3	18:b:71:ILE:HD12	1.95	0.49
19:c:49:VAL:HB	19:c:50:PRO:HD3	1.95	0.49
22:U:574:LYS:O	22:U:579:ARG:NH1	2.45	0.49
23:V:121:PHE:CZ	23:V:167:LEU:HD22	2.48	0.49
29:B:175:LYS:HG2	29:B:178:LYS:HD3	1.94	0.49
30:C:29:GLU:HG2	31:D:51:LEU:HD22	1.95	0.49
31:D:132:LEU:HB3	31:D:137:ASN:C	2.38	0.49
33:F:323:ASN:ND2	33:F:325:GLN:HG2	2.28	0.49
7:n:48:SER:HB2	7:n:51:ASP:HB2	1.95	0.49
7:n:135:ILE:HD13	7:n:163:ALA:HB2	1.95	0.49
10:q:9:GLY:HA3	10:q:12:TYR:CZ	2.48	0.49
13:t:138:ALA:HB3	13:t:147:GLN:HB2	1.95	0.49
15:f:244:GLU:O	15:f:248:LEU:HG	2.13	0.49
24:X:74:ARG:CG	24:X:75:PRO:HD3	2.43	0.49
24:X:339:ILE:HD11	24:X:387:ILE:HD11	1.95	0.49
28:A:179:GLY:H	28:A:353:HIS:CE1	2.30	0.49
31:D:143:LEU:HD13	32:E:64:LEU:CD1	2.43	0.49
33:F:151:VAL:HG13	33:F:163:THR:HA	1.94	0.49
33:F:183:GLU:HG2	33:F:235:LEU:HD22	1.95	0.49
33:F:221:LYS:NZ	33:F:321:GLN:HA	2.28	0.49
2:H:72:ILE:HG13	2:H:107:THR:HG23	1.93	0.49
5:L:93:LEU:HD21	12:S:73:LYS:HG2	1.95	0.49
6:M:107:PRO:HG2	6:M:110:HIS:HB3	1.95	0.49
10:Q:85:ARG:CD	10:Q:124:LEU:HB2	2.26	0.49
15:f:799:VAL:HG21	15:f:821:LEU:HD12	1.94	0.49
18:b:146:GLU:HG2	18:b:147:GLU:N	2.28	0.49
22:U:639:LEU:CD1	31:D:68:LEU:HD12	2.42	0.49
23:V:314:ARG:NH1	25:Y:378:ASN:O	2.45	0.49
31:D:412:GLN:O	31:D:412:GLN:NE2	2.45	0.49
2:H:150:ASP:OD1	2:H:153:GLY:N	2.32	0.48
2:H:152:SER:O	3:I:81:SER:OG	2.29	0.48
4:J:88:ARG:NH1	10:Q:70:ARG:HA	2.20	0.48
6:M:190:VAL:HG13	6:M:213:LEU:HD23	1.95	0.48
9:P:12:MET:HE3	9:P:150:CYS:SG	2.52	0.48
12:S:7:PHE:HZ	12:S:140:SER:HB2	1.77	0.48
5:l:97:PHE:O	13:t:94:ARG:NE	2.40	0.48
6:m:73:VAL:HG22	6:m:139:SER:HB2	1.94	0.48
15:f:86:THR:HB	15:f:155:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:419:LEU:HD22	15:f:822:VAL:HG12	1.94	0.48
15:f:887:PHE:HB3	15:f:900:LEU:HD12	1.96	0.48
18:b:53:THR:OG1	18:b:59:GLU:N	2.45	0.48
19:c:255:TYR:HE2	24:X:411:VAL:HG21	1.78	0.48
23:V:449:ALA:HA	23:V:458:VAL:HG13	1.94	0.48
29:B:153:ASN:HB3	29:B:160:ILE:HD12	1.95	0.48
30:C:140:VAL:HB	30:C:212:ILE:HG12	1.95	0.48
3:I:33:THR:HA	3:I:165:GLY:HA3	1.95	0.48
4:J:159:ASN:OD1	4:J:159:ASN:N	2.34	0.48
5:L:23:GLU:HA	5:L:26:MET:HE2	1.93	0.48
9:P:45:MET:HG3	9:P:87:LEU:HD11	1.95	0.48
9:P:118:LYS:HD3	9:P:119:PRO:HD2	1.95	0.48
10:Q:85:ARG:HD2	10:Q:124:LEU:H	1.78	0.48
11:R:8:PHE:CE1	11:R:13:ILE:HG12	2.48	0.48
11:R:158:ARG:O	11:R:162:GLN:HG2	2.13	0.48
12:S:194:ARG:NH1	12:S:205:GLU:OE1	2.46	0.48
1:g:122:SER:OG	1:g:156:PRO:O	2.31	0.48
15:f:136:GLU:HG3	15:f:137:ARG:H	1.78	0.48
15:f:219:LYS:HD3	15:f:258:LYS:NZ	2.28	0.48
15:f:683:GLU:CD	29:B:87:PRO:HB3	2.38	0.48
15:f:745:LEU:HA	15:f:748:LEU:HD12	1.95	0.48
22:U:217:CYS:SG	22:U:248:ILE:HG23	2.53	0.48
23:V:375:PHE:HA	23:V:378:VAL:HG22	1.94	0.48
26:Z:94:TRP:HE1	26:Z:109:ASN:CG	2.20	0.48
27:W:263:TRP:CZ2	27:W:295:LYS:HB3	2.47	0.48
30:C:215:SER:HA	30:C:249:ASP:HB2	1.96	0.48
30:C:400:SER:O	30:C:400:SER:OG	2.31	0.48
2:H:111:VAL:HA	2:H:114:VAL:HG12	1.95	0.48
10:Q:39:SER:OG	10:Q:40:GLU:N	2.45	0.48
1:g:122:SER:O	1:g:126:THR:HG23	2.13	0.48
3:i:190:LEU:O	3:i:194:ILE:HG13	2.14	0.48
7:n:179:ILE:HG13	7:n:184:VAL:HG23	1.95	0.48
20:d:31:LEU:HD11	22:U:19:LEU:HD12	1.94	0.48
22:U:21:GLU:O	22:U:25:HIS:ND1	2.46	0.48
23:V:475:ALA:O	23:V:478:GLN:NE2	2.40	0.48
33:F:253:GLY:HA3	33:F:286:ASP:O	2.14	0.48
4:J:42:VAL:HG12	4:J:210:VAL:HG22	1.93	0.48
11:R:52:CYS:O	11:R:56:GLU:HG2	2.13	0.48
2:h:43:GLY:HA3	2:h:184:LEU:HD21	1.95	0.48
14:k:70:ILE:HA	14:k:93:ARG:HG2	1.94	0.48
6:m:140:TYR:CZ	6:m:218:GLU:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:133:SER:HA	7:n:136:TYR:CE2	2.49	0.48
15:f:423:ASP:HB2	16:x:37:ASN:H	1.79	0.48
17:a:240:PHE:HE2	17:a:271:LYS:HE2	1.78	0.48
19:c:194:HIS:CD2	29:B:155:LYS:HD3	2.48	0.48
19:c:225:TRP:HA	26:Z:196:HIS:HD2	1.77	0.48
20:d:200:PHE:CG	20:d:205:LYS:HG2	2.48	0.48
22:U:552:ILE:O	22:U:585:THR:OG1	2.29	0.48
22:U:607:VAL:HB	31:D:68:LEU:HD11	1.95	0.48
25:Y:217:LYS:HE3	25:Y:253:LEU:HD21	1.95	0.48
25:Y:359:PRO:HG2	25:Y:364:TRP:HD1	1.77	0.48
31:D:370:ILE:HG22	31:D:372:GLY:N	2.27	0.48
32:E:148:VAL:HG13	32:E:149:ILE:HG13	1.95	0.48
33:F:120:LYS:O	33:F:136:VAL:HA	2.13	0.48
2:H:77:SER:OG	2:H:78:GLY:N	2.47	0.48
2:H:113:ARG:HH21	9:P:77:LYS:HB3	1.77	0.48
4:J:41:VAL:HG13	4:J:142:PRO:HB2	1.94	0.48
5:L:155:ASP:OD1	5:L:156:CYS:N	2.46	0.48
11:R:8:PHE:CE2	11:R:10:HIS:HB2	2.48	0.48
9:p:122:CYS:SG	9:p:123:SER:N	2.87	0.48
13:t:99:ARG:NH1	13:t:104:ASN:OD1	2.45	0.48
15:f:157:GLU:OE1	15:f:157:GLU:N	2.40	0.48
15:f:478:ARG:NH1	15:f:507:ASP:OD2	2.40	0.48
22:U:208:LEU:HD12	22:U:215:ASN:ND2	2.29	0.48
22:U:439:GLU:HB2	22:U:473:VAL:HG12	1.96	0.48
24:X:240:ASP:OD1	24:X:240:ASP:N	2.46	0.48
26:Z:255:ASP:HA	26:Z:258:VAL:HG22	1.94	0.48
27:W:148:THR:O	27:W:152:ILE:HG12	2.14	0.48
28:A:418:LYS:HG3	29:B:344:PRO:HG2	1.95	0.48
32:E:108:MET:SD	32:E:108:MET:N	2.78	0.48
2:H:33:ALA:N	31:D:417:TYR:OH	2.37	0.48
10:Q:118:MET:HE3	10:Q:122:ALA:HA	1.95	0.48
15:f:78:LEU:O	15:f:82:ILE:HG12	2.13	0.48
15:f:287:ASP:O	15:f:291:GLN:HG2	2.13	0.48
16:x:70:GLN:NE2	16:x:85:MET:SD	2.84	0.48
20:d:106:LEU:HG	20:d:111:ARG:HB3	1.94	0.48
22:U:802:TYR:CD1	22:U:892:LEU:HD11	2.49	0.48
22:U:834:SER:N	29:B:70:ASP:OD1	2.25	0.48
23:V:180:ARG:NH1	23:V:183:GLU:OE1	2.46	0.48
24:X:185:LYS:NZ	25:Y:244:ALA:HB3	2.28	0.48
27:W:220:GLU:HG2	27:W:221:LYS:H	1.78	0.48
29:B:224:LEU:HD23	29:B:351:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:197:THR:O	30:C:198:LEU:HG	2.14	0.48
6:M:106:ILE:HG12	6:M:111:LEU:HB2	1.96	0.48
7:N:39:ASP:OD1	7:N:39:ASP:N	2.45	0.48
8:O:171:SER:HB2	12:s:211:ARG:HH21	1.79	0.48
10:Q:19:ARG:HD3	10:Q:177:THR:HG23	1.96	0.48
11:R:12:VAL:HB	11:R:179:VAL:HB	1.95	0.48
13:T:214:MET:HE3	8:o:144:PRO:HB3	1.96	0.48
6:m:229:LYS:O	6:m:232:ARG:HB3	2.13	0.48
13:t:124:TYR:HB2	13:t:137:LEU:HD13	1.95	0.48
14:K:15:PHE:CD1	14:K:21:LEU:HB3	2.49	0.48
14:K:41:GLN:HB2	14:K:153:LEU:HB2	1.96	0.48
15:f:515:ALA:O	15:f:518:THR:OG1	2.31	0.48
18:b:22:LEU:HB2	18:b:23:PRO:HD3	1.96	0.48
20:d:93:ALA:O	20:d:97:GLN:NE2	2.46	0.48
22:U:179:TYR:CZ	22:U:183:LEU:HD11	2.49	0.48
22:U:347:ASN:HB3	22:U:813:TYR:CD1	2.49	0.48
22:U:378:CYS:HA	22:U:411:ILE:HA	1.95	0.48
22:U:507:VAL:HA	22:U:543:LYS:HD2	1.96	0.48
22:U:638:SER:HB2	30:C:43:ARG:HD2	1.95	0.48
22:U:658:ILE:HG12	22:U:763:VAL:HG11	1.96	0.48
22:U:833:LEU:HD23	29:B:69:LYS:HE3	1.96	0.48
24:X:285:GLU:OE2	24:X:288:LYS:NZ	2.45	0.48
25:Y:46:ARG:HA	25:Y:46:ARG:CZ	2.44	0.48
26:Z:174:HIS:HA	26:Z:177:ARG:CD	2.38	0.48
28:A:214:LEU:HB3	28:A:318:LEU:HD21	1.95	0.48
28:A:220:THR:O	28:A:223:THR:OG1	2.32	0.48
30:C:46:GLN:CG	31:D:65:GLN:O	2.56	0.48
30:C:53:ASN:OD1	31:D:75:ALA:HB3	2.14	0.48
30:C:168:PRO:HB3	30:C:183:PRO:HG2	1.95	0.48
31:D:132:LEU:HD23	31:D:139:LEU:HA	1.96	0.48
31:D:183:LEU:HD11	31:D:198:PRO:HB2	1.96	0.48
2:H:68:ILE:HD11	2:H:74:LEU:HD22	1.95	0.48
2:H:109:GLN:NE2	9:P:78:GLU:OE2	2.47	0.48
14:k:29:GLU:O	14:k:32:LYS:HG2	2.14	0.48
7:n:2:THR:H	7:n:17:ASP:HB3	1.78	0.48
7:n:187:GLN:OE1	7:n:187:GLN:N	2.47	0.48
11:r:97:MET:O	11:r:116:SER:N	2.45	0.48
15:f:505:MET:HE3	15:f:541:THR:HG21	1.96	0.48
15:f:677:HIS:HA	15:f:680:ARG:HB3	1.95	0.48
17:a:164:GLN:OE1	17:a:164:GLN:N	2.44	0.48
19:c:100:LYS:HA	19:c:105:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:722:ASP:OD1	22:U:723:ASP:N	2.43	0.48
23:V:228:ARG:HD3	23:V:257:ASN:ND2	2.29	0.48
26:Z:58:PHE:CE1	26:Z:68:TRP:HB2	2.49	0.48
27:W:117:ASP:CG	27:W:119:PRO:HD2	2.38	0.48
33:F:414:GLU:HG3	33:F:415:LEU:HG	1.94	0.48
33:F:427:VAL:HG23	33:F:428:GLN:HG3	1.96	0.48
3:I:90:LEU:HD22	3:I:114:LEU:HD22	1.96	0.48
10:Q:29:LYS:HE3	10:Q:32:HIS:HA	1.95	0.48
10:Q:56:PHE:CD2	10:Q:100:VAL:HG21	2.49	0.48
3:i:91:ARG:HD3	9:p:76:LEU:HB3	1.95	0.48
9:p:61:GLN:NE2	10:q:124:LEU:O	2.42	0.48
9:p:72:ASN:HA	9:p:75:GLU:HG2	1.96	0.48
15:f:99:LEU:HD23	15:f:106:LEU:HD11	1.96	0.48
15:f:343:LYS:HB3	15:f:381:VAL:HG11	1.96	0.48
15:f:459:CYS:O	16:x:79:GLY:N	2.46	0.48
15:f:840:LEU:HB3	15:f:842:VAL:HG23	1.96	0.48
23:V:111:TYR:CE2	23:V:115:LYS:HE2	2.49	0.48
25:Y:250:LEU:HD23	25:Y:257:ARG:HA	1.96	0.48
26:Z:17:LEU:HD23	26:Z:17:LEU:H	1.77	0.48
28:A:76:ALA:HA	28:A:80:LEU:HB2	1.95	0.48
29:B:125:THR:N	29:B:129:SER:O	2.47	0.48
29:B:178:LYS:HB2	29:B:246:THR:HG22	1.96	0.48
30:C:290:LYS:HD3	30:C:290:LYS:N	2.29	0.48
4:J:36:ARG:NH2	14:K:60:GLU:OE2	2.47	0.48
5:L:50:LYS:HD2	5:L:211:SER:HB2	1.94	0.48
6:M:186:CYS:O	6:M:190:VAL:HG23	2.14	0.48
7:N:133:SER:HA	7:N:136:TYR:CZ	2.49	0.48
8:O:98:LEU:HB2	8:O:113:ILE:HB	1.96	0.48
12:S:151:ASN:HD22	9:p:173:ASN:ND2	2.11	0.48
13:T:179:ARG:NH1	7:n:26:ILE:O	2.45	0.48
6:m:180:GLN:O	6:m:184:MET:HG2	2.14	0.48
14:K:199:LEU:HD12	14:K:210:LEU:HD22	1.96	0.48
19:c:37:ALA:HA	19:c:72:VAL:HG12	1.96	0.48
21:e:22:PHE:HZ	23:V:287:ARG:HG2	1.79	0.48
22:U:368:ALA:HB1	22:U:731:ILE:HB	1.96	0.48
23:V:407:VAL:HG22	23:V:422:ILE:HD11	1.95	0.48
25:Y:348:ASP:O	25:Y:352:GLU:N	2.46	0.48
25:Y:387:ILE:HD11	26:Z:279:LYS:HG3	1.96	0.48
26:Z:174:HIS:O	26:Z:177:ARG:HD3	2.14	0.48
27:W:375:MET:HE3	27:W:408:ARG:NH2	2.29	0.48
29:B:59:ARG:NH1	29:B:63:LEU:HB2	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:199:GLU:O	29:B:203:LEU:HG	2.14	0.48
31:D:406:VAL:O	31:D:408:LYS:NZ	2.44	0.48
32:E:171:LEU:HD23	32:E:298:LYS:HG3	1.96	0.48
1:G:230:LEU:HD23	1:G:234:GLU:HB3	1.96	0.47
3:I:91:ARG:HD3	9:P:76:LEU:HB3	1.96	0.47
11:R:58:LEU:HD12	11:R:61:ARG:HD3	1.94	0.47
13:T:100:ARG:HD3	13:T:128:LEU:HA	1.95	0.47
14:K:116:VAL:HG12	14:K:156:MET:HE2	1.94	0.47
15:f:166:VAL:HG13	15:f:184:LEU:HD23	1.94	0.47
20:d:105:PHE:HB2	20:d:166:PHE:CD2	2.48	0.47
22:U:63:VAL:HA	22:U:66:LYS:HB2	1.94	0.47
23:V:109:ASN:O	23:V:113:LEU:HD23	2.14	0.47
23:V:344:ASP:HB3	23:V:346:LEU:HD23	1.95	0.47
26:Z:136:GLU:HB3	27:W:448:LYS:HZ3	1.79	0.47
30:C:188:LEU:HB3	30:C:317:PHE:CE2	2.49	0.47
31:D:210:CYS:N	31:D:376:ASN:OD1	2.47	0.47
32:E:304:PRO:HG2	32:E:339:ASN:HA	1.96	0.47
12:s:1:ARG:NH1	12:s:2:PHE:H	2.11	0.47
14:K:22:PHE:C	14:K:24:VAL:H	2.23	0.47
15:f:128:VAL:HG11	15:f:154:TRP:CD1	2.49	0.47
15:f:137:ARG:HH22	15:f:172:GLU:HG3	1.78	0.47
19:c:172:HIS:CD2	19:c:173:GLU:H	2.32	0.47
22:U:580:ARG:HD3	22:U:771:PHE:HZ	1.78	0.47
22:U:701:ILE:HD13	22:U:809:SER:HA	1.95	0.47
24:X:342:PHE:HB3	24:X:345:VAL:HB	1.97	0.47
24:X:413:SER:O	24:X:417:LYS:HB2	2.14	0.47
27:W:407:ASP:O	27:W:411:GLY:N	2.46	0.47
29:B:230:THR:HG23	29:B:391:SER:HB2	1.95	0.47
30:C:56:VAL:CB	31:D:79:VAL:HG21	2.33	0.47
30:C:271:ARG:O	30:C:275:GLU:HG2	2.15	0.47
32:E:33:LEU:HD12	32:E:34:LYS:N	2.24	0.47
32:E:147:GLU:HG3	32:E:151:LEU:HG	1.97	0.47
33:F:152:GLY:N	33:F:162:GLU:O	2.46	0.47
2:H:45:VAL:HG22	2:H:212:ILE:HG22	1.96	0.47
2:H:83:TYR:HB2	2:H:132:VAL:HG21	1.97	0.47
4:J:90:GLU:HG3	4:J:110:TYR:CE1	2.50	0.47
5:L:99:PHE:HB2	13:T:87:ALA:HB1	1.96	0.47
10:Q:157:VAL:HG12	10:Q:161:ARG:HH12	1.79	0.47
12:S:46:LEU:HD12	12:S:72:LEU:HD12	1.95	0.47
13:T:92:LEU:O	13:T:96:MET:HG2	2.14	0.47
1:g:206:LEU:HD23	1:g:208:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:21:GLN:HG2	2:h:22:ILE:N	2.29	0.47
6:m:134:SER:HB2	6:m:153:PRO:HD3	1.96	0.47
10:q:85:ARG:HB2	10:q:118:MET:HE1	1.96	0.47
15:f:242:GLU:OE1	15:f:242:GLU:N	2.43	0.47
15:f:679:LEU:HD13	15:f:713:PHE:CD2	2.49	0.47
15:f:869:THR:HG23	15:f:871:PRO:HD2	1.96	0.47
20:d:144:MET:C	23:V:440:LYS:HZ1	2.22	0.47
24:X:194:ARG:HH21	24:X:214:SER:HB2	1.79	0.47
25:Y:379:ARG:O	25:Y:383:LEU:HG	2.15	0.47
29:B:236:ALA:O	29:B:239:VAL:HG22	2.14	0.47
9:P:58:THR:CA	10:Q:85:ARG:HH21	2.09	0.47
9:P:149:MET:HE2	9:P:173:ASN:HD22	1.80	0.47
1:g:127:GLN:NE2	2:h:128:ARG:O	2.48	0.47
2:h:45:VAL:HG22	2:h:212:ILE:HG22	1.97	0.47
3:i:194:ILE:HG12	3:i:236:LEU:HD23	1.96	0.47
4:j:87:ALA:O	4:j:90:GLU:HG2	2.13	0.47
14:k:206:MET:HG3	14:k:210:LEU:HB3	1.96	0.47
6:m:175:GLU:OE1	6:m:196:ILE:HD13	2.13	0.47
17:a:157:ASP:OD2	17:a:161:LYS:NZ	2.44	0.47
18:b:131:LEU:HD22	18:b:136:VAL:HG21	1.97	0.47
24:X:292:GLN:O	24:X:296:ASN:ND2	2.41	0.47
27:W:274:VAL:O	27:W:283:GLN:NE2	2.35	0.47
28:A:121:PHE:HA	33:F:87:PRO:O	2.14	0.47
28:A:368:ILE:HG23	28:A:370:PHE:HD2	1.80	0.47
29:B:200:SER:O	29:B:326:LYS:NZ	2.46	0.47
29:B:209:GLU:HA	29:B:212:GLU:HB3	1.96	0.47
32:E:72:LYS:HD3	32:E:78:ARG:CD	2.44	0.47
33:F:170:SER:HA	33:F:173:LYS:HE2	1.96	0.47
33:F:356:MET:N	33:F:356:MET:SD	2.87	0.47
3:I:25:MET:HG3	3:I:152:PRO:HD2	1.96	0.47
3:I:220:ASN:OD1	3:I:220:ASN:N	2.48	0.47
4:J:7:ILE:HG22	4:J:8:THR:H	1.80	0.47
15:f:469:TYR:O	15:f:481:SER:OG	2.28	0.47
19:c:220:LEU:HD13	26:Z:134:PRO:HA	1.94	0.47
19:c:277:LYS:HD2	19:c:282:ARG:HG2	1.95	0.47
20:d:229:GLN:HG3	20:d:231:LYS:HB2	1.95	0.47
27:W:413:ILE:HD12	27:W:415:PHE:CZ	2.49	0.47
28:A:121:PHE:CE1	28:A:123:VAL:HB	2.49	0.47
29:B:135:ILE:HG13	29:B:159:VAL:O	2.15	0.47
32:E:121:ASN:HD22	33:F:147:PRO:HD2	1.78	0.47
32:E:317:ALA:HA	32:E:320:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:GLN:HB3	1:G:150:GLN:HE21	1.80	0.47
6:M:41:CYS:HG	6:M:189:ILE:HG21	1.74	0.47
7:N:14:LEU:HD21	7:N:101:ALA:HB3	1.96	0.47
1:g:49:VAL:HG13	1:g:219:VAL:HG12	1.97	0.47
3:i:99:LEU:HD21	10:q:86:ARG:HE	1.79	0.47
14:k:121:LEU:HD12	14:k:123:PHE:HE1	1.80	0.47
5:l:152:ASN:HA	6:m:85:ARG:HH12	1.79	0.47
8:o:8:TYR:CE2	8:o:10:ASP:HB2	2.50	0.47
15:f:240:VAL:HG21	15:f:248:LEU:HD12	1.97	0.47
15:f:551:LYS:HG2	15:f:587:PHE:HB2	1.96	0.47
17:a:186:LYS:HA	17:a:193:GLN:HE22	1.80	0.47
21:e:27:TRP:HB2	23:V:355:ARG:H	1.79	0.47
22:U:243:LEU:HD21	22:U:915:LYS:HA	1.96	0.47
23:V:176:MET:HG3	23:V:217:VAL:HG22	1.96	0.47
25:Y:19:ILE:O	25:Y:23:ARG:HG3	2.15	0.47
26:Z:182:THR:HG22	26:Z:183:THR:N	2.29	0.47
28:A:194:PRO:HB3	28:A:208:PRO:HG3	1.97	0.47
33:F:62:VAL:O	33:F:66:LEU:N	2.47	0.47
2:H:107:THR:HB	2:H:140:ASN:CB	2.45	0.47
2:H:114:VAL:O	2:H:118:MET:HG2	2.15	0.47
3:I:45:LEU:HD13	3:I:75:SER:OG	2.14	0.47
3:I:114:LEU:O	3:I:117:ILE:HG22	2.15	0.47
5:L:66:VAL:C	12:S:77:HIS:HE2	2.23	0.47
5:L:94:ASP:O	5:L:98:VAL:HG22	2.14	0.47
6:M:4:GLY:HA3	33:F:299:GLU:H	1.77	0.47
6:M:66:LEU:HD13	6:M:214:SER:HB2	1.97	0.47
6:M:74:GLY:HA3	6:M:224:HIS:CE1	2.50	0.47
8:O:164:PHE:HZ	8:O:192:PRO:HB2	1.80	0.47
11:R:122:SER:OG	11:R:123:GLY:N	2.47	0.47
1:g:18:PRO:HA	2:h:24:TYR:CE1	2.50	0.47
5:l:158:ALA:HB1	5:l:172:LEU:HD22	1.97	0.47
6:m:215:TRP:CE3	6:m:227:VAL:HG22	2.50	0.47
6:m:215:TRP:CZ3	6:m:227:VAL:HG22	2.49	0.47
9:p:30:ILE:HG13	9:p:31:GLN:H	1.80	0.47
10:q:41:LYS:NZ	10:q:185:LYS:O	2.47	0.47
11:r:103:GLY:HA2	11:r:179:VAL:HG11	1.97	0.47
15:f:333:LEU:HD13	15:f:871:PRO:HB3	1.96	0.47
17:a:159:SER:OG	17:a:175:ASP:OD2	2.28	0.47
19:c:211:GLU:C	19:c:213:GLU:H	2.21	0.47
21:e:27:TRP:HA	23:V:355:ARG:NE	2.25	0.47
22:U:374:SER:OG	22:U:407:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:405:THR:OG1	22:U:445:ALA:HB2	2.14	0.47
22:U:550:VAL:HG22	22:U:768:GLN:HE22	1.80	0.47
22:U:558:GLY:H	22:U:589:ALA:HA	1.80	0.47
22:U:633:CYS:CB	22:U:659:CYS:SG	3.03	0.47
23:V:372:LEU:HA	23:V:399:ARG:CZ	2.45	0.47
23:V:407:VAL:HG21	23:V:437:ILE:HG21	1.97	0.47
23:V:487:HIS:O	23:V:490:SER:OG	2.25	0.47
24:X:190:LEU:HD21	24:X:214:SER:HA	1.96	0.47
24:X:271:VAL:HG11	24:X:288:LYS:HG2	1.96	0.47
26:Z:34:ARG:HH21	26:Z:102:HIS:HE2	1.61	0.47
27:W:44:ILE:O	27:W:48:LEU:HG	2.14	0.47
27:W:148:THR:OG1	27:W:168:GLU:OE1	2.33	0.47
27:W:236:HIS:HD1	27:W:237:GLU:CD	2.21	0.47
33:F:191:LEU:O	33:F:195:ILE:HG23	2.14	0.47
33:F:344:ARG:HB3	33:F:347:ARG:HB2	1.97	0.47
2:H:233:ILE:O	24:X:87:ARG:NH1	2.44	0.47
5:L:4:ASN:O	5:L:6:TYR:N	2.45	0.47
2:h:11:THR:OG1	2:h:122:THR:O	2.29	0.47
6:m:71:ARG:NH1	6:m:99:ARG:HE	2.13	0.47
8:o:186:LEU:HD23	8:o:189:TYR:HD1	1.80	0.47
15:f:263:PRO:HB2	15:f:891:THR:HB	1.97	0.47
15:f:834:ASP:HB3	15:f:840:LEU:HD11	1.97	0.47
17:a:194:GLN:NE2	17:a:225:LEU:O	2.43	0.47
18:b:18:ASN:ND2	18:b:25:ARG:HH12	2.13	0.47
19:c:46:ARG:HH11	32:E:104:THR:HG22	1.79	0.47
19:c:52:GLU:O	19:c:77:GLN:NE2	2.48	0.47
19:c:257:LYS:O	19:c:261:GLU:HG2	2.15	0.47
20:d:41:THR:HG22	20:d:44:THR:H	1.80	0.47
20:d:76:ALA:HB3	22:U:10:SER:HB2	1.96	0.47
22:U:54:PHE:CE2	22:U:56:SER:HB3	2.50	0.47
27:W:317:TRP:HB3	27:W:358:VAL:HG21	1.97	0.47
28:A:229:VAL:O	28:A:232:ARG:HG2	2.15	0.47
29:B:139:VAL:HG23	29:B:144:LEU:HD11	1.97	0.47
3:I:78:GLY:HA3	3:I:132:VAL:HA	1.96	0.47
11:R:137:GLY:HA2	10:q:166:GLU:CD	2.40	0.47
13:T:107:TRP:O	13:T:108:ASN:ND2	2.48	0.47
1:g:47:CYS:SG	1:g:221:THR:HG22	2.55	0.47
2:h:203:MET:HB2	2:h:208:ILE:HD11	1.97	0.47
2:h:223:PRO:HA	2:h:226:VAL:HB	1.96	0.47
3:i:3:ARG:HA	4:j:5:ARG:HH22	1.80	0.47
11:r:8:PHE:HE2	11:r:10:HIS:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:s:10:GLY:HA3	12:s:42:LYS:HE2	1.97	0.47
13:t:21:VAL:HG23	13:t:191:THR:HG22	1.97	0.47
14:K:200:ILE:HG23	14:K:241:ILE:HD12	1.95	0.47
15:f:673:ARG:HH22	28:A:59:ILE:HG13	1.80	0.47
15:f:886:GLU:HB3	15:f:906:TYR:CD2	2.48	0.47
22:U:135:ASN:HA	22:U:138:PHE:CE2	2.50	0.47
22:U:751:ARG:H	22:U:751:ARG:HD2	1.80	0.47
27:W:294:LYS:HD3	27:W:294:LYS:N	2.30	0.47
29:B:187:ILE:HG13	35:B:501:ADP:C6	2.50	0.47
1:G:40:VAL:HG13	1:G:179:LEU:HD11	1.97	0.47
4:J:20:GLU:O	4:J:24:GLU:HG2	2.15	0.47
7:N:162:LEU:HD11	7:N:197:PHE:CD1	2.50	0.47
1:g:43:ARG:HG2	1:g:164:LYS:O	2.15	0.47
6:m:151:ILE:HG12	6:m:157:SER:HB2	1.97	0.47
15:f:163:ALA:HB1	15:f:207:LEU:HD22	1.97	0.47
15:f:602:GLY:HA3	15:f:788:MET:HE1	1.96	0.47
17:a:77:VAL:HG21	17:a:110:ALA:HB1	1.96	0.47
28:A:148:GLN:HB2	28:A:150:HIS:CE1	2.50	0.47
32:E:55:GLN:HE22	32:E:109:ARG:NH1	2.12	0.47
3:I:240:HIS:O	3:I:244:GLU:HG2	2.15	0.46
4:j:65:LEU:HD13	4:j:88:ARG:HG3	1.97	0.46
9:p:107:PRO:HD2	9:p:124:LEU:HB2	1.97	0.46
13:t:91:TRP:CE3	13:t:92:LEU:HD22	2.46	0.46
15:f:127:SER:HA	15:f:139:CYS:HA	1.96	0.46
25:Y:157:ILE:HA	25:Y:160:ASN:HD21	1.79	0.46
28:A:411:GLU:HA	28:A:414:ASN:HD21	1.79	0.46
31:D:88:VAL:HA	32:E:80:VAL:HB	1.96	0.46
31:D:106:THR:HG21	32:E:78:ARG:CD	2.41	0.46
32:E:75:ASN:HD22	33:F:130:GLN:N	2.12	0.46
32:E:352:MET:HA	32:E:355:ILE:HB	1.97	0.46
33:F:132:TYR:CD2	33:F:158:TYR:HB3	2.50	0.46
5:L:56:LEU:HD11	14:K:182:GLN:HA	1.97	0.46
5:L:82:ARG:NH2	14:K:117:SER:OG	2.48	0.46
6:M:7:TYR:CD2	6:M:16:PRO:HD3	2.51	0.46
7:N:66:HIS:O	7:N:69:GLU:HG2	2.15	0.46
9:P:73:LEU:O	9:P:77:LYS:HG2	2.15	0.46
10:Q:19:ARG:NH1	10:Q:193:ASN:HD22	2.14	0.46
10:Q:81:ALA:HA	10:Q:104:LEU:HD13	1.96	0.46
6:m:71:ARG:HH11	6:m:105:ASN:HB3	1.80	0.46
15:f:604:GLY:HA2	15:f:661:ALA:HB2	1.97	0.46
19:c:75:MET:HG2	19:c:91:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:c:251:LEU:HD21	19:c:283:HIS:CG	2.50	0.46
25:Y:39:ASP:HA	25:Y:42:MET:HE3	1.98	0.46
31:D:278:GLN:H	31:D:278:GLN:CD	2.23	0.46
31:D:368:ASP:C	31:D:370:ILE:HG12	2.40	0.46
3:I:13:SER:HG	3:I:17:ARG:H	1.58	0.46
6:M:160:TYR:CG	6:M:163:CYS:HB2	2.50	0.46
2:h:9:SER:HA	2:h:125:GLY:HA2	1.97	0.46
14:k:202:LEU:O	14:k:206:MET:HG2	2.16	0.46
8:o:34:ILE:HG22	8:o:42:TYR:HD2	1.79	0.46
15:f:612:LEU:HB3	15:f:653:ALA:HB1	1.97	0.46
15:f:698:SER:OG	15:f:701:ASN:HB3	2.16	0.46
15:f:783:SER:HB2	15:f:787:LEU:HD13	1.96	0.46
17:a:211:PHE:O	17:a:339:ARG:NH1	2.48	0.46
17:a:318:GLY:HA2	17:a:321:LYS:HD3	1.96	0.46
19:c:52:GLU:HB3	19:c:113:HIS:CE1	2.49	0.46
19:c:104:ARG:HB2	26:Z:25:ARG:HD2	1.98	0.46
22:U:835:ILE:HG22	29:B:70:ASP:OD2	2.15	0.46
27:W:136:ILE:O	27:W:141:GLU:HB3	2.14	0.46
27:W:387:ASP:O	27:W:390:GLU:HG2	2.15	0.46
29:B:395:ILE:HD13	29:B:398:ILE:HD11	1.96	0.46
2:H:42:ASN:HB2	2:H:185:GLU:HB2	1.97	0.46
4:J:146:GLN:HG3	4:J:161:ILE:HG13	1.97	0.46
11:R:180:ARG:HH11	11:R:185:ILE:HG21	1.81	0.46
13:T:16:PHE:CE2	13:T:21:VAL:HG23	2.50	0.46
3:i:67:LYS:HE2	3:i:225:ILE:HD12	1.97	0.46
4:j:86:ARG:HG2	4:j:114:LEU:HD22	1.98	0.46
6:m:158:TYR:HB2	6:m:160:TYR:HE1	1.80	0.46
15:f:180:GLN:C	15:f:183:PRO:HD2	2.40	0.46
17:a:177:LEU:HD21	17:a:216:LEU:HB3	1.97	0.46
19:c:255:TYR:CD1	19:c:280:PRO:HG3	2.50	0.46
22:U:179:TYR:O	22:U:183:LEU:HG	2.15	0.46
22:U:832:VAL:HB	22:U:836:THR:HB	1.97	0.46
25:Y:377:LEU:HA	25:Y:380:VAL:HG22	1.97	0.46
28:A:38:GLN:HB3	28:A:42:SER:OG	2.15	0.46
28:A:120:LYS:HB2	33:F:90:VAL:HG12	1.97	0.46
28:A:164:MET:HE1	28:A:241:ILE:HD13	1.97	0.46
28:A:397:ILE:HG21	29:B:211:TYR:HB3	1.96	0.46
28:A:408:ASP:OD1	28:A:409:PHE:N	2.47	0.46
32:E:177:GLY:HA3	33:F:344:ARG:CZ	2.46	0.46
4:J:69:VAL:HG22	4:J:104:VAL:HG12	1.96	0.46
4:J:99:GLU:HG3	11:R:81:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:17:ASP:OD2	7:N:171:GLY:N	2.49	0.46
11:R:1:THR:N	11:R:169:TYR:O	2.49	0.46
11:r:184:TRP:HZ3	11:r:186:ARG:HG3	1.80	0.46
12:s:148:LEU:HD23	12:s:178:VAL:HG12	1.97	0.46
18:b:136:VAL:HG12	18:b:138:VAL:HG23	1.96	0.46
22:U:720:LYS:HA	22:U:727:LYS:HD2	1.97	0.46
24:X:369:ILE:HD12	24:X:374:PHE:HD2	1.80	0.46
27:W:263:TRP:CH2	27:W:295:LYS:HB3	2.51	0.46
28:A:411:GLU:HG3	28:A:415:LYS:HE2	1.98	0.46
30:C:66:LEU:HD12	30:C:66:LEU:O	2.16	0.46
30:C:336:MET:HA	31:D:195:GLY:HA3	1.97	0.46
30:C:371:LEU:HD11	31:D:187:HIS:HB3	1.96	0.46
32:E:328:TYR:HA	32:E:331:ILE:HD12	1.97	0.46
32:E:344:ARG:NH2	33:F:345:SER:O	2.49	0.46
12:S:21:ALA:HB3	12:S:198:VAL:HB	1.98	0.46
3:i:27:ALA:HA	3:i:30:HIS:ND1	2.30	0.46
14:k:163:VAL:HA	5:l:60:GLN:CD	2.40	0.46
10:q:4:LEU:HD23	10:q:132:HIS:HD2	1.81	0.46
18:b:92:VAL:HG12	26:Z:68:TRP:H	1.80	0.46
18:b:100:ARG:HE	18:b:101:GLN:N	2.14	0.46
22:U:693:LEU:HD12	22:U:696:ILE:HD13	1.97	0.46
27:W:300:PRO:HA	27:W:303:LYS:HE2	1.97	0.46
27:W:451:MET:O	27:W:455:LEU:HG	2.16	0.46
28:A:302:LEU:O	28:A:306:LEU:HG	2.16	0.46
28:A:331:LEU:C	28:A:334:PRO:HD2	2.41	0.46
30:C:250:GLU:OE2	30:C:296:ASN:ND2	2.49	0.46
30:C:265:GLY:O	30:C:268:GLU:HG3	2.16	0.46
33:F:223:VAL:HG22	33:F:350:ARG:HB2	1.98	0.46
4:J:66:ASP:OD1	4:J:92:GLN:NE2	2.49	0.46
4:J:210:VAL:N	4:J:218:LYS:O	2.49	0.46
8:O:159:ILE:O	8:O:163:ILE:HG13	2.16	0.46
11:R:21:THR:HG21	11:R:169:TYR:HD1	1.79	0.46
1:g:132:ARG:HB2	6:m:12:SER:HA	1.97	0.46
1:g:155:ASP:OD2	1:g:158:GLY:N	2.47	0.46
4:j:88:ARG:CZ	10:q:70:ARG:HA	2.46	0.46
13:t:1:THR:N	13:t:105:PRO:O	2.38	0.46
14:K:16:SER:HG	14:K:20:ARG:H	1.62	0.46
19:c:148:ILE:HG22	32:E:103:THR:CG2	2.46	0.46
19:c:195:GLY:HA3	19:c:199:HIS:CE1	2.50	0.46
22:U:552:ILE:HB	22:U:581:SER:OG	2.16	0.46
26:Z:192:THR:O	26:Z:196:HIS:ND1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:327:GLU:HG2	27:W:337:ALA:HB1	1.98	0.46
27:W:356:ASN:O	27:W:359:VAL:N	2.46	0.46
28:A:105:ASP:HA	28:A:111:TYR:HA	1.96	0.46
30:C:56:VAL:HG21	31:D:79:VAL:HG21	0.63	0.46
32:E:36:LEU:O	32:E:37:THR:C	2.57	0.46
33:F:388:THR:HG22	33:F:388:THR:O	2.15	0.46
1:G:83:MET:HE1	1:G:132:ARG:HH21	1.79	0.46
2:H:51:LYS:HE2	2:H:200:GLU:HG3	1.98	0.46
10:Q:56:PHE:O	10:Q:60:ILE:HG12	2.16	0.46
12:S:94:THR:HG21	14:K:102:THR:HA	1.98	0.46
2:h:196:LYS:HB3	2:h:203:MET:SD	2.56	0.46
8:o:51:ASP:HB3	8:o:94:ILE:HG23	1.98	0.46
14:K:184:VAL:HG21	14:K:201:ILE:HD11	1.98	0.46
15:f:267:ARG:HG3	15:f:787:LEU:HD11	1.98	0.46
15:f:446:LEU:HD13	15:f:483:PHE:HB3	1.97	0.46
15:f:646:MET:O	15:f:649:HIS:ND1	2.47	0.46
17:a:136:GLU:O	17:a:140:GLU:HG3	2.16	0.46
17:a:156:TYR:HB3	17:a:179:PHE:HB2	1.98	0.46
27:W:372:ARG:NH1	27:W:414:ASN:HB3	2.31	0.46
31:D:88:VAL:O	31:D:132:LEU:N	2.32	0.46
6:M:134:SER:HB2	6:M:153:PRO:HD3	1.97	0.46
12:S:113:LEU:HD23	12:S:198:VAL:HG12	1.98	0.46
3:i:72:MET:HG3	3:i:137:ILE:O	2.16	0.46
5:l:67:ASP:OD1	5:l:68:ASN:N	2.48	0.46
10:q:106:GLY:O	10:q:114:ALA:N	2.43	0.46
11:r:102:CYS:HB3	11:r:111:LEU:HD13	1.98	0.46
14:K:38:ILE:HD12	14:K:202:LEU:HD22	1.98	0.46
15:f:208:LEU:HA	15:f:211:ILE:HG12	1.98	0.46
18:b:51:LEU:HD11	18:b:71:ILE:HG23	1.98	0.46
20:d:62:SER:HB3	20:d:71:PHE:HB2	1.96	0.46
22:U:133:ILE:O	22:U:137:MET:HG2	2.15	0.46
22:U:422:LEU:O	22:U:425:THR:OG1	2.34	0.46
22:U:685:GLN:HB3	22:U:726:ALA:HA	1.98	0.46
22:U:722:ASP:HB3	22:U:727:LYS:HG3	1.97	0.46
23:V:314:ARG:HH12	25:Y:381:GLN:HB2	1.81	0.46
24:X:397:TYR:HB3	25:Y:365:GLN:OE1	2.16	0.46
30:C:117:ARG:HG2	30:C:118:ASN:H	1.80	0.46
30:C:147:THR:HA	30:C:205:HIS:CE1	2.51	0.46
32:E:64:LEU:HB3	32:E:68:LYS:HB3	1.98	0.46
32:E:348:THR:O	32:E:351:GLY:N	2.48	0.46
33:F:403:ALA:HA	33:F:406:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:GLY:HA2	2:H:165:LYS:HB3	1.97	0.46
4:J:79:ASP:O	4:J:83:VAL:HG23	2.16	0.46
5:L:56:LEU:HD13	14:K:167:ALA:HB3	1.98	0.46
7:N:164:MET:HA	7:N:170:SER:HB2	1.98	0.46
13:T:186:ARG:HH22	7:n:199:VAL:HG11	1.81	0.46
3:i:119:GLN:NE2	4:j:79:ASP:OD1	2.47	0.46
14:k:182:GLN:HB2	5:l:56:LEU:HD11	1.97	0.46
5:l:89:ARG:NH1	12:s:77:HIS:HB3	2.31	0.46
11:r:127:SER:HB3	11:r:136:TYR:HE1	1.80	0.46
13:t:167:ASP:O	13:t:171:ARG:HG3	2.16	0.46
15:f:827:PRO:HB2	15:f:829:MET:SD	2.55	0.46
19:c:122:LEU:HD21	19:c:142:ALA:HB1	1.97	0.46
19:c:234:TYR:O	27:W:422:ASN:ND2	2.49	0.46
20:d:187:GLU:OE1	23:V:452:ASN:ND2	2.48	0.46
22:U:889:LEU:HD23	22:U:892:LEU:HD13	1.97	0.46
23:V:470:ARG:HG3	23:V:473:GLN:HE21	1.81	0.46
27:W:19:ASP:OD1	27:W:20:TYR:N	2.49	0.46
27:W:141:GLU:OE1	27:W:141:GLU:N	2.49	0.46
27:W:207:LYS:HA	27:W:210:ASN:ND2	2.30	0.46
30:C:32:GLN:HA	31:D:55:GLU:OE1	2.16	0.46
30:C:127:LEU:HD12	30:C:128:PRO:HD2	1.98	0.46
30:C:189:TYR:CG	30:C:300:ILE:HD11	2.51	0.46
30:C:289:ILE:HG13	30:C:289:ILE:O	2.16	0.46
33:F:339:ASP:OD1	33:F:339:ASP:N	2.44	0.46
7:N:13:VAL:HG11	7:N:153:LEU:HA	1.98	0.45
7:N:29:ARG:HD2	13:t:209:TRP:CZ3	2.51	0.45
11:R:179:VAL:HA	11:R:184:TRP:HA	1.97	0.45
3:i:165:GLY:O	3:i:168:SER:OG	2.34	0.45
14:k:97:GLN:HB3	11:r:61:ARG:HG2	1.98	0.45
5:l:35:THR:HG23	5:l:48:ALA:HB2	1.97	0.45
6:m:169:ARG:HB2	6:m:173:LYS:NZ	2.31	0.45
10:q:16:ALA:HB2	10:q:180:VAL:HG12	1.97	0.45
12:s:99:ARG:HG3	12:s:104:TYR:CZ	2.51	0.45
16:x:77:PHE:HE1	16:x:98:CYS:HB3	1.81	0.45
17:a:47:ASP:O	17:a:49:CYS:N	2.46	0.45
17:a:224:SER:HA	17:a:227:ASN:HB2	1.98	0.45
25:Y:220:VAL:HG11	25:Y:249:VAL:HG21	1.97	0.45
29:B:218:PRO:HB2	29:B:220:LYS:HG2	1.98	0.45
29:B:423:LYS:O	29:B:426:VAL:HG12	2.16	0.45
30:C:83:LYS:HG2	30:C:105:ILE:HG12	1.98	0.45
30:C:273:MET:HE2	30:C:277:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:E:300:HIS:ND1	32:E:302:ASP:OD1	2.48	0.45
9:P:58:THR:CA	10:Q:85:ARG:NH2	2.76	0.45
11:R:68:LEU:HB3	14:K:93:ARG:HD3	1.98	0.45
16:x:95:GLN:HG2	16:x:96:ASP:H	1.81	0.45
17:a:146:PRO:HB2	26:Z:142:GLU:HG3	1.98	0.45
21:e:59:GLU:HA	21:e:62:LYS:HZ2	1.82	0.45
24:X:343:SER:N	27:W:406:VAL:O	2.47	0.45
29:B:79:ILE:HG12	29:B:83:GLU:OE1	2.17	0.45
1:G:115:CYS:SG	1:G:160:TYR:HB2	2.56	0.45
4:J:72:ALA:HB3	4:J:132:LEU:HD11	1.99	0.45
8:O:26:VAL:HB	12:s:185:ARG:HA	1.99	0.45
1:g:56:VAL:HG23	1:g:56:VAL:O	2.16	0.45
5:l:98:VAL:HA	13:t:94:ARG:HG3	1.98	0.45
5:l:130:VAL:C	5:l:149:PRO:HG3	2.42	0.45
9:p:61:GLN:OE1	10:q:85:ARG:HD2	2.16	0.45
11:r:194:ASP:HA	11:r:197:GLU:HG2	1.97	0.45
15:f:437:GLU:HB2	15:f:440:ILE:HG13	1.98	0.45
18:b:33:VAL:HG11	18:b:71:ILE:HG21	1.96	0.45
20:d:175:ARG:HH21	20:d:205:LYS:HD2	1.80	0.45
22:U:254:GLU:HB3	22:U:751:ARG:HD3	1.98	0.45
23:V:350:GLN:HG2	23:V:353:LEU:HD23	1.99	0.45
24:X:378:LEU:HD23	25:Y:311:TYR:CE2	2.51	0.45
26:Z:44:GLN:HG2	26:Z:45:LYS:N	2.30	0.45
29:B:113:GLU:H	29:B:123:VAL:HA	1.81	0.45
29:B:287:ILE:HG13	29:B:291:GLY:HA3	1.97	0.45
30:C:155:ASP:O	30:C:159:LYS:HG3	2.17	0.45
32:E:225:HIS:HB2	32:E:228:CYS:SG	2.56	0.45
33:F:227:GLY:O	33:F:333:ASN:HA	2.16	0.45
33:F:402:GLU:HA	33:F:405:MET:HE2	1.98	0.45
3:I:197:LEU:HA	3:I:200:THR:HG22	1.98	0.45
3:I:233:VAL:O	3:I:237:ILE:HG13	2.16	0.45
10:Q:108:ASP:HB3	10:Q:111:GLU:HG3	1.98	0.45
11:R:37:ILE:HD11	11:R:56:GLU:HB3	1.97	0.45
14:k:27:ALA:O	14:k:31:ILE:HG12	2.16	0.45
14:k:121:LEU:HD12	14:k:123:PHE:CE1	2.52	0.45
7:n:30:VAL:HG22	7:n:175:ARG:NH2	2.32	0.45
13:t:99:ARG:HG3	13:t:104:ASN:O	2.16	0.45
15:f:143:ARG:NE	15:f:158:TYR:OH	2.41	0.45
15:f:178:LYS:HA	15:f:181:ARG:HG3	1.98	0.45
15:f:442:SER:OG	15:f:476:THR:O	2.32	0.45
18:b:157:VAL:HG21	18:b:170:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:461:LEU:O	22:U:465:LEU:HD23	2.16	0.45
22:U:607:VAL:O	31:D:68:LEU:CD2	2.64	0.45
31:D:160:PRO:HB3	31:D:221:HIS:NE2	2.31	0.45
31:D:387:VAL:HG22	31:D:387:VAL:O	2.16	0.45
32:E:36:LEU:CG	32:E:37:THR:H	2.28	0.45
32:E:158:LEU:O	32:E:162:VAL:HG23	2.17	0.45
32:E:177:GLY:CA	33:F:344:ARG:CZ	2.95	0.45
32:E:264:MET:SD	32:E:265:ASP:N	2.89	0.45
33:F:221:LYS:HZ1	33:F:321:GLN:HA	1.80	0.45
33:F:286:ASP:OD1	33:F:287:GLU:N	2.48	0.45
3:I:214:ALA:HB2	3:I:227:VAL:HG12	1.98	0.45
7:N:42:PHE:CE1	7:N:184:VAL:HG21	2.51	0.45
7:N:134:TYR:HA	7:n:133:SER:O	2.16	0.45
10:Q:51:GLY:HA3	11:R:118:GLY:HA3	1.99	0.45
11:R:165:TYR:HA	9:p:205:ASP:HB3	1.99	0.45
12:S:91:MET:O	12:S:95:ILE:HG12	2.16	0.45
12:S:133:ASP:OD1	12:S:134:SER:N	2.49	0.45
3:i:87:THR:O	3:i:91:ARG:HG3	2.17	0.45
14:k:29:GLU:O	14:k:33:LEU:HG	2.15	0.45
11:r:149:VAL:HG12	11:r:178:HIS:HE1	1.81	0.45
22:U:486:MET:HE1	22:U:758:PRO:HG3	1.98	0.45
23:V:466:ILE:HG22	23:V:470:ARG:HH12	1.80	0.45
25:Y:310:SER:H	25:Y:358:ARG:NH1	2.14	0.45
27:W:231:ILE:O	27:W:235:GLN:HG2	2.17	0.45
28:A:142:VAL:HB	28:A:147:TYR:HA	1.99	0.45
28:A:224:LEU:H	28:A:224:LEU:HD22	1.81	0.45
31:D:115:ILE:HG13	31:D:139:LEU:HD23	1.97	0.45
31:D:411:GLU:HG2	31:D:412:GLN:N	2.28	0.45
32:E:180:LYS:HD2	32:E:278:ALA:HB1	1.97	0.45
33:F:55:MET:O	33:F:58:GLU:N	2.49	0.45
4:J:63:CYS:HB3	4:J:88:ARG:HH22	1.82	0.45
1:g:112:ASP:OD1	1:g:113:MET:N	2.50	0.45
5:l:103:LEU:HD22	5:l:108:LEU:HB2	1.98	0.45
5:l:196:ARG:HG3	5:l:239:ARG:HE	1.82	0.45
6:m:172:ALA:HB2	6:m:200:VAL:HG11	1.98	0.45
14:K:229:PHE:O	14:K:234:LEU:HB3	2.16	0.45
15:f:748:LEU:O	15:f:752:HIS:ND1	2.31	0.45
19:c:193:ILE:HG23	29:B:155:LYS:HZ2	1.81	0.45
27:W:315:MET:HE2	27:W:358:VAL:HG12	1.98	0.45
27:W:419:LYS:HG3	27:W:424:LEU:HB2	1.99	0.45
29:B:204:PRO:O	29:B:206:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:117:ARG:H	30:C:121:TYR:HA	1.80	0.45
2:H:58:ASP:OD1	2:H:60:ARG:HG2	2.17	0.45
2:H:150:ASP:CG	2:H:153:GLY:H	2.20	0.45
2:H:173:PHE:CE1	2:H:177:ARG:HG3	2.52	0.45
9:P:58:THR:O	10:Q:85:ARG:NH2	2.47	0.45
12:S:38:ARG:HH12	12:S:212:LYS:HG3	1.81	0.45
12:S:148:LEU:HD12	9:p:149:MET:HE2	1.98	0.45
2:h:219:ARG:NH1	2:h:221:LEU:HA	2.32	0.45
4:j:234:LYS:HA	4:j:237:GLU:HG2	1.98	0.45
9:p:26:ARG:HH11	9:p:186:ILE:HB	1.82	0.45
14:K:207:GLU:HG2	28:A:420:TYR:CG	2.52	0.45
15:f:239:TYR:HA	29:B:67:ARG:NH2	2.31	0.45
15:f:663:GLY:HA2	15:f:781:TYR:CZ	2.51	0.45
19:c:152:LYS:HG3	31:D:83:GLN:HG3	1.98	0.45
22:U:92:ASP:OD2	22:U:140:ARG:NH2	2.48	0.45
22:U:487:GLY:N	22:U:518:LEU:O	2.36	0.45
22:U:599:ILE:CG2	31:D:60:TYR:CZ	2.99	0.45
26:Z:174:HIS:C	26:Z:177:ARG:HG3	2.42	0.45
29:B:135:ILE:HD12	29:B:159:VAL:CG1	2.46	0.45
29:B:174:MET:HA	30:C:271:ARG:HH22	1.82	0.45
30:C:117:ARG:HD2	30:C:120:SER:OG	2.16	0.45
31:D:260:ALA:HB3	31:D:305:VAL:HG13	1.98	0.45
1:G:43:ARG:N	1:G:164:LYS:O	2.36	0.45
1:G:153:LYS:NZ	1:G:168:ALA:HB2	2.30	0.45
4:J:139:ASP:OD1	11:R:106:LYS:HD3	2.17	0.45
6:M:83:ASP:OD1	6:M:84:ALA:N	2.50	0.45
13:T:207:THR:OG1	13:T:209:TRP:NE1	2.50	0.45
3:i:28:ILE:HD13	3:i:133:SER:HB2	1.99	0.45
4:j:79:ASP:HA	4:j:82:ILE:HG12	1.98	0.45
14:k:73:HIS:CD2	14:k:74:ILE:HG13	2.52	0.45
10:q:37:LYS:HD3	10:q:188:ILE:HD12	1.99	0.45
12:s:36:HIS:HB3	13:t:132:TYR:CE2	2.52	0.45
14:K:229:PHE:HD2	14:K:234:LEU:HB2	1.81	0.45
15:f:175:ASP:OD1	15:f:175:ASP:N	2.50	0.45
15:f:845:ARG:N	15:f:881:GLU:O	2.46	0.45
22:U:750:SER:OG	22:U:751:ARG:N	2.50	0.45
22:U:798:PRO:HB2	22:U:800:VAL:HG23	1.97	0.45
23:V:306:ARG:HA	23:V:309:MET:HG2	1.99	0.45
25:Y:359:PRO:HB2	25:Y:364:TRP:HB2	1.98	0.45
30:C:49:ARG:CZ	31:D:73:LEU:HD11	2.47	0.45
30:C:80:MET:HE2	30:C:80:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:203:VAL:HA	30:C:206:HIS:HB2	1.98	0.45
30:C:325:ARG:NH2	30:C:348:ALA:O	2.30	0.45
30:C:333:SER:HA	30:C:336:MET:HE3	1.98	0.45
31:D:168:GLY:N	35:D:501:ADP:HN62	2.09	0.45
32:E:36:LEU:C	32:E:38:LYS:N	2.71	0.45
1:G:151:VAL:HG13	1:G:163:PHE:HA	1.99	0.45
3:I:6:ASP:N	3:I:6:ASP:OD1	2.50	0.45
5:L:109:VAL:HG22	5:L:134:ILE:HD12	1.99	0.45
5:L:166:GLN:H	5:L:166:GLN:CD	2.25	0.45
6:M:41:CYS:N	6:M:44:GLY:O	2.50	0.45
9:P:53:LEU:CB	9:P:60:VAL:HG13	2.47	0.45
1:g:180:GLU:HG2	2:h:54:SER:CB	2.47	0.45
10:q:86:ARG:NH1	10:q:90:ASP:HB3	2.32	0.45
15:f:409:SER:O	15:f:819:TYR:OH	2.34	0.45
15:f:776:LEU:HA	15:f:827:PRO:HA	1.98	0.45
15:f:776:LEU:HD22	15:f:825:MET:HG2	1.99	0.45
17:a:54:ASP:N	17:a:54:ASP:OD1	2.50	0.45
18:b:148:VAL:HG23	18:b:172:THR:HG23	1.98	0.45
19:c:122:LEU:HD13	19:c:196:LEU:HG	1.99	0.45
19:c:296:ILE:HD12	20:d:246:VAL:HG22	1.99	0.45
20:d:77:GLN:HE21	22:U:11:LEU:HD23	1.82	0.45
20:d:237:ILE:CG2	20:d:238:PRO:HD3	2.47	0.45
22:U:206:MET:SD	22:U:220:LEU:HD21	2.57	0.45
22:U:813:TYR:CE2	22:U:815:ALA:HB2	2.52	0.45
27:W:231:ILE:HG22	27:W:246:HIS:NE2	2.32	0.45
29:B:109:VAL:HB	30:C:94:LYS:HE2	1.99	0.45
31:D:349:THR:HG23	31:D:355:SER:HB2	1.99	0.45
33:F:65:GLU:O	33:F:69:MET:HB2	2.17	0.45
33:F:80:ILE:O	33:F:84:LYS:N	2.43	0.45
1:G:38:THR:HA	1:G:169:GLY:HA3	1.98	0.45
1:G:86:ASP:OD1	1:G:86:ASP:N	2.50	0.45
5:L:35:THR:HG21	5:L:73:SER:HB3	1.99	0.45
7:N:19:ARG:HB2	7:N:171:GLY:O	2.16	0.45
11:R:11:GLY:HA2	11:R:104:TRP:HZ3	1.82	0.45
1:g:147:GLN:HG3	1:g:150:GLN:OE1	2.17	0.45
3:i:18:LEU:HD12	3:i:20:GLN:NE2	2.29	0.45
14:k:141:LEU:HD12	14:k:156:MET:HG2	1.98	0.45
15:f:656:GLY:O	15:f:660:ILE:HG12	2.17	0.45
15:f:703:ARG:HB3	15:f:706:ILE:HG13	1.98	0.45
15:f:849:ALA:HA	15:f:862:ILE:HA	1.98	0.45
17:a:123:LEU:HD12	17:a:162:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:91:ARG:HD2	18:b:91:ARG:HA	1.73	0.45
19:c:137:SER:HB2	19:c:140:ALA:HB2	1.99	0.45
19:c:226:MET:HE2	26:Z:201:LEU:HA	1.99	0.45
20:d:44:THR:HA	20:d:47:GLN:HB3	1.99	0.45
20:d:92:SER:O	20:d:94:TYR:N	2.50	0.45
20:d:149:ASN:HA	20:d:152:PHE:CD2	2.52	0.45
22:U:381:THR:HA	22:U:412:HIS:CE1	2.51	0.45
26:Z:48:LEU:HD11	26:Z:92:VAL:HB	1.99	0.45
27:W:28:LEU:HD12	27:W:66:ILE:HD13	1.99	0.45
27:W:308:LEU:HA	27:W:313:GLU:OE2	2.17	0.45
29:B:140:ASP:OD1	29:B:140:ASP:N	2.39	0.45
29:B:265:LYS:HB3	29:B:268:ARG:NH2	2.32	0.45
30:C:212:ILE:HB	30:C:246:ILE:HA	1.99	0.45
31:D:82:ILE:O	31:D:83:GLN:HB2	2.16	0.45
32:E:236:ASP:OD2	32:E:279:THR:OG1	2.29	0.45
33:F:202:ILE:C	33:F:205:PRO:HD2	2.42	0.45
2:H:65:VAL:N	2:H:209:GLU:OE2	2.37	0.44
10:Q:102:LEU:HB2	10:Q:118:MET:HG3	1.98	0.44
12:S:64:LEU:HD21	12:S:92:LEU:HD11	1.98	0.44
3:i:27:ALA:HA	3:i:30:HIS:CE1	2.53	0.44
3:i:196:VAL:O	3:i:200:THR:HG22	2.17	0.44
14:k:52:LYS:HE2	14:k:61:PRO:HB3	1.99	0.44
12:s:156:LYS:HE3	12:s:156:LYS:HB2	1.83	0.44
18:b:91:ARG:HH12	18:b:130:ARG:HD3	1.82	0.44
19:c:79:GLY:HA3	33:F:79:LYS:O	2.16	0.44
20:d:8:GLU:HB3	20:d:18:LYS:HZ1	1.82	0.44
20:d:34:ASN:ND2	22:U:26:LYS:HE3	2.32	0.44
22:U:260:PHE:O	22:U:264:VAL:HG23	2.16	0.44
22:U:404:ALA:O	22:U:407:SER:OG	2.27	0.44
23:V:357:LEU:HD13	23:V:360:TYR:HD2	1.82	0.44
27:W:111:TYR:O	27:W:114:GLU:HG3	2.17	0.44
29:B:264:PRO:HG3	29:B:308:THR:HA	1.99	0.44
31:D:107:THR:N	32:E:77:PRO:HB3	2.32	0.44
3:I:124:PHE:O	3:I:127:LYS:NZ	2.45	0.44
12:S:148:LEU:HD11	9:p:148:GLY:C	2.42	0.44
3:i:14:PRO:HA	4:j:21:TYR:CE1	2.53	0.44
6:m:193:VAL:HA	6:m:196:ILE:HG22	1.99	0.44
13:t:74:GLU:HG3	13:t:83:TYR:CZ	2.52	0.44
15:f:698:SER:OG	15:f:701:ASN:O	2.35	0.44
17:a:198:PHE:CZ	17:a:230:ARG:HD2	2.52	0.44
17:a:217:LEU:HB3	17:a:241:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:101:LEU:HD23	20:d:166:PHE:CE1	2.52	0.44
20:d:147:SER:HB3	20:d:150:LYS:HB2	2.00	0.44
20:d:205:LYS:HZ1	20:d:209:TYR:HB2	1.82	0.44
22:U:413:LYS:HA	22:U:449:ILE:HA	1.98	0.44
30:C:56:VAL:CG2	31:D:79:VAL:CG1	2.95	0.44
30:C:97:VAL:HG21	30:C:121:TYR:C	2.42	0.44
32:E:81:VAL:HG11	32:E:100:LEU:HD22	1.99	0.44
4:J:116:GLN:NE2	14:K:84:ASP:OD1	2.50	0.44
6:M:160:TYR:CD1	6:M:163:CYS:HB2	2.52	0.44
10:Q:116:TYR:HB3	10:Q:124:LEU:HD11	2.00	0.44
3:i:194:ILE:HG21	3:i:240:HIS:HB2	2.00	0.44
5:l:150:SER:O	5:l:152:ASN:ND2	2.50	0.44
6:m:120:HIS:NE2	6:m:124:LEU:HD21	2.33	0.44
9:p:25:ASP:OD1	9:p:41:LYS:NZ	2.36	0.44
9:p:56:LEU:O	9:p:60:VAL:HG23	2.17	0.44
9:p:123:SER:HB2	9:p:137:VAL:HB	1.99	0.44
10:q:2:GLU:OE1	10:q:2:GLU:N	2.40	0.44
15:f:597:VAL:HA	15:f:660:ILE:HD11	1.99	0.44
15:f:907:ASP:N	15:f:907:ASP:OD1	2.51	0.44
17:a:89:ASP:HB3	17:a:92:VAL:HG12	1.97	0.44
17:a:122:LYS:HB3	17:a:131:THR:HG22	1.98	0.44
23:V:209:LYS:HA	23:V:212:TYR:HB3	1.99	0.44
27:W:227:TYR:HA	27:W:230:MET:HG3	1.99	0.44
28:A:239:ARG:NH1	28:A:275:ASP:OD2	2.50	0.44
30:C:128:PRO:HG2	30:C:130:LYS:HZ1	1.83	0.44
30:C:244:SER:HB2	30:C:289:ILE:HG22	1.99	0.44
30:C:297:ARG:HG3	30:C:297:ARG:O	2.17	0.44
31:D:372:GLY:HA2	31:D:410:ASP:OD2	2.18	0.44
4:J:28:LYS:C	4:J:28:LYS:HD3	2.42	0.44
2:h:29:VAL:HG13	2:h:77:SER:O	2.17	0.44
2:h:66:GLU:O	2:h:74:LEU:HD23	2.17	0.44
2:h:189:HIS:HA	2:h:233:ILE:HD13	2.00	0.44
3:i:37:ILE:HD11	3:i:44:LEU:HD12	1.99	0.44
3:i:123:GLN:NE2	4:j:125:ARG:HG3	2.31	0.44
3:i:134:LEU:HD12	3:i:136:TYR:CE1	2.53	0.44
7:n:33:LYS:HD3	7:n:45:ARG:HE	1.81	0.44
9:p:27:ARG:HB2	9:p:183:MET:HB2	1.98	0.44
10:q:102:LEU:HB2	10:q:118:MET:HB3	2.00	0.44
12:s:141:ALA:O	12:s:145:LEU:HD23	2.17	0.44
15:f:72:ARG:HB3	15:f:73:PRO:HD3	1.98	0.44
15:f:149:GLU:OE1	15:f:150:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:164:GLY:HA3	28:A:40:THR:HG21	1.99	0.44
15:f:261:ARG:HH21	15:f:263:PRO:CG	2.30	0.44
15:f:290:VAL:O	15:f:294:MET:HG2	2.18	0.44
19:c:32:TYR:HB2	19:c:68:ARG:HG2	1.99	0.44
19:c:251:LEU:HD22	19:c:279:ASP:HB2	1.98	0.44
22:U:592:GLY:HA2	22:U:628:ARG:HD3	1.99	0.44
23:V:216:ARG:NH1	23:V:253:LEU:HD23	2.32	0.44
23:V:240:LEU:HG	23:V:241:ARG:HE	1.83	0.44
27:W:268:LYS:HA	27:W:301:LYS:HG3	1.99	0.44
29:B:233:THR:O	29:B:234:LEU:C	2.61	0.44
30:C:49:ARG:O	30:C:53:ASN:ND2	2.46	0.44
31:D:173:GLN:C	31:D:175:GLN:H	2.26	0.44
32:E:37:THR:O	33:F:69:MET:HE3	2.18	0.44
33:F:172:VAL:HG11	33:F:270:ASP:C	2.42	0.44
33:F:184:GLN:OE1	33:F:185:TYR:N	2.51	0.44
3:I:29:GLY:O	3:I:166:ASN:HA	2.17	0.44
3:I:46:ALA:HA	3:I:213:ILE:HG22	1.97	0.44
4:J:132:LEU:HD12	4:J:132:LEU:O	2.18	0.44
4:J:157:LYS:HB3	4:J:176:TYR:CZ	2.52	0.44
9:P:29:GLY:HA2	9:P:35:VAL:HG23	1.98	0.44
9:P:58:THR:HG21	10:Q:121:LEU:HB3	1.98	0.44
10:Q:85:ARG:NE	10:Q:124:LEU:H	2.15	0.44
10:Q:145:ARG:O	10:Q:145:ARG:NH1	2.46	0.44
2:h:205:GLU:HB3	2:h:227:LYS:HB3	2.00	0.44
7:n:17:ASP:OD1	7:n:18:SER:N	2.50	0.44
8:o:54:MET:HG2	9:p:96:TYR:CE1	2.52	0.44
10:q:111:GLU:N	10:q:111:GLU:OE1	2.50	0.44
12:s:36:HIS:HB3	13:t:132:TYR:CZ	2.53	0.44
12:s:71:ARG:HD2	12:s:95:ILE:HD11	1.99	0.44
15:f:809:ILE:HG12	15:f:814:SER:CB	2.47	0.44
19:c:268:GLU:O	19:c:272:ILE:HG12	2.17	0.44
22:U:199:ARG:O	22:U:203:LYS:HG3	2.18	0.44
25:Y:64:GLN:CD	25:Y:64:GLN:H	2.26	0.44
25:Y:268:TYR:HA	25:Y:271:PHE:HB3	1.97	0.44
26:Z:110:GLU:HA	26:Z:113:LYS:NZ	2.33	0.44
27:W:159:VAL:HG12	27:W:196:VAL:HG22	2.00	0.44
29:B:165:ASP:C	29:B:167:THR:H	2.25	0.44
2:H:107:THR:HB	2:H:140:ASN:HB2	1.98	0.44
2:H:147:PHE:CD2	2:H:155:TYR:HB2	2.52	0.44
3:I:218:ARG:NH1	3:I:223:THR:OG1	2.50	0.44
6:M:186:CYS:HG	6:M:219:LEU:HD13	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:61:GLN:NE2	10:Q:124:LEU:O	2.44	0.44
14:k:91:LYS:HZ1	14:k:137:PHE:HZ	1.65	0.44
5:l:11:THR:HA	6:m:129:ARG:HD3	2.00	0.44
8:o:187:ARG:HB3	8:o:188:PRO:HD3	2.00	0.44
9:p:53:LEU:HD23	9:p:60:VAL:HA	2.00	0.44
9:p:107:PRO:HG2	9:p:124:LEU:HD12	1.99	0.44
15:f:63:LEU:HG	15:f:109:ILE:HD13	1.98	0.44
20:d:71:PHE:O	20:d:75:MET:HG2	2.16	0.44
20:d:175:ARG:HE	20:d:205:LYS:HD3	1.82	0.44
22:U:200:VAL:O	22:U:204:ILE:HG22	2.18	0.44
22:U:714:SER:O	22:U:718:ASN:ND2	2.51	0.44
23:V:181:TYR:HB3	23:V:221:LEU:HD21	1.99	0.44
23:V:285:TRP:HD1	23:V:315:LYS:HD2	1.83	0.44
25:Y:49:ASN:HA	25:Y:52:PRO:HG2	1.99	0.44
26:Z:19:VAL:HG11	26:Z:124:ILE:HD13	1.99	0.44
26:Z:136:GLU:HB3	27:W:448:LYS:NZ	2.32	0.44
27:W:298:GLU:OE1	27:W:298:GLU:N	2.42	0.44
29:B:284:ILE:HB	29:B:287:ILE:HG22	1.99	0.44
30:C:388:ALA:O	30:C:392:GLN:NE2	2.49	0.44
33:F:414:GLU:O	33:F:416:THR:N	2.47	0.44
8:O:147:GLU:CD	8:O:150:GLU:H	2.25	0.44
9:P:78:GLU:OE2	9:P:80:ARG:HB2	2.18	0.44
10:Q:131:ALA:H	10:Q:140:LEU:HD21	1.82	0.44
5:l:72:ILE:HD13	5:l:88:MET:HE1	1.98	0.44
5:l:196:ARG:HB2	5:l:205:LEU:HD13	1.99	0.44
10:q:160:LEU:HA	10:q:163:CYS:SG	2.58	0.44
12:s:136:LYS:NZ	12:s:137:ALA:O	2.48	0.44
20:d:158:ILE:HD12	20:d:164:THR:HA	2.00	0.44
23:V:115:LYS:HZ1	23:V:144:ASP:HA	1.82	0.44
23:V:285:TRP:CD1	23:V:315:LYS:HD2	2.52	0.44
25:Y:268:TYR:OH	25:Y:303:ALA:O	2.36	0.44
27:W:116:THR:OG1	27:W:117:ASP:N	2.50	0.44
28:A:384:GLU:O	28:A:388:VAL:HG23	2.17	0.44
29:B:246:THR:OG1	29:B:280:SER:HB2	2.18	0.44
29:B:285:ASP:HA	29:B:330:ALA:O	2.17	0.44
30:C:343:ASN:O	30:C:347:ILE:HG12	2.17	0.44
31:D:389:GLU:C	31:D:391:ARG:H	2.25	0.44
9:P:169:GLN:O	9:P:173:ASN:ND2	2.50	0.44
14:k:19:GLY:HA2	5:l:24:TYR:HB3	2.00	0.44
5:l:65:HIS:HA	5:l:221:PHE:HE2	1.83	0.44
9:p:66:ARG:NH1	9:p:70:ARG:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:r:113:TYR:O	11:r:120:ARG:HA	2.18	0.44
12:s:199:THR:HG23	12:s:201:GLU:H	1.83	0.44
15:f:266:LEU:HD22	15:f:294:MET:SD	2.57	0.44
15:f:560:LEU:O	15:f:564:LEU:HG	2.18	0.44
19:c:161:ARG:NE	19:c:203:ILE:HD11	2.33	0.44
22:U:638:SER:CB	30:C:43:ARG:HD2	2.48	0.44
23:V:166:TYR:HE1	23:V:206:VAL:HG13	1.82	0.44
23:V:442:ILE:HD12	23:V:450:SER:HA	2.00	0.44
26:Z:258:VAL:O	26:Z:262:LEU:N	2.51	0.44
28:A:206:ILE:HG22	28:A:207:GLU:HG2	1.98	0.44
28:A:397:ILE:HD13	29:B:211:TYR:HB3	2.00	0.44
29:B:184:TYR:CE2	29:B:240:ALA:HB1	2.53	0.44
31:D:81:ARG:O	31:D:82:ILE:C	2.60	0.44
31:D:132:LEU:HA	31:D:138:ALA:O	2.18	0.44
33:F:203:VAL:O	33:F:207:ASN:ND2	2.50	0.44
1:G:86:ASP:HB3	1:G:134:LEU:HB3	2.00	0.44
2:H:36:VAL:HG12	2:H:162:ALA:HB2	1.99	0.44
7:N:38:HIS:CG	7:N:39:ASP:H	2.36	0.44
7:N:162:LEU:HA	7:N:165:GLU:HG3	1.99	0.44
11:R:112:TYR:CE2	11:R:122:SER:HB2	2.53	0.44
1:g:222:VAL:O	1:g:222:VAL:HG13	2.18	0.44
3:i:134:LEU:HD12	3:i:136:TYR:HE1	1.82	0.44
4:j:195:LEU:O	4:j:199:VAL:HG12	2.18	0.44
9:p:8:GLY:HA2	9:p:141:THR:HG21	2.00	0.44
9:p:53:LEU:HB3	9:p:60:VAL:HG13	2.00	0.44
10:q:19:ARG:HH21	10:q:31:ASP:HB3	1.82	0.44
17:a:292:THR:HA	17:a:329:LYS:O	2.17	0.44
18:b:8:VAL:HG13	18:b:51:LEU:HD23	2.00	0.44
19:c:152:LYS:CG	31:D:83:GLN:HG3	2.47	0.44
20:d:202:THR:N	20:d:203:PRO:HD3	2.33	0.44
22:U:191:LYS:HA	22:U:194:ARG:HB3	1.99	0.44
22:U:436:ALA:HB1	22:U:472:ILE:HD13	2.00	0.44
22:U:591:CYS:SG	22:U:755:THR:HG21	2.58	0.44
24:X:344:ARG:HH21	27:W:409:LEU:HB3	1.83	0.44
29:B:140:ASP:O	29:B:144:LEU:HG	2.18	0.44
30:C:324:ALA:O	30:C:328:ILE:HG12	2.17	0.44
31:D:247:VAL:HG11	31:D:292:LEU:HA	1.99	0.44
31:D:387:VAL:HG13	32:E:164:ILE:CD1	2.48	0.44
33:F:121:CYS:HB3	33:F:133:PHE:CZ	2.53	0.44
33:F:322:PRO:C	33:F:324:THR:H	2.25	0.44
1:G:78:CYS:SG	1:G:140:LEU:HB3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ASP:OD2	8:O:72:ARG:NH2	2.43	0.43
1:G:211:LYS:O	1:G:213:SER:N	2.44	0.43
7:N:175:ARG:HG2	7:N:188:VAL:HG22	1.99	0.43
3:i:43:VAL:HG21	3:i:137:ILE:HB	2.00	0.43
14:k:12:VAL:HG21	14:k:124:GLY:HA2	1.99	0.43
12:s:138:GLY:HA2	12:s:142:SER:HB3	2.00	0.43
15:f:75:LEU:HD21	15:f:121:PHE:HB3	2.00	0.43
15:f:136:GLU:HG3	15:f:137:ARG:N	2.33	0.43
15:f:162:LEU:HD21	15:f:187:LEU:HD21	2.00	0.43
19:c:138:GLU:OE1	19:c:139:ARG:NH1	2.51	0.43
19:c:223:LYS:HD2	26:Z:132:GLY:O	2.17	0.43
29:B:262:ASP:H	29:B:265:LYS:NZ	2.15	0.43
31:D:167:ILE:HG12	31:D:169:GLY:H	1.82	0.43
32:E:61:LEU:N	32:E:70:ILE:O	2.51	0.43
1:G:119:ALA:HB2	1:G:160:TYR:HB3	2.00	0.43
7:N:29:ARG:HD2	13:t:209:TRP:HZ3	1.82	0.43
9:P:20:VAL:HG12	9:P:121:ILE:HD11	2.00	0.43
10:Q:38:MET:HE1	10:Q:60:ILE:HG22	2.00	0.43
2:h:224:THR:O	2:h:227:LYS:HG3	2.18	0.43
13:t:43:MET:HG3	13:t:64:LYS:HG3	2.00	0.43
15:f:606:VAL:HA	15:f:609:VAL:HG22	2.00	0.43
15:f:680:ARG:HE	28:A:64:GLY:N	2.16	0.43
17:a:373:ASP:HB2	20:d:247:ILE:HD12	2.00	0.43
24:X:110:CYS:HB2	24:X:133:LEU:HD21	2.01	0.43
26:Z:138:TYR:CE1	27:W:448:LYS:HD3	2.54	0.43
27:W:246:HIS:HA	27:W:249:ALA:HB3	1.99	0.43
28:A:120:LYS:HB3	28:A:120:LYS:HE2	1.65	0.43
29:B:53:THR:OG1	29:B:54:PRO:HD3	2.17	0.43
31:D:183:LEU:HB2	31:D:184:PRO:HD3	1.99	0.43
33:F:73:ILE:O	33:F:77:SER:N	2.31	0.43
10:Q:85:ARG:NE	10:Q:122:ALA:O	2.51	0.43
11:R:63:CYS:HB2	11:R:74:ILE:HG21	2.01	0.43
2:h:88:HIS:NE2	2:h:92:LYS:HE2	2.33	0.43
4:j:16:LEU:O	4:j:20:GLU:HG2	2.19	0.43
5:l:50:LYS:HB2	5:l:50:LYS:HE3	1.84	0.43
13:t:9:THR:HB	13:t:182:ARG:HB3	1.99	0.43
14:K:46:VAL:H	14:K:220:VAL:HB	1.83	0.43
14:K:199:LEU:HD11	14:K:215:ILE:HG21	2.00	0.43
15:f:240:VAL:HB	15:f:244:GLU:HG3	2.01	0.43
15:f:292:LYS:HE3	15:f:899:ILE:HD13	1.99	0.43
15:f:611:GLN:O	15:f:615:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:34:TRP:CZ3	17:a:68:GLU:HB2	2.53	0.43
18:b:20:ASP:OD1	18:b:25:ARG:HB2	2.18	0.43
24:X:74:ARG:HG2	24:X:75:PRO:HD3	2.00	0.43
25:Y:234:PRO:C	25:Y:236:LEU:H	2.24	0.43
26:Z:221:PRO:HD2	27:W:453:HIS:HB3	2.00	0.43
29:B:250:VAL:HB	29:B:284:ILE:HG22	2.00	0.43
31:D:391:ARG:NH2	31:D:397:LYS:HD2	2.33	0.43
1:G:165:ALA:HB1	1:G:179:LEU:HB3	1.98	0.43
1:G:171:LYS:HD2	1:G:206:LEU:HD21	2.00	0.43
2:H:59:GLU:HG2	2:H:206:ASP:HB2	1.98	0.43
3:I:33:THR:HA	3:I:165:GLY:CA	2.48	0.43
4:J:189:LYS:HG3	4:J:232:ILE:HG12	2.00	0.43
10:Q:101:ASN:HB3	10:Q:132:HIS:NE2	2.33	0.43
11:R:65:ILE:HG13	14:K:97:GLN:HG3	2.01	0.43
11:R:140:ASP:CG	10:q:170:ARG:HH21	2.26	0.43
13:T:25:ASP:OD1	13:T:25:ASP:N	2.49	0.43
4:j:65:LEU:HB2	4:j:69:VAL:HG12	2.00	0.43
4:j:148:ASP:OD2	4:j:152:THR:OG1	2.37	0.43
5:l:226:ASP:OD1	5:l:226:ASP:N	2.51	0.43
7:n:36:PRO:HB3	7:n:42:PHE:CZ	2.53	0.43
12:s:11:THR:HG22	12:s:141:ALA:H	1.83	0.43
15:f:233:LEU:O	15:f:237:VAL:HG23	2.18	0.43
15:f:607:LEU:HA	15:f:610:GLN:HG3	2.01	0.43
17:a:146:PRO:HB3	26:Z:143:GLU:HG3	1.99	0.43
19:c:222:LYS:HE3	26:Z:176:LEU:HD11	2.00	0.43
19:c:292:MET:HB2	26:Z:263:ALA:HB1	2.00	0.43
22:U:229:VAL:HG21	22:U:252:LEU:HD13	2.01	0.43
26:Z:234:PHE:HB2	27:W:438:LEU:HD23	2.01	0.43
28:A:261:PHE:HZ	28:A:306:LEU:HB3	1.84	0.43
29:B:288:ASP:OD2	29:B:330:ALA:N	2.51	0.43
31:D:92:PHE:CD1	31:D:103:VAL:HG12	2.54	0.43
33:F:203:VAL:HG12	33:F:207:ASN:ND2	2.33	0.43
1:G:115:CYS:SG	1:G:140:LEU:HD21	2.58	0.43
2:H:102:GLN:H	9:P:89:SER:HG	1.60	0.43
3:I:33:THR:HB	3:I:48:GLU:HB3	2.00	0.43
9:P:56:LEU:O	9:P:60:VAL:HG23	2.19	0.43
12:S:147:PRO:HA	12:S:150:ASP:OD1	2.17	0.43
13:T:51:LEU:HD13	13:T:112:ILE:HG12	2.01	0.43
13:T:145:LEU:HD12	8:o:132:LEU:HB3	2.01	0.43
2:h:221:LEU:HD22	2:h:225:GLU:HG3	1.99	0.43
4:j:42:VAL:HG22	4:j:210:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:30:TYR:N	13:t:33:LEU:O	2.49	0.43
15:f:607:LEU:HD21	22:U:840:LYS:CA	2.49	0.43
17:a:326:GLU:CD	27:W:373:ILE:HG13	2.43	0.43
18:b:44:ASN:O	18:b:47:ASN:ND2	2.52	0.43
22:U:501:LEU:HD22	22:U:516:LEU:HD11	2.00	0.43
24:X:347:ILE:HG13	24:X:358:LYS:NZ	2.33	0.43
25:Y:19:ILE:HD13	25:Y:43:ALA:HB3	2.01	0.43
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	2.00	0.43
29:B:357:ASP:OD1	29:B:359:LYS:N	2.50	0.43
30:C:114:VAL:HG21	30:C:123:LEU:HD22	2.00	0.43
31:D:273:LYS:HZ1	32:E:251:ARG:HD3	1.84	0.43
32:E:33:LEU:HD21	33:F:62:VAL:HG22	2.00	0.43
32:E:177:GLY:CA	33:F:344:ARG:NH1	2.82	0.43
33:F:249:LEU:HD21	33:F:271:ALA:HB1	1.99	0.43
3:I:49:ARG:CB	3:I:52:ILE:HD11	2.48	0.43
7:N:59:VAL:HG11	7:N:83:PHE:CE2	2.54	0.43
9:P:107:PRO:HG2	9:P:124:LEU:HB2	2.00	0.43
11:R:134:TYR:OH	9:p:33:GLN:HB3	2.18	0.43
11:R:143:TYR:HA	11:R:147:LEU:HD11	2.00	0.43
5:l:86:ASN:HA	5:l:89:ARG:HG2	2.00	0.43
5:l:184:LEU:HD12	5:l:185:ASN:N	2.33	0.43
11:r:98:GLY:HA2	11:r:115:ASP:HA	2.00	0.43
15:f:333:LEU:HD11	15:f:831:VAL:HG22	2.01	0.43
19:c:65:TYR:OH	22:U:543:LYS:HD3	2.19	0.43
19:c:172:HIS:CG	19:c:173:GLU:N	2.84	0.43
19:c:255:TYR:CD2	24:X:411:VAL:HG11	2.54	0.43
22:U:356:THR:HG22	22:U:717:ILE:HD11	1.99	0.43
27:W:345:GLU:O	27:W:348:GLU:HG2	2.19	0.43
27:W:384:LEU:HB3	27:W:388:GLU:HB2	1.99	0.43
30:C:113:ARG:O	30:C:127:LEU:N	2.52	0.43
30:C:227:GLY:HA3	30:C:265:GLY:HA3	2.00	0.43
32:E:75:ASN:ND2	33:F:130:GLN:N	2.67	0.43
2:H:72:ILE:CG1	2:H:107:THR:HG23	2.49	0.43
7:N:26:ILE:HB	13:t:179:ARG:HA	2.01	0.43
9:P:11:VAL:HG11	9:P:52:GLY:HA3	1.99	0.43
12:S:25:SER:OG	12:S:43:CYS:SG	2.53	0.43
3:i:68:LEU:HD12	3:i:72:MET:HG2	2.01	0.43
6:m:189:ILE:O	6:m:193:VAL:HG23	2.18	0.43
11:r:39:PRO:HA	11:r:184:TRP:HE1	1.84	0.43
13:t:72:ILE:O	13:t:76:LEU:HG	2.18	0.43
13:t:136:SER:HB2	13:t:150:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:48:LEU:HB2	14:K:218:ALA:HB3	1.99	0.43
15:f:680:ARG:HH21	28:A:63:THR:HB	1.83	0.43
17:a:137:ASP:O	17:a:141:MET:HG2	2.18	0.43
22:U:167:ILE:HD12	22:U:204:ILE:HG12	2.00	0.43
22:U:188:MET:HE3	31:D:49:GLN:HG2	2.00	0.43
23:V:148:ARG:HD2	23:V:148:ARG:O	2.17	0.43
24:X:162:ASP:OD1	24:X:163:LYS:N	2.52	0.43
27:W:259:GLU:OE2	27:W:262:LYS:HD3	2.19	0.43
28:A:176:ASP:H	28:A:227:ARG:HE	1.65	0.43
32:E:120:TYR:CZ	33:F:97:LEU:HD11	2.54	0.43
2:H:179:ASN:OD1	2:H:180:GLU:N	2.46	0.43
3:I:25:MET:HE2	29:B:435:PRO:HB3	2.01	0.43
3:I:28:ILE:HG13	3:I:152:PRO:HG2	2.01	0.43
4:J:80:ALA:O	4:J:84:ILE:HG13	2.18	0.43
8:O:164:PHE:O	12:s:38:ARG:NH2	2.51	0.43
11:R:137:GLY:C	10:q:142:ILE:HD11	2.43	0.43
1:g:37:LEU:HG	1:g:53:GLN:NE2	2.34	0.43
1:g:124:VAL:O	1:g:128:ASN:ND2	2.37	0.43
2:h:158:TRP:CD1	3:i:56:LEU:HD13	2.53	0.43
2:h:225:GLU:O	2:h:229:TYR:HD1	2.01	0.43
4:j:90:GLU:OE2	4:j:107:ILE:HG23	2.18	0.43
7:n:45:ARG:HB2	7:n:52:THR:HB	2.01	0.43
12:s:65:THR:O	12:s:69:GLU:HG2	2.18	0.43
15:f:845:ARG:HE	15:f:883:ALA:HA	1.83	0.43
20:d:22:GLU:O	20:d:26:LEU:HG	2.18	0.43
22:U:347:ASN:ND2	22:U:813:TYR:HB2	2.34	0.43
23:V:362:LEU:HD23	23:V:378:VAL:HG11	2.01	0.43
27:W:341:PHE:HB3	27:W:351:TRP:NE1	2.34	0.43
27:W:375:MET:HG3	27:W:386:VAL:HG22	2.01	0.43
28:A:229:VAL:HG21	28:A:237:PHE:CD1	2.53	0.43
30:C:89:VAL:O	30:C:93:GLY:N	2.52	0.43
31:D:265:ASP:OD1	31:D:266:GLU:N	2.52	0.43
31:D:326:ARG:HB3	31:D:327:LEU:HD12	1.99	0.43
33:F:263:ASP:O	33:F:267:LEU:HG	2.19	0.43
33:F:424:ILE:O	33:F:427:VAL:HG22	2.19	0.43
1:G:128:ASN:HA	2:H:127:VAL:HB	2.01	0.43
2:H:100:VAL:HG13	9:P:93:ASN:ND2	2.34	0.43
4:J:23:GLN:O	4:J:26:VAL:HG12	2.19	0.43
2:h:39:LYS:HZ1	2:h:144:PRO:C	2.26	0.43
3:i:179:TYR:CD2	4:j:53:LEU:HD22	2.54	0.43
4:j:115:LYS:O	4:j:119:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:p:50:TYR:HD2	9:p:190:ILE:HD11	1.84	0.43
10:q:77:PRO:HB3	10:q:106:GLY:HA3	2.00	0.43
12:s:125:ASP:OD1	12:s:128:GLY:N	2.35	0.43
15:f:262:PHE:N	15:f:263:PRO:HD2	2.34	0.43
15:f:590:PHE:HB2	15:f:649:HIS:HB3	1.99	0.43
15:f:666:ILE:HD11	29:B:68:ILE:HG12	2.01	0.43
17:a:64:ILE:HG22	17:a:68:GLU:OE2	2.19	0.43
19:c:31:VAL:HB	19:c:205:ILE:HD12	2.01	0.43
19:c:57:MET:HE3	19:c:69:VAL:HG21	2.00	0.43
19:c:191:ALA:HB1	19:c:197:ASN:HB2	2.00	0.43
19:c:193:ILE:HG12	29:B:155:LYS:HD2	1.99	0.43
22:U:649:ARG:HB2	22:U:683:VAL:HG21	2.00	0.43
24:X:331:LEU:HB3	24:X:364:LYS:HE3	2.01	0.43
24:X:397:TYR:CE2	25:Y:362:LYS:HG2	2.54	0.43
26:Z:233:VAL:O	26:Z:237:LEU:HG	2.19	0.43
27:W:313:GLU:OE1	27:W:313:GLU:N	2.45	0.43
27:W:340:VAL:HA	27:W:350:ARG:NH1	2.34	0.43
32:E:117:PRO:CG	33:F:95:GLU:H	2.30	0.43
33:F:82:VAL:HA	33:F:85:THR:HB	2.01	0.43
1:G:101:TRP:CG	1:G:109:ILE:HB	2.53	0.43
4:J:127:PHE:O	4:J:129:ILE:N	2.49	0.43
5:L:15:PRO:HA	6:M:25:TYR:CG	2.53	0.43
11:R:38:ASN:OD1	11:R:41:LEU:N	2.52	0.43
3:i:19:TYR:HB3	3:i:23:TYR:CZ	2.53	0.43
14:k:137:PHE:O	14:k:158:PRO:HB3	2.19	0.43
6:m:90:ILE:HG21	6:m:118:TYR:CE2	2.54	0.43
7:n:16:ALA:HB1	7:n:33:LYS:HB2	2.01	0.43
9:p:12:MET:HB3	9:p:146:MET:CE	2.49	0.43
10:q:103:LEU:HG	10:q:132:HIS:HD2	1.83	0.43
14:K:67:ILE:HG21	14:K:218:ALA:HB2	2.01	0.43
17:a:188:LEU:HB2	17:a:189:PRO:HD2	2.01	0.43
22:U:204:ILE:O	22:U:208:LEU:HG	2.19	0.43
23:V:489:MET:HE1	25:Y:388:ASN:HA	2.01	0.43
26:Z:189:GLN:HE22	26:Z:193:ASN:HD21	1.66	0.43
26:Z:196:HIS:HA	26:Z:199:LYS:HB2	2.00	0.43
28:A:83:ASP:O	28:A:86:THR:HG22	2.19	0.43
29:B:221:GLY:HA2	29:B:326:LYS:HG3	2.00	0.43
30:C:74:GLY:O	30:C:114:VAL:N	2.48	0.43
30:C:297:ARG:O	30:C:299:ASP:N	2.52	0.43
31:D:214:MET:HE2	35:D:501:ADP:C5	2.54	0.43
1:G:21:ARG:NH1	1:G:26:GLU:OE1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:THR:OG1	1:G:108:GLU:OE2	2.28	0.42
1:G:212:PRO:HB3	1:G:239:LEU:HD12	2.00	0.42
2:H:101:TYR:HE1	9:P:90:MET:HE2	1.83	0.42
2:H:126:GLY:O	2:H:128:ARG:N	2.52	0.42
4:J:16:LEU:O	4:J:20:GLU:HG2	2.17	0.42
4:J:76:LEU:O	4:J:129:ILE:HD13	2.19	0.42
4:J:191:VAL:HG11	4:J:208:LEU:HD21	2.00	0.42
10:Q:11:ASP:N	10:Q:11:ASP:OD1	2.50	0.42
12:S:16:ALA:HB2	12:S:121:VAL:HG23	2.01	0.42
12:S:28:ARG:NH2	12:S:213:ASP:O	2.52	0.42
1:g:215:ILE:HD11	1:g:235:ILE:HG23	2.01	0.42
4:j:119:THR:HG22	4:j:126:PRO:HB3	2.00	0.42
4:j:224:GLU:HA	4:j:227:LYS:HG2	2.01	0.42
5:l:204:ASP:OD1	5:l:205:LEU:N	2.51	0.42
10:q:21:ALA:O	10:q:28:MET:N	2.51	0.42
14:K:42:THR:OG1	14:K:43:SER:N	2.52	0.42
15:f:165:GLU:HA	15:f:168:LYS:HD2	2.01	0.42
15:f:182:GLU:HB2	15:f:183:PRO:HD3	2.01	0.42
18:b:92:VAL:HG12	26:Z:67:VAL:HA	2.00	0.42
18:b:161:ASN:ND2	18:b:168:SER:O	2.47	0.42
18:b:179:LEU:O	18:b:183:LEU:HG	2.19	0.42
19:c:265:MET:O	19:c:266:THR:OG1	2.36	0.42
21:e:17:ASP:N	21:e:17:ASP:OD1	2.51	0.42
22:U:138:PHE:O	22:U:142:LEU:HG	2.19	0.42
22:U:508:THR:O	22:U:511:ALA:N	2.52	0.42
22:U:684:ARG:HH11	22:U:726:ALA:HB1	1.83	0.42
22:U:904:LYS:HD3	22:U:912:ILE:HG13	2.00	0.42
26:Z:65:ASP:OD2	26:Z:102:HIS:HB2	2.18	0.42
26:Z:174:HIS:HA	26:Z:177:ARG:CG	2.49	0.42
28:A:182:GLU:O	28:A:186:LYS:HG2	2.19	0.42
28:A:241:ILE:HG22	28:A:244:GLU:H	1.84	0.42
29:B:144:LEU:HA	29:B:162:VAL:HG21	2.00	0.42
30:C:165:ILE:HD13	30:C:165:ILE:HA	1.91	0.42
31:D:391:ARG:CG	31:D:392:TYR:H	2.21	0.42
32:E:56:ILE:HG13	32:E:57:VAL:N	2.34	0.42
32:E:117:PRO:HA	32:E:120:TYR:HB3	2.01	0.42
32:E:313:LEU:HG	32:E:343:LEU:HD13	2.00	0.42
32:E:323:HIS:HB2	32:E:325:GLU:OE1	2.19	0.42
33:F:313:LEU:O	33:F:317:LEU:HG	2.19	0.42
4:J:132:LEU:HD22	4:J:159:ASN:HB2	2.00	0.42
10:Q:35:MET:HB3	10:Q:43:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:206:LEU:HG	1:g:208:ILE:HG23	2.00	0.42
3:i:115:CYS:SG	3:i:156:TYR:HB3	2.58	0.42
14:k:66:LYS:HA	14:k:78:MET:HE2	2.00	0.42
14:k:86:LYS:HE2	14:k:86:LYS:HB3	1.91	0.42
6:m:117:MET:HE3	6:m:117:MET:HB3	1.90	0.42
6:m:150:MET:HG3	6:m:163:CYS:SG	2.59	0.42
10:q:7:ILE:HD11	10:q:14:LEU:HD23	2.00	0.42
14:K:207:GLU:HA	28:A:420:TYR:CZ	2.54	0.42
15:f:612:LEU:HD13	15:f:653:ALA:O	2.19	0.42
15:f:762:VAL:O	15:f:766:GLN:HG3	2.19	0.42
17:a:90:PRO:HA	17:a:93:ALA:HB3	2.00	0.42
19:c:281:LYS:HG2	19:c:282:ARG:HH11	1.83	0.42
22:U:349:ASP:O	22:U:353:LEU:HG	2.19	0.42
22:U:474:ARG:HB3	22:U:508:THR:HG21	2.01	0.42
27:W:207:LYS:HA	27:W:210:ASN:HD21	1.84	0.42
29:B:149:SER:OG	29:B:163:LEU:HB3	2.19	0.42
30:C:260:GLU:OE1	30:C:260:GLU:N	2.47	0.42
32:E:25:ARG:NE	33:F:55:MET:HE3	2.34	0.42
32:E:42:LYS:HB2	33:F:73:ILE:HD11	2.00	0.42
32:E:309:ARG:HD3	32:E:338:PHE:O	2.19	0.42
32:E:344:ARG:NE	33:F:345:SER:OG	2.53	0.42
33:F:198:LEU:HD21	33:F:236:LEU:HD21	2.01	0.42
33:F:272:PHE:HE2	33:F:320:PHE:HE2	1.66	0.42
2:H:108:ALA:O	2:H:111:VAL:HG12	2.18	0.42
7:N:59:VAL:HG11	7:N:83:PHE:CZ	2.53	0.42
8:O:211:VAL:HG21	9:P:198:ARG:HD3	2.01	0.42
3:i:12:PHE:CE2	4:j:125:ARG:HB2	2.55	0.42
5:l:168:ALA:HB2	5:l:198:THR:OG1	2.19	0.42
8:o:28:ASP:OD1	8:o:29:LYS:N	2.51	0.42
17:a:278:MET:HE3	17:a:339:ARG:HD3	2.02	0.42
23:V:464:ILE:HG21	23:V:469:THR:HG23	2.01	0.42
24:X:126:ARG:O	24:X:130:GLU:HG3	2.19	0.42
24:X:206:LEU:O	24:X:209:THR:OG1	2.27	0.42
25:Y:163:LYS:O	25:Y:168:ILE:HG12	2.19	0.42
26:Z:7:GLN:HB3	26:Z:46:LYS:HB3	2.01	0.42
29:B:230:THR:HA	35:B:501:ADP:O2A	2.19	0.42
31:D:317:LEU:HB3	31:D:321:LEU:HD11	2.01	0.42
33:F:289:ASP:OD1	33:F:289:ASP:N	2.52	0.42
33:F:422:GLU:O	33:F:426:GLU:HG3	2.19	0.42
6:M:195:LYS:O	6:M:199:ILE:HG12	2.20	0.42
7:N:30:VAL:HG11	13:t:211:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:58:HIS:HB3	13:T:130:VAL:HG13	2.01	0.42
12:S:166:LEU:HG	12:S:170:ARG:HH11	1.83	0.42
2:h:109:GLN:O	2:h:113:ARG:HG2	2.19	0.42
7:n:21:THR:HG22	7:n:26:ILE:HA	2.00	0.42
13:t:97:TYR:HA	13:t:100:ARG:HG2	2.02	0.42
17:a:11:SER:HB3	17:a:22:TRP:CZ2	2.54	0.42
17:a:81:LEU:O	17:a:85:ARG:HG2	2.19	0.42
17:a:279:GLU:HA	17:a:282:PHE:CE2	2.55	0.42
20:d:252:GLN:NE2	23:V:488:ASN:OD1	2.52	0.42
22:U:78:LEU:O	22:U:82:LEU:HB2	2.18	0.42
24:X:417:LYS:HD3	24:X:417:LYS:HA	1.79	0.42
25:Y:26:LEU:HB3	25:Y:59:LYS:HD2	2.02	0.42
25:Y:101:ARG:HG2	25:Y:136:HIS:CE1	2.55	0.42
25:Y:312:ARG:HA	25:Y:356:THR:HG22	2.01	0.42
27:W:169:LEU:O	27:W:182:ARG:NH2	2.52	0.42
30:C:209:CYS:O	30:C:210:THR:HG23	2.19	0.42
31:D:85:ILE:CG1	31:D:86:PRO:HD2	2.38	0.42
32:E:249:ALA:HB1	33:F:261:ILE:HG12	2.00	0.42
2:H:19:LEU:O	2:H:22:ILE:N	2.52	0.42
7:N:172:GLY:HA2	13:t:209:TRP:CH2	2.55	0.42
9:P:28:PHE:HD2	9:P:36:THR:HG22	1.84	0.42
9:P:30:ILE:HG12	9:P:33:GLN:HG2	2.01	0.42
2:h:162:ALA:O	2:h:167:TYR:HB2	2.19	0.42
8:o:2:THR:HG21	8:o:162:GLY:HA3	2.02	0.42
10:q:3:TYR:OH	10:q:5:ILE:HD12	2.19	0.42
11:r:71:LYS:O	11:r:71:LYS:HG2	2.20	0.42
17:a:232:TRP:CZ3	17:a:253:THR:HA	2.54	0.42
17:a:338:PRO:HB2	26:Z:229:GLN:HA	2.02	0.42
18:b:51:LEU:HB2	18:b:62:THR:OG1	2.19	0.42
23:V:391:THR:HA	23:V:394:LEU:HD13	2.01	0.42
24:X:248:ILE:HD13	24:X:251:LEU:HD21	2.01	0.42
24:X:366:SER:HA	24:X:369:ILE:HG22	2.01	0.42
25:Y:231:LEU:HD12	25:Y:234:PRO:CG	2.49	0.42
25:Y:316:LEU:HA	25:Y:319:MET:HG2	2.00	0.42
27:W:151:THR:O	27:W:155:GLN:HG3	2.19	0.42
27:W:186:ILE:O	27:W:189:GLN:NE2	2.52	0.42
27:W:340:VAL:HG12	27:W:341:PHE:CD1	2.55	0.42
28:A:362:MET:HB2	28:A:364:VAL:HG22	2.00	0.42
29:B:141:LYS:HA	29:B:144:LEU:HD12	2.01	0.42
31:D:85:ILE:HG12	32:E:105:LEU:HD21	2.01	0.42
31:D:370:ILE:O	31:D:371:SER:OG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:GLU:O	1:G:226:LYS:HA	2.19	0.42
5:L:77:LEU:HD23	5:L:80:ASP:H	1.84	0.42
10:Q:4:LEU:HD22	10:Q:45:LEU:HB3	2.01	0.42
11:R:113:TYR:CZ	11:R:115:ASP:HB2	2.55	0.42
13:T:59:ASP:O	13:T:63:LEU:HD23	2.19	0.42
1:g:27:TYR:CZ	6:m:16:PRO:HA	2.54	0.42
14:k:8:TYR:O	14:k:10:ARG:N	2.52	0.42
7:n:14:LEU:HD23	7:n:44:CYS:SG	2.60	0.42
10:q:95:ARG:HG3	10:q:96:THR:HG23	2.01	0.42
15:f:195:ASN:HD22	15:f:204:ALA:HB2	1.84	0.42
15:f:494:ARG:HE	15:f:495:GLU:H	1.66	0.42
15:f:610:GLN:NE2	15:f:611:GLN:HG3	2.35	0.42
23:V:134:PHE:HD2	23:V:187:ILE:HD11	1.84	0.42
26:Z:6:VAL:HG12	26:Z:43:TRP:CE2	2.54	0.42
26:Z:23:PHE:HD2	26:Z:97:THR:HG21	1.84	0.42
27:W:187:LEU:HB3	27:W:225:LYS:NZ	2.34	0.42
28:A:380:SER:O	28:A:384:GLU:HB2	2.19	0.42
30:C:273:MET:HE1	30:C:309:GLY:HA3	2.00	0.42
2:H:72:ILE:HA	2:H:137:CYS:O	2.20	0.42
2:H:80:GLY:N	2:H:81:PRO:HD2	2.35	0.42
3:I:118:LYS:O	3:I:122:THR:HG22	2.19	0.42
6:M:72:HIS:H	6:M:72:HIS:CD2	2.38	0.42
10:Q:35:MET:HG3	10:Q:181:ARG:HD2	2.01	0.42
2:h:177:ARG:HG3	2:h:177:ARG:O	2.19	0.42
3:i:184:MET:HG3	3:i:189:ALA:HB2	2.02	0.42
14:k:215:ILE:HD11	14:k:234:LEU:HD21	2.01	0.42
5:l:168:ALA:O	5:l:172:LEU:HG	2.20	0.42
7:n:40:ARG:HG2	7:n:103:TRP:CE3	2.53	0.42
8:o:17:ASP:OD2	8:o:33:LYS:NZ	2.53	0.42
13:t:182:ARG:N	13:t:182:ARG:HD2	2.35	0.42
15:f:322:SER:HA	15:f:456:ARG:HB2	2.01	0.42
17:a:359:ASP:O	17:a:363:MET:HG2	2.19	0.42
19:c:59:GLY:HA3	19:c:69:VAL:HG22	2.01	0.42
22:U:117:ASP:OD1	22:U:192:GLN:HG3	2.20	0.42
23:V:487:HIS:O	23:V:491:VAL:HG23	2.20	0.42
30:C:42:LEU:HD22	31:D:66:LYS:HB2	2.01	0.42
30:C:64:GLN:OE1	30:C:67:GLN:NE2	2.52	0.42
30:C:68:GLU:O	30:C:118:ASN:ND2	2.52	0.42
30:C:198:LEU:C	30:C:200:ALA:H	2.26	0.42
30:C:199:LEU:O	30:C:203:VAL:HG22	2.19	0.42
31:D:367:PRO:HD3	31:D:403:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:E:234:GLU:OE2	32:E:236:ASP:HB2	2.20	0.42
33:F:124:ILE:HG21	33:F:153:VAL:HG21	2.00	0.42
33:F:139:LEU:HD23	33:F:161:LEU:HA	2.00	0.42
1:G:104:LYS:HB3	1:G:104:LYS:HE3	1.75	0.42
2:H:180:GLU:HB3	2:H:183:GLU:HG2	2.02	0.42
5:L:77:LEU:CD2	5:L:80:ASP:H	2.33	0.42
5:L:115:LYS:HE3	5:L:128:TYR:HE2	1.83	0.42
12:S:106:VAL:HG23	12:S:108:ASN:HD21	1.84	0.42
1:g:121:ILE:HG22	1:g:125:TYR:CZ	2.55	0.42
14:k:13:ASN:ND2	5:l:124:GLY:O	2.48	0.42
5:l:23:GLU:O	5:l:26:MET:HG2	2.19	0.42
6:m:45:VAL:HG23	6:m:146:ALA:HB1	2.02	0.42
7:n:133:SER:HA	7:n:136:TYR:HE2	1.85	0.42
15:f:322:SER:HB3	15:f:456:ARG:O	2.20	0.42
15:f:408:LEU:HB3	15:f:815:HIS:CE1	2.42	0.42
15:f:613:LEU:HA	15:f:616:CYS:SG	2.59	0.42
19:c:177:THR:HG23	22:U:364:VAL:HG23	2.02	0.42
20:d:26:LEU:HD13	22:U:19:LEU:HD21	2.01	0.42
20:d:92:SER:OG	20:d:93:ALA:N	2.51	0.42
23:V:471:GLU:N	23:V:472:PRO:HD2	2.34	0.42
24:X:344:ARG:HG3	24:X:386:ILE:HA	2.02	0.42
25:Y:291:HIS:HA	25:Y:295:TYR:CE2	2.54	0.42
25:Y:304:TYR:HD2	25:Y:343:LEU:HD21	1.84	0.42
29:B:247:PHE:CZ	29:B:249:ARG:HB2	2.55	0.42
29:B:339:PRO:HA	29:B:342:ILE:HB	2.02	0.42
32:E:39:GLN:HB2	33:F:69:MET:O	2.20	0.42
32:E:111:LEU:HD22	33:F:133:PHE:CE1	2.55	0.42
7:N:52:THR:HG22	7:N:96:ALA:HB1	2.02	0.42
9:P:205:ASP:OD2	11:r:19:ARG:NH2	2.53	0.42
12:S:187:VAL:HG12	8:o:19:ARG:NH1	2.35	0.42
1:g:81:THR:HG21	1:g:169:GLY:HA2	2.01	0.42
5:l:176:MET:HE3	5:l:176:MET:HB3	1.92	0.42
8:o:67:SER:HB3	8:o:74:PRO:HG3	2.01	0.42
13:t:88:ILE:O	13:t:92:LEU:HD23	2.19	0.42
15:f:62:ARG:HD2	15:f:70:LEU:HB3	2.01	0.42
17:a:81:LEU:HD11	17:a:117:ALA:HB2	2.01	0.42
18:b:140:ILE:HB	18:b:170:LEU:HD12	2.02	0.42
20:d:155:LYS:HB3	20:d:167:ILE:HB	2.02	0.42
22:U:665:ASN:O	22:U:666:LYS:HB3	2.20	0.42
22:U:792:ASN:OD1	22:U:793:LYS:N	2.53	0.42
22:U:826:GLU:HB3	29:B:84:GLN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:168:GLN:HB3	23:V:191:LEU:HB2	2.02	0.42
23:V:481:SER:O	23:V:484:LEU:HG	2.20	0.42
25:Y:337:PHE:HB2	25:Y:343:LEU:HD22	2.01	0.42
26:Z:40:LEU:HG	26:Z:91:ILE:HG12	2.01	0.42
27:W:231:ILE:HG13	27:W:232:GLN:N	2.35	0.42
28:A:232:ARG:HH12	28:A:271:LEU:HD13	1.83	0.42
29:B:227:PRO:HD2	29:B:353:PHE:HD2	1.83	0.42
2:H:107:THR:O	2:H:111:VAL:N	2.53	0.42
4:J:108:THR:HG22	4:J:133:ILE:HD13	2.02	0.42
5:L:71:GLY:HA3	5:L:221:PHE:CZ	2.54	0.42
6:M:163:CYS:SG	6:M:164:ALA:N	2.93	0.42
8:O:11:GLY:HA2	8:O:108:PRO:HB3	2.02	0.42
8:O:164:PHE:CZ	8:O:192:PRO:HB2	2.55	0.42
9:P:27:ARG:NH2	11:r:168:ALA:HB2	2.35	0.42
13:T:96:MET:HE3	13:T:127:MET:HA	2.02	0.42
14:k:17:PRO:HA	5:l:24:TYR:CE1	2.55	0.42
6:m:102:PHE:HB3	7:n:78:THR:HG23	2.01	0.42
7:n:112:TYR:CE2	7:n:122:ARG:HB2	2.54	0.42
13:t:4:PRO:HD3	13:t:107:TRP:CD2	2.54	0.42
15:f:511:SER:HB3	15:f:514:VAL:HG23	2.02	0.42
15:f:687:ARG:HG3	15:f:721:VAL:HG21	2.02	0.42
20:d:67:ASP:OD1	20:d:67:ASP:N	2.47	0.42
22:U:393:LEU:HA	22:U:393:LEU:HD23	1.83	0.42
22:U:557:TYR:CE1	22:U:757:MET:HE3	2.55	0.42
23:V:225:ASP:OD1	23:V:226:VAL:HG23	2.20	0.42
24:X:211:ASP:O	24:X:231:TYR:HB3	2.20	0.42
24:X:365:LEU:HD21	24:X:385:LEU:HD13	2.02	0.42
25:Y:101:ARG:NH2	25:Y:136:HIS:HB3	2.35	0.42
25:Y:342:ARG:HD3	25:Y:342:ARG:HA	1.77	0.42
28:A:327:LEU:HG	28:A:328:ASP:H	1.85	0.42
28:A:336:ARG:HA	28:A:336:ARG:HD2	1.86	0.42
29:B:75:GLU:O	29:B:79:ILE:HG22	2.19	0.42
29:B:120:HIS:HA	29:B:134:SER:HA	2.02	0.42
29:B:280:SER:OG	29:B:281:ILE:N	2.51	0.42
30:C:35:VAL:HG11	31:D:59:GLU:CA	2.44	0.42
30:C:235:PHE:CD2	30:C:276:LEU:HD13	2.48	0.42
31:D:85:ILE:O	31:D:86:PRO:C	2.63	0.42
31:D:293:LEU:HA	31:D:296:MET:HG2	2.02	0.42
33:F:253:GLY:N	33:F:254:PRO:HD2	2.34	0.42
2:H:109:GLN:O	2:H:113:ARG:HG2	2.20	0.41
3:I:114:LEU:HA	3:I:114:LEU:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:158:ALA:HB1	5:L:172:LEU:HD13	2.02	0.41
12:S:151:ASN:HD22	9:p:173:ASN:CB	2.33	0.41
8:o:103:VAL:HA	8:o:108:PRO:HA	2.01	0.41
13:t:135:PRO:HB2	13:t:154:LEU:HD13	2.02	0.41
13:t:156:LYS:HA	13:t:156:LYS:HE3	2.01	0.41
15:f:609:VAL:O	15:f:613:LEU:HG	2.20	0.41
15:f:699:VAL:HG13	15:f:779:CYS:HA	2.02	0.41
17:a:245:VAL:HG23	17:a:246:GLU:N	2.35	0.41
22:U:213:PHE:CG	22:U:214:ILE:N	2.87	0.41
22:U:521:LEU:HG	22:U:557:TYR:HE2	1.84	0.41
24:X:143:TYR:CZ	25:Y:252:SER:HB3	2.55	0.41
24:X:400:ALA:O	24:X:403:THR:OG1	2.30	0.41
25:Y:66:ASP:OD2	25:Y:70:LEU:HB2	2.20	0.41
28:A:329:PRO:C	28:A:333:ARG:HE	2.28	0.41
30:C:194:THR:HG23	35:C:501:ADP:H3'	2.02	0.41
30:C:391:MET:HB3	30:C:392:GLN:NE2	2.35	0.41
32:E:25:ARG:HE	33:F:55:MET:CE	2.33	0.41
32:E:33:LEU:HD22	32:E:37:THR:HG21	2.02	0.41
33:F:188:ILE:HA	35:F:501:ADP:N1	2.34	0.41
4:J:117:ARG:O	4:J:124:ARG:NH2	2.39	0.41
4:j:134:VAL:HG12	4:j:144:LEU:HD13	2.02	0.41
4:j:184:ASP:OD1	4:j:184:ASP:N	2.51	0.41
7:n:53:GLN:CD	8:o:119:THR:H	2.29	0.41
10:q:107:TYR:HA	10:q:113:PRO:HA	2.03	0.41
11:r:61:ARG:O	11:r:65:ILE:HG12	2.20	0.41
14:K:217:LEU:HD23	14:K:229:PHE:CD2	2.56	0.41
15:f:178:LYS:HD3	15:f:181:ARG:HG3	2.02	0.41
19:c:40:LYS:HD2	19:c:74:ALA:HB2	2.03	0.41
19:c:119:GLY:HA3	19:c:190:GLN:NE2	2.30	0.41
22:U:115:ASN:HD22	22:U:126:ILE:HD11	1.85	0.41
22:U:415:HIS:NE2	22:U:418:GLU:HB2	2.35	0.41
30:C:42:LEU:O	30:C:46:GLN:HG2	2.20	0.41
31:D:231:VAL:HG12	31:D:234:GLU:H	1.85	0.41
2:H:74:LEU:HD11	2:H:134:LEU:HB2	2.02	0.41
2:H:134:LEU:HD23	2:H:134:LEU:H	1.85	0.41
3:I:167:ASN:OD1	3:I:167:ASN:N	2.53	0.41
6:M:36:ALA:N	6:M:165:ILE:O	2.53	0.41
1:g:159:TYR:CG	1:g:159:TYR:O	2.73	0.41
4:j:166:LYS:HA	4:j:169:ARG:HG2	2.02	0.41
12:s:63:THR:HG21	13:t:97:TYR:CG	2.55	0.41
13:t:74:GLU:HG3	13:t:83:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:143:ARG:NE	15:f:151:LEU:HD11	2.35	0.41
17:a:149:THR:HG23	17:a:182:CYS:HB2	2.02	0.41
19:c:259:VAL:HG11	24:X:411:VAL:HG12	2.02	0.41
22:U:483:LEU:HD13	22:U:778:PHE:CZ	2.55	0.41
22:U:560:MET:HA	22:U:590:TYR:CE2	2.55	0.41
22:U:602:LEU:HD21	22:U:622:LEU:HB3	2.02	0.41
22:U:904:LYS:HB3	22:U:912:ILE:HG23	2.02	0.41
25:Y:138:LEU:HD23	25:Y:168:ILE:HG22	2.02	0.41
25:Y:367:GLN:O	25:Y:371:LYS:HG2	2.19	0.41
27:W:166:LEU:HD12	27:W:193:CYS:SG	2.59	0.41
27:W:336:PRO:O	27:W:340:VAL:HG23	2.20	0.41
27:W:359:VAL:HG11	27:W:392:PHE:HD2	1.85	0.41
29:B:232:LYS:NZ	29:B:235:LEU:HB2	2.35	0.41
32:E:39:GLN:HB3	33:F:73:ILE:CD1	2.50	0.41
32:E:72:LYS:HD3	32:E:78:ARG:NE	2.35	0.41
3:I:190:LEU:O	3:I:194:ILE:HG12	2.20	0.41
6:M:150:MET:HE3	6:M:150:MET:HB3	1.96	0.41
7:N:24:SER:HB2	13:t:141:TYR:CZ	2.55	0.41
11:R:40:TYR:OH	11:R:74:ILE:HG22	2.20	0.41
1:g:162:GLY:HA3	2:h:61:SER:HB3	2.02	0.41
4:j:35:VAL:HG12	4:j:42:VAL:HB	2.01	0.41
5:l:36:VAL:HG13	5:l:172:LEU:HD11	2.03	0.41
6:m:37:ILE:HD11	6:m:193:VAL:HG13	2.02	0.41
11:r:91:LYS:HE3	11:r:91:LYS:HB2	1.91	0.41
14:K:108:THR:HG22	14:K:110:GLU:H	1.86	0.41
15:f:514:VAL:O	15:f:518:THR:HG23	2.20	0.41
17:a:261:LEU:HD12	17:a:261:LEU:HA	1.87	0.41
19:c:266:THR:O	19:c:268:GLU:N	2.53	0.41
20:d:105:PHE:HB2	20:d:166:PHE:HD2	1.83	0.41
21:e:22:PHE:CD2	23:V:324:PHE:HB2	2.55	0.41
22:U:147:TYR:HA	22:U:150:ALA:HB3	2.01	0.41
22:U:250:PHE:CE1	22:U:328:ILE:HD12	2.56	0.41
22:U:524:LYS:HD3	22:U:559:ARG:NE	2.35	0.41
22:U:727:LYS:O	22:U:731:ILE:HG13	2.21	0.41
22:U:800:VAL:HB	22:U:880:ASN:HB3	2.02	0.41
23:V:394:LEU:HG	23:V:397:ARG:NH2	2.36	0.41
26:Z:23:PHE:CD2	26:Z:97:THR:HG21	2.55	0.41
26:Z:189:GLN:O	26:Z:192:THR:OG1	2.30	0.41
27:W:275:ILE:HD11	27:W:305:LEU:HA	2.02	0.41
28:A:229:VAL:HG22	28:A:232:ARG:CZ	2.49	0.41
28:A:404:ALA:HA	28:A:407:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:369:THR:HA	29:B:372:MET:HG2	2.01	0.41
32:E:200:SER:OG	32:E:233:ASP:O	2.33	0.41
2:H:78:GLY:HA2	31:D:417:TYR:CE1	2.56	0.41
2:H:203:MET:SD	2:H:230:LEU:HD21	2.61	0.41
5:L:80:ASP:OD2	5:L:126:ARG:NH2	2.54	0.41
6:M:31:GLU:O	6:M:167:LYS:HA	2.21	0.41
8:O:45:GLY:HA3	8:O:52:THR:HG21	2.03	0.41
1:g:138:MET:HB3	1:g:154:CYS:SG	2.59	0.41
3:i:69:ASN:OD1	3:i:72:MET:HB3	2.20	0.41
4:j:180:ALA:HB1	4:j:190:LEU:HD11	2.01	0.41
6:m:188:ASP:O	6:m:192:GLU:HG2	2.20	0.41
6:m:227:VAL:HG12	6:m:228:PRO:O	2.21	0.41
8:o:51:ASP:OD2	9:p:99:ARG:NH1	2.54	0.41
8:o:82:MET:HA	8:o:85:GLN:NE2	2.36	0.41
11:r:8:PHE:CE2	11:r:10:HIS:HB2	2.55	0.41
13:t:154:LEU:HD23	13:t:154:LEU:HA	1.82	0.41
15:f:99:LEU:HD22	15:f:129:LEU:HD11	2.01	0.41
17:a:116:THR:O	17:a:158:LEU:HD21	2.21	0.41
18:b:18:ASN:OD1	18:b:25:ARG:NH1	2.54	0.41
22:U:24:LEU:HA	22:U:27:LEU:HG	2.03	0.41
22:U:607:VAL:C	31:D:68:LEU:CD2	2.93	0.41
22:U:761:VAL:HA	22:U:764:LEU:HD12	2.02	0.41
24:X:341:PRO:O	27:W:406:VAL:HG12	2.20	0.41
25:Y:47:ASP:HA	25:Y:113:ARG:HH12	1.85	0.41
25:Y:50:MET:HB2	25:Y:70:LEU:CD2	2.50	0.41
25:Y:228:MET:SD	25:Y:263:LEU:HD13	2.61	0.41
28:A:387:SER:HB3	29:B:345:GLY:HA3	2.03	0.41
30:C:66:LEU:HA	30:C:70:GLY:N	2.36	0.41
30:C:113:ARG:HH21	30:C:129:ASN:HA	1.85	0.41
6:M:215:TRP:CG	6:M:227:VAL:HG12	2.56	0.41
7:N:46:SER:OG	7:N:97:GLY:O	2.37	0.41
7:N:114:VAL:HA	7:N:119:MET:O	2.20	0.41
10:Q:85:ARG:HD2	10:Q:124:LEU:N	2.36	0.41
2:h:34:PRO:HD2	2:h:49:GLU:OE2	2.20	0.41
4:j:36:ARG:HB2	4:j:144:LEU:HB2	2.02	0.41
4:j:107:ILE:O	4:j:111:ILE:HG13	2.20	0.41
14:k:221:GLN:OE1	14:k:221:GLN:N	2.53	0.41
5:l:238:GLU:HG3	5:l:239:ARG:H	1.85	0.41
6:m:23:VAL:O	6:m:27:MET:HG3	2.21	0.41
10:q:29:LYS:HD2	11:r:122:SER:O	2.21	0.41
10:q:39:SER:OG	10:q:40:GLU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:607:LEU:H	15:f:607:LEU:HD12	1.85	0.41
15:f:670:MET:HG3	29:B:71:TYR:CD2	2.55	0.41
15:f:806:VAL:HB	15:f:810:ILE:CG2	2.51	0.41
17:a:18:GLN:N	17:a:19:PRO:HD2	2.35	0.41
22:U:202:VAL:HG12	22:U:219:CYS:HB2	2.03	0.41
22:U:223:LEU:HD23	22:U:225:ASP:OD2	2.21	0.41
22:U:493:VAL:O	22:U:497:LEU:HD13	2.21	0.41
23:V:111:TYR:HE2	23:V:115:LYS:HE2	1.86	0.41
25:Y:294:TYR:CD1	25:Y:298:GLU:HB2	2.54	0.41
27:W:145:LEU:HD21	27:W:172:GLU:CD	2.44	0.41
29:B:193:GLN:O	29:B:197:ILE:HG22	2.21	0.41
29:B:406:ALA:HA	29:B:410:ARG:HB2	2.02	0.41
30:C:113:ARG:HB3	30:C:127:LEU:HB3	2.03	0.41
30:C:117:ARG:HG2	30:C:118:ASN:N	2.36	0.41
31:D:215:LEU:H	31:D:215:LEU:HD12	1.86	0.41
33:F:123:VAL:HG22	33:F:133:PHE:CD2	2.53	0.41
33:F:235:LEU:CD1	35:F:501:ADP:H2'	2.50	0.41
1:G:73:THR:HG23	1:G:75:ASN:H	1.85	0.41
4:J:120:GLN:O	4:J:124:ARG:NH2	2.53	0.41
7:N:36:PRO:HB3	7:N:42:PHE:CZ	2.56	0.41
9:P:178:ASP:OD2	9:P:181:SER:HB2	2.21	0.41
10:Q:4:LEU:O	10:Q:132:HIS:N	2.54	0.41
11:R:166:ARG:NE	10:q:144:ASP:OD2	2.50	0.41
13:T:34:ALA:O	7:n:166:ARG:NH1	2.54	0.41
1:g:23:TYR:HA	1:g:26:GLU:HG2	2.02	0.41
2:h:54:SER:O	2:h:56:LEU:N	2.54	0.41
3:i:111:VAL:HG22	3:i:136:TYR:CD2	2.52	0.41
4:j:23:GLN:HE22	4:j:148:ASP:HB2	1.85	0.41
4:j:35:VAL:HG23	4:j:158:ALA:HB2	2.01	0.41
6:m:27:MET:HA	6:m:30:VAL:HG12	2.02	0.41
10:q:62:LYS:HB2	10:q:62:LYS:HE2	1.91	0.41
10:q:90:ASP:OD1	10:q:91:CYS:N	2.53	0.41
10:q:104:LEU:HB2	10:q:116:TYR:HB2	2.03	0.41
11:r:3:THR:O	11:r:127:SER:OG	2.33	0.41
12:s:64:LEU:HD13	12:s:106:VAL:HG21	2.03	0.41
17:a:302:ILE:HD12	17:a:302:ILE:HA	1.94	0.41
19:c:146:ASP:OD1	19:c:148:ILE:HG12	2.21	0.41
23:V:338:LEU:HD12	23:V:398:LEU:HD12	2.03	0.41
23:V:357:LEU:O	23:V:361:PHE:N	2.46	0.41
23:V:494:MET:HE3	30:C:44:ARG:NH1	2.35	0.41
24:X:90:ARG:HE	24:X:128:ALA:HB1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:56:ALA:HA	25:Y:59:LYS:NZ	2.35	0.41
25:Y:275:LEU:HG	25:Y:296:VAL:HG12	2.03	0.41
25:Y:380:VAL:HG11	26:Z:265:LEU:HD11	2.01	0.41
28:A:277:ILE:HG23	28:A:280:ILE:HG13	2.01	0.41
28:A:321:THR:OG1	28:A:322:ASN:N	2.54	0.41
28:A:371:GLU:O	28:A:375:ARG:HG3	2.21	0.41
29:B:99:VAL:HG21	29:B:138:PHE:CD2	2.55	0.41
29:B:187:ILE:HG13	35:B:501:ADP:N1	2.36	0.41
29:B:260:LEU:HD23	29:B:260:LEU:H	1.85	0.41
32:E:317:ALA:O	32:E:322:LYS:NZ	2.54	0.41
1:G:70:PHE:HZ	1:G:88:ARG:NH1	2.19	0.41
1:G:103:TYR:HB2	7:N:61:TYR:CD1	2.55	0.41
2:H:73:GLY:HA3	2:H:218:PHE:CE1	2.55	0.41
4:J:136:PHE:HA	4:J:142:PRO:HA	2.03	0.41
6:M:102:PHE:HB3	7:N:78:THR:HG23	2.02	0.41
3:i:20:GLN:HG2	3:i:21:VAL:N	2.35	0.41
4:j:40:ILE:HG22	4:j:212:ARG:HG3	2.03	0.41
4:j:144:LEU:HB3	4:j:156:TRP:O	2.20	0.41
5:l:139:ASP:N	5:l:139:ASP:OD1	2.53	0.41
6:m:20:VAL:HG23	6:m:20:VAL:O	2.20	0.41
6:m:60:GLU:H	6:m:60:GLU:CD	2.29	0.41
9:p:164:PHE:CE1	9:p:198:ARG:HD2	2.56	0.41
11:r:160:ILE:HD13	11:r:160:ILE:HA	1.94	0.41
12:s:27:THR:OG1	12:s:192:ALA:HB3	2.20	0.41
14:K:206:MET:SD	14:K:215:ILE:HD11	2.61	0.41
15:f:429:ILE:HD12	15:f:432:TYR:HB2	2.03	0.41
15:f:553:THR:HA	15:f:556:ARG:HH12	1.85	0.41
17:a:22:TRP:CZ3	17:a:25:LEU:HD13	2.56	0.41
17:a:72:ASN:HA	18:b:17:ARG:NH2	2.33	0.41
19:c:151:VAL:HG13	19:c:152:LYS:N	2.35	0.41
20:d:183:GLU:OE1	20:d:215:TRP:NE1	2.54	0.41
22:U:323:LEU:H	22:U:323:LEU:HD12	1.85	0.41
22:U:627:PHE:CE1	22:U:755:THR:HG22	2.56	0.41
22:U:881:PRO:HG2	22:U:927:PRO:HB2	2.03	0.41
23:V:330:LYS:HG2	23:V:360:TYR:HE2	1.85	0.41
23:V:360:TYR:O	23:V:364:THR:HG23	2.20	0.41
24:X:401:LEU:HD11	25:Y:372:LYS:HG3	2.03	0.41
25:Y:17:LEU:HD22	25:Y:214:MET:HG2	2.03	0.41
25:Y:300:ARG:HA	25:Y:303:ALA:HB3	2.03	0.41
27:W:225:LYS:O	27:W:229:LEU:HD23	2.21	0.41
28:A:229:VAL:HG21	28:A:237:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:232:ARG:NH2	28:A:271:LEU:HB3	2.30	0.41
28:A:297:ARG:NH2	33:F:171:ARG:HG2	2.35	0.41
29:B:92:GLN:OE1	29:B:96:ARG:HB2	2.21	0.41
32:E:20:LYS:HA	32:E:23:ASP:HB2	2.02	0.41
32:E:49:ALA:HB1	33:F:159:LEU:HD22	2.02	0.41
32:E:70:ILE:HA	32:E:80:VAL:HG22	2.02	0.41
1:G:25:VAL:HG21	31:D:415:GLU:HG3	2.03	0.41
1:G:40:VAL:HG23	1:G:202:LEU:HD13	2.02	0.41
1:G:69:LEU:HD21	1:G:216:GLU:HB3	2.02	0.41
1:G:225:PRO:O	1:G:226:LYS:HB2	2.21	0.41
2:H:58:ASP:OD1	2:H:60:ARG:N	2.54	0.41
2:H:103:GLU:N	2:H:104:PRO:HD3	2.36	0.41
4:J:16:LEU:HB3	4:J:19:VAL:HB	2.02	0.41
6:M:186:CYS:SG	6:M:219:LEU:HD22	2.61	0.41
7:N:164:MET:SD	7:N:174:ILE:HG12	2.61	0.41
9:P:138:VAL:HG22	9:P:147:TYR:CE1	2.56	0.41
9:P:172:LEU:HD13	12:s:157:ASN:HD21	1.86	0.41
10:Q:85:ARG:CD	10:Q:124:LEU:H	2.33	0.41
11:R:166:ARG:HD3	11:R:166:ARG:HA	1.88	0.41
11:R:172:GLY:O	11:R:192:VAL:HG22	2.20	0.41
13:T:178:TYR:OH	13:T:208:ASN:N	2.48	0.41
1:g:12:HIS:CD2	6:m:6:GLY:HA3	2.56	0.41
1:g:80:MET:HE3	1:g:138:MET:HB2	2.02	0.41
1:g:119:ALA:HB1	2:h:84:ARG:NH2	2.35	0.41
5:l:65:HIS:CD2	12:s:77:HIS:HE1	2.39	0.41
5:l:85:CYS:HA	5:l:88:MET:HE2	2.03	0.41
8:o:80:ASN:HD21	8:o:119:THR:HG21	1.85	0.41
8:o:127:MET:C	8:o:131:SER:HB2	2.46	0.41
9:p:30:ILE:HG13	9:p:31:GLN:N	2.36	0.41
10:q:116:TYR:HB3	10:q:124:LEU:HD11	2.02	0.41
10:q:184:ASP:OD1	10:q:184:ASP:N	2.54	0.41
11:r:1:THR:O	11:r:130:SER:N	2.54	0.41
12:s:21:ALA:HB3	12:s:198:VAL:HB	2.03	0.41
14:K:108:THR:O	14:K:111:SER:OG	2.33	0.41
15:f:53:GLN:HB2	15:f:98:PHE:CE1	2.56	0.41
15:f:76:GLU:CD	15:f:79:ARG:HH22	2.29	0.41
15:f:237:VAL:HG13	15:f:245:ASN:OD1	2.21	0.41
15:f:316:ASP:O	15:f:320:ILE:HG12	2.21	0.41
15:f:345:PRO:O	15:f:763:ARG:NH2	2.52	0.41
15:f:848:GLN:OE1	15:f:878:GLU:HB3	2.20	0.41
17:a:290:GLN:HA	17:a:330:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:25:ARG:NH1	18:b:145:GLU:OE2	2.53	0.41
18:b:52:ILE:HG13	18:b:93:ALA:HA	2.02	0.41
18:b:71:ILE:HD12	18:b:71:ILE:H	1.86	0.41
19:c:39:LEU:HD12	26:Z:17:LEU:HD21	2.03	0.41
20:d:152:PHE:HE1	20:d:174:ILE:HG21	1.86	0.41
22:U:363:SER:HG	22:U:365:CYS:HG	1.69	0.41
22:U:550:VAL:O	22:U:554:LEU:HD23	2.21	0.41
22:U:595:ASN:O	22:U:599:ILE:HG13	2.21	0.41
22:U:827:LYS:HG2	29:B:85:MET:HE2	2.02	0.41
22:U:872:GLU:O	22:U:874:ASN:N	2.53	0.41
23:V:479:ARG:HD3	26:Z:265:LEU:HD13	2.03	0.41
23:V:482:PHE:HA	23:V:485:ASP:OD2	2.20	0.41
25:Y:179:ARG:HD3	25:Y:182:VAL:HG23	2.02	0.41
25:Y:235:ASP:O	25:Y:239:LYS:HG2	2.21	0.41
26:Z:191:ILE:O	26:Z:195:VAL:HG23	2.20	0.41
28:A:120:LYS:HZ1	33:F:153:VAL:HG23	1.86	0.41
29:B:111:THR:O	29:B:123:VAL:HG23	2.21	0.41
30:C:28:ILE:HD13	30:C:28:ILE:HA	1.96	0.41
30:C:83:LYS:O	30:C:98:ASP:HA	2.21	0.41
30:C:189:TYR:CZ	30:C:316:GLU:HB3	2.56	0.41
31:D:170:MET:SD	31:D:343:LEU:HD21	2.61	0.41
32:E:22:ILE:HD13	33:F:56:LYS:NZ	2.35	0.41
33:F:172:VAL:HG11	33:F:270:ASP:HB3	2.03	0.41
33:F:212:PHE:CD2	33:F:219:PRO:HG3	2.56	0.41
33:F:321:GLN:HB3	33:F:322:PRO:HD3	2.03	0.41
33:F:344:ARG:HB3	33:F:347:ARG:HG2	2.03	0.41
3:I:10:THR:HG23	3:I:10:THR:O	2.21	0.41
3:I:49:ARG:HB3	3:I:52:ILE:HD11	2.02	0.41
8:O:51:ASP:HB3	8:O:94:ILE:HG23	2.03	0.41
11:R:131:GLY:HA2	11:R:134:TYR:HD2	1.87	0.41
1:g:158:GLY:O	2:h:84:ARG:NH2	2.54	0.41
2:h:89:ARG:HD2	2:h:117:VAL:HG11	2.03	0.41
7:n:161:ALA:HA	7:n:164:MET:HG2	2.02	0.41
15:f:678:LEU:HB3	15:f:686:LEU:HD11	2.02	0.41
18:b:8:VAL:HG23	18:b:110:ILE:HG23	2.02	0.41
19:c:145:VAL:HA	19:c:156:VAL:O	2.21	0.41
23:V:211:TYR:OH	23:V:234:ARG:NH2	2.51	0.41
29:B:139:VAL:HG13	29:B:139:VAL:O	2.21	0.41
29:B:434:THR:O	29:B:435:PRO:C	2.63	0.41
30:C:393:LYS:HA	30:C:393:LYS:HD3	1.93	0.41
31:D:199:PRO:O	31:D:306:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:200:ARG:HH22	31:D:326:ARG:HA	1.86	0.41
32:E:194:ASN:HD22	32:E:227:PRO:HG2	1.85	0.41
3:I:86:LEU:HD13	3:I:130:PHE:CD2	2.56	0.40
3:I:114:LEU:HD23	3:I:136:TYR:OH	2.22	0.40
7:N:123:GLN:NE2	7:N:125:PHE:O	2.49	0.40
8:O:127:MET:C	8:O:131:SER:HB2	2.45	0.40
9:P:118:LYS:HD3	9:P:118:LYS:HA	1.86	0.40
3:i:3:ARG:NH2	14:k:125:GLU:OE1	2.50	0.40
3:i:43:VAL:HG23	3:i:137:ILE:HD12	2.02	0.40
7:n:84:LYS:HB2	7:n:120:MET:HB2	2.03	0.40
13:t:171:ARG:O	13:t:175:VAL:HG23	2.21	0.40
15:f:742:ALA:O	15:f:746:ARG:HG3	2.20	0.40
17:a:346:ILE:O	17:a:349:MET:HG2	2.21	0.40
22:U:158:ARG:HA	22:U:158:ARG:NH1	2.36	0.40
22:U:208:LEU:HD12	22:U:215:ASN:HD22	1.86	0.40
22:U:410:VAL:HG12	22:U:780:SER:HB2	2.03	0.40
23:V:325:LYS:O	23:V:328:VAL:HG12	2.20	0.40
23:V:361:PHE:O	23:V:364:THR:OG1	2.31	0.40
24:X:74:ARG:HA	24:X:77:LEU:HD12	2.03	0.40
26:Z:180:LYS:NZ	31:D:81:ARG:HH21	2.19	0.40
27:W:28:LEU:HD13	27:W:65:ARG:HE	1.86	0.40
27:W:88:MET:HA	27:W:130:MET:SD	2.60	0.40
28:A:80:LEU:HD12	28:A:80:LEU:HA	1.92	0.40
28:A:184:ILE:H	28:A:184:ILE:HG13	1.63	0.40
29:B:64:LYS:HE2	29:B:64:LYS:HB3	1.90	0.40
31:D:157:ASP:OD1	31:D:158:GLN:HG2	2.21	0.40
31:D:410:ASP:OD1	31:D:410:ASP:N	2.53	0.40
33:F:91:SER:O	33:F:149:ASP:HA	2.21	0.40
3:I:52:ILE:HG23	3:I:52:ILE:HD12	1.88	0.40
5:L:66:VAL:O	12:S:77:HIS:NE2	2.53	0.40
5:L:133:LEU:HD23	5:L:133:LEU:HA	1.87	0.40
6:M:185:THR:O	6:M:189:ILE:HG12	2.21	0.40
7:N:8:PHE:HB3	7:N:152:CYS:SG	2.61	0.40
10:Q:22:ALA:CB	10:q:172:ILE:HD12	2.51	0.40
1:g:51:VAL:HG23	1:g:217:VAL:HG22	2.02	0.40
2:h:17:GLY:HA3	3:i:27:ALA:HB2	2.03	0.40
4:j:82:ILE:HG13	4:j:83:VAL:N	2.37	0.40
14:k:32:LYS:HE2	14:k:32:LYS:HB3	1.87	0.40
14:k:197:SER:O	14:k:201:ILE:HG12	2.21	0.40
7:n:14:LEU:HD13	7:n:179:ILE:HD13	2.03	0.40
10:q:35:MET:HE3	10:q:45:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:127:MET:HE2	13:t:127:MET:HB3	1.93	0.40
17:a:369:HIS:HA	17:a:372:HIS:CE1	2.57	0.40
17:a:371:ALA:HA	20:d:247:ILE:HG21	2.04	0.40
20:d:166:PHE:HA	20:d:169:ILE:HG22	2.02	0.40
23:V:258:TYR:O	23:V:263:LEU:N	2.51	0.40
27:W:63:THR:O	27:W:67:LEU:HG	2.22	0.40
27:W:177:MET:HE3	27:W:177:MET:HB2	1.98	0.40
29:B:217:LYS:O	29:B:219:PRO:HD3	2.22	0.40
31:D:178:ARG:O	31:D:182:GLU:HG2	2.21	0.40
32:E:21:GLU:OE2	32:E:25:ARG:NH1	2.53	0.40
33:F:94:ILE:HB	33:F:123:VAL:HB	2.02	0.40
2:H:230:LEU:HD23	2:H:230:LEU:HA	1.95	0.40
5:L:137:TYR:CE2	5:L:217:LYS:HA	2.56	0.40
6:M:83:ASP:OD1	6:M:83:ASP:C	2.64	0.40
7:N:149:LYS:HE2	7:N:178:ALA:HB1	2.03	0.40
7:N:199:VAL:O	7:N:199:VAL:HG23	2.21	0.40
8:O:55:THR:O	8:O:59:ILE:HG12	2.21	0.40
10:Q:85:ARG:HE	10:Q:123:ALA:HA	1.86	0.40
1:g:211:LYS:HB2	1:g:214:GLU:HG3	2.03	0.40
14:k:220:VAL:HG22	14:k:226:PHE:HD1	1.86	0.40
5:l:69:HIS:CE1	5:l:70:ILE:HG13	2.56	0.40
5:l:133:LEU:HD21	5:l:159:MET:HB3	2.04	0.40
6:m:197:ILE:HA	6:m:200:VAL:HG22	2.02	0.40
7:n:103:TRP:CZ2	7:n:181:GLU:HG3	2.55	0.40
7:n:144:ARG:O	7:n:147:MET:HG3	2.21	0.40
11:r:51:ASP:HA	12:s:97:TYR:CE2	2.56	0.40
11:r:191:ASN:OD1	11:r:192:VAL:N	2.54	0.40
15:f:257:ARG:HH21	15:f:281:ILE:HA	1.85	0.40
15:f:394:ASP:HB2	15:f:397:LYS:HE3	2.03	0.40
17:a:100:THR:HA	17:a:103:LYS:HG2	2.02	0.40
17:a:371:ALA:O	17:a:375:LEU:HG	2.21	0.40
22:U:414:GLY:HA2	22:U:453:HIS:HE1	1.87	0.40
22:U:908:ILE:HD13	22:U:908:ILE:HA	1.96	0.40
26:Z:22:HIS:HA	26:Z:25:ARG:HG2	2.03	0.40
26:Z:38:VAL:HA	26:Z:94:TRP:HA	2.02	0.40
26:Z:96:HIS:O	26:Z:123:ILE:HA	2.21	0.40
27:W:169:LEU:HA	27:W:182:ARG:HH22	1.86	0.40
28:A:103:ASN:HB2	28:A:114:ASN:H	1.86	0.40
30:C:81:ASP:O	30:C:105:ILE:HD13	2.21	0.40
31:D:204:MET:HA	31:D:331:ILE:O	2.22	0.40
31:D:230:VAL:HG21	31:D:264:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:E:111:LEU:HA	32:E:112:PRO:HD3	1.89	0.40
32:E:215:ILE:HA	32:E:218:MET:SD	2.61	0.40
4:J:40:ILE:HD13	4:J:184:ASP:OD1	2.21	0.40
5:L:13:TRP:HZ3	6:M:29:ALA:HB2	1.87	0.40
7:N:84:LYS:HD2	7:N:120:MET:HB2	2.04	0.40
11:R:52:CYS:SG	11:R:97:MET:HG3	2.62	0.40
1:g:68:HIS:HE2	1:g:80:MET:C	2.26	0.40
2:h:25:ALA:O	2:h:29:VAL:HG23	2.22	0.40
2:h:53:LYS:HD2	2:h:56:LEU:HD11	2.02	0.40
3:i:164:ILE:HD12	3:i:164:ILE:HA	1.93	0.40
3:i:170:ALA:HB1	3:i:174:MET:HE3	2.04	0.40
6:m:65:ARG:O	6:m:77:VAL:HG22	2.22	0.40
7:n:34:LEU:O	7:n:34:LEU:HD12	2.21	0.40
15:f:285:CYS:HB2	15:f:290:VAL:HG11	2.04	0.40
15:f:556:ARG:HG2	15:f:590:PHE:CE2	2.57	0.40
15:f:737:ASN:HD21	15:f:773:LYS:C	2.26	0.40
17:a:4:VAL:HB	17:a:5:PRO:HD3	2.03	0.40
17:a:25:LEU:HG	17:a:37:LEU:HD11	2.03	0.40
17:a:138:VAL:HG11	17:a:155:PHE:HB2	2.03	0.40
17:a:294:GLU:O	17:a:298:LYS:HG3	2.21	0.40
17:a:351:ASP:O	17:a:354:GLU:HG2	2.21	0.40
19:c:34:SER:OG	19:c:70:ILE:HA	2.22	0.40
22:U:524:LYS:HE3	22:U:524:LYS:HB3	1.97	0.40
22:U:554:LEU:HD23	22:U:554:LEU:H	1.87	0.40
23:V:167:LEU:HD12	23:V:168:GLN:N	2.36	0.40
24:X:177:TYR:HB3	24:X:182:ASN:HB2	2.03	0.40
24:X:377:ILE:HD12	25:Y:312:ARG:HB2	2.04	0.40
27:W:182:ARG:HD2	27:W:182:ARG:HA	1.98	0.40
29:B:233:THR:HA	29:B:236:ALA:HB3	2.03	0.40
32:E:75:ASN:HD22	33:F:130:GLN:HA	1.85	0.40
33:F:225:MET:HG3	33:F:331:ALA:HA	2.03	0.40
33:F:369:HIS:CD2	33:F:397:LYS:HB2	2.56	0.40
3:I:52:ILE:HG22	3:I:52:ILE:O	2.21	0.40
4:J:16:LEU:HD12	4:J:16:LEU:HA	1.94	0.40
5:L:172:LEU:O	5:L:176:MET:HB3	2.22	0.40
6:M:69:VAL:HG11	6:M:75:MET:HE3	2.03	0.40
7:N:58:ALA:O	7:N:61:TYR:HB3	2.21	0.40
12:S:63:THR:O	12:S:67:ILE:HG13	2.22	0.40
12:S:148:LEU:O	12:S:151:ASN:OD1	2.40	0.40
1:g:132:ARG:HA	1:g:133:PRO:HD3	1.93	0.40
3:i:119:GLN:HB2	4:j:78:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:119:GLN:OE1	4:j:82:ILE:HD13	2.21	0.40
5:l:39:LYS:HA	5:l:44:ALA:HA	2.03	0.40
11:r:51:ASP:HA	12:s:97:TYR:HE2	1.86	0.40
12:s:70:ALA:O	12:s:74:MET:HG3	2.22	0.40
13:t:147:GLN:N	13:t:148:PRO:HD2	2.37	0.40
15:f:671:ALA:HB2	29:B:71:TYR:HE2	1.86	0.40
16:x:56:GLN:HE21	16:x:85:MET:HG2	1.86	0.40
17:a:326:GLU:OE1	27:W:373:ILE:HG13	2.21	0.40
19:c:50:PRO:HD3	32:E:53:VAL:HG12	2.04	0.40
19:c:298:GLN:HB2	26:Z:252:LYS:NZ	2.36	0.40
20:d:182:ILE:HG22	20:d:186:TYR:HE2	1.87	0.40
21:e:28:ALA:H	23:V:355:ARG:HE	1.70	0.40
22:U:361:ARG:HA	22:U:361:ARG:HD3	1.85	0.40
22:U:405:THR:HG23	22:U:444:TYR:HD2	1.87	0.40
23:V:302:TYR:CB	23:V:339:LEU:HD21	2.42	0.40
24:X:185:LYS:HZ3	25:Y:244:ALA:HB3	1.87	0.40
27:W:373:ILE:HG22	27:W:413:ILE:HD11	2.03	0.40
28:A:178:GLY:HA3	28:A:354:ILE:HG12	2.03	0.40
28:A:393:GLY:HA2	29:B:214:MET:HE2	2.03	0.40
29:B:211:TYR:O	29:B:215:GLY:N	2.55	0.40
31:D:189:GLU:H	31:D:189:GLU:HG2	1.72	0.40
31:D:237:GLN:CG	31:D:238:LYS:H	2.33	0.40
33:F:170:SER:OG	33:F:171:ARG:N	2.55	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	G	235/246 (96%)	217 (92%)	17 (7%)	1 (0%)	30 62
1	g	241/246 (98%)	229 (95%)	12 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	224/234 (96%)	197 (88%)	26 (12%)	1 (0%)	30	62
2	h	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
3	I	245/261 (94%)	232 (95%)	13 (5%)	0	100	100
3	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
4	J	235/248 (95%)	205 (87%)	27 (12%)	3 (1%)	9	39
4	j	236/248 (95%)	228 (97%)	8 (3%)	0	100	100
5	L	235/269 (87%)	226 (96%)	8 (3%)	1 (0%)	30	62
5	l	235/269 (87%)	229 (97%)	6 (3%)	0	100	100
6	M	236/255 (92%)	220 (93%)	15 (6%)	1 (0%)	30	62
6	m	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
7	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100
7	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
8	O	218/277 (79%)	212 (97%)	5 (2%)	1 (0%)	24	57
8	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
9	P	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	Q	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
10	q	194/201 (96%)	191 (98%)	3 (2%)	0	100	100
11	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
11	r	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
12	S	210/241 (87%)	205 (98%)	5 (2%)	0	100	100
12	s	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
13	T	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
13	t	214/264 (81%)	209 (98%)	5 (2%)	0	100	100
14	K	218/241 (90%)	207 (95%)	11 (5%)	0	100	100
14	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
15	f	815/908 (90%)	780 (96%)	35 (4%)	0	100	100
16	x	83/230 (36%)	81 (98%)	2 (2%)	0	100	100
17	a	371/376 (99%)	347 (94%)	24 (6%)	0	100	100
18	b	189/377 (50%)	177 (94%)	11 (6%)	1 (0%)	24	57
19	c	285/310 (92%)	254 (89%)	31 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	d	250/350 (71%)	211 (84%)	38 (15%)	1 (0%)	30	62
21	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
22	U	853/953 (90%)	801 (94%)	52 (6%)	0	100	100
23	V	442/534 (83%)	427 (97%)	15 (3%)	0	100	100
24	X	378/422 (90%)	366 (97%)	11 (3%)	1 (0%)	36	67
25	Y	378/389 (97%)	346 (92%)	31 (8%)	1 (0%)	36	67
26	Z	284/324 (88%)	256 (90%)	27 (10%)	1 (0%)	30	62
27	W	442/456 (97%)	417 (94%)	23 (5%)	2 (0%)	24	57
28	A	401/433 (93%)	351 (88%)	45 (11%)	5 (1%)	10	41
29	B	398/440 (90%)	338 (85%)	55 (14%)	5 (1%)	9	39
30	C	362/398 (91%)	315 (87%)	44 (12%)	3 (1%)	16	49
31	D	370/418 (88%)	308 (83%)	57 (15%)	5 (1%)	9	38
32	E	368/403 (91%)	340 (92%)	27 (7%)	1 (0%)	36	67
33	F	349/439 (80%)	309 (88%)	35 (10%)	5 (1%)	9	38
All	All	13230/15118 (88%)	12367 (94%)	824 (6%)	39 (0%)	37	67

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	164	LYS
6	M	104	TYR
29	B	256	ILE
29	B	435	PRO
30	C	87	VAL
33	F	170	SER
4	J	182	GLU
4	J	199	VAL
8	O	187	ARG
20	d	93	ALA
26	Z	144	VAL
28	A	73	ALA
28	A	172	VAL
28	A	206	ILE
29	B	205	LEU
31	D	164	TYR
31	D	172	ILE
25	Y	212	GLU

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Mol	Chain	Res	Type
28	A	108	ASP
29	B	253	SER
30	C	230	MET
30	C	246	ILE
31	D	151	ILE
32	E	112	PRO
27	W	117	ASP
27	W	140	ILE
31	D	231	VAL
33	F	137	ILE
33	F	326	VAL
33	F	136	VAL
5	L	63	ILE
4	J	98	VAL
2	H	32	GLY
18	b	23	PRO
28	A	177	VAL
31	D	406	VAL
33	F	279	ALA
24	X	318	ILE
29	B	145	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	201/210 (96%)	199 (99%)	2 (1%)	68	75
1	g	206/210 (98%)	206 (100%)	0	100	100
2	H	184/191 (96%)	183 (100%)	1 (0%)	81	80
2	h	190/191 (100%)	190 (100%)	0	100	100
3	I	205/221 (93%)	205 (100%)	0	100	100
3	i	210/221 (95%)	210 (100%)	0	100	100
4	J	201/211 (95%)	201 (100%)	0	100	100
4	j	202/211 (96%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	L	203/230 (88%)	201 (99%)	2 (1%)	68	75
5	l	203/230 (88%)	203 (100%)	0	100	100
6	M	195/212 (92%)	193 (99%)	2 (1%)	68	75
6	m	198/212 (93%)	198 (100%)	0	100	100
7	N	158/181 (87%)	158 (100%)	0	100	100
7	n	157/181 (87%)	157 (100%)	0	100	100
8	O	181/228 (79%)	181 (100%)	0	100	100
8	o	181/228 (79%)	181 (100%)	0	100	100
9	P	173/174 (99%)	173 (100%)	0	100	100
9	p	173/174 (99%)	173 (100%)	0	100	100
10	Q	167/171 (98%)	167 (100%)	0	100	100
10	q	167/171 (98%)	167 (100%)	0	100	100
11	R	156/202 (77%)	156 (100%)	0	100	100
11	r	156/202 (77%)	156 (100%)	0	100	100
12	S	177/199 (89%)	177 (100%)	0	100	100
12	s	178/199 (89%)	178 (100%)	0	100	100
13	T	179/215 (83%)	179 (100%)	0	100	100
13	t	179/215 (83%)	179 (100%)	0	100	100
14	K	187/203 (92%)	185 (99%)	2 (1%)	65	74
14	k	196/203 (97%)	196 (100%)	0	100	100
15	f	682/763 (89%)	682 (100%)	0	100	100
16	x	73/207 (35%)	73 (100%)	0	100	100
17	a	329/336 (98%)	329 (100%)	0	100	100
18	b	167/312 (54%)	167 (100%)	0	100	100
19	c	247/268 (92%)	247 (100%)	0	100	100
20	d	224/294 (76%)	224 (100%)	0	100	100
21	e	42/63 (67%)	42 (100%)	0	100	100
22	U	727/816 (89%)	727 (100%)	0	100	100
23	V	388/460 (84%)	388 (100%)	0	100	100
24	X	326/362 (90%)	326 (100%)	0	100	100
25	Y	320/344 (93%)	320 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Z	252/295 (85%)	252 (100%)	0	100	100
27	W	402/416 (97%)	402 (100%)	0	100	100
28	A	338/372 (91%)	334 (99%)	4 (1%)	63	73
29	B	333/385 (86%)	325 (98%)	8 (2%)	43	64
30	C	313/346 (90%)	313 (100%)	0	100	100
31	D	312/366 (85%)	309 (99%)	3 (1%)	68	75
32	E	323/353 (92%)	321 (99%)	2 (1%)	78	79
33	F	290/379 (76%)	289 (100%)	1 (0%)	86	83
All	All	11251/12833 (88%)	11224 (100%)	27 (0%)	85	85

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	69	LEU
1	G	86	ASP
2	H	71	HIS
5	L	38	LEU
5	L	99	PHE
6	M	23	VAL
6	M	215	TRP
14	K	31	ILE
14	K	210	LEU
28	A	102	ILE
28	A	222	LYS
28	A	223	THR
28	A	237	PHE
29	B	49	LEU
29	B	123	VAL
29	B	160	ILE
29	B	210	TYR
29	B	232	LYS
29	B	239	VAL
29	B	334	ILE
29	B	347	ILE
31	D	85	ILE
31	D	115	ILE
31	D	414	HIS
32	E	30	ARG
32	E	33	LEU

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Mol	Chain	Res	Type
33	F	134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	33	ASN
1	G	128	ASN
2	H	42	ASN
2	H	88	HIS
2	H	166	ASN
2	H	214	ASN
3	I	30	HIS
3	I	40	ASN
3	I	240	HIS
4	J	92	GLN
5	L	86	ASN
6	M	180	GLN
7	N	123	GLN
7	N	158	ASN
8	O	57	GLN
9	P	93	ASN
9	P	145	GLN
9	P	157	ASN
9	P	173	ASN
12	S	80	ASN
13	T	188	GLN
1	g	53	GLN
1	g	147	GLN
1	g	193	GLN
2	h	95	GLN
2	h	109	GLN
2	h	189	HIS
3	i	109	GLN
3	i	146	GLN
4	j	18	GLN
4	j	23	GLN
4	j	215	GLN
14	k	23	GLN
5	l	117	GLN
5	l	121	GLN
6	m	101	ASN
6	m	201	HIS

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Mol	Chain	Res	Type
8	o	62	ASN
8	o	193	ASN
9	p	93	ASN
9	p	173	ASN
10	q	27	GLN
10	q	71	ASN
10	q	87	ASN
11	r	119	ASN
11	r	151	GLN
12	s	77	HIS
12	s	151	ASN
12	s	157	ASN
13	t	3	ASN
13	t	188	GLN
14	K	114	GLN
14	K	152	GLN
14	K	178	GLN
14	K	221	GLN
15	f	43	GLN
15	f	148	GLN
15	f	323	ASN
15	f	473	ASN
15	f	566	HIS
15	f	605	ASN
15	f	724	ASN
15	f	815	HIS
16	x	56	GLN
17	a	10	GLN
17	a	36	GLN
17	a	143	ASN
17	a	168	ASN
17	a	219	HIS
17	a	249	GLN
17	a	337	GLN
18	b	101	GLN
19	c	194	HIS
19	c	237	HIS
20	d	10	ASN
20	d	47	GLN
20	d	97	GLN
20	d	109	GLN
20	d	221	ASN

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Mol	Chain	Res	Type
20	d	230	GLN
22	U	89	ASN
22	U	107	HIS
22	U	267	ASN
22	U	373	ASN
22	U	389	ASN
22	U	412	HIS
22	U	718	ASN
22	U	768	GLN
22	U	874	ASN
23	V	64	GLN
23	V	110	HIS
23	V	185	GLN
23	V	329	HIS
23	V	350	GLN
23	V	365	GLN
23	V	400	HIS
24	X	78	ASN
24	X	170	GLN
24	X	182	ASN
24	X	416	ASN
25	Y	306	GLN
25	Y	357	ASN
25	Y	388	ASN
26	Z	189	GLN
26	Z	193	ASN
26	Z	225	GLN
26	Z	282	ASN
27	W	96	GLN
27	W	99	GLN
27	W	156	ASN
27	W	395	ASN
28	A	44	GLN
28	A	150	HIS
28	A	296	GLN
28	A	314	ASN
29	B	181	GLN
29	B	332	ASN
29	B	425	ASN
30	C	67	GLN
30	C	206	HIS
30	C	270	GLN

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Mol	Chain	Res	Type
31	D	127	ASN
31	D	295	GLN
31	D	412	GLN
32	E	45	ASN
32	E	75	ASN
32	E	220	ASN
32	E	280	ASN
32	E	359	HIS
33	F	76	ASN
33	F	130	GLN
33	F	208	HIS
33	F	323	ASN
33	F	417	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
35	ADP	D	501	-	28,29,29	1.43	5 (17%)	43,45,45	1.91	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ADP	F	501	-	28,29,29	1.43	5 (17%)	43,45,45	1.87	8 (18%)
35	ADP	B	501	-	28,29,29	1.45	5 (17%)	43,45,45	1.85	9 (20%)
35	ADP	E	501	-	28,29,29	1.26	3 (10%)	43,45,45	1.79	7 (16%)
34	ATP	A	501	-	32,33,33	0.26	0	48,52,52	0.31	0
35	ADP	C	501	-	28,29,29	1.48	5 (17%)	43,45,45	1.89	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ADP	D	501	-	-	4/16/32/32	0/3/3/3
35	ADP	F	501	-	-	3/16/32/32	0/3/3/3
35	ADP	B	501	-	-	3/16/32/32	0/3/3/3
35	ADP	E	501	-	-	2/16/32/32	0/3/3/3
34	ATP	A	501	-	-	6/22/38/38	0/3/3/3
35	ADP	C	501	-	-	1/16/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	501	ADP	C5-C4	4.83	1.47	1.39
35	C	501	ADP	C5-C4	4.81	1.47	1.39
35	B	501	ADP	C5-C4	4.77	1.47	1.39
35	D	501	ADP	C5-C4	4.74	1.47	1.39
35	E	501	ADP	C5-C4	4.03	1.46	1.39
35	C	501	ADP	PA-O3A	2.82	1.62	1.59
35	E	501	ADP	C5-C6	2.82	1.48	1.41
35	F	501	ADP	C5-C6	2.74	1.48	1.41
35	D	501	ADP	C5-C6	2.72	1.48	1.41
35	C	501	ADP	C5-C6	2.71	1.48	1.41
35	B	501	ADP	C5-C6	2.69	1.48	1.41
35	F	501	ADP	C5-N7	-2.34	1.34	1.39
35	B	501	ADP	PA-O3A	2.32	1.62	1.59
35	B	501	ADP	C8-N7	2.31	1.36	1.31
35	D	501	ADP	C8-N7	2.30	1.36	1.31
35	B	501	ADP	C5-N7	-2.29	1.34	1.39
35	D	501	ADP	C5-N7	-2.29	1.34	1.39
35	C	501	ADP	C8-N7	2.28	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	501	ADP	C5-N7	-2.28	1.34	1.39
35	F	501	ADP	C8-N7	2.25	1.36	1.31
35	D	501	ADP	PA-O3A	2.05	1.61	1.59
35	F	501	ADP	PA-O3A	2.05	1.61	1.59
35	E	501	ADP	C5-N7	-2.03	1.35	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	501	ADP	C5-C4-N3	-6.40	117.91	126.72
35	F	501	ADP	C5-C4-N3	-6.23	118.14	126.72
35	D	501	ADP	C5-C4-N3	-6.13	118.28	126.72
35	C	501	ADP	C5-C4-N3	-6.00	118.46	126.72
35	B	501	ADP	C5-C4-N3	-5.84	118.67	126.72
35	F	501	ADP	N3-C4-N9	5.01	135.69	127.17
35	C	501	ADP	N3-C4-N9	4.83	135.38	127.17
35	D	501	ADP	N3-C4-N9	4.83	135.38	127.17
35	B	501	ADP	N3-C4-N9	4.67	135.12	127.17
35	E	501	ADP	N3-C4-N9	4.63	135.05	127.17
35	F	501	ADP	C2-N3-C4	3.81	121.13	111.83
35	D	501	ADP	C2-N3-C4	3.80	121.11	111.83
35	C	501	ADP	C2-N3-C4	3.71	120.88	111.83
35	B	501	ADP	C2-N3-C4	3.68	120.81	111.83
35	E	501	ADP	C2-N3-C4	3.65	120.74	111.83
35	D	501	ADP	C4-C5-N7	-3.46	106.63	110.58
35	B	501	ADP	C4-C5-N7	-3.43	106.66	110.58
35	C	501	ADP	C4-C5-N7	-3.35	106.75	110.58
35	D	501	ADP	O4'-C1'-N9	3.34	114.51	108.09
35	F	501	ADP	C4-C5-N7	-3.33	106.78	110.58
35	D	501	ADP	N3-C2-N1	-3.21	123.73	128.58
35	B	501	ADP	N3-C2-N1	-3.18	123.77	128.58
35	E	501	ADP	C4-C5-N7	-3.13	107.00	110.58
35	C	501	ADP	N3-C2-N1	-3.11	123.87	128.58
35	F	501	ADP	N3-C2-N1	-3.11	123.88	128.58
35	E	501	ADP	N3-C2-N1	-2.92	124.17	128.58
35	F	501	ADP	C3'-C2'-C1'	2.77	106.70	101.46
35	B	501	ADP	C4-N9-C8	2.68	108.55	105.74
35	C	501	ADP	C4-N9-C8	2.56	108.42	105.74
35	D	501	ADP	C5-N7-C8	2.55	107.46	103.45
35	B	501	ADP	C5-N7-C8	2.53	107.43	103.45
35	E	501	ADP	C3'-C2'-C1'	2.51	106.21	101.46
35	C	501	ADP	C5-N7-C8	2.47	107.33	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	501	ADP	C5-N7-C8	2.45	107.31	103.45
35	D	501	ADP	C4-N9-C8	2.45	108.31	105.74
35	B	501	ADP	C3'-C2'-C1'	2.44	106.09	101.46
35	C	501	ADP	C3'-C2'-C1'	2.41	106.02	101.46
35	F	501	ADP	C4-N9-C8	2.32	108.17	105.74
35	E	501	ADP	C5-N7-C8	2.29	107.05	103.45
35	C	501	ADP	C2'-C1'-N9	-2.25	107.72	113.30
35	B	501	ADP	C6-C5-N7	2.03	135.99	132.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 21 short contacts:

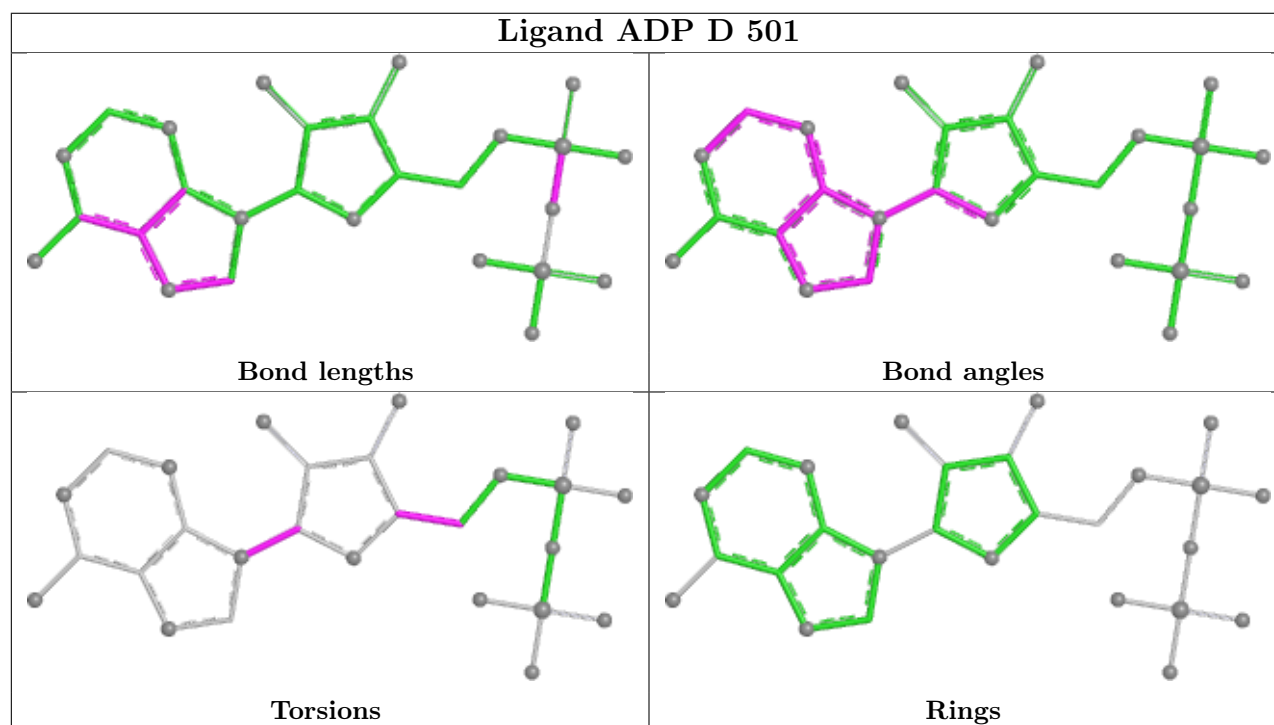
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	D	501	ADP	4	0
35	F	501	ADP	4	0
35	B	501	ADP	5	0
35	E	501	ADP	1	0

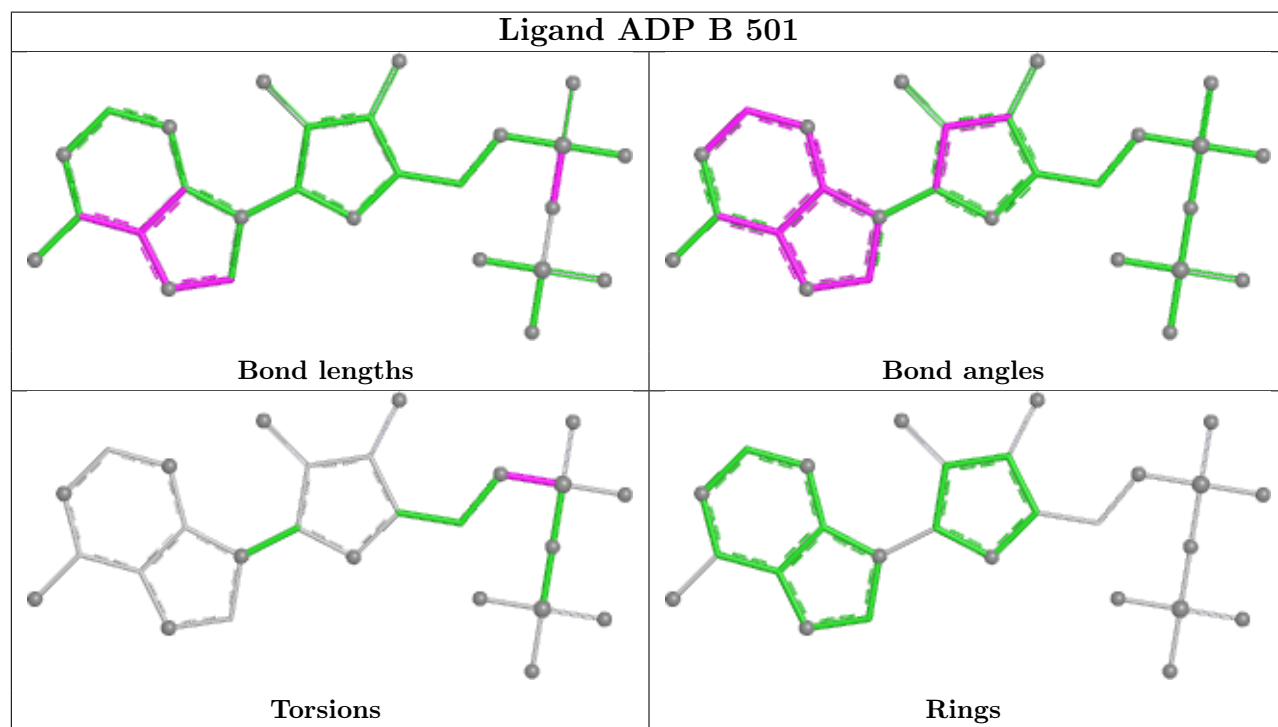
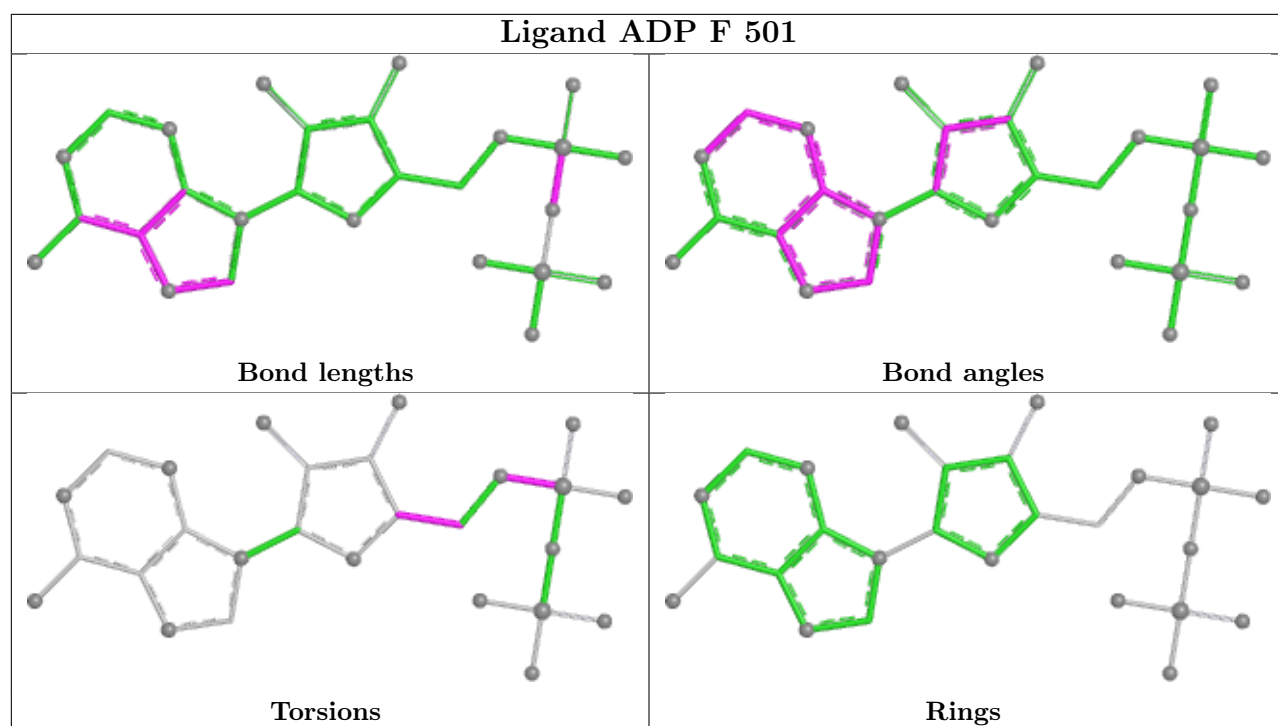
Continued on next page...

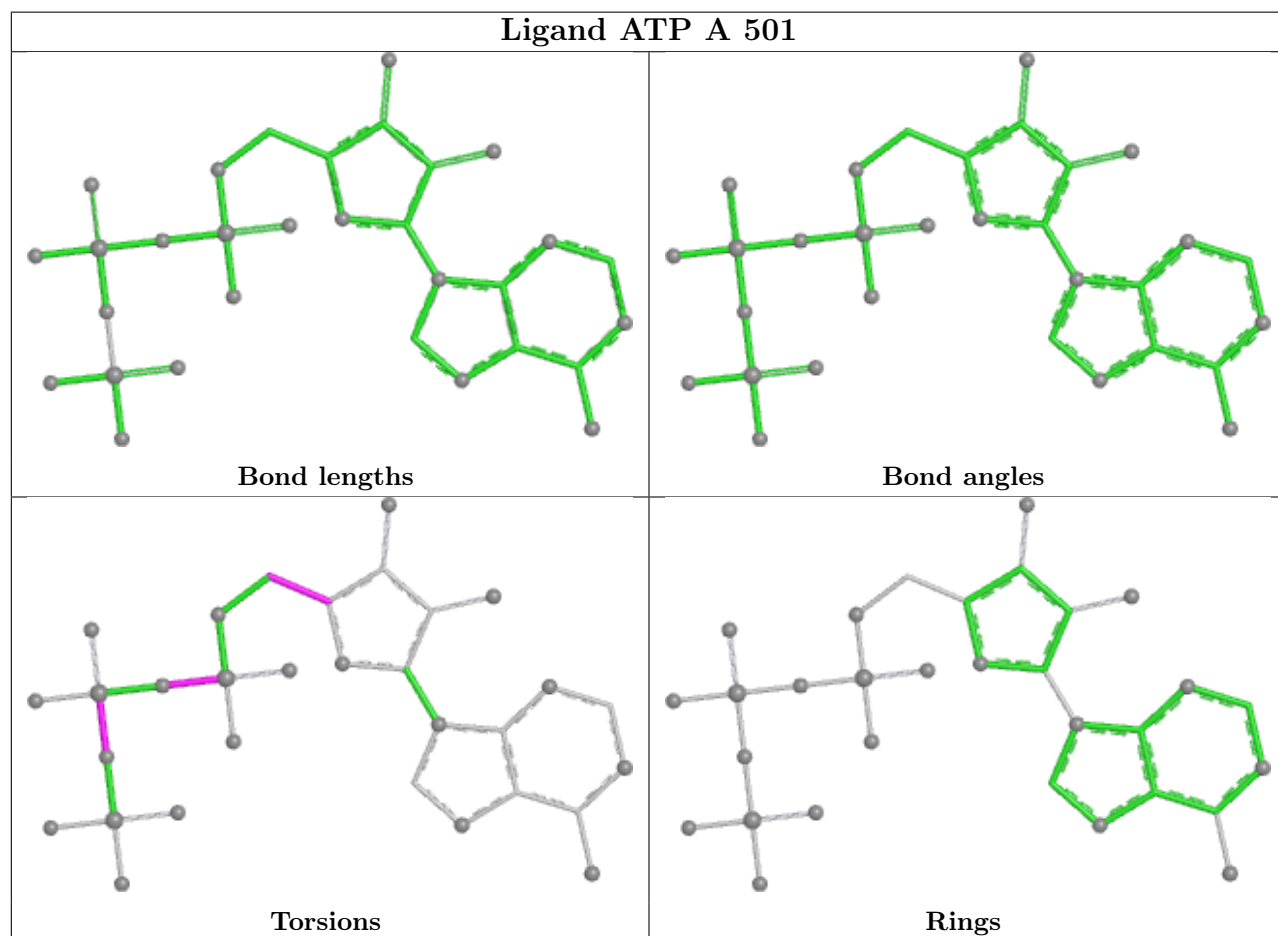
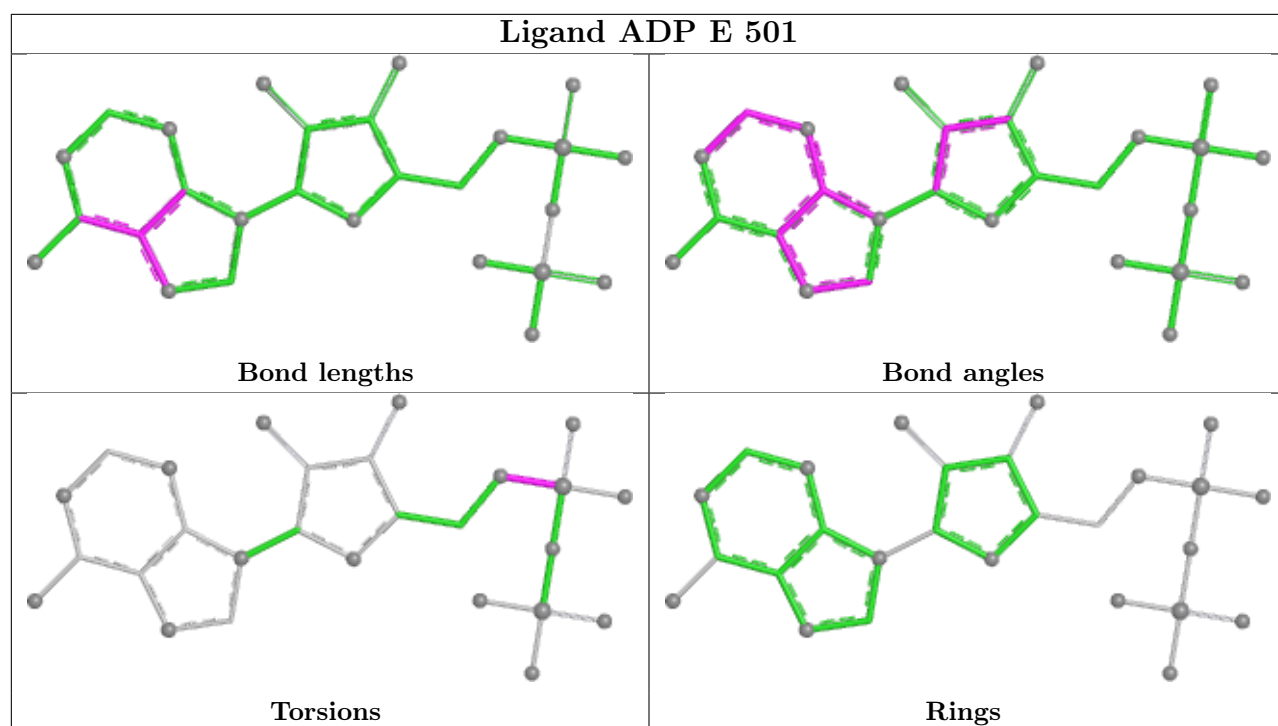
Continued from previous page...

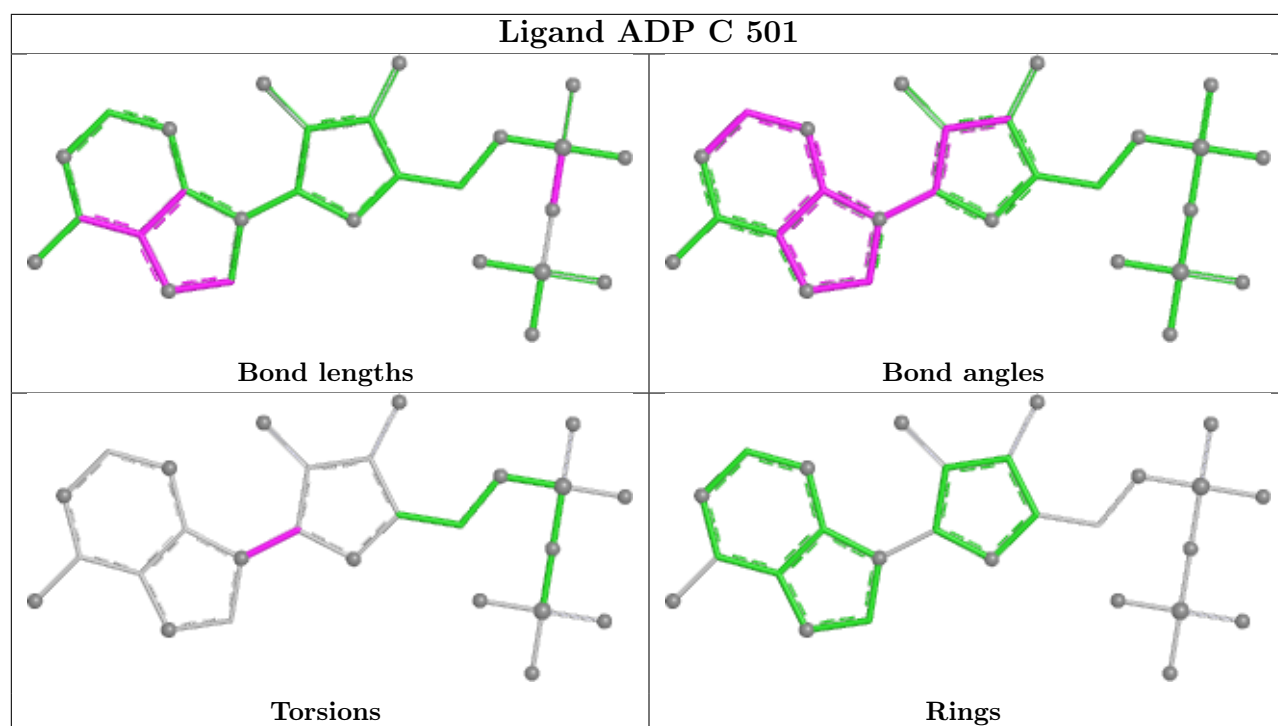
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	501	ATP	1	0
35	C	501	ADP	6	0

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](#)

There are no chain breaks in this entry.

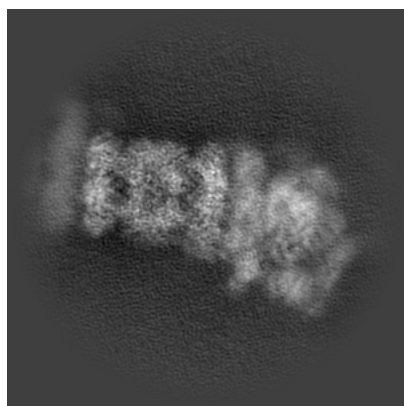
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52193. These allow visual inspection of the internal detail of the map and identification of artifacts.

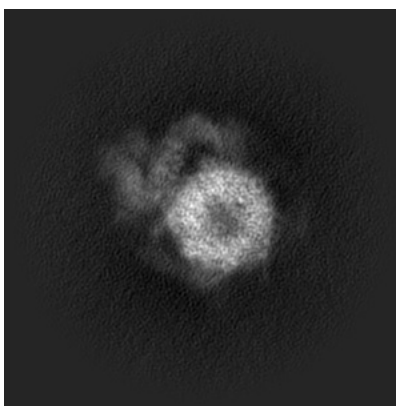
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

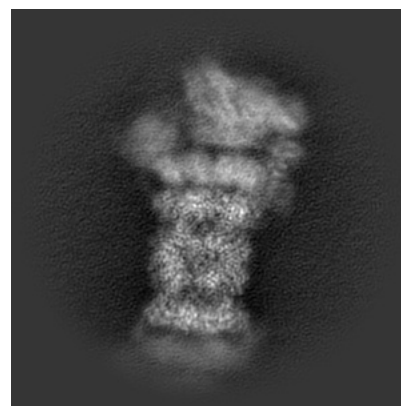
6.1.1 Primary map



X

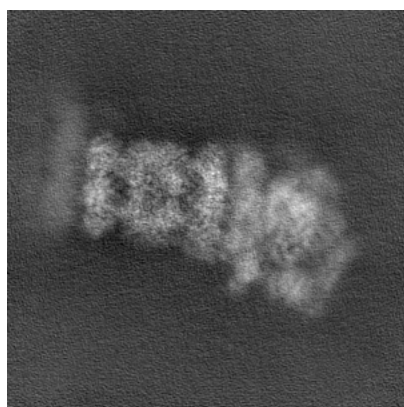


Y

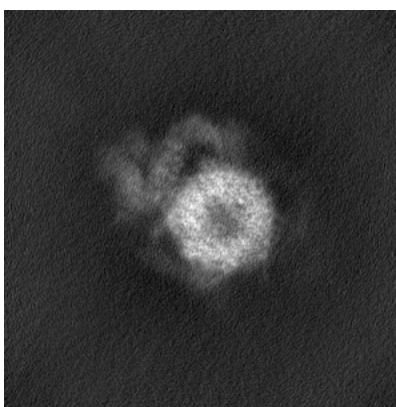


Z

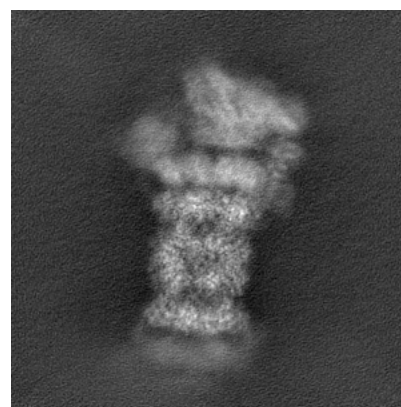
6.1.2 Raw map



X



Y

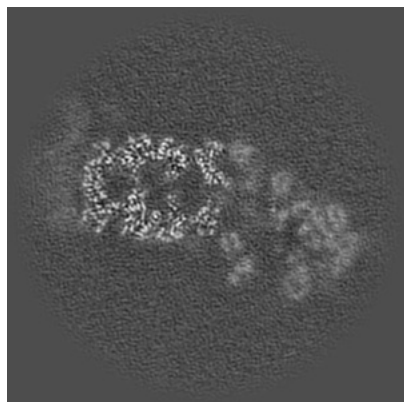


Z

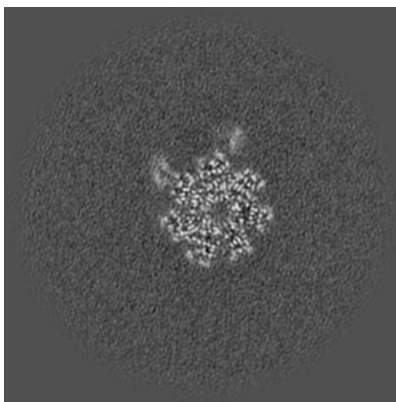
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

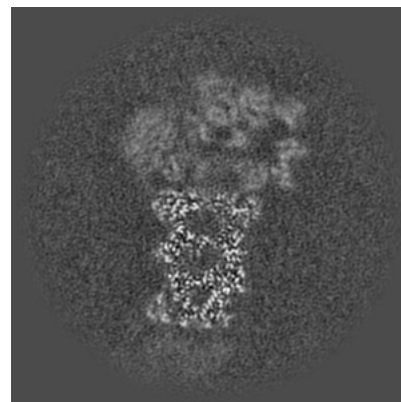
6.2.1 Primary map



X Index: 150

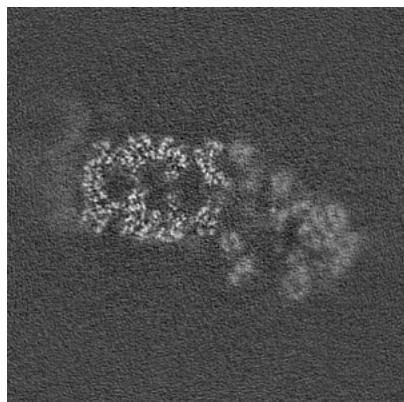


Y Index: 150

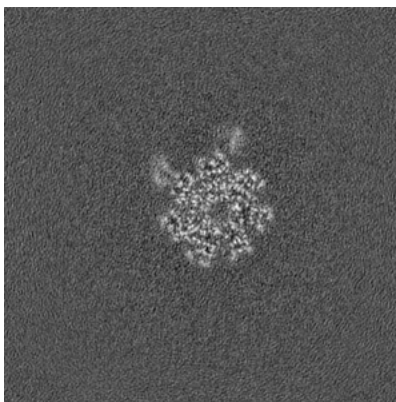


Z Index: 150

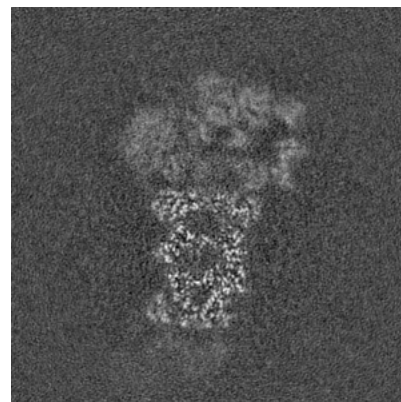
6.2.2 Raw map



X Index: 150



Y Index: 150

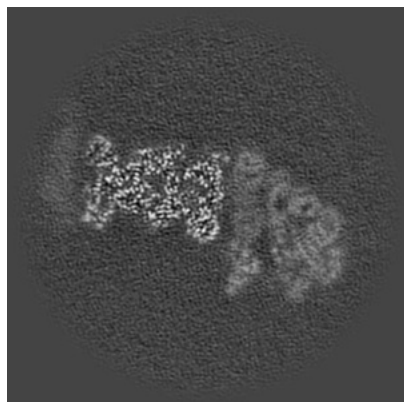


Z Index: 150

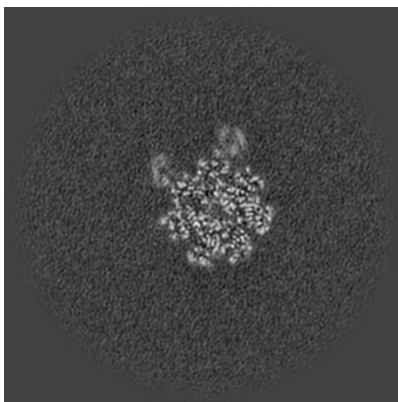
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

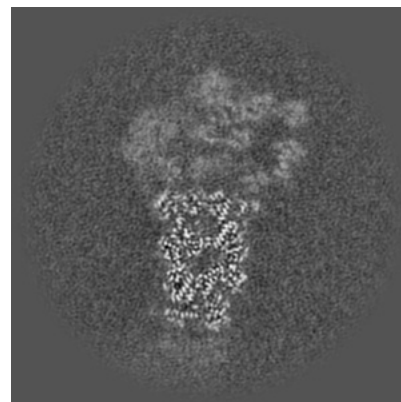
6.3.1 Primary map



X Index: 161

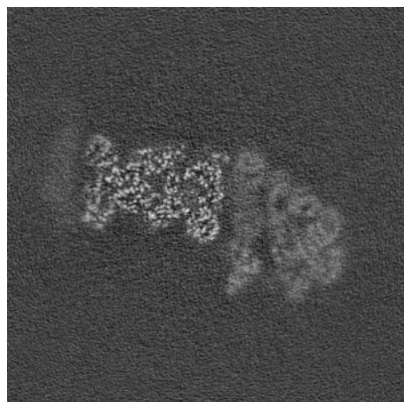


Y Index: 152

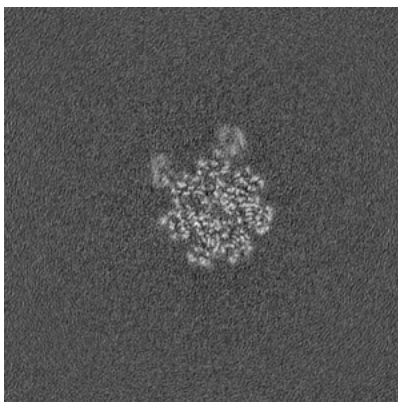


Z Index: 147

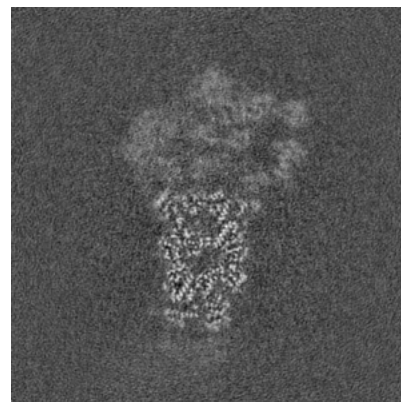
6.3.2 Raw map



X Index: 161



Y Index: 152

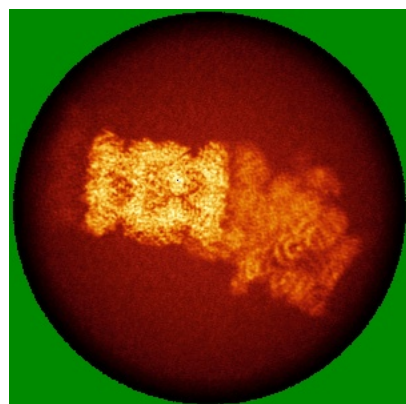


Z Index: 147

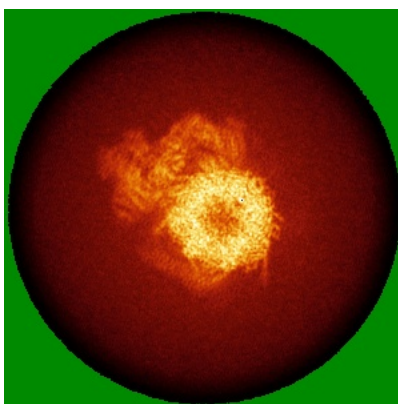
The images above show the largest variance slices of the map in three orthogonal directions.

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

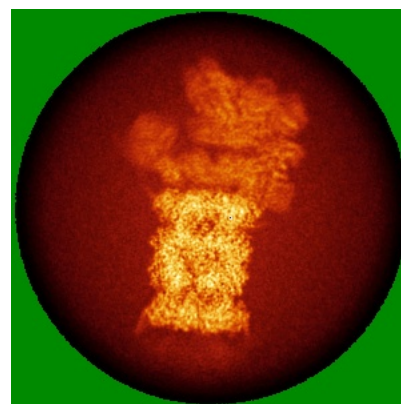
6.4.1 Primary map



X

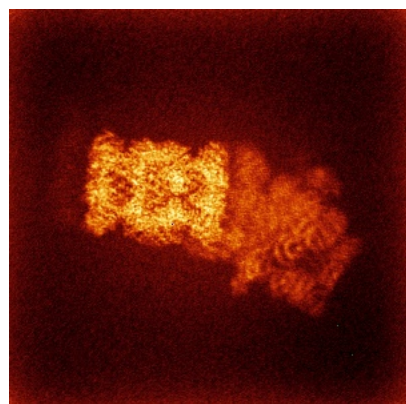


Y

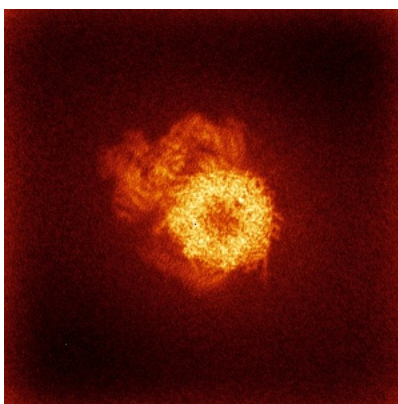


Z

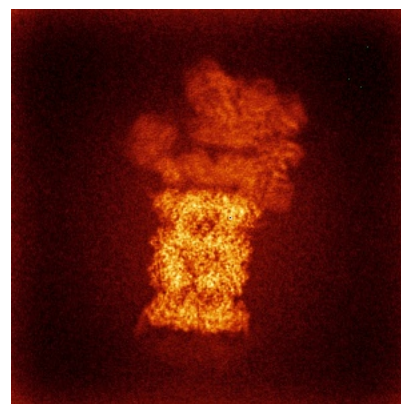
6.4.2 Raw map



X



Y

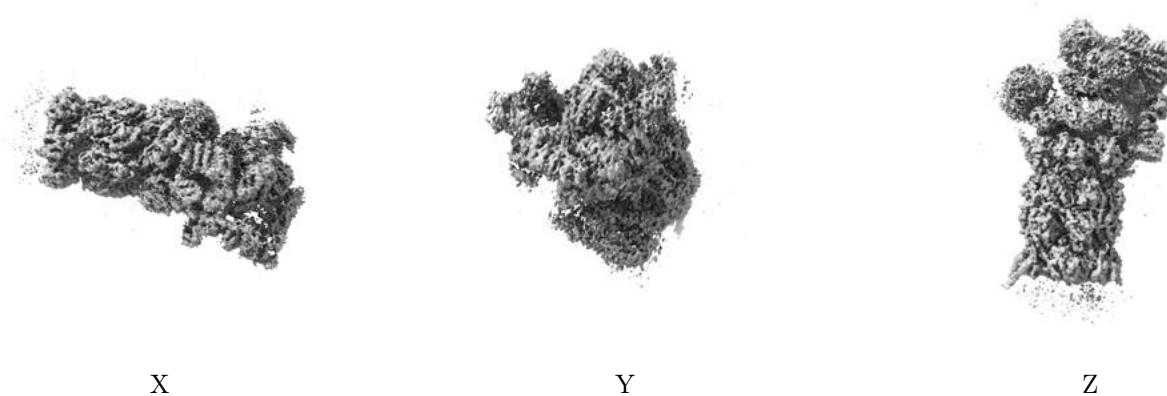


Z

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

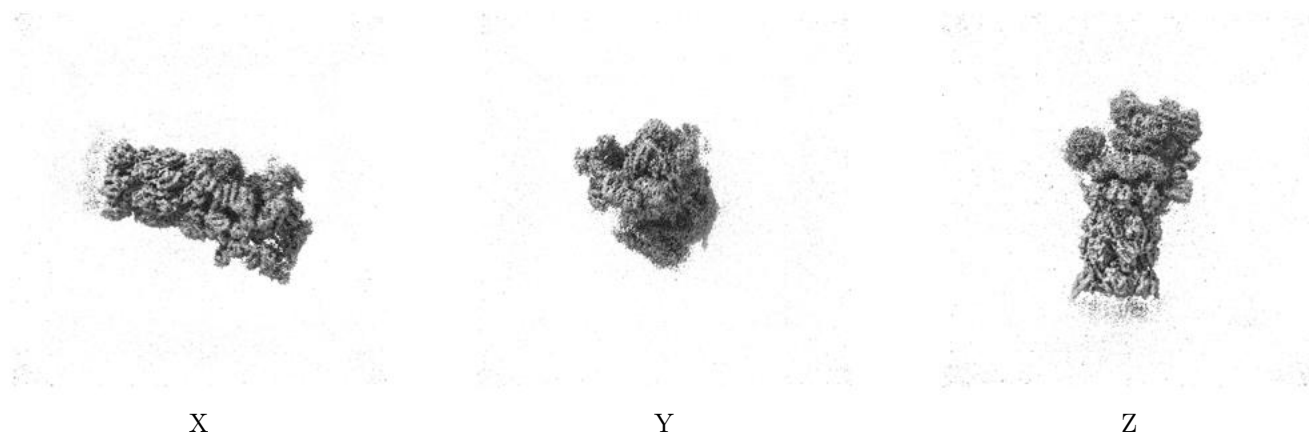
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

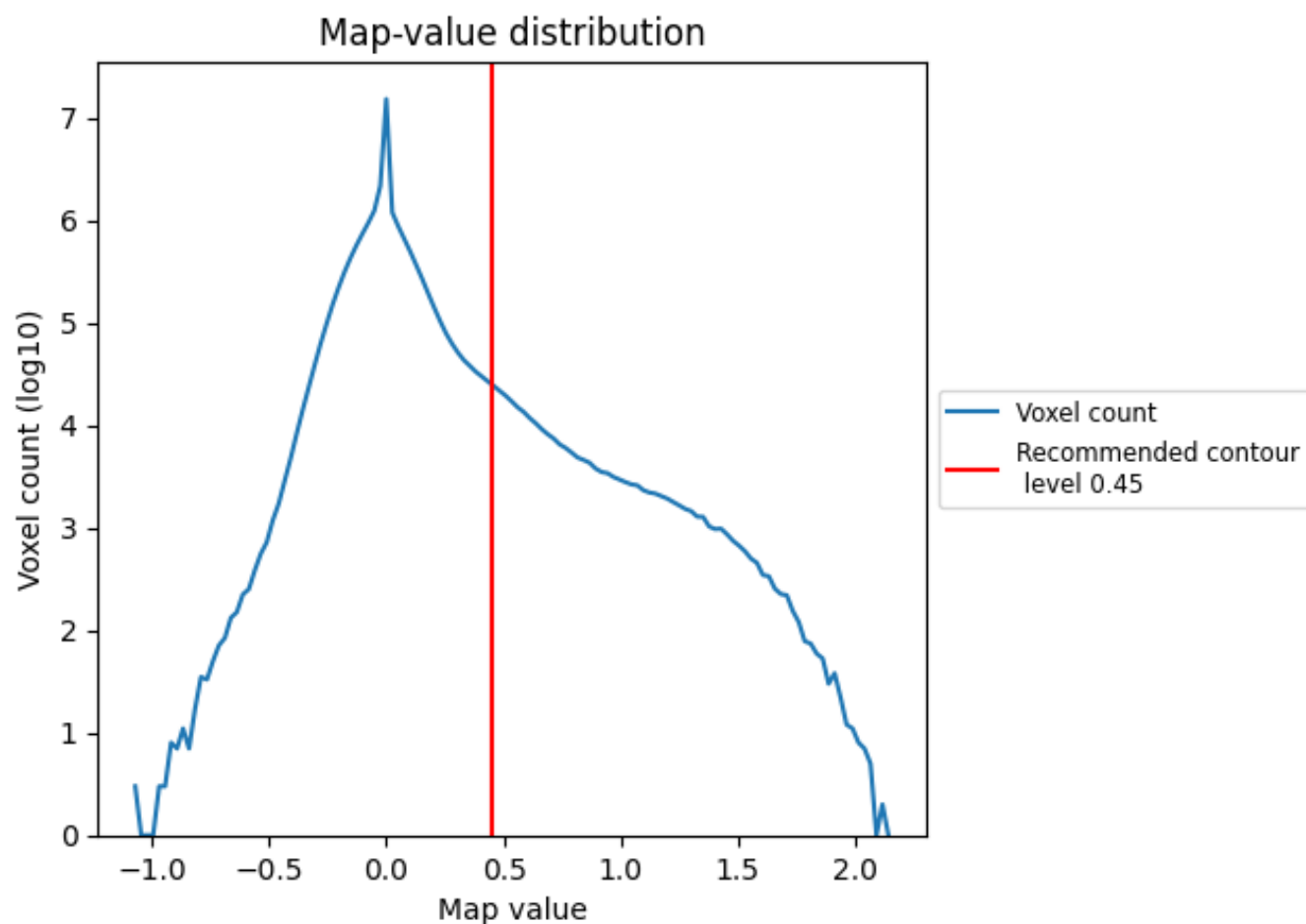
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

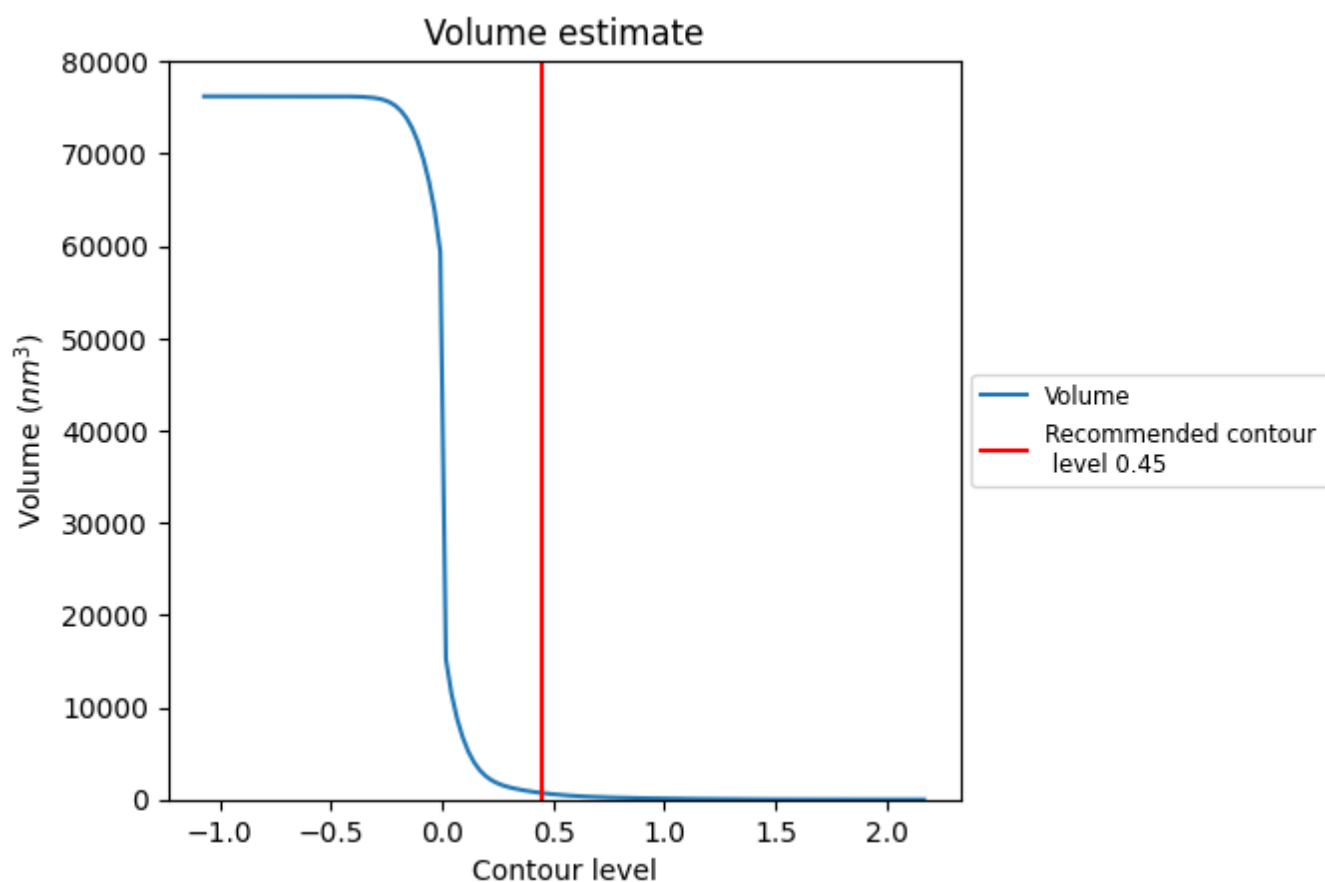
This section contains the results of statistical analysis of the map.

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.

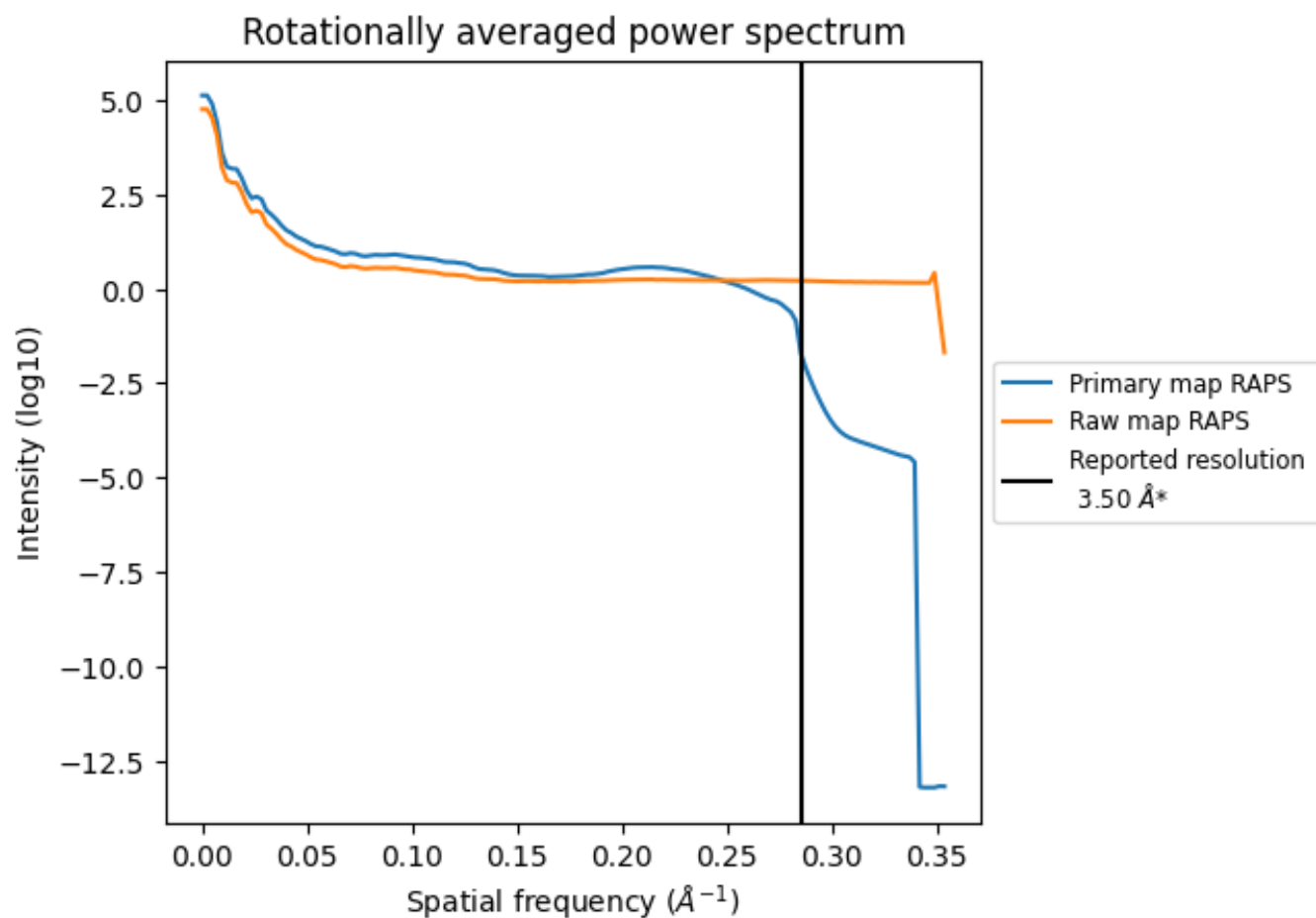
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 707 nm³; this corresponds to an approximate mass of 639 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 ⓘ

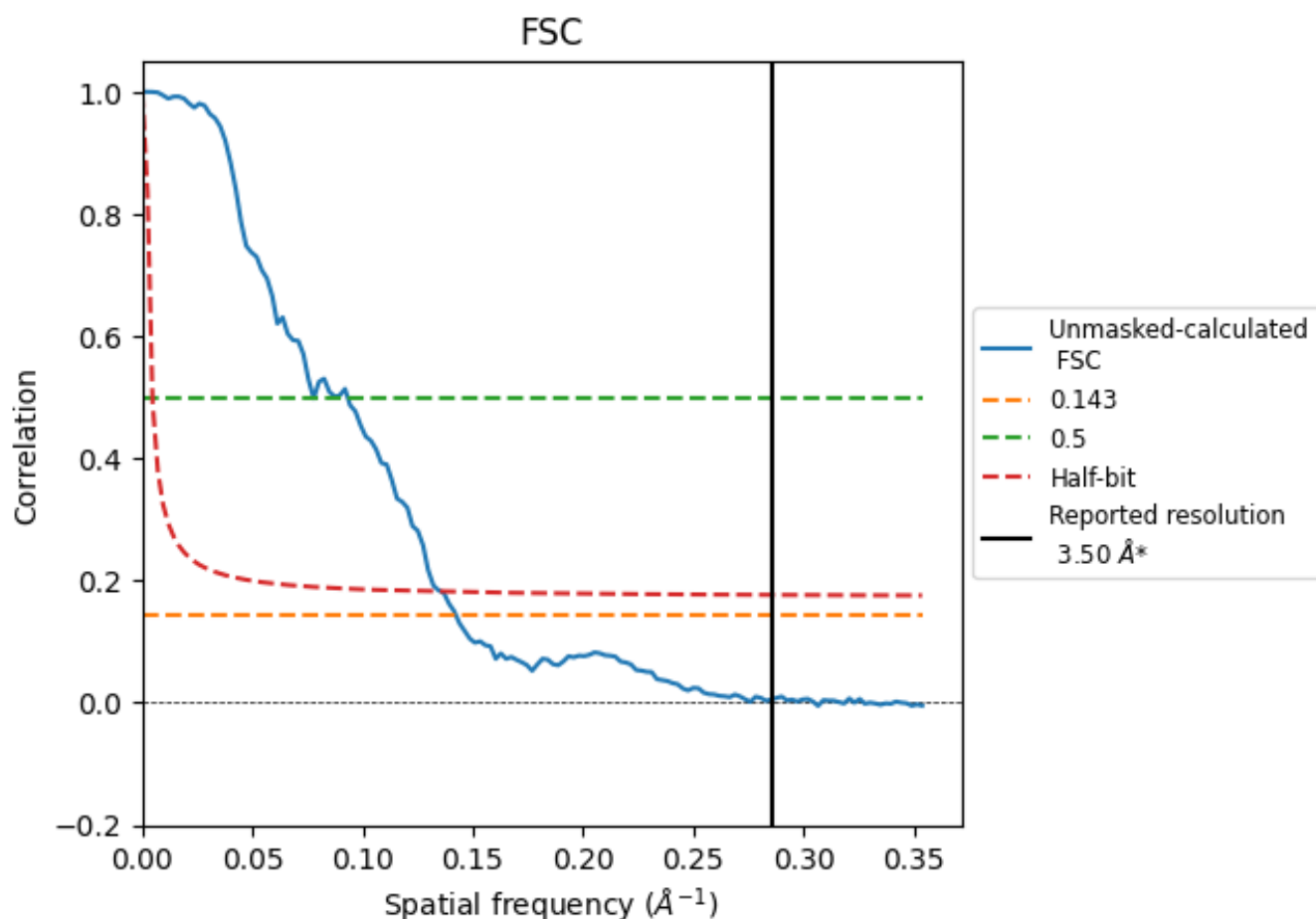


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

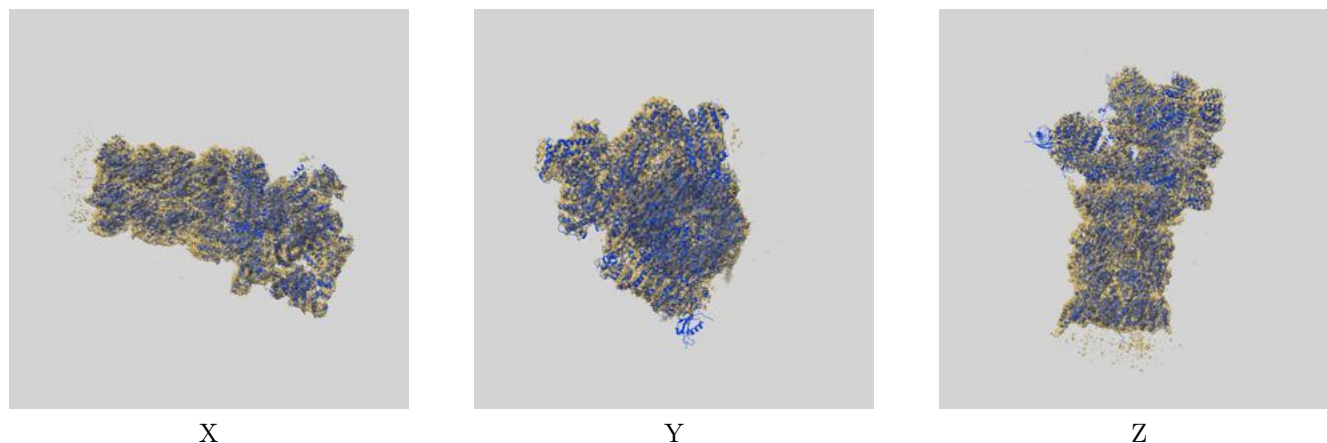
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.03	12.87	7.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.03 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52193 and PDB model 9SZT. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



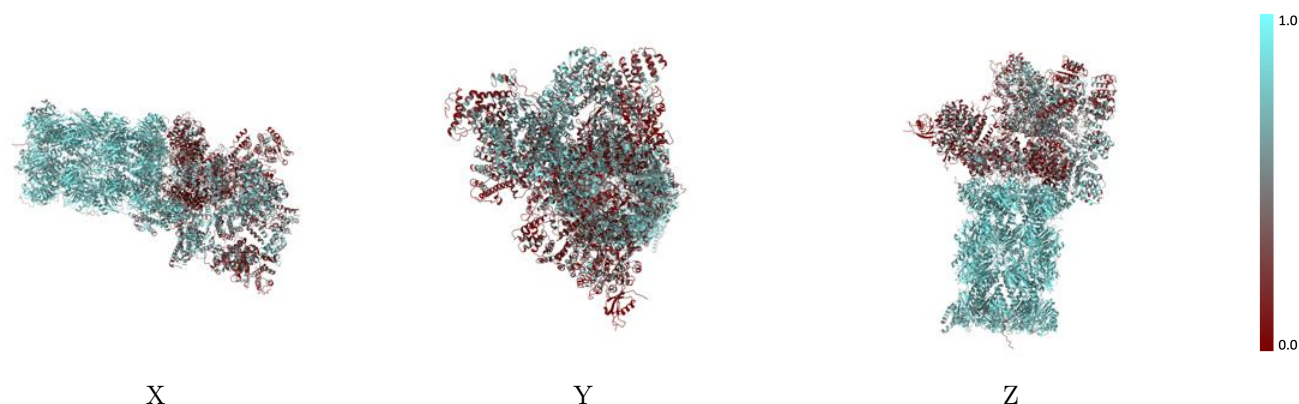
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



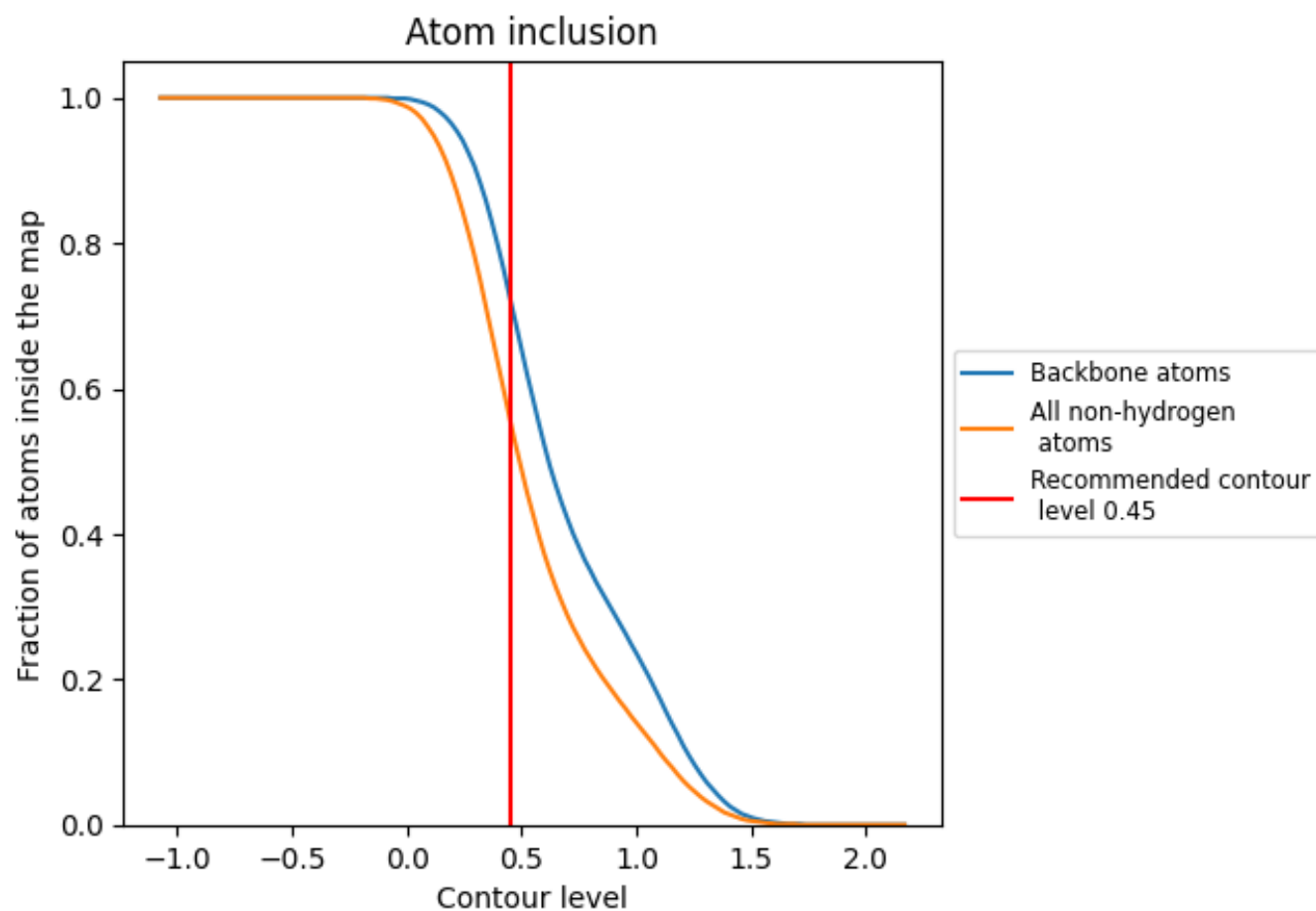
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 56% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5570	 0.2350
A	 0.2980	 0.0840
B	 0.3190	 0.1180
C	 0.3690	 0.1320
D	 0.2030	 0.0980
E	 0.1840	 0.0510
F	 0.2960	 0.0730
G	 0.7780	 0.3830
H	 0.7570	 0.3640
I	 0.7510	 0.3740
J	 0.7170	 0.3310
K	 0.7590	 0.3660
L	 0.7840	 0.3940
M	 0.7840	 0.3810
N	 0.8060	 0.4150
O	 0.8250	 0.4180
P	 0.8230	 0.4260
Q	 0.8100	 0.4220
R	 0.8460	 0.4250
S	 0.8230	 0.4230
T	 0.8230	 0.4130
U	 0.4040	 0.0960
V	 0.3840	 0.1090
W	 0.5770	 0.1670
X	 0.6090	 0.2250
Y	 0.5590	 0.1520
Z	 0.4550	 0.1190
a	 0.4260	 0.1070
b	 0.2220	 0.0580
c	 0.4300	 0.1110
d	 0.2790	 0.0810
e	 0.3250	 0.0810
f	 0.2620	 0.0800
g	 0.7170	 0.3410
h	 0.7160	 0.3360



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Chain	Atom inclusion	Q-score
i	 0.7170	 0.3190
j	 0.7230	 0.3350
k	 0.7280	 0.3430
l	 0.7600	 0.3540
m	 0.7480	 0.3470
n	 0.8120	 0.4110
o	 0.7990	 0.3970
p	 0.8010	 0.4040
q	 0.8140	 0.4100
r	 0.8340	 0.4190
s	 0.8010	 0.4060
t	 0.8020	 0.4110
x	 0.0030	 0.0290